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ENVIRONMENTAL RESEARCH DIVISION
TECHNICAL PROGRESS REPORT

January 1984 - December 1985

T. M. Beasley, Division Director

May 1986

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ABSTRACT

Technical progress in the various research and assessment activities of Argonne National Laboratory's Environmental Research Division is reported for the period 1984-1985. Textual, graphic, and tabular information is used to briefly summarize (in separate chapters) the work of the Division's Atmospheric Physics, Environmental Effects Research, Environmental Impacts, Fundamental Molecular Physics and Chemistry, and Waste Management Programs. Information on professional qualifications, awards, and outstanding professional activities of staff members, as well as lists of publications, oral presentations, special events organized, and participants in educational programs, are provided in appendices at the end of each chapter.

CHAPTER 1. DIVISION DIRECTOR'S OVERVIEW

In previous years, separate technical progress reports were issued to update activities within each program of the Environmental Research Division at Argonne National Laboratory. In 1985, Division Management concluded that a single, less detailed, report should be prepared. In addition to publication economies, such a report would bring together a synoptic view of the Division's scientific capabilities. This report is the result of that decision. As with all such reporting changes, there will necessarily be an initial unevenness in both style and content; some programs will stress work still in progress, while others will speak principally to work largely completed. In time, however, a more balanced presentation will certainly emerge.

The reporting period spans two years: 1984-1985. The report is arranged along structural lines as illustrated in the following organizational chart. Each of the scientific chapters is followed by appendices outlining staff qualifications, professional activities and awards, and special events organized by the staff, as well as a listing of their publications and oral presentations.

While the organizational chart reflects my directorship of the Division, I undertook those responsibilities in November 1985. Prior to that time, the stewardship of the Division was in the capable hands of Dr. P. F. Gustafson, acting Division Director, and Dr. A. J. Dvorak, Associate Division Director. It was under Dr. Gustafson's supervision that the work reported here was carried out. Argonne continues to benefit from Dr. Gustafson's expertise in his new responsibilities in the office of the Associate Laboratory Director for Energy, Environment and Biological Research (EEBR), Dr. Harvey Drucker.

This introduction would not be complete without special mention of the efforts by the editorial staff of the Division in preparing this report. We are indebted to John DePue, Dimis J. Wyman, Kerri Schroeder, Lorenza Ceballos, and Amie George for their professionalism and the infectious good humor they displayed throughout the enterprise.

T. M. Beasley, Director
Environmental Research Division

ENVIRONMENTAL RESEARCH DIVISION
Programmatic Organization

APPENDIX 1-A. STAFF QUALIFICATIONS
Division Management and Support Staff

Name	Position	Highest Degree	Major	Year Received	Institution
<u>DIVISION MANAGEMENT</u>					
Beasley, Thomas M	Division Director (Fall 1985 - present)	Ph.D.	Oceanography	1968	Oregon State University
Gustafson, Philip F.*	Acting Division Director (until Fall 1985)	Ph.D.	Physics	1958	Illinois Institute of Technology
Dvorak, Anthony J.	Associate Director	Ph.D.	Plant Ecology	1973	University of Oklahoma
Tuma, Leroy A.	Assistant Director	A.A.	Mechanical Engineering	1948	Morton Junior College
<u>SUPPORT STAFF</u>					
DePue, John D.	Technical Editor	M.S.	Biology	1974	Texas A&I University
Wyman, Dimis J.	Technical Editor	M.S.	Botany	1969	University of Minnesota
Yuan, YuChien	Radiological Analyst	Ph.D.	Nuclear Engineer	1976	Northwestern University
Zielen, Albin J.	Computer Scientist	Ph.D.	Physical and Inorganic Chemistry	1953	University of California-Berkeley

*No longer a member of the Division.

CHAPTER 2. ATMOSPHERIC PHYSICS PROGRAM

<u>Program Staff</u>	<u>Title</u>
M.L. WESELY	Program Manager
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R.L. COULTER	Meteorologist
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P. FRENZEN	Senior Meteorologist
R.L. HART	Scientific Associate
P.E. HESS	Scientific Associate
M.-S. HONG	Postdoctoral Appointee
I.-Y. LEE	Meteorologist
B.M. LESHT	Physicist
T.J. MARTIN	Scientific Associate
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2.1 PROGRAM OVERVIEW

M.L. Wesely (Program Manager)

Research by the Atmospheric Physics Program took a few new directions during 1984 and 1985. Processes of dry and wet deposition important in delivery of acidifying substances to the surface gradually became the dominant topics of our studies. This led to greater emphasis on atmospheric chemistry, although the underlying nature of most of the research projects was still physics. Some work retained its explicit orientation toward atmospheric physics, notably experimental studies of transport and dispersion in the lower atmosphere and application of associated remote sensing systems. Even some of this work, however, was devoted to issues of "acid rain." Together with numerical modeling studies of long-range transport and deposition, research for the national acid deposition program comprised over 70% of the work in this group. A few projects on aquatic physical processes and on application of models to problems in environmental engineering were added to our activities as a result of transfer of two staff members from other programs in the Environmental Research Division.

The scientific expertise of the staff members of the Atmospheric Physics Program reflects the activities described above. As a group, the staff is familiar with most aspects of atmospheric processes of transport, transformation, diffusion, and deposition of airborne acidifying substances. For example, our capabilities in experimental and theoretical micrometeorology have been applied in studies of dry deposition to evaluate the air-surface exchange of trace substances. Techniques to measure wet as well as dry deposition have been employed for both intensive, comprehensive measurement and routine monitoring. The micrometeorological studies overlap with experimental investigations of transport and dispersion in the planetary boundary layer, for which we have developed and applied advanced Doppler acoustic sounding systems.

In atmospheric numerical modeling, we have extensively investigated acidification and scavenging processes involving cloud physics and chemistry. Our experience in atmospheric numerical modeling also involves long-range and short-range transport and diffusion, which requires an understanding of mixing processes in the lower atmosphere. Our trajectory modeling has been a productive means of describing transport and deposition of trace substances over continental distances and multiyear time scales. Our short-range modeling has provided descriptions of transport and diffusion of materials from isolated sources, including the purposeful release of obscurants. In addition, our expertise in analysis of aquatic systems, including the capability to model heat exchange via industrial cooling ponds, ecosystems in the Great Lakes, and the behavior of trace substances in the Great Lakes, is well established. To complement this, we have developed and used experimental techniques to measure the physical processes responsible for transport of suspended sediment in the benthic boundary layer.

This chapter summarizes the orientation and progress of projects in the Atmospheric Physics Program. Greater technical detail is given for ongoing work than for completed tasks. More thorough accounts of the completed research can be found in the peer-reviewed scientific literature and Argonne topical reports listed at the end of this chapter in Appendix 2-E.

2.2 AIR-SURFACE DRY EXCHANGE

2.2.1 Summary

Our studies of air-surface exchange associated with dry deposition are focused on two topics: numerical modeling and routine measurement of fluxes from the atmosphere. Much of the Program's effort is devoted to carrying out two or three intensive field experiments each year to measure the fluxes of sulfur and nitrogen compounds over selected types of surfaces. Data from the field experiments are interpreted to develop parameterizations of deposition velocities (downward fluxes divided by concentrations at specified heights). Surface resistances to uptake of each substance are determined and described in terms of local surface and micrometeorological conditions. The mathematical expressions produced are used in numerical modeling as well as in evaluation of fluxes at sites where dry deposition is to be measured routinely.

For modeling, a dry deposition "module" has been developed and is periodically improved for use in the Regional Acid Deposition Model (RADM) by the National Center for Atmospheric Research. For routine measurement, the parameterizations are derived for application at three core research sites, one of which is operated at Argonne. Here, additional experiments on dry deposition processes are carried out; activities include testing of monitoring systems and proposed monitoring methods. Practically all of this work is performed for the National Acid Precipitation Assessment Program.

2.2.2 Dry Deposition Parameterization Experiments

*M.L. Wesely, D.L. Sisterson, D.R. Cook, R.L. Hart, F.T. DePaul,
and P. Frenzen*

Many micrometeorological experiments on dry deposition have been conducted by Argonne over the past few years. Those listed in Table 2.1 represent field efforts carried out since 1983 at one of three core research sites established to develop and test techniques to measure dry deposition routinely. These experiments usually took place over a period of about two weeks. Several other experiments were conducted to address specific questions with regard to surface conditions, diurnal variations, or chemical species. Preliminary data processing for most of the experiments has been completed, but of the research efforts listed in Table 2.1, final data analysis and

Table 2.1 Locations, dates, and pollutant flux measurements by Argonne for each of the dry deposition comparison experiments

Site	Dates	Conditions; Fluxes Measured ^a
PSU ^b	February 1-10, 1983	Bare soil, some snow in furrows; SO_4^{2-} , fine particles, O_3 , CO_2 .
ATDD ^c	April 25-May 8, 1983	Early leaf stage of deciduous forest; SO_4^{2-} , fine particles, O_3 , CO_2 .
ANL ^d	July 25-Aug. 4, 1983	Lush grass; SO_2 , SO_4^{2-} , O_3 , fine particles, CO_2 .
PSU	January 17-27, 1984	Snow-covered surface; SO_2 , SO_4^{2-} , NO_x , O_3 , CO_2 .
ATDD	June 11-12, 1984	Active deciduous forest; SO_2 , SO_4^{2-} , fine particles, O_3 .
PSU	July 19-25, 1985	Mostly senescent oats and barley with corn-grass mixture upwind; SO_2 and O_3 .

^a Sensible heat and latent heat fluxes, as well as surface stress, were measured for all experiments.

^b Rock Springs research site near University Park, PA, operated by the Pennsylvania State University (PSU).

^c Oak Ridge research site, near the Walker Branch Watershed in Tennessee, operated by the Atmospheric Turbulence and Diffusion Division (ATDD) of NOAA/ARL.

^d Argonne research site, operated by Argonne National Laboratory (ANL).

interpretation have been completed only for the 1983 PSU experiment. Some results from that experiment are reported by Wesely et al. (1985).

The experiments listed in Table 2.1 were joint efforts by Argonne, the Atmospheric Turbulence and Diffusion Division (ATDD) of the National Oceanic and Atmospheric Administration (NOAA) Air Resources Laboratory (ARL), the Pennsylvania State University (PSU), and other invited participants. The parameterizations derived from these comparison experiments will be applied in conjunction with routine local measurements, such as described in Section 2.2.5, to estimate fluxes throughout the year.

2.2.2.1 Dry Deposition Intercomparison Experiments

Field intercomparisons were conducted under the sponsorship of the U.S. Environmental Protection Agency (EPA) in September 1981 and June 1982 to facilitate development of practical methods for routine monitoring of dry deposition. Analysis of the data gathered was completed in 1984, and the results were published in 1985.

The two experiments, each a month long, were hosted by the Illinois State Water Survey. They were conducted above a grass field in central Illinois. Argonne provided the primary micrometeorological data set for use by the participants, who came from 14 institutions in the United States and Canada. The results are summarized by Dolske and Gatz (1985) and the accompanying articles in the same journal issue.

One of the main direct comparisons produced was for sulfate fluxes and deposition velocities. Mathematical expressions for the deposition velocities in terms of micrometeorological variables were developed (Wesely et al. 1985). Average daily deposition velocities obtained by Argonne with the eddy-correlation technique varied from 0.09 to 0.26 cm s⁻¹ over a three-week period. Systematic differences among different types of surrogate surfaces were obtained by other participants: many of the small, relatively smooth surfaces placed just above the grass produced estimates of sulfate fluxes within a factor of two of that obtained by Argonne. However, these findings might not be applicable to different conditions, especially to different natural surfaces.

2.2.2.2 Participation in the TULLA Experiment

Three staff members of the Atmospheric Physics Program participated in collaborative, dry deposition experiments in the Black Forest area of southwestern West Germany during March 1985. The purpose of our participation was to use Argonne equipment and techniques to measure dry deposition of SO₂ and O₃ in support of the West German TULLA program. ("TULLA" is a German acronym indicating studies of the transport and transformation of air pollutants in the state of Baden-Württemberg and from surrounding countries.) The dry deposition experiments were carried out in collaboration with the Karlsruhe Nuclear Research Center and three West German universities, as well as with the Atmospheric Turbulence and Diffusion Division (ATDD) of NOAA/ARL.

The dry deposition experiments were conducted in two phases. During the first two weeks of March, both Argonne and ATDD measured SO₂ and O₃ fluxes above a flat field of patchy grass and bare soil in order to compare instrument performance and calibrations. For the second two weeks, when the main experiments of TULLA were conducted, ATDD moved to a forested site in order to increase spatial sampling. Several days worth of good data were collected by Argonne over the nonforested site. Deposition velocities varied mostly in response to local atmospheric conditions, solar radiation, and the wetness of the soil surface.

2.2.2.3 Effects of Humidity on Particle Flux Measurements

A study was conducted during 1984 at Argonne's deposition monitoring site to investigate the effects of humidity on particle flux measurements. One goal was to determine if the growth and shrinkage of fine particles due to condensation and evaporation as the particles are subjected to different ambient relative humidities cause errors in the estimates of particle fluxes obtained by application of a micrometeorological gradient technique. Also investigated was the suggestion that particle deposition might be enhanced by rapid growth of particles and subsequent gravitational settling when the particles are swept very close to wet surfaces where the relative humidity approaches 100% (Slinn and Slinn 1980).

Measurements of submicron particle concentrations were alternately taken at heights of 1.0 and 8.5 m above a grassy surface at Argonne's deposition monitoring site. The measurements were taken of two size ranges corresponding to diameters of 0.01 to 0.07 μm and 0.07 to 0.7 μm . The particle flux was calculated by application of an aerodynamic-gradient technique. Relationships from Hänel (1972) were adopted to describe the effects of relative humidity on the size of particles in thermodynamic equilibrium with the surrounding moist air. Details of the experiment and data analyses are given by DePaul and Sisterson (1985).

A total of 168 twenty-minute runs were taken during appropriate meteorological conditions. No significant effects of surface or atmospheric humidity on the particle fluxes were detected in the cases analyzed. These analyses were limited by measurement inaccuracies to cases when relative humidity was less than 98% at the two heights measured. Peak deposition values were seen in the afternoon, and minimum values were seen at night, as has been observed previously in eddy-correlation measurements by Argonne (Wesely and Hicks 1979; Wesely et al. 1982, 1985). There was some tendency for the fluxes to be directed slightly upward at night over wet grass.

2.2.2.4 Measurements of Nitric Oxide Fluxes

Nitric oxide (NO) fluxes were measured by the eddy-correlation technique at Argonne's deposition monitoring site (Sisterson et al. 1984; Cook and Cobourn 1984). The chemiluminescent NO analyzer used in the measurements was built at Argonne (Drapcho et al. 1983) and follows the basic concept and operation as described by Kley and MacFarland (1980). The detection limit (where the signal-to-noise ratio is unity) is 40 ppt of NO. Only concentrations greater than 0.1 ppb, nonplume conditions, and wind directions with good fetch requirements were included in the data base. Nitric oxide concentrations were sampled at 8.0 m above a grassy surface at a rate of 20 s^{-1} and averaged over 25 minutes on selected days from October 1983 through May 1984. The data base consists of 256 data-collection periods.

Preliminary results indicate that the NO fluxes measured at a height of 8.0 m are not usually representative of fluxes at the surface. Rapid reactions of NO with O_3 and the photochemical production of NO from NO_2

apparently produce a substantial change of flux with height, as discussed by Fitzjarrald and Lenschow (1983). Also, there is evidence that NO is produced at the surface when ambient concentrations of NO₂ are high. Additional interpretation of these results is underway.

2.2.2.5 Use of Fast-Response Instrumentation

Fast-response sensors are essential for eddy-correlation measurements. At heights of 5 to 10 m at fixed surface installations, sensors with an exponential time response of one second can be used if adjustments are computed to compensate for inadequate detection of all the flux-carrying eddies (Wesely 1983). Sensors with such a frequency response have been used in many of the dry deposition experiments conducted by the Atmospheric Physics Program. The flux estimates are routinely adjusted to compensate for poor instrument frequency response; the data are considered acceptable if the adjustments computed are less than 30%. Considerable effort has been spent by Argonne staff and collaborators over the past several years to develop fast-response sensors for use from fixed towers. These include flame-photometric sensors for gaseous and particulate sulfur and chemiluminescent detectors for nitrogen oxides and ozone.

Fast response in chemical sensors is often achieved at the expense of signal-to-noise ratio. Wesely and Hart (1985) performed an analysis to show that a small signal-to-noise ratio results in increased scatter in run-to-run variability of eddy-correlation flux estimates, but usually does not systematically bias the estimates. For example, sulfur and nitrogen sensors used in past experiments were sufficiently noisy that 5 to 20 times the number of data-collection periods or length of total averaging times were required to achieve the same statistical significance as obtained with sensors having very low noise levels.

Cup anemometers of novel design featuring fast response and, for their type, a unique ability to sense only horizontal components of the wind have been used for micrometeorological field research by this group for a number of years (Frenzen and Hart 1970). However, relatively poor starting-stalling speeds were found to limit the use of the anemometers in field studies of dry deposition where light-wind regimes can be important. Therefore, an improved version of the instrument was developed using hemispherical cups rather than conical cups. This change resulted in a larger front-to-back drag coefficient difference and a corresponding increase in driving torque. When mounted on a commercial anemometer base equipped with a 20-slot photo-chopper readout, this anemometer has a stalling speed less than 0.5 m s⁻¹ and a distance constant of 0.45 m.

2.2.2.6 ASDEP Research Needs

A concerted, multilaboratory effort was made during 1984 and 1985 to identify crucial gaps in knowledge about dry deposition. This resulted in preparation of several reports and summaries, including the Air-Surface Dry

Exchange Processes (ASDEP) proposal (Wesely 1984), an informal document entitled "Tracer-Simulated Dry-Deposition of Environmental Pollutants (TDEP)," and an earlier version of these documents that included aspects of both ASDEP and TDEP in a critical review. It is clear that the amount of information available is insufficient for many chemical species important in acid deposition. Even for chemical substances whose dry deposition has been studied extensively, the available information is usually restricted to deposition above uniform surfaces in flat terrain. Additionally, the distribution of deposition of materials in deep vegetative canopies is poorly understood. This limits our ability to determine the causes of damage to vegetation.

The ASDEP-TDEP studies suggest the need for a program to measure and parameterize dry deposition velocities above large areas of nonuniform terrain typical of landscapes in the Northeast. A combination of aircraft, tracer, and surface measurements to determine directly the deposition over areas tens of kilometers square has been proposed. Results would be compared to estimates based on measurements at scattered sites and associated calculations that sum the dry deposition components to different types of surfaces. Detailed inventories of surface conditions and some numerical modeling of local transport and diffusion would be necessary. Adjustments to the surface-based parameterizations currently in use would be derived on the basis of the nature and extent of surface nonuniformities and irregularities.

2.2.3 Numerical Module Development

C.M. Sheih and M.L. Wesely

Because dry deposition results in substantial removal from the atmosphere and accounts for a large portion of the sulfur and nitrogen compounds delivered to the surface, the Regional Acid Deposition Model (RADM) being developed by the National Center for Atmospheric Research (1985) for the National Acid Precipitation Assessment Program must include a description of the dry deposition processes. Sheih et al. (1979) compiled available formulae and data to produce a computer module to describe dry deposition over the eastern United States and surrounding regions. The main components of the module are a FORTRAN subroutine and land-use map. For RADM, this work has been modified to expand the geographical domain considered and to incorporate new research findings acquired during the last several years. These modifications have incorporated O_3 , NO plus NO_2 , and HNO_3 into the module; only SO_2 and particulate sulfur were addressed in the earlier version.

The deposition velocity v_g for a gas at height z over land is computed from the equations given by Wesely and Hicks (1977) as:

$$v_g = ku_*[\ln(z/z_o) + 2(D_h/D_g)^{2/3} + ku_*r_g - \psi_c]^{-1}, \quad (2-1)$$

where k is the von Karman constant, u_* is the friction velocity, z_0 is the surface roughness scale length, D_h and D_g are the molecular diffusivities for heat and the gas of interest, respectively, ψ_c is the stability correction function for the gas, and r_g is the surface resistance to the uptake of the gas. The deposition velocities of sulfate particles over water and land are computed from:

$$v_p = ku_*[\ln(z/z_0) + ku_*r_p - \psi_c]^{-1}, \quad (2-2)$$

where r_p is the surface resistance for particle uptake.

To determine deposition velocities with these equations, the parameters that must be specified are surface roughness, molecular diffusivity, stability correction function, friction velocity, and surface resistance. The actual values used for the surface roughness and resistance depend on the season for which the calculations are being conducted and on which of 11 possible land-use types occur in the area of interest.

The land-use data used in the present study cover an area from 52 to 134 degrees longitude and 24 to 55 degrees latitude. The area is divided into a matrix of 328×186 (longitude by latitude) grid cells with increments of $1/4$ and $1/6$ degree longitude and latitude, respectively. Data for each grid cell contain longitude and latitude coordinates of the cell and the percentage of the areas covered by the 11 land-use types in the cell. A sample map of dry deposition velocities for HNO_3 for summer daytime conditions is shown in Figure 2.1.

RADM has successfully utilized these features of the dry deposition module to compute deposition of SO_2 , SO_4^{2-} , and HNO_3 over the eastern United States for three days in the spring (Walcek et al. 1986). Domain-averaged mid-day deposition velocities were found to be 0.5 cm s^{-1} for SO_2 , 0.2 cm s^{-1} for sulfate, and 2.5 cm s^{-1} for HNO_3 .

Most Eulerian models provide sets of atmospheric parameters that are meant to be averages over entire grid cells. For example, the mesoscale meteorology model of RADM gives one average profile of wind speed, temperature, and humidity per grid square of 80 by 80 km. From these profiles, the fluxes of momentum, heat, and moisture required for input to the dry deposition module must be derived in order to compute deposition velocities using Equations 2-1 and 2-2. In the current version of the module used in RADM, grid-averaged fluxes are derived from the profiles with semi-empirical equations designed to avoid time-consuming iterative calculations that are necessary with conventional micrometeorological formulae. Grid-averaged fluxes might not be adequate, however, because friction velocity and other such factors can vary strongly within each grid square.

For each grid cell in RADM, a new average friction velocity is estimated on the basis of a grid-averaged wind speed and a surface roughness computed as the logarithmic average of those obtained from the land-use map. To calculate

friction velocities over each land-use type, the products of wind speed and friction velocity are assumed constant at a specified height between 10 and 40 m. This provides both realistic variations in local friction velocity above each grid cell and a distribution of wind speed that, when averaged, is consistent with the grid-averaged wind taken from RADM. The heat and moisture fluxes important in computing the Monin-Obukhov length are assumed constant and equal to the grid averages. This is a deficiency of the process, but a small one compared with the practice of assuming constant friction velocity, or alternatively, wind velocity.

Achievement of methods to measure dry deposition routinely with few skilled personnel and limited equipment has long been an objective of the National Acid Precipitation Assessment Program (NAPAP). A workshop report (Hicks et al. 1980) strongly recommends three measurement techniques for

further investigation: techniques of eddy accumulation, modified Bowen ratio, and variance. Recent research for the EPA on the variance technique and for DOE on the modified Bowen ratio technique is summarized below. With these two micrometeorological techniques, deposition is measured indirectly and is compared with fluxes over the surface measured directly by eddy correlation. Other approaches, such as surface sampling and mass-budget calculations, are important potential measurement techniques. However, these other approaches are less well established than micrometeorological techniques and suffer from the same general problems of possibly being too difficult and expensive for routine application.

2.2.4.1 Variance Technique

A description of the current status of work on the variance technique is provided by Ellestad et al. (1985). The most common type of variance technique is the standard deviation ratio, where the flux F_c of the scalar (trace substance) quantity c of interest is set equal to:

$$|F_c| = |F_s| \sigma_c / \sigma_s, \quad (2-3)$$

where the σ 's represent standard deviations and s is the reference scalar quantity with flux F_s .

Commensurate with typical scales of turbulence and limitations of stationarity in the atmospheric surface layer, data-collection periods are usually about 30 minutes. This approach assumes a type of similarity between the behavior of turbulent fluctuations of c and s . This assumption is valid if the fluctuations c' and s' are highly correlated in the range of frequencies sampled. As shown by Wesely (1983), this seems to be the case for most scalar quantities over many surfaces. The standard deviation ratio method represented by Equation 2-3 strongly resembles the modified Bowen ratio technique described below, for which local differences in concentrations measured across the same height interval are substituted for the σ 's in Equation 2-3.

An evaluation of the standard deviation ratio method with use of ozone variance and flux data collected over a field of soybeans is illustrated in Figure 2.2. As is typical for variance techniques, the direction of the flux, hence the sign of F_c , is not determined. (Other means must be taken to determine whether the flux is directed upward or downward.) It appears that humidity (q) provides a much better comparison than temperature (T), possibly because of the effects of local advection from a nearby field of maize. While temperature may not be a good choice for the reference scalar quantity at many sites, the difficulty of obtaining reliable fast-response (greater than 1 Hz) humidity measurements on a routine basis may prevent its use as the reference scalar quantity also.

Figure 2.2. Comparison of ozone fluxes 5 m above a soybean canopy as inferred from variance measurements versus eddy-correlation measurements, with stable and unstable atmospheric conditions as identified. Each point represents data obtained simultaneously over a 30-minute period.

As described by Ellestad et al. (1985) there are several alternative methods to Equation 2-3 that allow inference of fluxes from variance measurements. For most of the techniques suggested, there is the requirement that the sensors for the chemical species have rapid speed of response in a frequency range where nonatmospheric sensor noise is insignificant. However, many chemical sensors are noisy at the high frequencies. To overcome this obstacle, one approach might be to use at least three noisy signals for different chemical species: c_1 , c_2 , and c_3 . If the atmospheric turbulent fluctuations are perfectly correlated, then c_1' can be expressed as ac_2' and as bc_3' , where a and b are fixed numerical values for each data-collection period. Then it is easily shown that the atmospheric signal alone would produce a standard deviation for c_1 of:

$$\sigma_{c_1} = (\overline{c_1'c_2'} \overline{c_1'c_3'} / \overline{c_2'c_3'})^{1/2}. \quad (2-4)$$

Investigations involving Equation 2-4 will proceed with data amassed during previous experiments, especially those at the three core monitoring sites. Once σ_c is determined, Equation 2-4 or alternative approaches will be applied.

2.2.4.2 Modified Bowen Ratio Technique

Deposition velocities for SO_2 and O_3 were determined for a grassy surface at Argonne's deposition monitoring site using a tram system and employing the modified Bowen ratio and bulk aerodynamic techniques. The goals of this study were (1) to develop a system for the reliable, routine estimation of surface fluxes of trace substances, and (2) to evaluate the modified Bowen ratio and bulk aerodynamic micrometeorological techniques.

The modified Bowen ratio technique is derived from the assumption that eddy diffusivity for trace substances is the same as for heat and yields:

$$F_c = (H/\rho c_p) \Delta c / \Delta T, \quad (2-5)$$

where H and F_c are the sensible heat and contaminant fluxes, ΔT and Δc are the differences in potential temperature and contaminant concentrations between two heights, and ρ and c_p are the density and heat capacity of dry air, respectively.

The concentrations of SO_2 and O_3 were measured at 1.0 and 8.5 m using a tram system described by Sisterson et al. (1984). Heat flux values were measured directly by eddy correlation and were estimated using the bulk aerodynamic technique with temperature difference measured between the same heights as for the gas concentrations. Preliminary results indicate that the method is reliable and sufficiently accurate to obtain pollutant flux and deposition velocity estimates on a routine basis.

2.2.4.3 Methods to Monitor Atmospheric Stability

It was not uncommon 20 years ago to infer atmospheric stability by very simple means, such as using rough correlations with insolation, cloudiness, and wind speed. Now, however, much more precise methods are available (Pasquill and Smith 1983). For routine measurements at dry deposition monitoring sites, other approaches that do not rely on intensive micro-meteorological measurements are usually suggested. In one case, a bulk Richardson number, R_b , is calculated based on measurements of wind speed, a mean temperature difference, and knowledge of the values of the aerodynamic surface roughness length and zero-plane displacement height for the site. In many cases, the latter two values can be inferred with reasonable accuracy from the nature of the surface.

The bulk Richardson number approach was used successfully by Wesely et al. (1985) to apply parameterizations of deposition velocity for sulfate over grass for periods of a few weeks. Figure 2.3 shows a comparison of the relationship derived from theoretical relationships and from actual measurements at the 1981 Dry Deposition Intercomparison Experiment. This relationship is specific to heights of measurement above the zero-plane displacement height and to the value of surface roughness length. The slight offset seen between predictions and observations in the figure is probably due to the effect of humidity flux on z/L (height divided by the Monin-Obukhov length).

The main difficulty with the bulk Richardson number approach is to obtain sufficiently accurate measurements of the temperature difference on a routine basis. At the Argonne deposition site, continuous measurements have been taken successfully for over two years. The required accuracy can be obtained with commercially available systems over short vegetation or relatively smooth surfaces. Over very rough surfaces such as forests, however, the magnitudes

Figure 2.3. Plot of bulk Richardson number measured (dots) and calculated (solid line) on the basis of profile equations employing estimates of surface roughness versus z/L derived from eddy-correlation measurements. The dashed line is an empirical fit to the observations.

of the temperature difference are often too small to be of use. Furthermore, utilization of the bulk Richardson number approach above very tall vegetation is often prohibited by the inaccuracy of estimates of the zero-plane displacement heights.

An alternative is to measure the standard deviation of horizontal wind direction fluctuations (σ_θ), which have long been used as a rough estimator of atmospheric stability. Several disadvantages, however, should be kept in mind. At night, for example, meandering can cause excessively large values of σ_θ ; during the day, the height of the planetary boundary layer has an effect. Hence, there is not always a one-to-one relationship between σ_θ and z/L . Fluctuations of vertical wind velocity or direction are partially immune to some of these difficulties, but are more difficult to measure adequately on a routine basis.

2.2.5 Operation of ANL Dry Deposition Monitoring Station

D.L. Sisterson, R.L. Hart, D.R. Cook, and M.L. Wesely

The deposition monitoring site at Argonne is one of three sites that have been established in the United States to develop and test the concentration monitoring method and other approaches for calculating dry deposition. The Argonne site is taken to be representative of the Midwest; a site operated by the Atmospheric Turbulence and Diffusion Division of NOAA/ARL near the Oak Ridge National Laboratory Walker Branch Watershed is considered representative

of the forested Southeast; and the third site, operated by The Pennsylvania State University at the Rock Springs research site, is taken to be representative of the hilly Northeast.

Routine monitoring of NO and NO₂ (Columbia Scientific Industries Model 1600 Oxides Analyzer), O₃ (Dasibi Ozone Monitor Model 1003-AH), and SO₂ (Monitor Laboratories Inc. Model 8850 Sulfur Oxide Analyzer) began at the Argonne core site in July 1983. Instrumentation calibrations and routine zero and span checks are being performed using a Columbia Scientific Industries CSI Model 1800 Programmable Gas Phase Titration Calibrator. All real-time pollutant concentration sensors sample air through a common PFA Teflon line 15 m long with the intake at 8.0 m leading to a spherical Pyrex glass manifold. For the period July 1983 through June 1985, a 12-mm (1/2-inch) I.D. Teflon line was used with unassisted flow. The flow rate of the combined instrumentation through the sample line was approximately 3 L min⁻¹, and the lag time was 2-3 minutes. Starting in July 1985, a 6-mm (1/4-inch) I.D. Teflon line was used, with assisted flow at the manifold giving a combined flow rate through the sample line of approximately 9 L min⁻¹. This yielded a lag time of approximately 15 seconds. Zeros were performed every other day for the first several months to check drift of the instrumentation. Currently, zeros performed once a week are sufficient to correct for zero drift. Spans are irregularly performed every other month. Calibrations are performed when spans are not within 10% of the calibration span gas value or when instruments are shut down for repairs or maintenance.

Meteorological information on wind speed, wind direction, ambient temperature, and dew-point temperature are determined at a height of 10 m on another tower 50 m west of the deposition monitoring building. In addition, temperature difference (between 1.0 and 8.5 m) is measured on the tower adjacent to the deposition monitoring building. A quality assurance plan is implemented for all chemical and meteorological instrumentation.

A Campbell Scientific Model CR7 data logger is used for data acquisition and preprocessing. A program developed for this system applies calibrations and takes half-hour averages of data for all the sensors listed above. In addition, the logger computes and takes half-hour averages of relative humidity and computes standard deviations of the air chemistry data. With an algorithm supplied by Campbell, half-hour, vector-averaged wind speed and direction and standard deviation of the wind direction also are obtained. Finally, the daily maximum value of each chemical species is reported, along with the time of occurrence and the wind direction at that time. Both hard copy and cassette tape output are produced.

The cassette tapes produced by the logger are read into a DEC 11/73 computer for editing and further processing. Zero offset and calibration slope corrections are applied to the data, and data considered unreliable because of equipment malfunction are appropriately flagged. Atmospheric stability (calculated using iterative bulk-aerodynamic techniques from wind speed, temperature difference, and an estimate of surface roughness) and half-hour averages of global radiation are added to the data record. Monthly

summaries of the data are produced. These include a tabulation of the data by day, a tabulation of monthly averages by hour, time-series plots of the half-hour averages (e.g., see Figure 2.4), and wind directional "roses" of wind speed, frequency distribution, and concentration.

A number of meteorological variables are also measured approximately 450 m east of the core site, as described by Hart (1984).

Figure 2.4. Sample plot of monthly pollutant concentrations measured at the Argonne core site.

2.3 EXPERIMENTAL STUDIES OF ACID PRECIPITATION

2.3.1 Summary

Experimental sampling studies of surface wet deposition that were initiated during the Multistate Atmospheric Power Production Pollution Study (MAP3S) were completed in recent years under the new NAPAP Processing of Emissions by Clouds and Precipitation (PRECP) program. The Atmospheric Physics Program recently has been extensively involved in multilaboratory field experiments under the PRECP program. Our efforts have been focused on determining how the wet deposition of acidic and other pollutants depends upon inputs to individual storms (1) by understanding the chemical and physical processing of emissions by clouds and precipitation, (2) through analysis of appropriate data, model development and testing, and laboratory and field studies, and (3) for applications in the definition of relationships between pollutant releases and subsequent deposition. To date there have been two field experiments. The first experiment was conducted in April and May 1985, with operations centered in Columbus, Ohio. The second experiment took place in June 1985, with operations centered in Oklahoma City, Oklahoma. An overview of Argonne's participation in those two experiments is presented in

this section. Also discussed are Argonne's involvement with the next PRECP experiment (in January 1986) and some of the results of surface precipitation sampling studies recently completed by the Atmospheric Physics Program.

2.3.2 PRECP Experiments

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2.3.2.1 April Experiment (PRECP I)

The purpose of the PRECP I field experiment (April 1 - May 3, 1985) was to obtain information about the vertical extent of and scavenging ratios for sulfur and nitrogen oxides and for oxidant species in the vicinity of precipitating and nonprecipitating clouds. The study involved the use of two research aircraft and two stationary, instrumented motor homes. The center of operations for the experiment and the research aircraft was Columbus, Ohio. Three major types of experiments were attempted. Mobile sampling by aircraft to obtain data for determination of "improved" scavenging ratios for key sulfur and nitrogen species was the focus of one part of the study. Because the spring of 1985 was one of the driest springs in decades in the Midwest and Northeast, the mobile sampling activities were extensive. The second type of experiment was carried out in cooperation with the EPA-funded Philadelphia Experiment, which involved ground sampling of precipitation in southeastern Pennsylvania and southwestern New Jersey. Both motor homes were located in the Philadelphia area for this experiment. The third experiment consisted of two-airplane documentary flights in precloud air and in clouds in a pollution receptor area (defined by Syracuse-Albany-Whiteface Mountain) of upstate New York. The site of the experiment is located in a low emission area approximately 500 km downwind of major source regions.

The Argonne motor home, equipped with instrumentation listed in Table 2.2, was to provide air-quality and meteorological support for interpretation of precipitation chemistry for samples collected as part of the Philadelphia Experiment. The instantaneous air-quality data (i.e., ozone, sulfur dioxide by flame-photometry and pulsed-fluorescence, and nitrogen oxides) were averaged over 15-minute periods. Pollution, dosage, and wind roses were constructed from these data. An example of a concentration rose is shown in Figure 2.5. Because the hourly, instantaneous wind speed and direction data used to construct the pollution roses were assumed to be representative for one hour (two 30-minute average periods on either side of the time of the wind measurement), information is given in 30-degree arcs to allow for the variability of wind direction.

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Table 2.2. Characteristics of instruments mounted in the Argonne mobile research facility to measure air chemistry during the April PRECP experiment

Variable	Instrument	Units	Technique	Type	Limit of Detection	Accuracy
SO ₂	ANL Meloy Suifur Analyzer Model 285	ppb	flame photometric	15 min avg	1 ppb	±0.5 ppb
SO ₂	ANL Thermo Electron Analyzer Model 43	ppb	pulsed fluorescent	15 min avg	2 ppb	±1 ppb
SO ₂	PNL Barringer Correlation Spectrometer IV	ppb	vertical integration	15 min avg	1 ppb	±5%
O ₃	BNL Dasibi Analyzer Model AH-1003	ppb	UV absorption	15 min avg	1 ppb	±5%
NO _x , HNO ₃	BNL modified Monitor Laboratory Model 8840 Analyzer	ppb	chemi-luminescent	15 min avg	0.1 ppb 0.2 ppb	±10% ±20%
NO ₃ , SO ₄ , NH ₄	ANL Modified Lundgren Cascade Impactor	µg/m ³	IR Spectro-photometry	2 hr int avg	0.1 µg 3.0 µg 1.0 µg	±20% ±20% ±20%
Aerosols	ANL TSI Electrical Aerosol Analyzer Model 3030	part./m ³	particle charging	15 min avg	1 particle	
	Size Ranges (µm)					
	0.0100 to 0.0178					±15%
	0.0178 to 0.0316					±10%
	0.0316 to 0.0562					±10%
	0.0562 to 0.100					±10%
	0.100 to 0.178					±10%
	0.178 to 0.316					±10%
	0.316 to 0.562					±20%
	0.562 to 1.000					±30%
Aerosols	ANL Climet Optical Particle Counter Model 208A	part./m ³	light scattering	15 min avg	1 particle	
	Size Ranges (µm)					
	0.3 to 0.5					±1%
	0.5 to 0.7					±1%
	0.7 to 1.0					±1%
	1.0 to 2.0					±1%
	2.0 to 3.0					±1%
	3.0 to 5.0					±1%
	5.0 to 10.0					±1%

Figure 2.5. Concentration roses for the April PRECP Experiment.

2.3.2.2 June, PRESTORM Experiment (PRECP II)

Members of the Atmospheric Physics Program participated in the PRECP II field study in Oklahoma during June 1985. PRECP was operated as part of the PRESTORM program, which was a large multilaboratory operation designed to investigate the life cycle of complexes of thunderstorms on several different scales. PRECP activities were concentrated on subsets of the larger squall lines that passed near the Oklahoma City area. Activities of this group were limited primarily to monitoring near-surface atmospheric concentrations of SO_2 and O_3 , estimating the integrated burden of sulfur and nitrogen dioxide above the sampling site, collecting hi-vol particulate samples, and aiding in the collection of event and sequential rain samples from the precipitation collection network established around Oklahoma City.

Analysis of the data is not yet complete, but some preliminary observations can be made. Measured values of SO_2 concentrations were very small. Both near-surface and integrated burden measurements were usually below the detectable limit, with the possible exception of some early morning values. Ozone concentrations were generally near 40 ppb. Some of the most interesting data may have been collected during passage of a squall line. Estimates of the nitrogen dioxide burden above the site during the passage are being used along with aircraft measurements to estimate the production of NO and O_3 by lightning.

2.3.2.3 Planning for Winter Experiment (PRECP III)

The third PRECP field experiment will be held in the Syracuse area from January 13 through February 7, 1986. Instead of having one field manager,

this PRECP experiment has three co-field managers--one representative each from Pacific Northwest Laboratories, Argonne National Laboratory, and Brookhaven National Laboratory. The emphasis of this experiment is similar to the past two--i.e., to obtain improved scavenging ratios (using inflow air pollution concentrations rather than surface-measured concentrations to reduce the variability of the computed ratios) and outflow-to-inflow air pollution concentration ratios. Feasibility studies will be conducted to determine relative scavenging rates of orographic and lake-effect storms since meteorological fields may be determined fairly well, as opposed to the case for mesoscale frontal systems.

After the termination of the January PRECP experiment, PRECP participants will join the Genesis of Atlantic Lows Experiment (GALE) already in progress and will contribute research aircraft as well as a precipitation chemistry sampling network to operations centered in eastern North Carolina. In the event of a major GALE episode, the winter PRECP experiment investigators will participate in the Syracuse area since a GALE episode will bring conditions favorable for a PRECP frontal experiment.

2.3.3 Surface Precipitation Sampling Studies at Argonne

D.L. Sisterson, B.M. Lesht, B.E. Wurfel, S.A. Johnson,* and R. Kumar**

2.3.3.1 Methodology of Acidity and pH Measurements

Studies conducted at Argonne have shown that significant errors in precipitation acidity determinations can result from improper use of pH electrodes, where the overall uncertainty in measurement may be at best ± 0.10 pH units (Sisterson and Wurfel 1984). The most critical problem is the streaming potential. The sample should be agitated but then allowed to come to full rest; the pH measurement is then made in the quiescent solution. If further accuracy is desired, the liquid-junction potential, resulting from the differences in ionic strength between standard buffers and samples, can be eliminated by calibrating the electrode in solutions of dilute strong acids of known pH. This is preferable to the addition to the sample of an inert salt such as KCl, which may be used to increase the ionic strength of the sample but which in turn affects the measured pH. Furthermore, the Debye-Huckel correction for hydrogen ion activity to concentration can improve the measured pH.

The overall verification of the pH electrode performance or the free acidity of the sample is critical in assessing the actual errors associated with pH measurements. A dilute strong acid solution may be used to verify absolute pH measurement after routine calibration of the electrode in standard buffers. Titration and the use of Gran's method to independently determine the hydrogen ion concentration of a solution may also be used to verify pH

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electrode determinations of free acidity for samples with values less than pH 5.0. For samples with pH values greater than 5.0, weak acids (carbonic acid) may significantly contribute to the free acidity, and Gran's method is no longer applicable since it assumes only strong acids contribute to free acidity. For such samples, the pH measurements can only be verified by dilute strong acid solutions of known pH or by inference from simulations of detailed titration curves.

2.3.3.2 Event Versus Weekly Sampling for Wet Deposition

The chemical differences between weekly and event precipitation samples were investigated at Argonne from April 1980 through March 1982 and the results were published in 1985 (Sisterson et al. 1985a). Event samples were combined and weighted by precipitation amount over the corresponding weekly period. They were compared annually and seasonally for both years as well as separately. Much of this study addressed fundamental questions that arise when comparing analytical determinations made by two laboratories using different analytical techniques. Objective criteria were developed to determine data outliers so that any apparent differences were not due to a few atypical precipitation samples. An extensive data-screening protocol based on collection and analysis was developed to eliminate questionable samples.

Laboratory analyses were conducted for H^+ , Ca^{2+} , Mg^{2+} , NH_4^+ , SO_4^{2-} , and NO_3^- concentrations, and field measurements were made for pH and conductivity. In addition, the 1980-1981 samples were titrated to determine the total, strong, and weak acid concentrations. Although seasonal and annual precipitation amounts were different for the two years, the general patterns of event and weekly sample ion concentrations were similar. Weekly samples had significantly less $[NH_4^+]$ (where the brackets designate concentration) and higher laboratory pH in all seasons and more $[SO_4^{2-}]$ in every season but summer. Weekly samples had significantly more $[Ca^{2+}]$ and $[Mg^{2+}]$ during seasons with little precipitation. Event and weekly $[NO_3^-]$ were never significantly different. The weekly samples had more total acidity in the spring but less in the summer. The observed differences may be attributed to chemical degradation of the weekly samples while waiting collection and during shipment between field and laboratory. Since the magnitude of the differences will depend on the various ion concentrations in the precipitation (which can be expected to be a function of geographic location) as well as on the time the sample remains "unpreserved" while waiting chemical analysis, these results may differ from site to site.

2.3.3.3 Physical Scavenging

Precipitation chemistry and the chemical composition and mass loading of atmospheric aerosols (0.3 to 1.0 μm aerodynamic diameter) were examined for 25 individual precipitation events during a 12-month period (Sisterson et al. 1985b). Aerosol and precipitation data were used to (1) determine the influence of the precipitation event on the mass loading and the chemical composition of the fine-particle aerosol, and (2) calculate the apparent

scavenging ratios of sulfate and ammonium ions. Two distinct types of aerosol behavior were observed. In one, the concentration of aerosol particles was observed to decrease during the rain but to recover quickly after the event. In the other, the aerosol particle concentration was found to increase either during or just after the rain. The meteorology associated with each precipitation event was examined in detail to determine the factors responsible for the observed behavior of the aerosol particles. The decrease in particle mass concentration in the first type of behavior was attributed to local precipitation scavenging of particles, with the subsequent recovery caused by advection of other portions of the same air mass to the sampling location. The second type of behavior, an increase in fine-particle concentration during or after precipitation, was apparently caused by an increase in relative humidity from less than 70% to greater than 90% (generally 100%) at the time the increase was observed.

The calculated scavenging ratios for sulfate and ammonium ions were observed to lie in the range 100 to 3000. Although the computed ratios were found to be within the general range of those measured by other researchers for convective and stratiform precipitation systems, the ratios were substantially higher in those cases where the aerosol mass in the 0.3 to 1.0 μm size range had increased during or after precipitation. The scavenging ratios reported may have been affected by limiting consideration to the size range sampled.

2.3.3.4 Urban Versus Rural Wet Deposition

Precipitation samples collected at Chicago's lakefront and at Argonne National Laboratory (approximately 40 km southwest of Chicago) from June 1981 through May 1982 were analyzed to investigate urban influences on local precipitation chemistry (Sisterson 1982, 1983). The Argonne and Chicago sample pairs were stratified into four wind direction categories (SW, SE, NW, NE) according to the 6-hour average wind direction prior to precipitation. The data were divided into two time periods: June-November 1981 (summer-fall) and December 1981-May 1982 (winter-spring). The calculated wet deposition values for each wind quadrant were normalized by the total precipitation amount received by each quadrant for summer-fall and winter-spring to minimize some of the potential effects of spatial variability of convective and stratiform storms.

Samples collected in Chicago had greater normalized deposition of all constituents (Ca^{2+} , Mg^{2+} , K^+ , Na^+ , NH_4^+ , Cl^- , NO_3^- , SO_4^{2-} , H^+ from pH) except H^+ regardless of wind direction or time period. This is explained by increased NH_4^+ and Ca^{2+} in the Chicago samples, which apparently had more neutral ammonium sulfate and more soil-derived calcium (both of which affect precipitation acidity). The cold-month precipitation (winter-spring) generally had higher normalized deposition values than did warm-month precipitation. This may be due to the removal of more pollutants from the atmosphere by the less efficient, but longer duration, stratiform precipitation than by the more efficient, but shorter duration, convective

precipitation. Warm-month southeast and southwest quadrants had the "dirtiest" precipitation; the northwest quadrant had the "cleanest". This was expected because the "dirtiest" source region for Argonne is for southerly winds that draw air from the Ohio River Valley. The "cleanest" wind direction is from the northwest. Cold months showed little variation in normalized deposition by wind direction for all constituents. This is explained by the dominance of stratiform precipitation for winter-spring; precipitation occurs for longer time periods with significant changes in wind direction throughout, and source/receptor relationships are unclear. Data obtained in this study have been used in another urban versus rural precipitation chemistry study by Lipfert et al. (1984).

2.4 TRANSPORT AND DIFFUSION IN THE ATMOSPHERIC BOUNDARY LAYER

2.4.1 Summary

Research on vertical and horizontal transport and diffusion of trace substances in the lower atmosphere continued during 1984 and 1985. A principal part of this effort was investigation of the physics of transport and diffusion in drainage flows that occur above complex terrain during stable nocturnal conditions. This work was carried out under DOE's Atmospheric Studies over Complex Terrain (ASCOT) project, a multiyear program that has included two large multilaboratory investigations. In 1980, the flows on the slopes and outflow region of a large (approximately 5-km-wide) basin were studied near Anderson Creek in northern California. This was followed in 1984 by a study concentrated on investigation of flows down a long (15-km), well-defined valley that included several tributaries along its length. In each of these efforts, the Atmospheric Physics Program made measurements with both remote and in-situ sensing systems to gather information on the physics of such flows. The information is being utilized by ASCOT to develop models capable of describing atmospheric dispersion of trace substances above such terrain.

Vertical transport of material from the well-mixed layer into nonprecipitating cumulus clouds, and thence to the free troposphere above, was studied as part of the EPA-sponsored Venting Experiment (VENTEX) effort to produce parameterizations of boundary-layer processes for the Regional Acid Deposition Model (RADM). The Atmospheric Physics Program participated in this effort under EPA funding, with a small amount of supplementary funding from DOE in 1985. Argonne efforts were concentrated on studying relationships of the large (approximately 1-km) eddy structure of the mixed layer to the life cycle of cumulus clouds.

Analysis has continued on the data collected during past experiments on transport and diffusion in the lower atmosphere. Reports summarizing techniques and data were produced for two large experiments (Rush and DeWitt) investigating the behavior of the atmospheric boundary layer conducted prior to 1984. Additionally, analysis was completed for experiments on dispersion of substances emitted near street level in urban street canyons.

2.4.2 Studies of Flow over Complex Terrain

R.L. Coulter and T.J. Martin

The 1984 ASCOT field program was conducted along Brush Creek Canyon, approximately 100 km northeast of Grand Junction, Colorado, from September 17 to October 5. It involved scientists from 20 laboratories and universities, some foreign, in an effort to measure and understand the physics governing the mass, momentum, and energy fluxes out of Brush Creek Canyon during nocturnal drainage flow conditions.

Several cross-valley lines of measurement were established along the lower 10 km of the canyon. Along each line, tethered sonde and sodars were used to measure wind, temperature, and moisture profiles. Surface towers were established along each line and at several sidewall locations to measure turbulence parameters, and a Doppler lidar was positioned to map the distribution of the along-valley wind component in vertical cross-valley planes every 300 m along the canyon.

The contribution of tributary canyons to the Brush Creek Canyon mass flux was estimated through laser anemometer, sodar, and tethered sonde measurements of winds and temperatures within Pack Canyon. Finally, smoke and tracer releases from well up Brush Creek Canyon and at ridgetop level above Pack Canyon were used to visualize the drainage flow and to estimate the integrated flow characteristics.

Two measurement sites were operated by Argonne personnel. The primary site was within Brush Creek Canyon in terrain with a slope of 1.5 degrees, on the floor of the main canyon about 1.5 km downstream from Pack Canyon. A multifrequency Doppler sodar (Coulter and Martin 1985b) was used to obtain continuous profiles of winds, and instruments on a 10-m tower were used to measure eddy fluxes of heat, momentum, and moisture. The multifrequency operation of the sodar provided a threefold increase in sample rate over conventional sodars. This increased the stability of variance estimates of the wind components and permitted determination of accurate mean wind profiles every five minutes.

A tethered sonde and the ANL minisodar were located in Pack Canyon, approximately 1 km above the confluence of Pack and Brush Creek Canyons. The high frequency (5.2-kHz) minisodar (Coulter et al. 1984a; Coulter and Martin 1985a) was operated in a single axis mode, pointed along the axis of Pack Canyon (slope about 12 degrees) at an elevation angle of about 35 degrees. Because of its portability, the minisodar was placed within the washed-out gully central to the tributary. Thus, the drainage wind component could be examined in detail and from locations not possible with conventional sodars.

Six coordinated ASCOT experiments were performed (see Table 2.3), five of which included release and tracking of tracers. The evolution of the drainage flow in the main canyon for the night of September 17 - 18, 1984, at the main

Table 2.3. Overall features at the ANL Brush Creek site during experimental periods of ASCOT 1984^a

Exp. No.	Date	Average Drainage Flow			Mesoscale Wind Direction (deg)	Conditions
		Depth (m)	h (m)	U ($m\ s^{-1}$)		
0	9/17-18	400	100-125	5-6	45-200	Clear, very stable; flow weakens after 0200 hr
1	9/19-20	350	100	4.5	180	Clear, stable, steady conditions
2	9/25-26	300	80	4.0	180	Partly cloudy, less stable, steady flow
3	9/27-28	400	100	8.0	270	Near neutral, unsteady, channeling flow after gust front at 2300 hr
4	9/29-30	300	80	6.0	180	Partly cloudy, stable, steady
5	10/05-06	300	80	3.0	360	Near neutral: weak unsteady flow

^a The maximum speed and its height are listed under U and h, respectively. All experiments lasted from about 2300 to 1100 hours on the following morning. Tracers were released during experiments 1 through 5.

Argonne site in Brush Creek Canyon is shown in Figure 2.6. Downslope winds (approximately 310 degrees) developed quite early and increased rapidly early in the evening to form a "jet" with magnitudes greater than $6\ m\ s^{-1}$ by 2200 hours (Mountain Standard Time). Winds remained from this direction to a depth of nearly 500 m, almost ridgetop height, despite an opposing synoptic wind field above the ridgetops. A weakening of the flow after 0130 hours was followed by synoptic winds progressing to lower elevations after 0300 hours. Complete flow reversal occurred just after sunrise as the upper walls of the canyon were heated. Drainage depths, maximum wind speeds, and steadiness of the flow varied considerably from night to night (Table 2.3), as did the large-scale meteorological conditions.

In contrast to the well-established drainage flow above the floor of the main canyon, the Pack Canyon drainage wind component was highly variable (Figure 2.7), even periodic, particularly at heights above 25 m. These characteristics were evident to some extent on all experimental nights. The small averaging time utilized with the minisodar (20 seconds) allowed detection of frequent flow reversals, alternating with surges in the downslope flow component. Such dynamic features may be related to the small-scale

Figure 2.6. Wind speed and direction contours for the night of September 17-18, 1984, at the main ANL site in Busch Creek Canyon.

Figure 2.7. Time series of downslope component of wind at the Pack Canyon location for September 18. Each time series is at a successively greater height above the surface.

topographic features of Pack Canyon. Another feature of the flow was the considerable delay in onset of upslope flow within Pack Canyon after the flow reversal began in Brush Creek Canyon. As shown in Figure 2.7, upslope flow in Pack Canyon on September 18 did not occur until 1030 hours, fully three hours after flow reversal occurred in Brush Creek Canyon.

Preliminary estimates of the mass flux from Brush Creek and Pack Canyons indicate that tributaries may contribute as little as 10% or as much as 70% of the total drainage in Brush Creek Canyon. Accurate estimates of these values require the incorporation of data from tethersondes, laser anemometers, towers, and the minisodar into the tributary estimates. Those estimates are presently being evaluated.

2.4.3 Studies of PBL Entrainment

R.L. Coulter and T.J. Martin

Argonne studies of entrainment of air from the well-mixed layer into the free troposphere above continued in 1984 and 1985. These studies began in 1982 with a scoping experiment in central Illinois (the VOICE experiment, see Coulter et al. 1983), expanded in 1983 to a detailed look at the convective boundary layer in central Oklahoma (BLX83, see Coulter et al. 1984b), and continued with the VENTEX 1984 and 1985 projects in Kentucky. These last two studies were devoted principally to investigation of cumulus cloud development at the top of the mixed layer.

The VOICE study showed that acoustic remote probing techniques can be used to help parameterize the unstable planetary boundary layer (PBL) through examination of vertical velocity statistics (Coulter and Underwood 1984). Time-lapse photography synchronized to sodar vertical velocity measurements during BLX83 showed that fair-weather cumulus clouds quite often are the visually observable part of "thermal plumes" whose roots begin within 50 m of the surface. In the VENTEX experiments, flights of free-flying balloons through thermal plumes and into the cumulus clouds were included to obtain vertical profiles of wind velocity and temperature up to and above cloud height.

During BLX83, two cameras fitted with lenses to give 90-degree fields of view were pointed vertically and located 500 m from the sodar receiver. They were operated synchronously at intervals from 33 to 262 seconds (see Coulter et al. 1983). The data from both cameras were used to calculate cloud height and cloud position through digitization and subsequent analysis of simultaneous photographs. The times of cloud position above the sodar were then compared to the times of thermal plume passage above the vertically pointing sodar receiver. Thermal plumes are very well defined regions of rising air in the convective PBL, with mean widths of 1 to 2 km and with velocity increasing with height up to about 300 m (Coulter and Thoma 1982). In general, thermal plumes grow with height (Lenschow and Stephens 1979), but the most active region of the thermal tends to decrease in size with increased

height above the velocity maximum as the plume expands. When the thermal reaches the condensation level, a cumulus cloud is formed. Thus, the air that is processed through the cloud has its source near the bottom of the well-mixed layer and may have higher concentrations of moisture and pollutants than does air surrounding the thermals. When the conditions are appropriate, the latent heat release associated with condensation may enable the cloud to grow on its own and eventually lose its dependence on the thermal plume for its energy.

Analysis of the thermal plume-cloud events during BLX83 in conditions of forced convection has led to the conclusions that (1) 78% of cumulus clouds were located at the top of thermal plumes that in turn extended nearly to the surface, and (2) 45% of the thermal plumes were associated with cumulus clouds at any one time.

It is not expected that all observed cumulus clouds would be associated with thermal plumes since some were dissipating, in which case there should be no source below. In some other cases, the thermal plume tilts with height due to wind shear within the PBL. In this case, the cloud would not be directly above the base of the thermal but might still be associated with it.

The second conclusion above must depend upon the moisture and temperature profile during the observations. Continued analysis of the data from VENTEX could make it possible to quantify this result as a function of the controlling meteorology.

During the VENTEX 1984 and 1985 field studies, the camera positions were modified so that a single vertically pointing camera was located at the sodar receiver and a second camera, tilted at 45 degrees, was located approximately 1 km away. This procedure simplified identification of cloud position relative to the sodar and allowed the separated camera to be used to estimate cloud base, height, and size. Figure 2.8 shows the vertical velocity, temperature, and moisture profile within a thermal plume and through the cloud at its top as derived from sodar and free-flying balloon data. Cloud inflow velocities of approximately 2 m s^{-1} are evident in this case. The inflow velocities measured with the balloons were highly dependent upon the location of the entry point of the balloon into the cloud.

Through use of the multifrequency capabilities of the Doppler sodar, we were able to measure the three-dimensional wind profile on short time scales during the VENTEX experiments. As shown by Coulter and Martin (1985b), these data can be used to estimate the convergence field that exists around thermal plumes. The vertical velocity field associated with the thermals increases rapidly with height (Coulter and Thoma 1982); thus there should be a compensatory change in the horizontal wind field to satisfy the continuity equation. An analysis was carried out by Coulter and Martin (1985b) on the basis of a model that assumes a circularly symmetric thermal plume in the horizontal plane, with symmetric inflow around the edge of the thermal. Results from this crude model indicate that the change in horizontal wind field through the thermal should be about 33% of the change in the vertical

Figure 2.8. Profile of vertical velocities averaged through a thermal plume using sodar data and a "snapshot" of the vertical velocity, temperature, and moisture profile near the center of the plume and through cloud level using airsonde data.

wind field. The sodar measurements yield a value of 25%, which is very encouraging with regard to the quality of the sodar data. This may imply that a large percentage of the variation in the crosswind component of the horizontal wind field, including the variance in the wind direction, can be related to the field of thermal plumes.

Through the course of the PBL entrainment experiments, a large data set has been amassed detailing the structure of the vertical and (to a lesser extent) horizontal wind field in the convective boundary layer. A complete analysis of all the data will take some time and effort; the potential results insofar as detailed knowledge of the dominant scales and processes controlling the transport of pollutants in the PBL are large.

2.4.4 Results from Past Experiments on the Mixed Layer

R.L. Coulter, D.L. Sisterson, and M.L. Wesely

2.2.4.1 The Rush Experiment

The Rush field experiment, conducted October 3-14, 1977, provided information on the daytime growth and initial decay of the mixed layer of the lower atmosphere over farmland in southeastern Indiana. Detailed structure of the planetary boundary layer (PBL), during conditions typical of autumn, was described with data obtained by high-resolution miniature-radiosonde, sodar,

and lidar systems. Sensible heat flux and surface stress data measured over unharvested senescent maize were used to characterize the lower boundary conditions.

In addition, ozone and fine submicron particle fluxes were determined in conjunction with a concurrent multiorganizational sulfur box-budget study, called Atmospheric Mass Balance of Industrially and Naturally Emitted Sulfur (AMBIENS). The methods of observation and data reduction for both the Rush experiment and the Atmospheric Physics Program's contribution to AMBIENS were summarized, and the data obtained were reported in tabular form in a series of appendices (Sisterson et al. 1983). These results can be used to test models of the behavior of the planetary boundary layer, such as variation of the mixed layer heights during the daytime.

2.4.4.2 The DeWitt Experiment

The DeWitt field study was conducted July 10-21, 1979, near Champaign, in central Illinois. It provided detailed information on the structure of the lower 2 km of the atmosphere and surface boundary conditions over flat farmland planted mainly with soybeans and maize. Mean wind and temperature profiles in the lower atmosphere were measured by in-situ soundings with high-resolution miniature radiosondes tracked optically up to heights of at least 2 km and with an instrument package carried aloft up to 500 m by a kytoon. Argonne sodar and University of Wisconsin lidar remote-sensing systems were used simultaneously to measure the height and depth of the entrainment zone at the top of the boundary layer as a function of time of day. Both systems were also used to measure profiles of mean wind velocity and some statistics of velocity fluctuations. At the surface, standard meteorological surface observations and measurements were made of solar and net radiation, and eddy fluxes of momentum, heat, water vapor, and ozone over a local maize canopy.

The DeWitt field study topical report (Coulter et al. 1986) summarizes observational and data-reduction techniques and presents the final processed data in a series of appendices. The results can be used to test models of the behavior of the planetary boundary layer, such as the influences of surface fluxes and entrainment aloft on the variation of mixed-layer height and mixing processes in the boundary layer.

2.4.5 Dispersion in Urban Street Canyons

C.M. Sheih and F.T. DePaul

A field study of trace-substance dispersion from an urban street canyon was undertaken to (1) determine the processes by which pollutants emitted at street level are transported out of the canyon, and (2) quantify the net rate of pollutant exchange between the canyon and the upper air. The experiments were performed when the ambient wind direction was nearly perpendicular to the street for a canyon of approximately equal building heights on both sides.

The street canyon had an aspect ratio of about 1.5 for the building height to the street width. These flow conditions were studied because they were known to result in the largest street-level concentrations of pollutants, and hence the largest exposure for pedestrians. To examine trace-substance transport within the canyon, mean wind velocities were determined by analyzing the trajectories of tracer balloons released in the canyon and photographed in rapid sequence. The results were reported by Sheih et al. (1985). The trajectories indicate the presence within the canyon of a primary vortex cell, provided the ambient wind velocity exceeds 1.5 to 2.0 m s⁻¹. The measurements collected during the experiments indicate that while pollutant mixing within the canyon occurs rapidly by mean wind advection, the final transport of material normally to the roof-level plane is accomplished by turbulent motions.

An artificial tracer, SF₆, was used at the field site to determine the net rate of trace-substance exchange between the street canyon and upper air. The gas was released at a regulated rate near the street for a period until its mean concentration reached a stable value. Then the emission was ended to permit study of the trend of the reduction in the tracer concentration at several locations within the canyon. The results have been reported by DePaul and Sheih (1985). Retention times, defined as the length of time for a pollutant concentration to reduce to 37% of its original value, were computed from measurements of tracer decay. The retention times were found to vary between 0.7 and 3.8 minutes for ambient winds between 1.7 and 4.5 m s⁻¹. The vertical flux near midblock was quantified by a ventilation velocity, which represents the average ret velocity of SF₆ transported out of the canyon. The ventilation velocities were computed from the retention times and found to range between 15 and 80 cm s⁻¹. Meteorological measurements of the ambient flow were also taken, and a semiempirical formula for predicting street-level pollutant concentrations was developed from the data.

2.5 ATMOSPHERIC NUMERICAL MODELING

2.5.1 Summary

Numerical modeling studies in the Atmospheric Physics Program cover a wide range of temporal and spatial scales. They range from diagnostic studies of cloud microphysics and chemistry, which focus on droplets of submicron size and some chemical processes with rate constants of fractions of a second, to the continental and annual deposition isopleths produced with long-range transport and deposition models. The diagnostic models are necessary for mechanistic understanding and for analysis of experimental results; the second approach has its greatest application in assessment of past, current, and potential future loading and associated policy analysis.

In addition, two projects have evaluated model performance in simulating transport and diffusion over long distances but short temporal scales. Transport and diffusion are associated with one component of uncertainty;

other components examined include climatological variability from year to year and changes in key rates of processes parameterized. Such studies of uncertainty and sensitivity are essential parts of any model-development effort.

The flow in a typical street canyon has been investigated with inexpensive, indirect measurements from balloon photography, and the data have been used in both conceptual development and verification of a numerical model. The development of a module for simulation of dry deposition in a highly sophisticated Eulerian model of regional acid deposition has been described in Section 2.2.3.

Two quite different local environmental problems related to energy production have been examined in modeling studies. In the first study, the noise propagation and resulting community impacts of nuclear power plants have been modeled, and a method for regulatory assessment has been developed. In the second study, cooling tower plume dispersion, including possible fogging, icing, shadowing, and salt drift, has been modeled and a user's guide developed.

2.5.2 Long-Range Transport and Dispersion

J.D. Shannon and B.M. Lesht

The Atmospheric Physics Program has been engaged for some years in modeling of long-range transport and deposition of air pollutants, primarily (but not exclusively) those pollutants related to acid deposition. The models have been used extensively to calculate deposition fields and source-receptor relationships for policy analysis (e.g., Streets et al. 1985). The primary modeling vehicle has been the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) model. ASTRAP predicts seasonal average atmospheric concentrations and cumulative wet and dry deposition, with the primary limiting assumption being that of linearity between emissions and deposition (Shannon 1981, 1985). In reprogramming of effort by Task Group C of the National Acid Precipitation Assessment Program (NAPAP), however, the direct financial support of Lagrangian model development was cut in half in FY 1985, and the project was ended at the close of the fiscal year. In separate projects, some limited applications and model uncertainty studies have continued through the first quarter of FY 1986 as tasks for the scheduled 1985 NAPAP Assessment (which will appear in 1986).

Net horizontal flux budgets have been calculated recently with ASTRAP. In the study, the United States and Canada are treated as a single source region, and the fluxes are calculated for transport across eight segments of the Atlantic Coast, plus segments along the Gulf of Mexico, Mexico, the Pacific Coast, and the Far North (Shannon 1984). Typical results, as shown in Table 2.4, are in excellent agreement with the partly measured and partly modeled net horizontal fluxes of Galloway et al. (1984).

Table 2.4. Transboundary sulfur flux estimates

Segment	ASTRAP	Galloway et al. (1984)
Atlantic Coast (deg lat. N)		
25-28	70	100
28-33	450	410
33-38	1,300	860
38-43	2,200	1,500
43-48	870	930
48-53	340	350
53-58	170	90
58-60	120	30
25-60	5,500	4,300
Gulf of Mexico	670	
Mexico	150	
Pacific Coast	120	
North of 60 deg N	260	

A continuing task is the estimation of the variation in deposition or source-receptor relationship arising solely from climatological variability, and the estimation of trends with simulations using historical records of emissions and meteorology. Unfortunately, the available long-term trend data, particularly for wet-only sampling, are very sparse. In addition, the horizontal, vertical, and seasonal resolution of emission data becomes poorer and requires more assumptions (such as effective emission heights) as one goes back in time.

ASTRAP has been used to examine annual variability and compare U.S. and Canadian contributions to cross-border fluxes. Net fluxes across the U.S.-Canada border, the Atlantic Coast as a whole, and the remainder of the exterior border components, as in Table 2.4, have been calculated and results will be presented in 1986. For this approach, fluxes originating from U.S. and Canadian emissions are calculated separately, since the sources near the southern borders of Ontario and Quebec on both sides of the border are difficult to describe and differentiate simultaneously. The results are shown in Figure 2.9. It appears that year-to-year variability can be as large as 20% of the mean, and fluxes from the United States appear to be approximately three times the fluxes from Canada. Simulations also indicate that for 1976 to 1981, climatological variability of fluxes was considerably larger than emissions-related variability.

Figure 2.9. Estimates of the annual net sulfur flux across the United States-Canada border for 1976-1981 for anthropogenic emissions from the United States (hatched) and from Canada (solid).

2.5.3 Cloud Microphysics and Chemistry

I.-Y. Lee and M.-S. Hong

The Modeling Of Cloud Acidification Processes (MOCAP) model has two versions: one version for warm clouds and a second for deep convective clouds. For the first version, details in spectral evolution of cloud droplets and raindrops are computed considering condensation and coagulation. For the second version, all the cloud microphysical processes are parameterized in terms of cloud bulk properties. For both versions, the in-cloud chemical processes are constructed under the assumptions (1) that the cloud droplets form on condensation nuclei whose water-soluble portion is composed of H_2SO_4 , $(\text{NH}_4)_2\text{SO}_4$, and NH_4NO_3 ; (2) that the cloud water is in equilibrium with gas-phase NH_3 , CO_2 , and HNO_3 ; and (3) that the production of sulfate is due mainly to oxidation of S(IV) by ozone and hydrogen peroxide.

Results from MOCAP applied to warm clouds are described in articles by Lee and Shannon (1985) and Lee (1986). Briefly, the simulations produce dynamic characteristics typical of fair-weather cumulus clouds. The in-cloud decrease in SO_2 concentration occurs mainly in the upper part of the cloud, where the decrease approaches 10%. The corresponding SO_2 decrease in the near-cloud environment is about 2% during the 30 minutes of real-time simulation. The dominant SO_2 oxidation pathway is kinetic oxidation by H_2O_2 . The results from runs to test sensitivity to the input concentrations of H_2O_2 show that the hydrogen peroxide concentrations reach a steady state value during the very early stages of cloud development. Thereafter, the cloud water acidity is controlled mainly by oxidation of dissolved SO_2 by ozone. The amount of SO_2 uptake increases with the increase of the liquid water mixing ratio. However, the pH field shows that low acidity corresponds to high liquid water content and vice versa, indicating that the dilution by liquid water overcompensates for the increase in uptake of acidifying species.

The cloud microphysical processes in the second version of MOCAP are parameterized in terms of cloud dynamic and physical parameters, as presented in Figure 2.10. The rates for autoconversion (Berry and Reinhardt 1974), evaporation of raindrops (Ogura and Takahashi 1971), accretion of cloud by rain and of cloud and ice by snow (Lin et al. 1983), melting of snow (Ogura and Takahashi 1971), and raindrop freezing (Hales and Easter 1982) are chosen among formulas currently in use in many storm models and based on compatibility with the model parameters produced by MOCAP. The formation of cloud droplets and ice crystals due to condensation and sublimation, respectively, is computed under the assumption that clouds, liquid, or ice form under a quasaturated state. If air is oversaturated, part of the excess water vapor must be condensed or sublimated, while the remainder must be exactly sufficient to maintain a saturated state at the raised temperature that results from the release of latent heat of condensation or sublimation. If air is unsaturated and if liquid water or ice is available, evaporation must occur. Test runs have been made in order to improve understanding of the physical and chemical properties associated with deep convection. Our preliminary results show good qualitative agreement between simulated and observed temporal trends in precipitation from the well-known OSCAR experiment conducted in 1981.

Figure 2.10. Temporal variation of various interconversion rates of cloud microphysical parameters.

2.5.4 CAPTEX Model Evaluation Workshop

*J.D. Shannon, B.M. Lesht, A.J. Policastro, I.-Y. Lee, and M. Wastag**

A workshop on evaluating models of long-range transport and diffusion with surface data from the Cross-Appalachian Tracer Experiment (CAPTEX) was hosted by the Atmospheric Physics Program on November 4 and 5, 1985. The CAPTEX field program, conducted in September and October of 1983, consisted of seven releases of an inert, nondepositing tracer. Five of the releases were made from Dayton, Ohio, and the others were from Sudbury, Ontario. A network of approximately 80 surface samplers with 6-hour resolution, centered in Pennsylvania and New York, provided the observations to which model simulations were compared. Additional samples from airborne sensors were used diagnostically, but not in statistical evaluation (Ferber 1984).

At the time of the workshop, results from five models had been submitted for evaluation. The models were ARL and ARL-BAT from the Air Resources Laboratory, LRTAP from the Ontario Ministry of the Environment, ARPPA from the Tennessee Valley Authority, and a particle-in-cell model from In-Young Lee of the Atmospheric Physics Program.

The evaluation consisted of three primary phases. First, model performance was quantified with a set of statistical tests recommended by the Woods Hole Workshop sponsored by the American Meteorological Society (Fox 1981, 1984), but with the number of statistical tests reduced to eliminate redundancies. The evaluations were concentrated on examining scatter plots, observed and predicted frequency distributions, and distributions of residuals. Many of the tests compared "unpaired" data, since experience has shown that even a small error in short-term orientation of a narrow plume can produce major differences between observed and predicted values when space and time are considered simultaneously in statistical analyses.

A second evaluation effort was concentrated on comparing the distribution of residuals from all models for a particular release, or for all releases for a particular model. Box plots, a form of bar graphs, were used extensively to depict the distributions of residuals in terms of mean, median, percentiles, and confidence about the mean. The box plots provided visual comparisons that summarized performance differences more effectively than did columns of numbers. An example of a box plot is shown in Figure 2.11.

A third evaluation involved comparing observed and modeled dosage patterns across the network for entire experiments and for 12-hour or 24-hour portions of experiments. The pattern comparisons thus far have been entirely subjective, but a literature search is underway to find objective tests for such comparisons. Because a number of modelers had not submitted results by the date of the workshop, the time for submission was extended until the first quarter of calendar year 1986. It is expected that eventually about ten

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models of varying complexity will be evaluated. A workshop report that will include the evaluation of the additional models is scheduled to be prepared during the first half of 1986.

Figure 2.11. An example of a box plot of residual distributions for the the ARL model for all CAPTEX releases. The outer limits of the error bars indicate the 90 and 10 percentiles; dashed lines give the medians; circled crosses denote the means; the vertical extent of the boxes shows the 95% confidence limits; and the box widths are proportional to sample sizes.

2.5.5 Dispersion of Military Smoke-Obscurants

A.J. Policastro, L. Coke, M. Wastag,* W.E. Dunn*, J. Liljegren*, and G. DeVaul*

The dispersion of military smoke-obscureants was examined on behalf of the U.S. Army Medical Bioengineering Research and Development Command to predict deposition rates and dosages to civilians and indigenous plants and wildlife resulting from the use of military smokes in field training exercises. The study had two objectives: (1) to carry out a comprehensive field experiment program to obtain high-quality data on the deposition rates and dosages resulting from smokes emitted by specific military smoke-generating devices,

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and (2) to use those field data, in conjunction with results that can be synthesized from other studies of smokes, to evaluate the performance of predictive models.

A series of fog-oil smoke releases were made at Dugway Proving Ground during March and April 1985. Detailed source measurements, as well as in-situ plume measurements and supporting meteorological data, were acquired during these tests. Dosage, deposition, and particle-size distributions were measured at up to 50 locations in the plume, ranging from 20 m to 1,000 m from the source. The plume samples were found to be almost entirely aerosol, with a less than 1% vapor fraction. Moreover, the droplet sizes had a log-normal distribution with a mass median diameter of 1.0 to 1.6 μm . Isopleth maps of dosage at 1.5 m above the ground were obtained for each test. The data will be used to provide baseline information for toxicology studies and to provide the basis for evaluation and improvement of smoke transport models.

In the model evaluation portion of the program, four Gaussian models were tested with field data from three trials during Smoke Week tests held in previous years by the U.S. Army. Although these data were not obtained for the explicit purpose of model evaluation, they represent the best data available outside of the current project for model testing. The Smoke Week data were collected during fog-oil trials. In a typical trial, 10-100 dosage samplers were set out along one or two transects approximately normal to the plume centerline at distances of about 50 to 80 m downwind. Model-data comparisons, such as illustrated in Figure 2.12, revealed that all four models were within factors of two to three in predicting dosages at each of the rows of samplers (Policastro et al. 1985a). The measurements from our studies differ from the Smoke Week tests in that our data involve longer runs of the smoke generator, greater distances downwind, and include particle sizing and deposition measurements.

2.5.6 Evaluation of Short-Term, Long-Range Transport Models

A.J. Policastro, M. Wastag, L. Coke*, R.A. Carhart*, and W.E. Dunn**

In the March 1980 Federal Register, the U.S. Environmental Protection Agency (EPA) published a request for submission of long-range transport models for possible inclusion in the next revision of EPA's "Guideline on Air Quality Models." Eight models have been accepted as candidates for consideration: RTM-II, MESOPUFF, MESOPUFF-II, MESOPLUME, MSPUFF, RADM, MTDDIS, and ARPPA. These models predict short-term averages (3, 12, 24 hours) of SO_2 , sulfates, and particulates over distances of 20 to 1000 km from single or multiple sources. Argonne has been contracted by EPA to evaluate the performance of these models with field data. An important component in the evaluation is the use of statistics recommended by the American Meteorological Society, coupled

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Figure 2.12. Comparison of dosage predictions of four models with field data from Smoke Week III, Trial 19, for sample lines 60 m (above) and 100 m (below) downwind of the point source. The source and the dosage samplers were at heights of 1.7 to 2.0 m, respectively, above the ground.

with supplementary graphical methods, to quantify and interpret the performance of the models. Data bases used to test the models represent single pollutant sources in which concentrations above background can be detected over mesoscale distances. The major application of the models in the EPA regulatory framework is for Prevention of Significant Deterioration (PSD) analyses for pristine (Class I) areas. Long-range transport models are required in calculations made at distances beyond 20 to 50 km, the limits of applicability of straight-line Gaussian models.

The eight models are being evaluated with two data bases. The first data base encompasses two tracer releases from Norman, Oklahoma, in July 1980, with samplers located on 100- and 600-km arcs. The second data base includes 15 data cases of two- to six-day periods of release of krypton-85 from the Savannah River Plant. Transport distances to samplers for the Savannah River Plant cases varied from 28 to 144 km. The period of study for the data was from October 1976 to July 1977.

Early work (PolICASTRO et al. 1983) involved the testing of two models, RTM-II and MESOPUFF, with krypton-85 tracer plume data taken at the Savannah River Plant during the period 1976-1977. Fifteen datasets covering between one and twelve 10-hour periods are used for model testing. Thirteen samplers within 144 km of the tracer release points provided 10-hour averages of krypton-85 concentrations. Conclusions drawn from the early work included the observation that sizeable errors often exist in the direction of the predicted plume and that there is a tendency to underestimate the amount of horizontal spreading. Model performance statistics are poor when points are paired in space and time, because of the errors in predicted plume orientation. Application of unpaired statistics revealed slightly better performance. The commonly used American Meteorological Society performance statistics do not permit the separation of the effects of errors of directionality and dispersion. Methods to evaluate statistically the correctness of the ground concentration pattern irrespective of point by point performance are being examined.

Seven of the eight models have been run with the July 8, 1980, tracer release data from Norman, Oklahoma. The release occurred during a three-hour period from nozzles that were about 1 m above ground level. For this test, a meteorological grid of 1000 km (east-west) by 800 km (north-south) was established. The grid included 24 surface stations and 8 upper-air stations. A grid size of 20 km x 20 km was used for meteorological modeling (wind field and mixing heights).

The model predictions indicated that the observed plume at the 600-km arc arrived ahead of each of the eight predicted plumes by at least one to about nine hours. For the 100-km arc, some models predicted arrival before the observed plume; some of the model predictions lagged the observed plume. A spatial offset existed as well, due largely to the assumptions made in the meteorological preprocessor (wind field prediction). Comparisons of predicted and observed concentrations on a paired basis in time and space were poor because of this time-lag and spatial offset problem. On an unpaired basis,

however, the peak predictions were within a factor of two of the observed (comparing the average of the highest 25 observed to highest 25 predicted) for five of the seven models tested at Oklahoma. A method to evaluate the capability of the models to predict the correct ground concentration pattern (located apart from the observed ground concentration pattern) is currently underway. Such a method would supplement model evaluation procedures using the American Meteorological Society statistics.

2.5.7 Dispersion in Urban Areas

C.M. Sheih

The use of diesel-powered automobiles has attracted considerable attention because they consume about 25% less fuel by volume than gasoline engines of the same power (e.g., Paul 1979). On the other hand, the potential impact upon the environment from increased use of diesel-powered cars is not clear. Compared with gasoline engines, diesel engines produce less carbon monoxide and total hydrocarbons. However, they generate a new spectrum of hazardous, potentially carcinogenic substances, such as benzopyrene (Santodonato et al. 1978). The most obvious emission increase from diesel engines is particulate matter. In addition, more than 90% of the mass of diesel emissions is in the form of particles of diameters less than 1 μm . These sizes are generally considered respirable because they are capable of passing into the pulmonary alveoli without significant impaction or removal in the upper respiratory track.

To study the impact of a potential increase in diesel emissions on atmospheric particle concentrations and size distributions, we conducted numerical simulations of particle dispersion over Chicago and surrounding suburban areas. The numerical model used is an Eulerian model developed earlier by Sheih (1977) that solves a system of finite-difference equations containing the mechanisms of thermal coagulation, advection, turbulent diffusion, and surface dry deposition. Twenty-one particle diameters with a uniform logarithmic increment are used to simulate the range of particle diameter from 0.001 to 100 μm . In this study we compared the simulated particle concentrations of vehicular emission (i.e., Paul 1979) for a "base" year and for a year after a projected dramatic increase in diesel emissions. The results indicated that the projected increase in diesel emissions would affect mainly the accumulation mode (diameter near 0.2 μm), whose concentration would be increased by about a factor of ten, while the concentration of particles of the Aitken nuclei mode (diameter near 0.02 μm) would be reduced significantly due to more active coagulation.

Parts A, B, and C of Figure 2.13 show contours of simulated concentrations of total, fine, and coarse particles, respectively, where the particle diameter dividing the two modes is 1 μm . The value 75 $\mu\text{g m}^{-3}$ of the contours represents the current primary air quality standard for annual average particulate concentrations. Figure 2.13(A) shows that only a small

area near an intersection of major highways exceeds the air quality standard. The pattern is shifted slightly southward from the intersection due to a high volume of trucking operations in this warehouse and industrial area. For the fine particle mode in Figure 2.13(B), no area exceeds the standard, and the contour of the maximum concentration is $40 \mu\text{g m}^{-3}$. This is further reduced to $20 \mu\text{g m}^{-3}$ for the coarse particle mode. The corresponding contours of particle concentrations with the emissions projected for the year 2000 show that the impact of the assumed increase in diesel emissions would be very significant for both total and fine particles but quite minor for coarse particles. The projected increase in diesel emissions would result in the air quality standard being exceeded in the entire city of Chicago and in some of the surrounding suburban areas.

Figure 2.13. Simulated contours (solid lines) of concentrations ($\mu\text{g m}^{-3}$) of (A) total, (B) fine, and (C) coarse particles for the year 1983. The $75 \mu\text{g m}^{-3}$ is the primary air-quality standard for annual average values. Dashed lines represent major highways.

2.5.8 Mathematical Modeling of Noise Impacts from Nuclear Power Plants

A.J. Policastro, R. Liebich, and W. E. Dunn**

The U.S. Nuclear Regulatory Commission (NRC) must provide an independent assessment of the impact of noise from the operation of each nuclear power plant under review for a construction or operating license. This NRC review includes determination of the impact of noise on the residents in the community surrounding the plant and verification that applicable community noise-control regulations are satisfied. Argonne has been aiding NRC in this review for four years.

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The NRC work is divided into two parts. The first part is ongoing and involves the development of a standard review plan by which guidance is provided to the NRC review staff in the preparation of the noise section of environmental impact statements. Acceptable methods are delineated for the modeling of noise propagation from such equipment as cooling towers, transformers, transmission lines, and loudspeakers. Recommendations are also given with respect to acceptable noise measurement instrumentation, methodologies for the monitoring of ambient noise, and the monitoring of the subsequent increased noise levels from plant operation. It is expected that the standard review plan document would be requested by applicants as guidance in their development of a noise monitoring and modeling program that would be acceptable to NRC.

The standard review plan consists of two documents. Part I provides a summary of the plan for administrators. It is aimed at providing information as to the threshold of acceptability of impacts from the various equipment at the plant site, and it also defines the conditions under which detailed modeling of noise impacts is necessary. The need for a detailed noise analysis depends largely on the kinds of major noise-making equipment at the site, as well as the location of the nearest noise-sensitive areas. Part II of the standard review plan is a detailed handbook of acceptable modeling and monitoring methodologies.

A major component to the modeling methodology presented in the handbook is the application of a noise prediction model (Dunn et al. 1983) based on the Edison Electric Institute Environmental Noise Guide. The computer model developed by Dunn et al. predicts noise levels from an arbitrary number of outdoor/indoor sources and receiver locations in the community. The model includes the effects of sound attenuation with distance along with molecular and anomalous attenuation based on ambient temperature and humidity. In addition, the attenuation caused by the ground, trees, and other vegetation can be simulated. The frequency, temporal, and directional characteristics of all noise sources are treated. Model predictions are made in terms of octave band sound pressure levels at any receptor and in terms of several indicators of community noise impacts. Separate calculational methods (outside the framework of the computer model) are presented to model noise from the transmission lines and from the power plant loudspeaker system.

The second part of the project has been completed and involved the application of this review methodology to about a dozen NRC licensing cases in which noise impacts were thought to be significant. Operational noise levels were predicted and likely community impacts were projected for the following plants: Catawba, Shearon Harris, Limerick (including the Point Pleasant and Bradshaw reservoir pumphouses), Bellefonte, Braidwood (nuclear site and pumphouse), Millstone, River Bend, Beaver Valley, and Vogtle. A description of these applications, including the results of the modeling, was included in the environmental impact statements published by the NRC for these nuclear power plants (operating license stage).

2.5.9 Cooling Tower Plume Dispersion--SACTI User's Manual

A.J. Policastro, L. Coke, M. Wastaq,* R.A. Carhart,* W.E. Dunn,*
P. Gavin,* and B. Boughton**

Siting and licensing studies for power plants that will use cooling towers must include consideration of such environmental effects as the general appearance of vapor plumes, salt-drift deposition, plume-induced fogging and icing at ground level, and shadowing (blocking the sun's rays). Work done during 1979-1982 at Argonne and at the University of Illinois led to the development of extensively validated models that predict vapor and drift plumes for a given set of meteorological data and tower conditions. These models, however, did not take seasonal and annual variations into account.

The purpose of this project was to develop the theory and provide a user's guide (Policastro et al. 1984) for a mathematical model for the prediction of the seasonal and annual physical impacts of cooling tower plumes, drift, fogging, icing, and shadowing. The model, Seasonal-Annual Cooling Tower Impacts (SACTI), is intended to provide predictions for use in the licensing of power plants with cooling towers. The submodels for these physical impacts provide improvements in theory and performance compared with existing methods.

The seasonal-annual methodology employs a new technique that reduces the available meteorological record at a site to approximately 30 to 100 categories. The plume submodels are then run once for a representative of each category, and the results are summed to provide predictions for a season or the year.

The model allows the treatment of any number of natural- or mechanical-draft cooling towers in any geometrical orientation. The model is easy to use and requires a minimal amount of user input. It is set up to run with a TDF-14 or CD-144 ground-level meteorological tape or standard NRC meteorological tape.

The model encompasses four computer codes in which the output of one is the input to the next. In this way, intermediate output that may be informative is saved and may be examined. The use of a sequence of four codes permits more flexibility to the user and provides the opportunity to better define the type and scale of printed output.

The model has been applied in two case studies, one for a site with three nearly colinear natural-draft cooling towers, and the other for a site with two linear mechanical-draft cooling towers oriented parallel to each other. Input and output of the codes were presented by Policastro et al. (1984).

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2.6 STUDIES OF AQUATIC SYSTEMS

2.6.1 Summary

The Atmospheric Physics Program's research on aquatic systems is divided among three major study areas: (1) aquatic ecosystem modeling, (2) analysis of Great Lakes water-quality surveillance data, and (3) in-situ observations of the physical and sedimentological conditions within the benthic boundary layer in the Great Lakes. Although seemingly disparate, our work in each of these areas is directed toward understanding the effects and fate of toxic and nutrient contaminants on aquatic ecosystems, in particular the Great Lakes. Two of the projects, ecosystem modeling and analysis of Great Lakes water-quality data, have been supported by the Environmental Protection Agency's Great Lakes National Program Office. The third project, benthic boundary layer observations, has been supported by the National Oceanic and Atmospheric Administration's Great Lakes Environmental Research Laboratory. All three projects are conducted with the close cooperation and participation of scientists from the sponsoring agencies.

Because the overall size of these three projects is small (less than one person-year of effort in FY 1985 and FY 1986), part of our approach has been to combine those aspects of the three subprojects that relate to common processes of general importance. In this sense, we use the aquatic ecosystem modeling work (subproject 1) as a method of expressing tentative hypotheses whose predictions can be examined using the water-quality data and historical information analyzed as part of subproject 2. Since our field work (subproject 3) is concentrated on studies related to the transport of particle-bound contaminants, we hope to use the results of that work both to improve our model parameterization and to quantify the uncertainty associated with particle-related processes in aquatic ecosystem models.

Another component of our aquatic systems research is application of a three-dimensional grid model to describe the thermal performance of ultimate heat sink (UHS) cooling ponds. This work has been done for the U.S. Nuclear Regulatory Commission. The advantage of the model lies in the ability to determine the detailed character of the flow field, whether it be one, two, or three dimensional. Existing models require a-priori knowledge of the character and dimensionality of the flow field in such ponds. Evaluation of the model has been accomplished by comparison of predictions with data from field and laboratory ponds.

2.6.2 Aquatic Ecosystem Modeling

B.M. Lesht

Nutrient-driven eutrophication, or the overfertilization of phytoplankton due to anthropogenic phosphorus loadings, has been a concern in the Great Lakes since the early 1960s. Our efforts in aquatic ecosystem modeling began as a project to implement a numerical model of nutrient-based eutrophication

of Lake Michigan (Lesht 1982a). This model was used to examine the likely outcome of different nutrient-loading strategies on the long-term water quality of the lake under the assumptions that both nutrient loading and within-lake removal processes are stochastic. We used Monte-Carlo techniques to quantify the uncertainty in the model forecasts associated with variability in the loading and within-lake removal processes. The results of this study (Lesht 1984a, 1984b) show that water quality in Lake Michigan can be expected to continue to improve.

Work with the dynamic eutrophication model led to development of a time-dependent, multi-segment, mass-balance model for contaminants in all of the Great Lakes (Lesht 1985). This model can be used to examine the effects of contaminant loading and within-lake removal processes (associated with particulate settling) on the Great Lakes as a system, thereby recognizing that conditions (either contamination or control) occurring in one of the lakes can affect the other lakes as well.

We are currently using the time-dependent, multi-segment, mass-balance model in a study of the effects of uncertainty in nutrient loading and removal processes on determining optimal strategies for basinwide phosphorus control on the Great Lakes. Previous studies (Chapra et al. 1983) have used a steady-state version of the multi-segment mass-balance model with phosphorus concentration and loading information from the mid 1970s to determine an optimal basinwide strategy for phosphorus control. In our work (Fontaine and Lesht 1985), the time-dependent model is coupled with a linear programming optimization routine to find the least-cost allocation of phosphorus controls across the entire basin. The questions we wish to answer include (1) how does one select an optimal strategy for phosphorus control under uncertain conditions, and (2) what are the likely results of both current and projected treatment strategies given that the processes controlling the results are stochastic?

Some of the early results of this work are presented in Table 2.5, which shows the estimated added annual cost (above those calculated by Chapra et al. 1983) for several phosphorus treatment scenarios. Scenarios 5 and 6 in this table are examples of strategies developed under the assumption of uncertainty. The Optimal Treatment Strategy for Stochastic Conditions (OTSSC) - Scenario 5, for example, is based on the maximum treatment capacity and allocation determined after 100 Monte-Carlo iterations of the mass-balance model. Scenario 6 is a treatment allocation based on the average capacity determined in similar Monte-Carlo fashion.

We expect that the techniques we develop for examining phosphorus-control strategies also will be applicable to strategies for control of toxic materials in the Great Lakes. We furthermore expect that our sensitivity analysis will demonstrate that there is a need to improve basic understanding of the processes responsible for within-lake removal of particle-bound pollutants.

Table 2.5. Estimated added annual cost for several hypothetical phosphorus control scenarios

Treatment	Description	Added Annual Cost (millions of dollars)
1	No additional treatment over mid-1970s levels	0
2	Optimal treatment levels based on nonstochastic simulation with updated (1985) conditions	49
3	Treatment levels specified by the 1978 Canada-U.S. agreement	440
4	All potential treatment capacity utilized (Chapra et al. 1983)	908
5	Optimal treatment levels based on maxima of stochastic simulations	652
6	Optimal treatment levels based on average of stochastic simulations	19

2.6.3 Analysis of Great Lakes Surveillance Data

B.M. Lesht

Control of phosphorus is just one of the national goals for restoring and improving the quality of the Great Lakes that were delineated in the 1978 Water Quality Agreement between the United States and Canada. Part of this agreement requires that the parties conduct water-quality surveillance programs to collect data necessary for the ongoing assessment of the condition of the Great Lakes, as well as for improving understanding of the Great Lakes ecosystem. Much of these data are collected by the U.S. Environmental Protection Agency's (EPA) Great Lakes National Program Office. Argonne has cooperated with EPA on analysis and interpretation of the data collected in 1983 and 1984 from lakes Erie, Huron, and Michigan. The general goals of the program and our analyses are to (1) determine the present state of the lakes in terms of nutrient concentrations, (2) use the recently collected data along with historical information to evaluate water-quality trends and variability in the three lakes, and (3) compare the recent observations with forecasts made using dynamic eutrophication models and historical loading estimates.

The complete analysis of the 1983 data was reported by Lesht and Rockwell (1985). We determined that in general, the conditions of the three lakes had improved since they were last surveyed in the late 1970s. Total phosphorus concentrations in lakes Michigan and Huron remained well below the target levels established in the water-quality agreement. Total phosphorus levels in the eastern and central basins of Lake Erie also were declining, although the

concentration in the western basin had not changed over the last several years. There is some evidence to suggest that this may be due to phosphorus regeneration from the sediments in the western basin.

All three lakes showed an increase in the concentration of nitrate-nitrite nitrogen, which may be a result of increased (or uncontrolled) loading or of reduced uptake due to phytoplankton growth, which is limited by the lower concentrations of available phosphorus. Seasonal depletion of epilimnion nitrate-nitrite, an indirect measure of eutrophication, was slightly (although not significantly) lower in Lake Michigan. The concentration of reactive silica in the water in Lake Michigan, where silica depletion has been a concern, had remained stable or increased slightly over ten years.

Simulations using nutrient-based eutrophication models of the three lakes were moderately successful in predicting the 1983 observations when initialized with historical data and forced with estimates of annual phosphorus load. Notable discrepancies between model predictions and field observations were found in Lake Michigan and in the western basin of Lake Erie. In both cases, the models underpredicted total phosphorus concentrations observed in 1983. The likely cause of this underprediction in both cases is a poor parameterization of the within-lake loss terms of the models.

We are continuing these analyses with the 1984 surveillance data collected by the Great Lakes National Program Office. Of considerable interest will be comparison of the 1984 data with the data collected in 1983 using identical sampling techniques and analytical methods. We also hope to conduct a preliminary evaluation of year-to-year variability in several water-quality indicators using these data.

2.6.4 Benthic Boundary Layer Experiments

B.M. Lesht

2.6.4.1 Benthic Nepheloid Layer in Southern Lake Michigan

Our analysis of surveillance data collected from lakes Michigan and Huron in 1983 and 1984 shows that after stratification, the concentrations of both nutrients and particulates in the region just above the sediment-water interface were enriched relative to the overlying waters. This enrichment is due to settling of particulate matter through the thermocline into the hypolimnion. These particulates subsequently are prevented from mixing with the overlying epilimnetic water due to gravitational stability. However, the particulate matter does not leave the water column, but remains in suspension in a layer near the bottom that may be 10-15 m thick. This layer, which is defined by an elevated concentration of particles and, hence, turbidity, is termed the "benthic nepheloid layer" and has been the focus of our deep-water field studies in recent years. Since many contaminants of concern are associated with lake sediments, especially the suspended, fine-grained sediments, observations of the behavior of the sediments in the benthic

nepheloid layer are essential for the development of any complete model of pollutant dispersal and fate in the Great Lakes.

To conduct these analyses, we make in-situ observations of horizontal current velocity, water temperature, and turbidity within 1 m of the sediment-water interface. The observations are made with sensors mounted on an aluminum tripod (Lesht 1982b). We made two deployments of the instrumented tripod in Lake Michigan in 1984 (Table 2.6). Both were conducted in waters 75 m deep--the first in late spring before stratification, the second in the early fall after maximum stratification. The first deployment took place in conjunction with the deployment of a string of sediment traps by the Great Lakes Environmental Research Laboratory (NOAA) and with a profiling near-bottom water sampler (Clemson University). The second deployment was done in conjunction with a large-scale experiment in lake circulation conducted by the Great Lakes Environmental Research Laboratory.

Table 2.6. Summary of deployments of Argonne instrumented tripod, 1984-1985

Deployment	Dates	Location ^a	Depth	Hours of Data
840203	26 April - 15 May 1984	42° 21.61'N 86° 39.76'W	75 m	456.5
840205	4 October - 25 October 1984	43° 01.11'N 86° 25.15'W	75 m	503.75
850203SC	11 July - 7 August 1985	42° 23.5'N 82° 34.0'W	6.5 m	648
850206SC	11 September - 9 October 1985	42° 24.5'N 82° 41.7'W	7m	660

^aThe 1984 deployments were in Lake Michigan; the 1985 deployments were in Lake St. Clair.

The basic results of the first deployment are illustrated in Figure 2.14. Near-bottom current speed during the observation period was generally low, below 0.04 m s^{-1} . There was one episode of higher flow (30 April) during which the horizontal speed reached 0.12 m s^{-1} . Although the concentration of total suspended material (TSM) as inferred from the transmittance measurements increased steadily during the deployment, there was very little correlation between transmittance and current speed. The bottom water temperature also increased steadily during the deployment, warming from 2.2°C to 3.4°C . The temperature record implies that the water column was slightly stable and not completely mixed vertically. Comparison of the total suspended material data to horizontal sediment flux showed that the observed variations in TSM seemed to be related to flows from the south and west of the tripod. This implies that the advection of already suspended material

accounted for most of the observed TSM signal. The vertical sediment fluxes measured by the sediment traps (Figure 2.15) show the expected pattern of high flux near the bottom. This flux, however, apparently was not due to local resuspension, but to flux from the advected nepheloid layer.

Figure 2.14. Horizontal current speed, total suspended material, and water temperature within 1 m of the bottom at 75-m depth in southern Lake Michigan during April and May 1984.

Figure 2.15. Vertical sediment flux at the 75-m depth in southern Lake Michigan during April and May 1984.

Our preliminary analysis of the results of this first deployment and the later, October, excursion suggested that the benthic nepheloid layer is not loaded by material resuspended in deep water. However, the concentration of material in the nepheloid layer does increase during the stratified period, probably as a result of advection of particles from shallower depths and by more or less constant resuspension of recently deposited, easily eroded sediments.

These observations also showed that the deeper waters of the Great Lakes are not quiescent, even after stratification. Clearly the material comprising the nepheloid layer is kept in suspension and the bottom flows can be quite variable and responsive to surface wind forcing. As a result, the concentration of material suspended within the nepheloid layer fluctuates as the layer is mixed into the overlying waters and reforms during less energetic conditions.

2.6.4.2 Benthic Boundary Layer in Lake St. Clair

We currently are using the instrumented tripod in a study of the benthic boundary layer and sediment transport pattern in Lake St. Clair, a shallow (maximum depth of 10 m) lake between the St. Clair River (which drains Lake Huron) and the Detroit River (which feeds Lake Erie). This river-lake system is one of two channel systems (St. Mary's River, draining Lake Superior into Lake Huron, is the other) that are being studied by an international consortium under the auspices of the Upper Great Lakes Connecting Channels Study (UGLCCS).

This study is jointly funded by the United States and Canada. The overall goal of the study is to define and quantify the pathways by which pollutants move between the upper Great Lakes. Our initial role is to provide data on the relationship between resuspension and transportation of sediments within Lake St. Clair and meteorological forcing.

We conducted two field experiments in Lake St. Clair during 1985 (Table 2.6). The first experiment was only partially successful because one channel of the two-axis current meter failed. However, we were able to infer some interesting features of the flow-sediment interaction. We found, for example, that turbidity is well correlated with the variance of the one operational current meter channel, which should be an analog to surface wave activity. We also found that the episodes of high current variability are very short, usually lasting only two or three hours. Further interpretation will be done when supplemental data from a Canadian meteorological buoy near the experiment location becomes available. Data from the second Lake St. Clair deployment has not been analyzed as yet. All sensors operated normally, however. More deployments in Lake St. Clair will be made during 1986.

2.6.5 Mathematical Modeling of Ultimate Heat Sink Cooling Pond Thermal Performance

A.J. PolICASTRO, M. Wastag, W.E. Dunn,* and R.A. Carhart**

The mathematical modeling of the thermal performance of ultimate heat sink (UHS) cooling ponds should account for the major physical mechanisms involved in the flow and surface heat transfer, including the interaction between the thermal and hydraulic aspects of the flow. It is often assumed that the small, heavily loaded, irregularly shaped nature of the UHS pond has the same character flow field as normal cooling ponds used for power plant cooling. Such ponds are generally vertically stratified, with a top layer consisting of the discharged warm water and the bottom layer consisting of cold water. In both types of ponds, water is removed through a bottom intake to support the recirculation process.

The U.S. Nuclear Regulatory Commission has established stringent safety standards on the design of cooling ponds as ultimate heat sinks for nuclear power plants. A typical UHS cooling pond is irregularly shaped, covers an area of about 30 to 60 acres, and has an average depth of 6 to 20 ft. The UHS pond would be heavily loaded during operation, running as much as 15 to 20 MW per acre. The intake temperature of the pond must be kept low enough to ensure the operation of safety-related equipment in the plant during and after emergency shutdown.

On behalf of NRC, we evaluated the adequacy of existing models of UHS thermal performance and characterized the behavior of UHS ponds. We addressed the following sets of questions:

- (1) Are the commonly used engineering formulas for surface heat transfer applicable to small, hot ponds that can reach temperatures as high as 160°F (71°C) during operation?
- (2) What is the structure of the flow field in these UHS ponds? More specifically, are such hot ponds strongly stratified as is commonly assumed? Also, what are the relative contributions of wind stress, discharge/intake flow, and buoyant convective motions to the thermal-hydraulics of these ponds?

To answer the first question, we made calculations to test the common engineering formulas for surface heat transfer for three hot pond experiments at Raft River, as reported by Athey (1982). The Ryan-Harleman Model (Ryan and Harleman 1973) performed very well with these data, indicating that no further improvements were warranted.

To answer the second set of questions, we modified the three-dimensional numerical model of Paul and Lick (1983) to treat UHS cooling ponds and then verified the modified model with relevant laboratory and field data. The Paul

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model was modified in the following ways: (1) a time-dependent heat load was added, (2) the Ryan-Harleman method was added to treat the time-dependent heat transfer, (3) boundary conditions at the intake were chosen to represent specified intake velocities which varied with time, and (4) an updated treatment of surface wind stress was added.

The modified model was verified using a laboratory experiment carried out by Cerco (1977) and with field data measured at the H.B. Robinson cooling pond in South Carolina (Carolina Power & Light Company 1979). The model performed very well in representing the main features of the temperature pattern and in predicting the measured intake temperatures.

Application of the revised model indicated surprising results (PolICASTRO et al. 1985b), as applied to a typical UHS case (Catawba UHS cooling pond). Figure 2.16 illustrates the predicted flow field at the surface of the Catawba pond at the time of peak intake temperature. The modeling revealed that the balance of physical mechanisms for the cooling of UHS cooling ponds is quite different than for ponds used in normal power plant cooling. The small, heavily loaded, irregularly shaped nature of a UHS pond will, in most cases, lead to a vertically mixed pond with only a one-dimensional (longitudinal) variation in pond temperature. Strong convective circulations resulting from the buoyancy of the discharge and the strong discharge/intake flow are supplemented by the removal of heat from the surface, leading to a breakdown in vertical stratification.

Figure 2.16. Surface horizontal velocities of Catawba UHS cooling pond at time of peak intake temperature after a hypothetical reactor accident.

The Paul-ANL model is proposed for use in the analysis of future UHS cooling ponds; such a model can be used to determine the detailed character of the flow field (whether it be one-, two-, or three-dimensional). It is not possible to categorize the flow field with certainty a priori for all pond designs. A methodology is presented in Policastro et al. (1985) for the use of zero-, one-, and three-dimensional models in analyzing UHS pond performance.

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APPENDICES FOR CHAPTER 2
Atmospheric Physics Program

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APPENDIX 2-A. STAFF QUALIFICATIONS
Atmospheric Physics Program

Name	Position	Highest Degree	Major	Year Received	Institution
Cook, David R.	Scientific Assistant	M.S.	Meteorology	1977	The Pennsylvania State University
Coulter, Richard L.	Meteorologist	Ph.D.	Meteorology	1976	The Pennsylvania State University
DePaul, Frank T.*	Postdoctoral Appointee	Ph.D.	Environmental Engineering	1984	Illinois Institute of Technology
Frenzen, Paul	Senior Meteorologist	Ph.D.	Meteorology	1964	The University of Chicago
Hart, Richard L.	Scientific Associate	B.S.	Mathematics	1970	Illinois Institute of Technology
Hong, Min-Sun	Postdoctoral Appointee	Ph.D.	Chemical Engineering	1985	University of Iowa
Hess, Paul E.	Scientific Associate	B.S.	Physics	1958	Wheaton College
Lee, In-Young	Meteorologist	Ph.D.	Meteorology	1975	University of California-Los Angeles
Lesht, Barry M.	Physicist	Ph.D.	Geophysical Sciences	1977	The University of Chicago
Martin, Timothy J.	Scientific Associate	B.A.	Physics	1974	Beloit College
PolICASTRO, Anthony J.	Mechanical Engineer	Ph.D.	Civil Engineering	1970	Columbia University
Shannon, Jack D.	Meteorologist	Ph.D.	Meteorology	1975	University of Oklahoma
Sheih, Ching-Ming	Meteorologist	Ph.D.	Aerospace Engineering	1969	The Pennsylvania State University
Sisterson, Douglas L.	Assistant Meteorologist	M.S.	Atmospheric Science	1975	University of Wyoming
Wesely, Marvin L.	Meteorologist	Ph.D.	Soil Science	1970	University of Wisconsin

*No longer a member of the Division.

APPENDIX 2-B. OUTSTANDING PROFESSIONAL ACTIVITIES AND AWARDS
Atmospheric Physics Program

R.L. COULTER--named member of American Meteorological Society Committee on Atmospheric Measurements.

P. FRENZEN--appointed Professor, Department of Geophysical Sciences, University of Chicago (Joint Appointment); named member of American Meteorological Society Committee on Boundary Layer and Turbulence; session chairman (Flow over Complex Terrain) at American Meteorological Society Seventh Symposium on Turbulence and Diffusion, November 1985; named member of Environmental Protection Agency Peer Review Committee on Urban Particulate Modeling Program; Visiting Scientist, CSIRO Division of Environmental Mechanics, Canberra, Australia, February-March 1984.

B.M. LESHT--named chairman of International Joint Commission's Lake Michigan Task Force.

A.J. POLICASTRO--appointed special representative by Electric Power Research Institute to evaluate new West German technology on stack gas discharge from cooling towers.

J.D. SHANNON--named member of American Meteorological Society Committee on Radioactivity and Atmospheric Chemistry; became Certified Consulting Meteorologist; named member of Interagency Task Force on Acid Precipitation; named chairman of EPA Peer Review Committee on Regional Particulate Modeling Program; session co-chairman (Acid Rain) American Institute of Chemical Engineers Annual Meeting, November 1985.

D.L. SISTERSON--named Secretary and subsequently Vice-Chairman of Subcommittee #2 (Methods and Quality Assurance) of National Atmospheric Deposition Program.

M.L. WESELY--named member of Electric Power Research Institute Peer Review Panel on the Integrated Forest Study; named member of Steering Committee for DOE's PRECP program; named coordinator of Air-Surface Dry Exchange Processes proposal for DOE.

D.R. COOK, R.L. HART, AND M.L. WESELY--Invited participants in West German "TULLA" program, March 1985.

APPENDIX 2-C. SPECIAL EVENTS ORGANIZED
Atmospheric Physics Program

- R.L. COULTER organized Environmental Research Division Seminar (Speaker: W. Mach, Florida State University; Title: On the inversion of temperature and humidity profiles over a water surface: work in progress), 15 March 1984, Argonne National Laboratory.
- R.L. COULTER organized Environmental Research Division Seminar (Speaker: L. Kristensen, Risø National Laboratory; Title: The effects of line averaging on solar flux measurements with a sonic anemometer near the surface), 20 March 1984, Argonne National Laboratory.
- P. FRENZEN organized briefings on atmospheric research at Atmospheric Physics Program, Environmental Research Division, 26 July 1984, Argonne National Laboratory.
- M.L. WESELY organized PRECP workshop for U.S. Department of Energy, 9-11 October 1984, Argonne National Laboratory.
- R.L. COULTER organized Division Seminar (Speaker: Roland Stull, University of Wisconsin; Title: Transilient turbulence: theory and applications), 21 May 1985, Argonne National Laboratory.
- J.D. SHANNON organized and co-hosted summer institute on Acid Rain Control: Developing a Consensus for Action, 14-16 August 1985, Argonne National Laboratory.
- J.D. SHANNON organized and hosted CAPTEX Model Evaluation Workshop, 5-6 November 1985, Argonne National Laboratory.
- P. FRENZEN organized and taught two-day workshop for Division of Educational Programs, Introduction to Micrometeorology, 16-17 November 1984, Argonne National Laboratory.
- D.R. COOK provided a workshop for the Weather Merit Badge for the Boy Scouts of America and gave demonstrations on wet and dry deposition for the Argonne Explorer Post, Fall 1985, Argonne National Laboratory.

APPENDIX 2-D. EDUCATIONAL PROGRAM PARTICIPANTS
Atmospheric Physics Program

- T. FRANK DEPAUL. Illinois Institute of Technology. Postdoctoral Appointee. Conducted field research on dry deposition of fine particles. January 1984 - February 1986.
- MIN-SUN HONG. University of Iowa. Postdoctoral Appointee. Conducted research on numerical modeling of atmospheric chemical processes. August 1985 - present.
- MARY LIAW. North Central College, Illinois. Faculty Research Leave Participant. Conducted research on atmospheric lightning and in-cloud production of nitrogen oxides. June-December 1985.
- ADAM W. BURNETT. Ohio University. Thesis Parts Program. Conducted research on influence of synoptic conditions on local air chemistry. July 1985 - present.
- SARA WOOD. University of Western Illinois. Thesis Parts Program. Conducted research on influence of local sources on air quality. March 1985 - present.
- CHRISTOPHER A. BADALI. The Pennsylvania State University. Undergraduate Research Program. Conducted research on acidic wet deposition and remote sensing. June - August 1985.
- ADAM W. BURNETT. Aquinas College, Tennessee. Undergraduate Research Program. Conducted research on acoustic remote sensing of fair weather clouds. June - August 1984.
- JANICE L. COEN. Grove City College, Pennsylvania. Undergraduate Research Program. Conducted research on acidic wet deposition and remote sensing. June - August 1985.
- KAREN J. KOWALEWSKY. State University of New York at Oswego. Undergraduate Research Program. Conducted micrometeorological studies of dry deposition. June - August 1984 and 1985.

STANLEY K. LENGERICH. Ball State University, Indiana. Undergraduate Research Program. Conducted research on environment of outdoor exposure chambers. September - November 1985.

MARK A. MILLION. University of Iowa. Undergraduate Research Program. Conducted research on numerical modeling of long-range transport and deposition. June - August 1985.

MICHAEL A PEZZIMENTI. Stockton State College, New Jersey. Undergraduate Research Program. Conducted research on micrometeorological and boundary-layer physical processes. June - August 1984.

MICHAEL P. NORTH. Eastern Illinois University. Undergraduate Research Program. Conducted research on simulation of atmospheric dispersion with minicomputers. June - August 1985.

MARK E. SCHNEIDER. University of Maine. Undergraduate Research Program. Conducted research on atmospheric numerical modeling of long-range transport and deposition. September - December 1985.

FREDERICK L. WASMER. University of Illinois. Undergraduate Research Program. Conducted research on numerical simulation of atmospheric dispersion. June - August 1985.

APPENDIX 2-E. PUBLICATIONS AND ORAL PRESENTATIONS 1984-1985
Atmospheric Physics Program

1. Refereed Journal Articles*

1984

Boer, R., E. Eloranta and R.L. Coulter. Lidar observations of mixed layer dynamics: Tests of parameterized entrainment models of mixed layer growth rate. Journal of Climate and Applied Meteorology 23:247-266 (1984). [EPA]**

Schatzmann, M. and A.J. Policastro. An advanced integral model for cooling tower plume dispersion. Atmospheric Environment 18(4):663-674 (1984). [EPRI]

Schatzmann, M. and A.J. Policastro. Effects of the Boussinesq approximation on the results of strongly-buoyant plume calculations. Journal of Climate and Applied Meteorology 23(1):117-123 (1984). [EPRI]

Schatzmann, M. and A.J. Policastro. Plume rise from stacks with scrubbers: A state-of-the-art review. Bulletin of the American Meteorological Society 65(3):210-215 (1984). [EPRI]

Sheih, C.-M. A comparison of wind speed shears for frontal and undisturbed synoptic conditions. Boundary-Layer Meteorology 28:329-342 (1984). [DOE/DSE/PNL]

Sisterson, D.L. and B.E. Wurfel. Methods for reliable pH measurements of precipitation samples. International Journal of Environmental Analytical Chemistry 18:143-165 (1984). [DOE/OHER, EPA/ORD]

*For published material, the names of all Environmental Research Division authors are underlined. (Included are Division members who participated in a project but left the Division before the results were published.)

**Funding agency (abbreviations are spelled out at the end of this appendix). In cases where no funding agency is listed, the publication was not related to any specific funded project.

Wesely, M.L. and J.D. Shannon. Improved estimates of sulfate dry deposition in eastern North America. Environmental Progress 3(2):78-81 (1984). [EPA/ESRL]

1985

DePaul, F.T. and C.M. Sheih. A tracer study of dispersion in an urban street canyon. Atmospheric Environment 19:555-559 (1985). [DOE/OHER]

Lee, I.-Y. and J.D. Shannon. Indications of nonlinearities in processes of wet deposition. Atmospheric Environment 19:143-149 (1985). [DOE/OHER]

Lesht, B.M. Time-dependent solution of multi-segment mass balance models of contaminants in the Great Lakes. Journal of Great Lakes Research 11(2):182-189 (1985). [EPA/GLNPO]

Ruff, R.E., K.C. Nitz, F.L. Ludwig, C.M. Bhumralkar, J.D. Shannon, C.M. Sheih, I.-Y. Lee, R. Kumar and D.J. McNaughton. Evaluation of three regional air quality models. Atmospheric Environment 19:1103-1115 (1985). [EPRI]

Sheih, C.M., B.J. Billman and F.T. DePaul. A method for measuring mean wind velocities in a canyon with tracer balloons. Boundary-Layer Meteorology 32:401-410 (1985). [DOE/OHER]

Sheih, C.M. and F.L. Ludwig. A comparison of numerical pseudodiffusion and atmospheric diffusion. Atmospheric Environment 19:1065-1068 (1985). [DOE/OHER]

Sisterson, D.L., S.A. Johnson and R. Kumar. The influence of humidity on fine-particle aerosol dynamics and precipitation scavenging. Aerosol Science & Technology 4(3):287-300 (1985). [DOE/OHER, EPA/ASRL]

Sisterson, D.L., B.E. Wurfel and B.M. Lesht. Chemical differences between event and weekly precipitation samples in northeastern Illinois. Atmospheric Environment 19(9):1453-1469 (1985). [DOE/OHER, EPA/ASRL]

Streets, D.L., B.M. Lesht, J.D. Shannon and T.D. Veselka. Climatological variability: effect on strategies to reduce acid deposition. Environmental Science and Technology 19:887-893 (1985). [DOE/OEA, EPA/ASRL, EPA/ADAS]

Wesely, M.L., D.R. Cook, R.L. Hart and R.E. Speer. Measurements and parameterization of particulate sulfur dry deposition over grass. Journal of Geophysical Research 90:2131-2143 (1985). [EPA/ASRL]

2. Books, Book Chapters, and Collections of Conference Proceedings

1984

Gillani, N., J.D. Shannon and D.E. Patterson. Transport processes. Chapter A-3, In: The Acidic Deposition Phenomenon and Its Effects: Critical Assessment Review Papers. Vol. 1: Atmospheric Sciences. A.P. Altschuller and R.A. Linthurst (eds.). EPA-600/8-83-016AF. U.S. Environmental Protection Agency. 1984. pp. 3-65 through 3-101. [DOE/OHER, EPA/ESRL]

3. Reports

1984

DePaul, F.T. and C.M. Sheih. A Study of Pollutant Dispersion in an Urban Canyon. ANL/ER-84-1. Environmental Research Division, Argonne National Laboratory. 1984. [DOE/OHER]

Easter, R.C., M.T. Dana, J.M. Thorp, K.M. Busness, J.M. Hales, G.S. Raynor, C.M. Benkovitz, R.L. Tanner and J.D. Shannon. Overview of the Oxidation and Scavenging Characteristics of April Rain (OSCAR) Experiment. PNL-4869. Battelle Pacific Northwest Laboratory. 1984. [EPA/ESRL]

Lesht, B.M. Ten-Year Forecasts of Water Quality in Lake Michigan Using a Deterministic Eutrophication Model. ANL/ER-84-2. Environmental Research Division, Argonne National Laboratory. 1984. [EPA/GLNPO]

Lesht, B.M. Lake Michigan Eutrophication Model: Calibration, Sensitivity, and Five-Year Hindcast Analysis. ANL/ER-84-3. Environmental Research Division, Argonne National Laboratory. 1984. [EPA/GLNPO]

Radiological and Environmental Research Division Annual Report, January-December 1982. Atmospheric Physics. ANL-82-65, Part IV. 1984. [DOE]

Ruff, R.E., K.C. Nitz, F.L. Ludwig, C.M. Bhumralkar, J.D. Shannon, C.M. Sheih, I.-Y. Lee, R. Kumar, D.J. McNaughton and G.R. Hilst. Regional Air Quality Model Assessment and Evaluation. Report EA-3671, Project 1630-21. Electric Power Research Institute. 1984. [EPRI]

Wesely, M.L. (editor). Air-Surface Dry Exchange Processes. ANL/ER-TM-84-4. Environmental Research Division, Argonne National Laboratory. 1984. [DOE/OHER]

Wesely, M.L., D.R. Cook and R.L. Hart. ANL Micrometeorological Measurements of Surface Fluxes at the 1982 Dry Deposition Intercomparison Experiment. Data summary report of EPA-sponsored experiment; submitted to Illinois State Water Survey. 1984. [EPA/ESRL]

1985

Ellestad, T.G., R.E. Speer, B.B. Hicks and M.L. Wesely. Development of Direct Methods for Measuring Dry Deposition: A Progress Report. Informal report to the U.S. Environmental Protection Agency. 1985. [EPA/ASRL]

Environmental Research Division Annual Report. Atmospheric Physics. January-December 1983. ANL-83-100, Part IV. Argonne National Laboratory. [DOE]

Lesht, B.M. Observations of Near Bottom Conditions Within the Benthic Nepheloid Layer in Southern Lake Michigan. Summary Report to the Great Lakes Environmental Research Laboratory, National Oceanic and Atmospheric Administration. 1985. [NOAA/GLERL]

Lesht, B.M. and D.C. Rockwell. The State of the Middle Great Lakes: Results of the 1983 Water Quality Survey of Lakes Erie, Huron, and Michigan. ANL/ER-85-2. Environmental Research Division, Argonne National Laboratory. 1985. [EPA/GLNPO]

Policastro, A.J., M. Wastag, W.E. Dunn, J. Leylak, P. Gavin and R.A. Carhart. Mathematical Modeling of Ultimate Heat Sink Cooling Ponds. NUREG/CR-4120, ANL/ES-143. Prepared for U.S. Nuclear Regulatory Commission. 1985. [NRC/NRR]

Shannon, J.D. User's Guide for the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) Model. Report 600/8-85/016. U.S. Environmental Protection Agency. 1985. [EPA]

4. Published Conference Papers

1984

Coulter, R.L., T.J. Martin and K.H. Underwood. A comparison of velocity techniques with field data. In: Proceedings of the Second International Symposium on Acoustic Remote Sensing of the Atmosphere and Oceans, 29 August - 1 September 1983, Rome, Italy. 1984. pp. IX:1-15. [Peer reviewed] [DOE/OHER]

Coulter, R.L., M.L. Wesely, K.H. Underwood and T.J. Martin. Heat flux derived from sodar amplitude and frequency data. In: Proceedings of the Second International Symposium on Acoustic Remote Sensing of the Atmosphere and Oceans, 29 August - 1 September 1983, Rome, Italy. 1984. pp. XXXVI:1-18. [Peer reviewed] [EPA/ASRL]

Frenzen, P. and D.L. Sisterson. An untapped midwestern wind energy resource: Nocturnal low-level wind maxima. In: Trends in Electric Utility Research, C.W. Bullard and P.J. Womeldorff (eds.). (Proceedings of a conference organized by the Midwest Universities Energy Consortium, 4 April 1984, Chicago, IL.) Pergamon Press. 1984. pp. 169-182. [DOE]

Knudson, D.A. and Jack D. Shannon. Meteorologically induced uncertainty in modeling of long-range source/receptor relationships. In: Transactions, the Meteorology of Acid Deposition, an APCA Specialty Conference, 16-19 October 1983, Hartford, CT (1984). pp. 358-366. [Peer reviewed] [EPRI]

Policastro, A.J., M. Wastag, J.D. Shannon, R. Carhart and W. Dunn. Evaluation of two short-term-range transport models with field data. In: Transactions, the Meteorology of Acid Deposition, an APCA Specialty Conference, 16-19 October 1983, Hartford CT. (1984). pp. 513-527. [Peer reviewed] [EPA/OAQPS]

Shannon, J.D. Climatological variability in modeling of long-term regional Transport and deposition of air-pollutants. In: Fourth Joint Conference on Applications of Air Pollution Meteorology, American Meteorological Society, 16-19 October 1984, Portland, OR (1984). pp. 178-181. [EPA/ESRL]

Shannon, J.D. Simulation modeling of atmospheric deposition of sulfur from biogenic and anthropogenic emissions. In: Transactions, An APCA Specialty Conference, Environmental Impact of Natural Emissions, 7-9 March 1984, Research Triangle Park, NC. 1984. [Peer reviewed] [DOE/OHER, EPA/ESRL]

Sheih, C.-M. An evaluation of wind field interpolation schemes used in studies of regional-scale pollutant transport. In: Transactions, the Meteorology of Acid Deposition, an APCA Specialty Conference, 16-19 October 1983, Hartford, CT. pp. 324-329. [EPRI]

Underwood, K.H. and R.L. Coulter. Vertical velocity statistics and spectra from a doppler sodar. In: Proceedings of the Second International Symposium on Acoustic Remote Sensing of the Atmosphere and Oceans, 29 August - 1 September 1983, Rome, Italy. 1984. pp. X:1-12. [Peer reviewed] [EPA/ASRL]

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Frenzen, P. Some problems in applications of the turbulent kinetic energy balance equations over land and sea. Seminar presented at the Department of Meteorology, U.S. Naval Postgraduate School, 22 February 1984, Monterey CA. [Scientists, faculty members] [ANL/OTD]

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Frenzen, P. The role of the divergence terms in the turbulent energy equation. Seminar presented to Atmospheric Physics Group at Los Alamos National Laboratory, 19 July 1984. [Scientists, program managers] [ANL/OTD/BER]

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*For oral presentations, the person who made the presentation is underlined.

**Audience for the presentation.

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Shannon, J.D. Modeling of long-range transport and dispersion. Presented at Meteorology Roundtable, Department of Geophysics, University of Chicago, 7 March 1985, Chicago, IL. [Faculty, graduate students] [DOE/OHER]

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Shannon, J.D. and B.M. Lesht. Examination of historical trends in sulfur deposition - a modeling approach. Presented at 1985 Annual Meeting, American Institute of Chemical Engineers, 12 November 1985, Chicago, IL. [Scientists] [DOE/OHER]

Sheih, C.M. A sulfur dry deposition module. Presented at TDEF/ASDEP Working Group Meeting, 8 January 1985, U.S. Department of Energy Headquarters, Germantown, MD. [Scientists & Program Managers] [DOE/OHER]

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Wesely, M.L. Summary of ASDEP. Presented at TDEF/ASDEP Working Group Meeting, 8 January 1985, U.S. Department of Energy, Germantown, MD. [Scientists, program managers] [DOE/OHER]

Wesely, M.L. Overview of Argonne-related programs. Presented at Global Effects Program Meeting, 13 February 1985, Santa Barbara, CA. [Scientists, program managers] [ANL/OTD]

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Wesely, M.L. Dry deposition research needs. Presented at NAPAP Peer Review of Regional Acid Deposition Model and Supporting Components, 25-29 March 1985, Raleigh, NC. [Program managers, scientists] [DOE/OHER]

Wesely, M.L. Practical aspects of dry deposition measurements. Presented at Workshop on Methods for Acidic Deposition Measurements, U.S. Environmental Protection Agency, Electric Power Research Institute, and U.S. Geological Survey, 2 May 1985, Raleigh, NC. [Scientists, program managers] [EPA/ASRL]

Wesely, M.L. Experience at Argonne National Laboratory on dry deposition measurements. Presented at Workshop on NCAR Micrometeorological Facility, National Center for Atmospheric Research, 10 June 1985, Boulder, CO. [Scientists] [EPA/ASRL]

Wesely, M.L. Proposed research for air-surface dry exchange program. Presented at Meeting of Special Committee on NAPAP Dry Deposition Research Needs, 24 June 1985, Washington, DC. [Scientists, program managers] [DOE/OHER]

Wesely, M.L. Dry deposition parameterizations, monitoring intercomparison, and development of variance methods. Presented at National Acid Precipitation Assessment Program Peer Review, 11 September 1985, Boulder, CO. [Scientists, program managers] [EPA/ASRL]

Wesely, M.L. Dry deposition research experiments. Presented at National Acid Precipitation Assessment Program Peer Review, 11 September 1985, Boulder, CO. [Scientists, program managers] [EPA/ASRL]

Wesely, M.L. Influence of climatology on atmospheric deposition process. Presented at Atmospheric Deposition Workshop, Great Lakes National Program Office, U.S. Environmental Protection Agency, 20 November 1985, University of Minnesota, Minneapolis, MN. [Scientists, program managers] [EPA/GLNPO]

CODES FOR FUNDING AGENCIES

EPA = U.S. Environmental Protection Agency
EPRI = Electric Power Research Institute
DOE = U.S. Department of Energy
DSE = Division of Solar Energy (in U.S. Department of Energy)
PNL = Pacific Northwest Laboratories
OHER = Office of Health and Environmental Research (in U.S. Department of Energy)
ORD = Office of Research and Development (in U.S. Environmental Protection Agency)
GLNPO = Great Lakes National Program Office (in U.S. Environmental Protection Agency)
ASRL = Atmospheric Sciences Research Laboratory (in U.S. Environmental Protection Agency)
ADAS = Acid Deposition Assessment Staff (in U.S. Environmental Protection Agency)
ESRL = Environmental Sciences Research Laboratory (in U.S. Environmental Protection Agency)
NOAA = National Oceanic and Atmospheric Administration
GLERL = Great Lakes Environmental Research Laboratory (in National Oceanic and Atmospheric Administration)
NRC = U.S. Nuclear Regulatory Commission
NRR = Office of Nuclear Reactor Regulation (in U.S. Nuclear Regulatory Commission)
OAQPS = Office of Air Quality Planning and Standards (in U.S. Environmental Protection Agency)
DEP = Division of Educational Programs (at Argonne National Laboratory)
OTD = Office of the Director (at Argonne National Laboratory)
DOD = U.S. Department of Defense
BNL = Battelle National Laboratory
OEA = Office of Environmental Analysis
BER = Biological and Environmental Research (at Argonne National Laboratory)

CHAPTER 3. ENVIRONMENTAL EFFECTS RESEARCH PROGRAM

CHAPTER 3. ENVIRONMENTAL EFFECTS RESEARCH PROGRAM

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3.1 PROGRAM OVERVIEW

T.M. Beasley, Acting Program Manager

The investigations of the Environmental Effects Research Program (EERP) for 1984 and 1985 generally represented a continuation of ongoing projects drawing on the staff's expertise in the fields of environmental radiochemistry, analytical chemistry, and basic plant sciences.

Aquatic radiochemistry research focused on those factors that determine the mobility of transuranic elements in both fresh and saline water systems. Central to the prediction of the long-term fate of these radioelements is the systematic study of the influence of such chemical variables as pH, dissolved organic carbon, and particle concentrations and compositions on the partitioning of their different valence states between "particulate" and "dissolved" phases. Substantial progress has been made in these topics through a combination of controlled laboratory experiments and field measurements.

The terrestrial ecology group continued studies on the effects of ozone, sulfur dioxide, drought, and acidic rain on agricultural crops and plant-soil systems important to the economic base of the central states. A fundamental understanding of the impacts of these entities on different plant species is required so that informed decisions can be made on energy-generation strategies using fossil fuels.

The soil-plant processes program intensified work on characterizing the influence of the mycorrhizal relationship as a stress-tolerance strategy in plants. Emphasis has been placed on identifying those physiological and morphological characteristics of a host that are affected by the mycorrhizal fungus. Research has also been initiated on how this root-fungus association modifies or influences the soil in which it grows, thereby altering both soil structure and pore space.

Finally, collaborative work between EERP staff and investigators within and outside of Argonne continued to be both stimulating and productive.

The following chapter sets out, in brief form, the results of the previous two years' effort, with frequent reference to the open literature publications and topical reports detailed in Appendix 3-E.

3.2. BEHAVIOR OF TRANSURANIC ELEMENTS IN NATURAL WATERS

3.2.1 Summary

W.R. Penrose

The transuranics project is a long-term study of the influence of the chemistry of natural waters on the behavior of actinide elements. In general, we are interested in natural processes that remove or immobilize actinides--in the wake of a spill or during long-term storage, for example. Chief among

these natural processes is adsorption onto particles from solution. Most of the water chemistry factors with which this project is concerned affect this adsorption process in some way: oxidation state of the actinides, the presence of natural or artificial complexing agents, and the nature of the adsorbing substance.

The research done under this project is generally a combination of field and laboratory work. Field situations are exploited in which actinide contamination is already present; since these situations are very scarce, the generality of the results is determined when necessary by laboratory experiments. For example, anomalous movements of americium and plutonium in groundwater near Los Alamos have been shown by laboratory experiments to be due to stable complexes of the element.

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3.2.2 Source Effects on Actinide Movement in Groundwater

D.M. Nelson and K.A. Orlandini

Americium and plutonium are generally considered to bind tightly to rock and soil surfaces, and transport of more than a few meters is unusual. In the Mortendad Canyon near Los Alamos National Laboratory, however, these elements were found to be moving rapidly through groundwater to distances at least 3.4 km from the discharge point (Nelson et al. 1983). Moreover, americium was seen to be moving at a far greater rate than plutonium; this is opposite to the order of mobility predicted from first principles.

Since the last annual report, other sources of known groundwater contamination have been examined to attempt to establish the generality of the phenomenon. Laboratory experiments have also been carried out to characterize the chemical nature of the actinides in the Mortendad Canyon groundwater.

The two locations of known groundwater contamination are at Hanford, Washington, and Sheffield, Illinois. The Hanford location has some interesting similarities with the Los Alamos location. Hanford is in an area of low rainfall, so that the presence of groundwater at all is due to the contaminated effluents. The soil is very porous and the groundwater flow rates are high.

Analysis of samples from Hanford showed that, in contrast to Los Alamos, oxidized plutonium was a major dissolved species both in the water being discharged and within the groundwater. Because oxidized plutonium is generally more poorly sorbed than reduced plutonium, its presence might be expected to result in increased transport of plutonium. This was not the case. Plutonium concentrations measured 10 m from the discharge are a factor of about 10^3 lower than those in the discharge; at 200 m, they are lower by a factor of 10^4 to 10^5 . This rapid decrease in concentration would be expected if plutonium existed as simple species in rapid equilibrium with one another

and with their surroundings. As the most strongly sorbed species (probably Pu(IV)) are removed from the water, the remaining dissolved species would redistribute in an attempt to restore equilibrium. The net result would be rapid sorption of the entire plutonium inventory.

Also in contrast to Los Alamos, americium at Hanford behaves almost exactly like reduced plutonium. Its distribution between dissolved and particulate forms and its decrease in concentration with distance from the discharge are almost the same as that of reduced plutonium. We have measured americium and plutonium in a number of surface waters and have found that, in general, americium distributions tend to be very similar to those found for reduced plutonium and for thorium. Because americium follows this trend at Hanford, this generalization may be useful in groundwaters as well as in surface waters.

We also examined the former commercial low-level waste disposal site at Sheffield, Illinois. This site has a number of features that make it attractive for study. First, it has been used as a disposal area for plutonium-bearing wastes. Second, it is in an area where the water table is sufficiently high to make migration in groundwater a possibility. Third, and most importantly, the subsurface flow of water at the site has been studied and the direction of movement is known. In fact, the flow of groundwater can be observed by means of elevated concentrations of tritium in observation wells ringing the site.

We collected water samples from the sump of one burial trench (T18), one monitoring well in the middle of the trenches (V), two monitoring wells (563 and 575) near the centerline of the tritium plume and down-gradient from the trenches, the deep well supplying drinking water to the site office, and a seep (or spring) at the base of the hill on which the trenches are located. Each water sample was filtered through 0.45- μ m membranes, and the plutonium concentration was measured in both water and filter.

Plutonium concentrations were very low in all of the samples, being about equal to our detection limit (Table 3.1). These concentrations should be compared with those found in a typical uncontaminated surface water, such as Lake Michigan: 0.27 femtocuries per liter (fCi/L) dissolved plus 0.08 fCi/L associated with particles. Also listed for comparison in Table 3.1 are the concentrations of natural ^{232}Th found in the samples. It is interesting to note that a higher fraction of plutonium than thorium is in the dissolved fraction, indicating plutonium may be more soluble (and hence potentially more mobile) than expected for a tetravalent actinide. Alternatively, the low, but apparently non-zero concentrations of plutonium in the dissolved fraction could be mere artifacts, with the true concentrations even lower.

We conclude from these measurements that the waste disposal sites at Hanford and Sheffield are functioning very well in their capacity to retain plutonium. The situation in the Mortendad Canyon at Los Alamos, then, is anomalous. Laboratory experiments were designed to attempt to resolve the observations.

An experiment in which groundwater was filtered through progressively finer filters showed the ambient plutonium in the Mortendad groundwater to be almost entirely (> 85%) associated with particles that passed through a 0.45- μm membrane filter but that were retained by a 0.025- μm membrane (Table 3.2). In contrast, while some of the ambient americium (about 25%) was associated with this size of particles, the majority passed through not only the 0.025- μm membrane, but also 100,000 and 10,000 molecular-weight cutoff ultrafiltration membranes. Thus, plutonium was associated with the largest size class of colloids, while most americium was either in solution or associated with very small colloids.

Table 3.1. Concentrations of plutonium and thorium in groundwater at Sheffield, Illinois

Source ^a	^{239,240} Pu (fCi/L)		²³² Th (fCi/L)	
	Dissolved	Particulate	Dissolved	Particulate
T18 sump	0.172 $\pm$ 0.034	0.106 $\pm$ 0.023	5.5 $\pm$ 1.2	16.1 $\pm$ 0.5
V	0.167 $\pm$ 0.050	1.21 $\pm$ 0.20	0.23 $\pm$ 0.12	112 $\pm$ 2
Well 563	0.026 $\pm$ 0.006	0.081 $\pm$ 0.030	0.03 $\pm$ 0.01	9.3 $\pm$ 0.2
Well 575	0.011 $\pm$ 0.003	0.053 $\pm$ 0.006	0.03 $\pm$ 0.01	8.5 $\pm$ 0.1
Seeps	0.012 $\pm$ 0.003	0.031 $\pm$ 0.005	0.005 $\pm$ 0.02	3.5 $\pm$ 0.1
Office Well	0.019 $\pm$ 0.005	0.013 $\pm$ 0.005	0.03 $\pm$ 0.01	0.12 $\pm$ 0.02

^a Locations of sources are identified in the text.

Table 3.2. Concentrations of Pu and Am in size fractions of Mortendad Canyon, Los Alamos, groundwater for March-April 1983^a

Particle Size Class	Plutonium (fCi/L)		Americium (fCi/L)	
	Dissolved	Particulate	Dissolved	Particulate
> 0.45 μm	-	350 $\pm$ 5	-	345 $\pm$ 24
> 0.45 μm	4,540 $\pm$ 103	520 $\pm$ 8	7,247 $\pm$ 72	249 $\pm$ 5
0.025 to 0.45 μm	670 $\pm$ 28	3,870 $\pm$ 22	5,249 $\pm$ 68	1,998 $\pm$ 13
100,000 daltons to 0.025 μm	648 $\pm$ 50	22 $\pm$ 3	5,191 $\pm$ 52	56 $\pm$ 3
10,000 to 100,000 daltons	230 $\pm$ 16	240 $\pm$ 10	3,103 $\pm$ 50	790 $\pm$ 14

^a Errors shown are counting errors only.

In another experiment, the water was spiked with tracer amounts of $^{242}\text{Pu}(\text{IV})$ and $^{243}\text{Am}(\text{III})$ immediately after filtration. The distribution of these tracer isotopes among the various smaller particle size classes was quite unlike the distribution of the ambient isotopes (Table 3.3). Much less tracer plutonium was associated with the large colloids, while much less tracer americium passed through the entire filter array. This indicates that the distributions of plutonium and americium among the particle size classes were not determined by the rapid sorption properties of the elements, but rather were dominated by processes having much slower kinetics. The distribution of plutonium among the size fractions smaller than $0.025\ \mu\text{m}$ was approximately the same for the tracer and ambient isotopes, indicating an equilibrium distribution may have been reached for those size classes. This was not true for americium.

Table 3.3. Exchange experiment with Mortendad Canyon groundwater^a

Particle Size Class	Ratio $^{242}\text{Pu}/^{239}, ^{240}\text{Pu}$		Ratio $^{243}\text{Am}/^{241}\text{Am}$	
	Dissolved	Particulate	Dissolved	Particulate
0.025 to $0.45\ \mu\text{m}$	6.95	0.18	0.61	0.99
100,000 daltons to $0.025\ \mu\text{m}$	7.10	2.48	0.60	2.74
10,000 to 100,000 daltons	7.07	5.74	0.37	1.68

^a Spikes of ^{242}Pu and ^{243}Am were added to the same samples of groundwater used in the experiment of Table 3.2. The concentrations of the spikes were measured separately from those of the ambient isotopes.

Since these elements are present at concentrations far too low for the precipitation of pure compounds to occur, their ultimate removal from solution must depend on their association with some larger particle. This is true whether they are present in true solution or are associated with some colloidal particle. To test the extent to which these radionuclides are available for sorption to other phases, an aliquot of water from the previous experiment was equilibrated for one week with some Lake Michigan sediment. Water that had already passed through the $0.025\text{-}\mu\text{m}$ filter was used so that sorption processes could be differentiated from simple flocculation of the larger colloids. This fraction is the one in which the tracer and ambient isotopes of plutonium had appeared to be near equilibrium. These sorption studies support that thesis. Both isotopes of plutonium were strongly sorbed ($K_D > 10^5$) and had similar oxidation state distributions ($\sim 50\%$ oxidized), indicating there was probably a rapid exchange of plutonium atoms among the various forms. In contrast, while the tracer americium isotope was strongly sorbed ($K_D = 4 \times 10^5$), the ambient isotope was much more weakly sorbed ($K_D = 5 \times 10^3$).

We conclude from these studies that the ambient americium is primarily sequestered in a low molecular weight form that neither exchanges with other forms nor sorbs to surfaces. While the origin of this form is not known for certain, it is probably present in the discharge and is probably not produced in the environment. It is most likely a very stable chelate produced somewhere within Los Alamos which passes unchanged through the treatment plant and through potential adsorbers in the subsurface environment. The ambient plutonium is associated with higher molecular weight inorganic colloids composed largely of amorphous silica. Again, the origin of this form is not certain. A reasonable hypothesis would be that it results from the dissolution of some natural siliceous material by the high pH effluent and then subsequent reprecipitation of this material. The bulk of the plutonium and that fraction of the americium not associated with the chelate are then incorporated into this colloidal silica and are carried downgradient with the groundwater. This uncharged colloid is slowly removed from solution, accounting for the greater removal of plutonium relative to americium. We feel that the mobility of both elements is largely decoupled from the chemistry of the groundwater and that their behaviors could not be predicted from any geochemical model using equilibrium thermodynamics.

3.2.3 Measurement of ^{237}Ac - ^{227}Th in Groundwater

D.M. Nelson and K.A. Orlandini

Our studies of ^{239}Pu and ^{241}Am in groundwater at Los Alamos (Mortendad Canyon) have shown americium to be far more mobile than plutonium. When the observation was first made it was not known whether this phenomenon was caused by differences in the intrinsic environmental chemistry of the two elements or by differences in their initial chemical forms. If the difference was intrinsic, these observations might have arisen because plutonium was present as Pu(IV) and americium as Am(III) . Since different actinide elements in the same oxidation state generally have very similar chemical properties, comparable differences in mobility should be present for any combination of one trivalent and one tetravalent actinide.

A particularly interesting pair of isotopes to compare would be ^{227}Ac and ^{227}Th . They are members of the ^{235}U decay chain and are therefore ubiquitous in the environment. Since ^{227}Ac (half-life = 21.8 years) decays to ^{227}Th (half-life = 18.7 days) they must also be present at the same total concentration. Any difference in concentration (between the two elements) observed in a groundwater sample must therefore be caused by differences in sorption to those parts of the system that are not sampled, i.e., the soil or rock matrix. Thus, if ^{227}Ac and ^{227}Th were measurable in groundwater, a general method would be available to compare the sorption behavior, and hence mobility, of trivalent and tetravalent actinides.

We have investigated the feasibility of measuring ^{227}Ac and ^{227}Th in groundwater using water from a deep well near Argonne (West Chicago well #5).

This is a challenging analytical problem for several reasons. First, the concentrations are quite low. Second, ^{227}Ac decays by emission of a very low energy beta particle, which can not be measured directly in low background counters, and so ^{227}Ac must be measured by ingrowth of ^{227}Th . Third, while ^{227}Th decays by alpha emission, and hence should be capable of being counted on low background alpha counters, its alpha energies are indistinguishable (on a silicon surface barrier detector) from those of ^{224}Ra and ^{212}Bi . These are daughters of ^{228}Th and are almost always present at concentrations far higher than those of ^{227}Th . The most practical method of detecting ^{227}Th under these circumstances is via the alpha emission of ^{215}Po (half-life = 1.8 seconds), a daughter farther down the decay chain. The alpha energy of this isotope is 7.38 MeV and has no interferences. On our detectors the background at this energy is ≤ 1 count per 10,000 minutes. Of course, proper corrections must be made for the ingrowth and decay of ^{223}Ra (half-life = 11.3 days), the first daughter of ^{227}Th . The maximum count rate of ^{215}Po occurs about three weeks after a ^{227}Th source has been isolated, so the optimum counting conditions are to start two weeks after separation and count for two weeks.

In this feasibility study, we passed the water through a 0.45- μm membrane filter as it was being collected. Both ^{227}Ac and ^{227}Th were immediately isolated from the filtered water by coprecipitation with 1 milligram per liter (mg/L) of $\text{Fe}(\text{OH})_3$, which was then also removed by filtration. The two filters (one containing the original particulate activity, the other the original dissolved activity) were then dissolved in 8 M HNO_3 , and the ^{227}Th was isolated by passage through AG1x8 anion exchange resin columns. The ^{227}Th fractions were electrodeposited and counted as outlined above. The raffinates (containing the ^{227}Ac) were set aside for 30 days to allow ingrowth of more ^{227}Th . After the 30-day period, the thorium was again isolated by ion exchange, electrodeposited, and counted. Chemical recoveries were monitored using internal standards of ^{229}Th for the first thorium extractions and ^{230}Th for the second.

The results of these measurements (Table 3.4) show that both ^{227}Ac and ^{227}Th are detectable in this water (using 100-L samples). No significant difference is seen between the concentrations of these two isotopes, implying both are sorbed to the rock matrix in this system to the same extent. This in turn implies similar mobilities for the two elements. The high fraction of the activity associated with the particulate matter in this water implies strong sorption for both elements. Based on the mass of particulate matter found in this water (0.13 mg/L), the K_d values would be approximately 10^7 . Strong adsorption of ^{228}Th can be demonstrated directly in this system by comparing its concentration with that of its parent, ^{228}Ra . The ^{228}Ra concentration in this water is ~ 3 pCi/L, so that at least 99.9% of the ^{228}Th has been removed from the water phase (including the suspended particulates) and transferred to the rock matrix. Since the distribution of ^{228}Th between the suspended particles and the dissolved phase is about the same as the corresponding distributions of ^{227}Ac and ^{227}Th , it is reasonable to assume that 99.9% of each of these isotopes is also sorbed to the rock matrix.

Table 3.4 Concentrations of actinium and thorium
in West Chicago well water

Nuclide	Concentration (fCi/L)			% Particulate
	Particulate	Dissolved	Total	
^{227}Ac	0.38 ± 0.03	0.27 ± 0.04	0.65 ± 0.05	58
^{227}Th	0.25 ± 0.03	0.37 ± 0.05	0.62 ± 0.06	40
^{228}Th	1.58 ± 0.05	1.05 ± 0.05	2.63 ± 0.07	60

These experiments demonstrate the feasibility of measuring ^{227}Ac and ^{227}Th in groundwater. In the one water tested, no differences in sorption were noted. This supports the conclusion of another section of this report that the high mobility of ^{241}Am at Los Alamos is a source effect and is not related to an intrinsic difference between trivalent and tetravalent actinides.

3.2.4 Cycling of Actinide Elements in B Pond, South Carolina

D.M. Nelson, K.A. Orlandini, S. Nakayama, and A.K. Luttermann**

Redox transformations in the environment can affect the behavior of actinide elements in several ways, two of which are of paramount importance. First, the materials with which these elements interact can be altered in both character and amount. For example, the oxidized forms of iron and manganese (Fe_2O_3 and MnO_2), which are excellent adsorbers, can be reduced to the more soluble Fe^{+2} and Mn^{+2} ions, which, if anything, might be expected to compete with the actinides for sorption sites on other substrates. Stronger reducing conditions can eventually lead to the production of new solids, e.g., FeS , which are again excellent adsorbers. Secondly, redox-induced changes in actinide behavior may involve changes in the oxidation state of the actinide itself. Both effects may occur concurrently in any real system undergoing a change in redox potential, making the task of correct interpretation doubly difficult.

An ideal location at which to unravel these interconnected effects would be a periodically anoxic system containing measurable concentrations of several actinide elements. Such a system exists on the Savannah River Plant site. Pond B is a former reactor cooling lake that was contaminated with conveniently measurable concentrations of $^{239,240}\text{Pu}$, ^{241}Am , and ^{244}Cm during the early 1960s. It is an impounded lake with an area of about 1 km^2 and a maximum depth of 12 m. During the winter the lake water is isothermal and

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saturated with oxygen; during the summer (May-October) the lake is thermally stratified, and the bottom waters become anoxic. Since natural ^{232}Th and ^{228}Th are also measurable in the lake, the behaviors of actinide elements that are always tetravalent (thorium), always trivalent (curium), or potentially variable (plutonium, americium) could be studied. Both temporal and spatial gradients of redox conditions could be studied.

In our study, we measured concentrations of $^{239,240}\text{Pu}$, ^{241}Am , ^{244}Cm , ^{228}Th , and ^{232}Th in both dissolved and particulate fractions of water from B Pond during two anoxic cycles. This work was done in cooperation with J.E. Pinder and J.W. Bowling of the Savannah River Ecology Laboratory, and J.J. Alberts of the University of Georgia Marine Institute. Samples were filtered through 0.45- μm membranes in the field before coming in contact with the atmosphere to avoid redox changes occurring during phase separation.

The behavior of plutonium, thorium, and americium appeared to be almost identical throughout the seasonal cycle. The ratios of these elements to one another, both in solution and on particles, were nearly invariant. Each element did change concentration in a systematic fashion, with concentration minima in the dissolved phase occurring in the late fall, after breakup of the summer stratification. Dissolved concentrations increased during the winter and remained uniform top to bottom. After the lake stratified in the spring, the total concentrations in the surface water decreased rapidly, and concentrations in the deeper water increased. This redistribution occurred before the bottom water became anoxic, suggesting that it was driven by simple settling of particles through the water column. Vertical profiles of total concentration then remained relatively unchanged throughout the summer, even after the system became anoxic.

Some transfer of activity from the suspended particles to the dissolved phase did occur, with the distribution coefficients (K_D) being three- to ten-fold lower in the anoxic water than in the oxygenated water. Even in the anoxic waters, the K_D s were quite high, $> 250,000$. Inventories of ^{239}Pu , ^{241}Am , and ^{232}Th in the water column showed little change and no clear trend during the seasonal cycle, supporting the contention that remobilization of these elements from the sediments during the anoxic period is not a significant process. The consistent behaviors of these three elements also strongly suggests that redox transformations of the actinides between the (III) and (IV) states are not important factors regulating behavior. The differences in dissolved/particulate partitioning that did occur were almost certainly due to changes in the adsorber.

In contrast to this straightforward cycling of plutonium, americium and thorium, we found a very puzzling picture for curium. For most of the period of this study, curium behaved exactly like the other three elements. However, in August 1984, at the peak of the anoxic period, the concentrations of dissolved curium were very high at all depths within the pond. Differences between curium and the other three elements were most pronounced in the surface waters, where the K_D for curium was almost 100 times lower than the K_D s for the other three. The phenomenon did not repeat during the summer of

1985. Unusually high concentrations of curium had been found in the pond area once before, during November 1983, indicating it does occur with some regularity.

We conducted laboratory tracer experiments and found no significant difference in K_D between Am and Cm as a function of pH or organic carbon content of the water. Experiments in which pH was varied were conducted in waters collected from Lake Michigan, which is low in dissolved organic carbon (DOC) (~ 1 mg/L), and from Saganashkee Slough, Illinois, which is comparatively high in DOC (~ 20 mg/L). The pH was adjusted in the range of 4 to 9 with HCl and NaOH. Each sample was equilibrated with tracer isotopes of americium and curium, and with Lake Michigan sediment (~ 20 mg/L) by stirring for three to four days. The samples were filtered (0.45- μ m membranes), the pH measured, and concentrations of americium and curium determined in both dissolved and particulate fractions.

Experiments in which DOC was varied were conducted with waters collected from a small pond on the Argonne site and from Volo Bog, Illinois, two waters of moderate to high DOC concentration but possibly quite different DOC character. The organic matter (> 1000 molecular weight) in these waters was concentrated by ultrafiltration and then recombined in various proportions with the respective ultrafiltrates to form a series of waters of varying DOC concentration. Each water was then equilibrated as above, but at constant pH (8.3 for the Argonne pond and 7.8 for Volo Bog).

Distribution coefficients (K_D = activity on the solids, dpm/g, divided by the activity in solution, dpm/mL) were then calculated for americium and curium for each water. The relationship between the K_D of americium and that of curium is presented in Figure 3.1. Variations in pH or DOC concentration produced large and systematic variations in K_D for both americium and curium, with low pH and high DOC producing low values of K_D . However, there were no large systematic differences between americium and curium over a three order of magnitude variation in K_D .

We can offer no good explanation for this anomalous "solubility" of curium in the environment. The aqueous chemistries of the two elements give no reason to suspect substantial differences in environmental behavior. Perhaps a biological mechanism is responsible for returning complexed curium, but not americium, to the water. The only other study where curium and americium behaviors have been followed in some detail (Pond 2513 at Oak Ridge) also showed curium to be significantly less particle-reactive than americium. We have also not discounted the possibility that an extraneous source may be periodically adding curium to the system. While no recorded discharges are occurring, it is possible that input from the atmosphere or some unmonitored aqueous source exists. No matter what its origin, the excess curium seems to display quite different behavior from the other actinides studied, i.e., much lower K_D , suggesting an investigation into its chemical form is warranted.

Figure 3.1. K_D values of americium and curium onto a standard (Lake Michigan) sediment, using water and dissolved organic carbon from various sources. Symbols indicate sources of DOC: crosses, Volo Bog; circles, ANL pond; squares, Saganashkee Slough; and triangles, Lake Michigan.

3.2.5 Speciation of Actinide Elements in High-Carbonate Natural Waters

D.M. Nelson and K.A. Orlandini

Carbonate ion forms strong complexes with many metals, including actinides. The formation constants of these complexes tend to be similar for all actinide elements of a given oxidation state. However, large differences are observed between oxidation states. For those actinides having more than one possible oxidation state (uranium, neptunium, plutonium, and americium), the formation of carbonate complexes will increase the relative stability of those oxidation states having the strongest complexes. The concentration of carbonate ion in a natural water may, therefore, be an important factor in determining the distribution of oxidation states. Since the sorption properties of the various oxidation states (and complexes) can be quite different from one another, the partitioning of the actinide elements between dissolved and particle-associated forms could in turn be influenced by the carbonate concentration.

We have investigated the sorption properties of several actinide elements onto calcium carbonate from solutions containing carbonate ion and, as expected, found substantial differences among oxidation states. These differences were then used as the basis of a scheme to identify which

oxidation state (of the multivalent actinides) was actually present under specific conditions. Calcium carbonate is an ideal substrate to use in such separations because it is not directly involved in any redox transformations and is present as a natural constituent in some natural waters. Differences in sorption between trivalent and tetravalent actinides are illustrated in Figure 3.2. In these experiments, promethium (^{145}Pm) was used as a convenient analog for the actinides in their (III) oxidation state. Plutonium (^{237}Pu) was added and presumably remained in the (IV) oxidation state. Sorption was reported as a distribution coefficient, or K_D , defined as the concentration of the tracer in the solid phase (dpm/kg) divided by the concentration of the tracer in the dissolved phase (dpm/L). Throughout the range of carbonate concentrations studied, promethium was sorbed more strongly by CaCO_3 than was plutonium. The K_D s for both elements decreased dramatically at elevated carbonate concentrations, with that for Pu(IV) decreasing first. Between carbonate concentrations of 0.05 and 0.5 mole/L, the K_D s are sufficiently different to allow a reasonably complete separation of these two elements. By analogy, any trivalent actinide or lanthanide should be separable from any tetravalent actinide using a simple one-step equilibration with a properly chosen amount of CaCO_3 .

Figure 3.2. K_D of promethium (III) and plutonium (IV) as a function of the sodium carbonate concentration.

This method was then used to investigate changes that could occur in the oxidation states of several actinides after addition to carbonate solutions. Two media were used, a natural, high-carbonate water collected from Mono Lake, California, and a solution of NaCO_3 in deionized water having a carbonate concentration (~ 0.32 mole/L) equal to that of Mono Lake. These waters were spiked with ^{244}Cm (which can only exist in the III state), ^{243}Am (which was added as III but which could possibly oxidize to the IV state), ^{242}Pu (which was added as IV but which could possibly reduce to the III state or oxidize to the V or VI states), and ^{228}Th (which can only exist in the IV state). A tracer amount of each isotope was added to each water, subsamples were with-

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drawn periodically, and the sorption of each isotope to CaCO_3 was measured.

The results of these experiments showed curium and americium to be sorbed nearly identically and to approximately the extent (80%-90% using 0.8 g CaCO_3/L) predicted by the earlier experiments with promethium, confirming the utility of Pm(III) as an analogue for the trivalent actinides. Both plutonium and thorium were much more poorly sorbed (only a small percentage sorbed under the above conditions). No significant change in sorption was observed over the course of several weeks, nor was any difference observed between Mono Lake water and the simple carbonate solution. The similarity between the sorption of plutonium and that of thorium confirms our supposition that the plutonium remained in the (IV) state with no appreciable reduction to the (III) state. Likewise, the similarity between curium and americium indicates no oxidation of the latter beyond the (III) state. Our results contradict the earlier studies of Cleveland et al. (1983), who reported rapid reduction of a majority of Pu(IV) to the (III) state. We feel their results are an artifact of the method they used to make the (III)-(IV) separation, namely, extraction with TTA from dilute acid. The similarity noted between the sorption from Mono Lake water and that from NaCO_3 solution indicates that the behaviors of the actinides in that lake are largely controlled by the actions of their carbonate complexes.

The sorption to calcium carbonate of the ambient $^{239,240}\text{Pu}$ and ^{241}Am in Mono Lake (introduced as fallout from nuclear weapons testing) was also determined. Results of these measurements were consistent with the previously discussed tracer studies, i.e., ^{241}Am was sorbed almost quantitatively, while $^{239,240}\text{Pu}$ was hardly sorbed at all. This shows that even for very long equilibration times (two decades had elapsed since their introduction) the observed oxidation states are the same as those found in the shortest-term tracer studies.

3.2.6. Investigation of Neptunium Behavior in Natural Waters

D.M. Nelson and J.O. Karttunen

Although neptunium is a relatively minor component of the radioactive waste produced in the nuclear energy cycle, it is important because of the long life of its principal isotope, ^{237}Np , and its propensity to exist in the relatively "soluble" pentavalent oxidation state. Because the actinide elements have similar chemical properties when in the same oxidation state, the behavior of neptunium in the environment is expected to have some similarity to that of plutonium, which also has a relatively stable (V) oxidation state. The major difference is expected to be an even greater stability of the (V) oxidation state relative to the (IV) state and hence less overall sorption to particulate phases. Our earlier studies have shown that for plutonium, even in systems where Pu(V) is the major dissolved form, removal from solution is due almost exclusively to sorption of Pu(IV) to particles. We have now conducted a series of experiments to determine whether

removal of neptunium from solution involves a similar process. Neptunium-235, a 410-day half-life isotope decaying by electron capture and gamma-ray emission, was used at tracer concentrations ($< 10^{-10}$ M) throughout these studies.

Our first goal was to devise consistent techniques to (1) produce neptunium tracer solutions of known oxidation state, and (2) measure the separate oxidation states quantitatively. Stock solutions of $^{235}\text{Np(IV)}$ and $^{235}\text{Np(V)}$ were produced by heating in 9 M HBr and 1 M HNO_3 , respectively. Oxidation state separations were accomplished using the rare earth fluoride precipitation technique, modified so that no "holding oxidant" was present. Solutions to be tested were made 1 M in H_2SO_4 , 0.0007 M in La^{+++} , and 0.3 M in HF. The resulting LaF_3 precipitate, carrying the Np(IV) , was removed by filtration. The supernate was then made 0.01 M in FeSO_4 to reduce the Np(V) remaining in solution to Np(IV) , and a second LaF_3 precipitate was generated to collect the original Np(V) fraction. This procedure resulted in clean separations; the first precipitate contained 98%-99% of the Np(IV) and the second contained 98%-99% of the Np(V) . Analysis of the tracer solutions showed each to be $> 98\%$ in the specified oxidation state. The oxidation state of neptunium sorbed to particles was measured by first retaining the particles on a filter, leaching the neptunium from the particles with 1 M H_2SO_4 , and finally carrying out the LaF_3 separation as described above.

Experiments in which Np(IV) tracer was added to filtered Argonne pond water showed a rapid conversion to Np(V) , unlike the behavior of Pu(IV) , which shows little or no conversion in the absence of particles over the same time periods. While the conversion was rapid ($\sim 50\%$ oxidized in the first 30 minutes), it did not follow first-order kinetics--i.e., the oxidation rate slowed progressively with time so that after four days there was still $\sim 5\%$ Np(IV) .

Other experiments done in the presence of natural Lake Michigan sediments (63 mg/L) showed oxidation kinetics similar to those found in the absence of particles. These experiments showed a rapid initial sorption of neptunium (presumably as Np(IV)) followed by a gradual conversion of both dissolved Np(IV) and sorbed neptunium to dissolved Np(V) . The sorption of neptunium was shown to obey the laws of mass action, with the amount sorbed being directly proportional to the amount of adsorber. The K_D describing the sorption process had a value of ~ 1500 in both Lake Michigan water and Argonne pond water. This is a factor of about 200 lower than the values of K_D for total plutonium in the same waters. In those two waters, about 90% and 30% (respectively) of the dissolved plutonium is typically present as Pu(V) , with the remainder being Pu(IV) . For neptunium, the dissolved Np(IV) is essentially unmeasurable, being typically 1%-2% of the total dissolved concentration (equal to the sensitivity of the method).

We attempted to influence the distribution of neptunium between the (IV) and (V) oxidation states by adjusting the concentration of oxygen dissolved in the water. These experiments were uniformly unsuccessful. Even in water flushed with high-purity nitrogen, spiked with Np(IV) , and equilibrated under

nitrogen atmosphere, the dissolved Np(IV) concentrations constituted less than 2% of the total. Thus, it appears that dissolved oxygen is not, itself, the oxidant directly responsible for the conversion of Np(IV) to Np(V).

Although dissolved Np(IV) concentrations were very low, the neptunium leached from the particles in these experiments was primarily Np(IV). This was true for those experiments spiked with Np(V) as well as for those spiked with Np(IV). The only exceptions were some experiments done under nitrogen atmosphere in which the carbon dioxide balance was upset, resulting in precipitation of calcium carbonate. Calcium carbonate is an excellent adsorber of pentavalent actinides and as might be expected, the overall sorption in those experiments was anomalously high, with large amounts of Np(V) present in the particulate phase.

Because the concentrations of dissolved Np(IV) were generally below our detection limit (i.e., could not be distinguished from the low level of Np(V) contamination) it was not possible to rigorously test the hypothesis that the K_D of Np(IV) is equal to the K_D of Pu(IV). Only one water, that with a very high concentration of dissolved organic carbon, had enough Np(IV) in solution at equilibrium for a reliable measurement of Np(IV) K_D . In that water the K_D of Np(IV) was almost identical to the K_D of Pu(IV).

These experiments show, as we had suspected, that the sorption behavior of neptunium is very similar to that of plutonium. The only substantive difference appears to be the increased stability of the (V) oxidation state, i.e., the ratio of Np(V) to Np(IV) in solution is several hundred times greater than the corresponding ratio for plutonium.

3.2.7 Reactive Sites for Actinides on Natural Sediments and Humic Acids

W.R. Penrose and M.W. Findlay, Jr.

Sediments and suspended particles in natural waters are responsible for the binding and ultimate removal of many trace substances, including heavy metals and hydrophobic organic compounds. Practically nothing is known, however, of the structure and mechanisms of the sites on natural particles that are responsible for this binding. Most work to date has been centered on more tractable model systems, such as hydrated iron oxides. Humic substances play a role in both modulating toxicity of trace metals and controlling their binding and sedimentation reactions, and they have been more intensively studied. However, even with these, there is still no clear picture of how a random polymer, produced by the decay of organic matter, can bind metals and organic substances as tightly as humic acids do.

Our work has been concerned with measuring the specificity and amount of binding sites for actinides and lanthanides on sediments and humic substances. This laboratory has established the role of dissolved organic matter in modulating the binding of actinides to particles. The purpose of this research has been to identify other interactions among constituents of natural waters that may influence the operation of natural controls on

actinide concentrations. We incidentally discovered that both sediments and humic acids can mediate the conversion of Pu(V) to the (IV) oxidation state.

The tools available for investigating scarce binding sites are fairly limited. A productive approach is to force two or more ions to compete for the same binding site. In these experiments, the binding of actinides or lanthanides to a natural sediment is measured while the concentration of a rare earth ion is increased. At the higher concentrations, the lanthanum displaces all of the rare earth and most of the actinide (Figure 3.3). The steepness of the curve describing the competition between La and Gd implies that both ions occupy the same sites, and that the sites for trivalent ions have a narrow range of binding energies. The binding properties of the tetravalent ions (Pu and Th) are affected less by the increasing concentrations of trivalent ions. This implies that the tetravalent ions occupy some, but not all, of the trivalent sites over a broader range of binding energies. The reciprocal experiment--increasing the concentration of the actinide in the presence of a tracer concentration of lanthanide--cannot be done because of the low solubility of the tetravalent actinides.

A more interesting phenomenon has been the reduction of Pu(V) to Pu(IV) by sediments and humic acids. The oxidation state distributions of such trace elements as As, I, Se, Mn, and Fe, as well as Pu, are major factors determining their fates in the environment. With the exceptions of Fe and Mn, however, very little is known of the agencies that bring about the interconversion of oxidation states.

Plutonium in the (V) state is stable indefinitely in neutral, particle-free solution. When particles of natural sediment are present, however, Pu(V) is rapidly reduced to the (IV) state in a nearly first-order fashion. If these sediments are treated with high heat to remove organic material, or if inorganic materials such as goethite (α -FeOOH), kaolin, silica, or alumina are substituted, the reduction reaction occurs at a much slower rate or not at all.

Like the binding of Pu, the reduction reaction is inhibited by low concentrations of rare earths. Figure 3.4 shows the results of increasing concentrations of Nd on the reduction of Pu(V). The affinity constant of Nd for the reducing site is $4.5 \times 10^7 \text{ M}^{-1}$, whereas the average affinity constant for neodymium binding to the same sediments is $5.0 \times 10^5 \text{ M}^{-1}$. Thus, only the highest-affinity binding sites are responsible for the reduction reaction.

Normally, the binding of trace metals to substances with heterogeneous surface characteristics is quite complex. Even "simple" substances such as iron oxides have a variety of sites that are capable of binding trace metals; these sites are distributed across a range of binding energies. This distribution is often referred to as an "affinity spectrum." In most cases--for example, the binding of copper to humic acids--the amount of metal bound increases slowly and irregularly across many orders of magnitude of free metal concentration. This curve can be deconvoluted mathematically to derive the

Figure 3.3. The binding of gadolinium, plutonium, and thorium to Lake Michigan sediments as a function of lanthanum concentration. Binding is expressed as the K_D (the ratio of radioactivity per unit weight of sediment to activity per unit volume of liquid).

Figure 3.4. The effect of increasing neodymium concentration on the reduction of Pu(V) by Lake Michigan sediments. The points shown are actual data; the solid line is a best fit to the data by a simple one-constant mass-action equation: $K = [MS]/([M] \cdot [S])$ where M is metal ion; S is the concentration of binding site on sediment; and K is the binding or affinity constant of site S.

affinity spectrum. In the case of rare earths, however, the binding curve follows the simple mass-action model for a single type of binding site (Figure 3.4). It is as if only one configuration of functional groups out of the infinity of possibilities was able to bind lanthanides. This is also true for the effect of rare earths on the reduction of Pu(V).

3.2.8 Effect of Dissolved Organic Carbon on the Physicochemical Behavior of Iron in Natural Waters

*K.A. Orlandini and M.A. Wahlgren**

There is a wealth of information in the literature of limnology and soil chemistry which indicates that natural organic compounds affect the concentration, bioavailability, mobility, and speciation of most detectable metal ions. The organic materials most frequently implicated in these interactions are the humates and fulvates. That these organic materials have some effect on the behavior of metal ions is evident from the measurements of stability constants in a variety of physicochemical conditions.

A recent field study of North American lakes identified an inverse linear correlation between plutonium, thorium, and uranium distribution coefficients and the dissolved organic carbon present in the subject lakes (Wahlgren and Orlandini 1982). A similar relationship was observed for fallout-derived americium in natural waters (Nelson and Orlandini 1985). Evidence from the literature and the authors' own observations indicating enhancement of trace element solubility with increasing amounts of dissolved organic matter suggested that the relation between metal-ion distribution coefficients and dissolved organic carbon was not limited to the actinide elements.

Because of the common occurrence of iron in adsorptive metal oxide coatings and the significance of iron as a micronutrient in natural aquatic systems, measurements were made of the concentrations of iron in both suspended particulates and the waters with which these particulates were in equilibrium. Our observations of a systematic relationship between iron and the dissolved organic carbon in a variety of natural waters across at least two climatic zones are presented here.

Some indirect evidence of this relationship appeared in a study made by Jackson and Hecky (1980), who showed an inverse linear relationship between primary productivity and dissolved organic matter in Canadian reservoirs and lakes. The data suggested that the soluble micronutrient iron was being made unavailable with increasing amounts of dissolved organic carbon. A more direct piece of evidence relating the distribution coefficient of iron and dissolved organic carbon was presented in a paper by Intskirveli et al. (1977). That experimental work showed that the uptake of iron tracer onto Dowex 50 cation resin varied inversely with the concentration of natural organic matter obtained from surface waters in Russia.

*Collaborator; affiliation is listed in the front of this chapter.

Figure 3.5 shows a plot of distribution coefficient versus dissolved organic carbon (DOC) for iron occurring in natural waters. Distribution coefficients represented by open circles were calculated from field data available in published reports and from the authors' measurements on field samples. The linear plot included on the figure and represented by closed circles was the result of laboratory experiments using iron-59 radiotracer, silica gel as the adsorber, and rain water to which was added natural organic matter concentrated and recovered from surface water by ultrafiltration techniques (Nelson et al. 1985).

There was no difference in the measured distribution coefficient whether the iron was first adsorbed to the silica gel or first added to the solution containing the DOC of choice before equilibrating the two phases.

These observations are consistent with the observations made for plutonium and americium in natural aquatic systems. The apparent similarity of the behavior of plutonium to that displayed by iron in natural systems suggests that the latter element can provide useful information on the behavior and fate of plutonium in these same systems.

Figure 3.5. Plot of distribution coefficient (K_D) of iron versus dissolved organic carbon (DOC) in natural water. Symbols: open circles = ambient iron in field samples; filled circles = laboratory experiments using ^{59}Fe .

3.2.9 Effects of Seasonal Changes in Dissolved Organic Compound Composition upon the Distribution of Trace Metals in a Productive Lake

M.W. Findlay and W.R. Penrose

In natural waters, dissolved organic carbon compounds play a significant role in determining the mobilization and distribution of trace metals. This is primarily due to the chelating properties of some dissolved carbon compounds, especially humic substances derived from the decay of dead organisms. The inclusion of organic carbon as a known agent in the mobility of actinides and other trace metals requires that its properties not change with season, or that at least they change in a predictable way. In normally productive waters, much of the organic matter is generated during summer plankton blooms. One might expect that the chemical and metal-binding properties of the organic carbon would change with time as the organisms grew, senesced, and decayed. We therefore decided to sample a highly productive lake several times over a season and to characterize the organic matter in those samples, particularly with respect to the ability to bind metals.

The lake chosen was Saganashkee Slough, near Argonne National Laboratory. This lake has an average depth of one meter and has a relatively small watershed relative to its surface area. In the summer of 1985, the lake level fell through evaporation so that there was no outflow after June. Thus, the organic matter in the lake at this time, plus that generated by photosynthesis, was present throughout the season.

Samples of Saganashkee water have been collected approximately monthly beginning in April 1985. Dissolved organic material with a nominal size over 1000 daltons was concentrated by ultrafiltration. This fraction was separated into humic (HA) and nonhumic compounds by adsorption chromatography. Additionally, the molecular weight distributions were studied using gel chromatography.

Preliminary results from the characterization of the "dissolved" organic compounds (DOC) are given in Table 3.5. There appear to be several trends in physical parameters from April through October, although more than one season's worth of data will be required to draw any definite conclusions.

The level of total DOC increased from 13 mg carbon (C)/L in April to a peak of 26.6 mg C/L in July, and then fell off through the fall. The concentrations of the > 1000-dalton compounds, however, increased steadily through October, for both the humic and nonhumic fractions. Curiously, though, the extinction coefficient at 250 nm (E^{250}), which increases with the number of chromophore groups, peaked in the summer and appeared to decrease through the fall for all fractions. The E_2/E_3 ratio ($\text{abs}^{250}/\text{abs}^{365}$) for the humic fraction seemed to be increasing in the fall, while that of the nonhumic fraction remained constant.

Experiments to study the binding of lanthanides and actinides to sediment are being conducted, initially using gadolinium to represent trivalent lanthanides and actinides. On samples collected from mid-spring through late

Table 3.5. Summary data for 1985 Saganashkee Slough samples

Parameter	Sample Date							
	4/22/85	5/13/85	6/12/85	7/17/85	8/23/85	9/26/85	10/29/85	11/25/85
Water temperature (°C)	21.5	21.5	18	25.5	24.5	16.5	12	1.5
pH							7.2	
Alkalinity (mg/L CaCO ₃)	92	90					90	
Conductivity (µmhos)	250	250						
Total susp. solids (mg/L)	34		109		88.1		50	35
Susp. solids % ash	64		70		62.7	78		74
TOC (< 35 µm)	15	15.3	21.9	38.2	40.8		21.7	16.8
DOC (< 0.45 µ)	13	15.6	16.4	26.6	24.5	18.2	19.5	16.8
DOC (< 1000 MW)	10.9	5.5						
DOC (> 1000 MW)	4.5	6	3.9	5.6	8.8	8.6	8	6.1
Ratio (>1000/<0.45)	0.35	0.38	0.24	0.21	0.36	0.47	0.41	0.36
<u>> 1000 MW FRACTION</u>								
<u>Total:</u>								
DOC (mg C/L)	4.5	5.95	3.9	5.6	8.82	8.56	8	6.1
E ₂ /E ₃ ^a	6.2	6.7	6.7	7.3	7.4	8.8	8.4	7.8
ε[250] ^b (A ²⁵⁰ ·mg ⁻¹ ·L·cm ⁻¹)	0.021	0.031	0.03	0.052		0.026	0.022	0.025
<u>Humic (retained on XAD7):</u>								
DOC	2.4	3.4	2.2	3.5	4.9	4.7	5.7	3.9
E ₂ /E ₃	6.3	6.4	6.3	6.5	6.6	8.2	6.9	6.9
ε[250]	0.033	0.032	0.033	0.033	0.042	0.032	0.021	0.025
<u>Nonhumic (XAD7 eluate):</u>								
DOC	2.3	2.5	1.7	2.1	3.8	4.7	4.5	1.9
E ₂ /E ₃	10.5	9.4	9.7	9.2	7.8	8.5	8.5	14.4
ε[250]	0.015	0.015	0.016	0.021	0.023	0.009	0.01	0.021
Humic/nonhumic	1.04	1.35	1.3	1.7	1.68	1	1.26	2.05

^aThe ratio $\text{abs}^{250}/\text{abs}^{365}$; measurements made at pH of ~ 9-9.5; adjusted with NaOH.

^bAbsorbance, or extinction coefficient, measured at 250 nm, pH ~ 9-9.5 in NaOH.

summer, no substantial changes have been observed in the effects of DOC levels on the partitioning of metals between dissolved and adsorbed species (see Figure 3.6). It is not yet known if the slightly greater slope of the April data is important, or even seasonally reproducible.

We plan to continue collecting samples through at least one full seasonal cycle, and possibly for an additional year. We will look for seasonal or long-term changes in the organic constituent, along with any corresponding changes in metal/organic compound interactions. Additional chemical characterization will include functional group analysis and size distribution of the more easily measured transition metals, such as copper and iron.

These experiments indicate that the properties of dissolved organic carbon that are relevant to trace metal mobility do not change drastically throughout a season, in spite of very high inputs of photosynthetically generated organic carbon. We hope to prove that estimates of actinide mobility can be made based solely on simple measurements, without the need to do detailed characterization of the constituents of the water.

Figure 3.6. Effects of Saganashkee Slough DOC (>1000 d) on the binding of lanthanides to sediment. K_d is the distribution coefficient for Gd in a 20 mg/L sediment suspension (pH = 6.0; MES buffer). DOC is expressed in mg C/L. [Sample dates: closed circles = 4/22/85; cross = 6/12/85; square = 8/23/85; hexagon = 10/29/85; open circle = 11/25/85]

3.3 NATIONAL CROP LOSS ASSESSMENT NETWORK

3.3.1 Summary

L.W. Kress

The National Crop Loss Assessment Network (NCLAN) was established by the U.S. Environmental Protection Agency (EPA) in 1980 to investigate the impacts of ozone (O_3), sulfur dioxide (SO_2), and nitrogen dioxide (NO_2) on the yield of important agricultural crops. Most research has been limited to effects of O_3 , although some work on interactions of $O_3 + SO_2$ and $SO_2 + NO_2$ has been accomplished with additional assistance from the Electric Power Research Institute (EPRI). Argonne National Laboratory has been responsible for the research in the Central States Region of the United States and has investigated the impacts of O_3 or $O_3 + SO_2$ on field corn, soybean, winter wheat, grain sorghum, and alfalfa. Winter wheat is the only crop in which significant cultivar variability in O_3 sensitivity has been identified.

The objective of the current studies at Argonne is to examine how drought stress affects the sensitivity of soybeans to O_3 . The hypothesis is that drought-stressed plants will be less sensitive to stress from O_3 .

Studies of O_3 and SO_2 effects on alfalfa and field corn, and O_3 and water stress effects on soybean are described in the following sections.

3.3.2 Effects of Ozone and/or Sulfur Dioxide on Alfalfa Yield and Select Rhizosphere Parameters

L.W. Kress and A.-C. McGraw

This study, funded jointly by EPA and EPRI, was designed to evaluate the effects of ozone (O_3) and/or sulfur dioxide (SO_2) on the yield of alfalfa and on select rhizosphere parameters.

The experimental design was a randomized complete block with two replications of five O_3 x four SO_2 treatments. The O_3 treatments were charcoal filtered (CF), nonfiltered (NF), 1.5 x NF, 2.0 x NF, and 2.5 x NF. The SO_2 treatments were zero, low-frequency distribution, medium-frequency distribution, and high-frequency distribution. There also was a nonchambered plot in each block replication.

Ozone was added to ambient air in the chambers whenever ambient O_3 was above 0.03 ppm between 0800-2000 CDT and in the absence of rain. The average length of the daily O_3 exposures was 8.5 hours on the 43 days when O_3 was actually dispensed during the 53-day exposure period. The SO_2 treatments began on 14 August (3 days/week) and differed not only in the hourly concentrations (ranging from 0.05-0.85 ppm), but also in the total hours of exposure (ranging from 1-6 hours) on each day.

An analysis of covariance of alfalfa top dry weight (using the pre-treatment harvest weight as the covariate) indicated no significant main or second-order effects on yield. In an analysis of variance, there were no significant effects of pollutant treatment on concentrations of reducing sugars, sucrose, or starch in leaves or stems. Additionally, linear and quadratic regressions were not significant for any of the measured above-ground variables regressed with increasing levels of pollutants.

Rhizosphere soil samples were collected in October after a final above-ground harvest, and were processed for quantitative determination of vesicular-arbuscular mycorrhizae and rhizobia (root-fungus and root-bacteria symbioses, respectively), nematodes, and for roots. Samples were collected from within each open-top fumigation chamber and from ambient control plots (AMB).

Linear relationships were not evident between increasing dosages of O_3 or SO_2 and any of the rhizosphere parameters measured. Ozone had little effect on the community of mycorrhizal fungi or on mycorrhizae, reduced rhizobia nodule biomass, and increased nematode populations (Figure 3.7). Sulfur dioxide had very few effects on any rhizosphere parameters measured. However, the combination of O_3 and SO_2 resulted in several significant ($p < 0.05$) positive (nematode populations) and negative (rhizobia nodule biomass and abundance) synergistic responses. In all, ten species of mycorrhizal fungi were detected; eight species were identified and two were unidentified, with the genus Glomus clearly a dominant.

Rhizosphere components of the ecosystem can be affected quite markedly by single or dual exposure to O_3 and SO_2 . Ozone and SO_2 affected root/microbe variables differentially, and the effects were not primarily negative. One overriding effect was the buildup of populations of soilborne nematodes in association with O_3 , and especially with the combination of O_3 and SO_2 . Carbon substrate associated with the indigenous pool of soil organic matter, soil microorganisms, and with alfalfa roots could have affected nematode populations. Conceivably, nematode populations could be an important predictor of the sensitivity of a system to pollutants.

Minimal effects of pollutants on the mycorrhizal and rhizobial symbioses were observed; however, there were several anomalies in the data. The presence of a chamber resulted in a significant decrease in spore population densities of mycorrhizal fungi. Additionally, in the absence of even ambient levels of pollutants, spore populations decreased significantly and rhizobia nodule biomass increased significantly. Chamber and charcoal filtering effects on relevant parameters emphasize the difficulty in conducting field studies. Lastly, cumulative effects of exposure to pollutants could not be ruled out for effects on the below-ground ecosystem.

Figure 3.7. Effects of fumigant exposure on rhizosphere population densities of mycorrhizal fungi and nematodes, and rhizobia nodules associated with field-grown alfalfa (* = $p < 0.05$). The response variables were measured after exposure to seasonal average concentrations (ppm) of O₃: - AMB = 0.042, CF = 0.018, NF = 0.039; and measurements were averaged from the O₃-amended (0.053, 0.067, 0.083) plots or from plots receiving dosages (ppm-hours) of SO₂ (2.00, 5.45, 13.60).

3.3.3 Effects of Ozone and Sulfur Dioxide on Corn

L.W. Kress, P.M. Irving, H.J. Smith, and W. Prepejchal

Field corn (*Zea mays* L.) is the most important agricultural crop in the United States, and the major production areas are subjected to potentially damaging concentrations of O₃. A study completed in 1981 at Argonne was used to develop a model for the impact of O₃ on grain yield of field corn. A Weibull model predicted losses of 2.6% at 0.06 ppm O₃ and 16.3% at 0.10 ppm O₃.

(Kress and Miller 1985). The ambient O_3 concentrations throughout most of the Midwest are 0.04-0.06 ppm.

The present study was funded jointly by EPA and EPRI to determine (1) the exposure-response relationship between daily O_3 exposure and yield of four field corn hybrids; (2) the exposure-response relationship between simulated point source SO_2 exposure and yield of four field corn hybrids; and (3) the potential interaction of daily O_3 exposure and intermittent SO_2 exposure on yield of the four corn hybrids.

Forty-four plots were planted in late May, with six plants of each of the four hybrids per plot. The experimental design was a randomized complete block with two replications of seven O_3 x three SO_2 treatments. The O_3 treatments were charcoal filtered (CF), nonfiltered (NF), and five levels of proportional addition above the nonfiltered. The SO_2 treatments were zero, medium-frequency distribution, and high-frequency distribution. Open-top chambers (Heagle et al. 1979) were established over the plots on 10 June, and the O_3 treatments began on 16 June. There also was a nonchambered plot (AA) in each replication. Ozone was added to all of the NF chambers whenever ambient O_3 was above 0.03 ppm between 0800-2000 CDT, in the absence of rain. The average length of the daily O_3 exposures was 9.2 hours for 80 days when O_3 was actually dispensed during the 82-day exposure period. The SO_2 exposures began on 1 July and differed not only in the hourly concentrations, but also in the total hours of exposure (78 hours for the medium and 147 hours for the high treatments). Exposures lasting 4 to 6 hours occurred two or three times per week in the high treatment. Exposures lasting 3 to 5 hours occurred one or two times per week in the medium treatment. Several physical and physiological measurements were made during the season; following harvest, measurements were made for plant height, stem circumference, total grain yield, weight per 100 seeds, cob length, cob weight, and percent of cob with kernels.

The data from this study are currently being analyzed. A preliminary evaluation indicates that the responses to O_3 are very similar to those observed previously at Argonne (Kress and Miller 1985). A test of heterogeneity of yield response to O_3 indicates that there is significant variation among hybrids (Figure 3.8). There appears to be little effect of SO_2 alone on yield, but SO_2 tends to cause greater O_3 -induced yield reductions at the lower O_3 concentrations. The most O_3 -sensitive hybrid (FR20A x FR35) also exhibits an O_3 x SO_2 interaction such that the O_3 causes greater yield reduction at the intermediate SO_2 level (7.45 ppm-hrs) than at either the control level (0.08 ppm-hrs) or the high level (17.60 ppm-hrs) (Figure 3.9).

Figure 3.8. Relative yield response of four field corn hybrids exposed to ozone (O_3) in open-top chambers for 12-hours/day for 82 days. Yield was calculated at 100% for 0.025 ppm O_3 as an assumed natural background concentration.

Figure 3.9. Relative yield response to ozone (O_3) of one field corn hybrid at three SO_2 dosages. Plants were exposed to daily O_3 and intermittent SO_2 treatments for 82 days.

3.3.4 Effects of Ozone and Water Stress on Soybeans

L.W. Kress, P.M. Irving, W. Prepejchal, and H.J. Smith

The influence of water deficits on plant growth and development is one of the most commonly studied aspects of plant physiology. Processes such as transpiration, photosynthesis, and enzyme activity are known to be affected by water stress and ozone (O_3) alike. It is generally believed that plants are less sensitive to O_3 when subjected to water stress. The objective of this study was to determine the influence of drought stress (applied during podfill) on the O_3 sensitivity of field-grown soybeans. An examination of various physiological processes may help in interpreting yield results from our study and may aid in the understanding of the mechanisms associated with both ozone and drought stress.

Utilizing specially designed rain-exclusion covers, a $5 O_3 \times 2 H_2O \times 2$ replication (plus open plots, wet and dry) study was completed with "Corsoy-79" soybeans. Proportional O_3 additions were performed during a 0800-2000 CST 12-hour window from 23 June to 17 September 1985. The O_3 treatments were open plot (AA), charcoal filtered (CF), nonfiltered (NF), and three levels of proportional addition above nonfiltered. Prior to 6 August, all plots were exposed to ambient rainfall. During July, all plots were also irrigated twice with a total of 5.08 cm H_2O . Rain was excluded from all plots beginning on 6 August at the initiation of podfill. The nonstressed plots were irrigated six times with a total of 7.62 cm H_2O in August and 7.62 cm in September. Harvest of the soybeans was concluded on 14 October.

Soil moisture to a 15-cm depth was monitored using a surface neutron probe. Differences in soil water content between irrigated and nonirrigated plots were evident in early August, soon after rainfall was eliminated. In the dry plots, soil moisture levels dropped from 25% in early August to about 6% in mid-September, while the wet plots remained above 15% moisture. In addition to measuring seed and stem yield, we also evaluated plant development, photosynthesis, leaf chlorophyll, soil respiration, mycorrhizal infection, and leaf water potential.

Differences between wet and dry plots in leaf water potential, which was determined with a Scholander pressure chamber, were not observed until late August. It is believed that the cool, humid conditions occurring during August were responsible for the lack of an effect of the low soil moisture levels on leaf water potential in the dry plots. By early September, however, leaf water potential in the dry plots was as low as -20 bars, while the wet plots never had water potentials below -9 bars.

Photosynthetic carbon fixation on the basis of unit leaf area was reduced by more than 50% ($p = 0.0001$) in the dry plots compared with the wet ones in late August. This appeared to be related to reduced stomatal conductance. Drought had no effect on leaf chlorophyll content; however, plants treated with the highest O_3 level in both wet and dry plots had reduced chlorophyll content compared with all other O_3 levels.

The above- and below-ground portions of the plant appeared to respond differently to O_3 depending on soil moisture conditions. Fine root mass of drought-stressed soybeans was significantly greater ($p = 0.02$) than that of irrigated plants. Root mass of drought-stressed plants was negatively affected by ozone, whereas no effect was observed on plants in irrigated plots. Shoot weight was negatively affected by O_3 concentrations in the well-watered plots and unaffected by O_3 in the drought-stressed plots, although overall shoot weight was lower in plants affected by drought conditions compared with irrigated plants.

Our results suggest that drought conditions result in reduced carbon fixation in leaves, but increased carbon allocation to the roots of soybeans. The drought-induced stimulation of root growth was apparently suppressed by the O_3 exposure. Conversely, the irrigated plots exhibited greater sensitivity to the O_3 in above-ground vegetative biomass accumulation.

A preliminary evaluation of the yield data shows (Table 3.6) that the drought stress reduced seed yields an average of 23%, but not dry stem weights. Ozone reduced the yields of well-watered plants up to 17% for seed yield and 30% for stem weight, but these reductions were not significant. For drought-stressed plants, O_3 reduced seed yield (by 6.6%) only in the 2.0 x NF treatment. Individual seed weights were reduced by the O_3 about equally in wet and dry treatments, but in the dry treatments, seed number was increased in all treatments compared to CF. The drought stress had a rather severe

Table 3.6. Relative yield responses of soybean exposed to O_3 and drought stress in open-top field chambers, 23 June - 28 September, 1985

H ₂ O Treatment	O ₃ Treatment	O ₃ Concentration (ppm)	Yield			
			kg/ha	100 Seed wt (g)	Seed #/Meter	Dry Stem wt/Meter
Wet	AA	0.041	4,464	14.9	1,304	92
	CF	0.014	3,664	14.9	1,068	85
	NF	0.040	3,391	14.4	1,029	59
	1.33 x NF	0.052	3,509	14.1	1,072	67
	1.67 x NF	0.063	3,377	13.9	1,062	72
	2.0 x NF	0.076	3,029	12.9	1,024	59
Dry	AA	0.041	3,899	13.9	1,222	101
	CF	0.017	2,450	13.1	813	62
	NF	0.041	2,758	12.6	956	73
	1.33 x NF	0.053	2,613	12.4	910	71
	1.67 x NF	0.064	2,590	13.1	867	63
	2.0 x NF	0.079	2,283	11.5	862	63

effect on yield (primarily seed number) in the CF treatment, with photosynthate apparently being shifted to root development. Considering only the four NF treatments, the response to O_3 was more severe in the dry plots (-17.5%) than the wet plots (-10.8%).

3.4 ACID RAIN STUDIES

3.4.1 Summary

P.M. Irving

Field studies for two major research efforts to examine the effects of acidic rain on terrestrial ecosystems were completed in 1984. The studies, conducted in Argonne's Microcosms for Acid Rain Studies (MARS) Facility, were funded by the Electric Power Research Institute (EPRI) and the Environmental Protection Agency (EPA).

The EPRI project (Sections 3.4.2 through 3.4.4) was a large, multidisciplinary study to examine the effects of acidic rain on two plant/soil systems. Components of this study included vegetative production and nutrient composition; soil microbial activity; nutrient cycling and partitioning; and chemistry of soil, soil water, and groundwater. Both episodic and cumulative effects were examined during the two years of experimental treatments with simulated rain. Data have been analyzed for a number of experimental parameters and the results are included in this report. Other information, such as input-output budgets for major nutrients, is still being analyzed.

The work funded by the EPA (Section 3.4.5) was part of a larger multi-laboratory project to determine the effects of acidic rain on major crops. Information from the Argonne project will be used to determine future protocol for the design of experiments and to aid in the extrapolation of data for regional crop loss assessments. The effect of temporal variations in rainfall acidity was examined at Argonne because current experimental design in most acidic rain studies does not include temporal variations in rainfall acidity even though such variations occur under ambient conditions. The work performed in 1983 was duplicated in 1984 in order to confirm experimental results. The 1984 data and combined results are presented in this report.

3.4.2 Nutrient Content and Production in Two Plant/Soil Systems Treated with Simulated Acidic Rain

P.M. Irving, W. Prepejchal, C. Davis,* and C. Nolt*

Hay crops (i.e., grass-legume mixtures), which are fourth in importance in the United States according to value and acreage harvested, are potentially sensitive to acidic precipitation because of their perennial nature and

*Collaborator; affiliation is listed at the front of this chapter.

typically low level of management. Therefore, a timothy (Phleum pratense) - red clover (Trifolium pratense) mixture was grown in our field research facility for studies of acidic-rain effects on soil/plant systems (Irving et al. 1983a). Plant production data for 1984 and cumulative yield and nutrient content for the combined years of 1983 and 1984 for the two soil types utilized in our studies are summarized in this section.

The growth of timothy was much more vigorous than that of the red clover for both soils in 1984, the second year of rainfall simulation. Although the clover was well nodulated, timothy, with its greater water-use efficiency, normally has a competitive advantage over time when planted in mixtures with clover. Vegetation on the Alvin soil was harvested three times during the 1984 growing season--in June, July, and September. The LaHogue soil was harvested twice--in June and August. Although both soils were fertilized with phosphorus and potassium prior to seeding in 1983, the LaHogue soil had significantly lower levels of the major plant nutrients than did the Alvin soil (Table 3.7). This accounts for the fewer harvests and overall lower cumulative yields of the LaHogue soil compared with the Alvin soil (Table 3.8).

There were no treatment effects on yield for the Alvin soil based on analysis of variance; however, cumulative yield of timothy (1983 and 1984 harvests combined) in the LaHogue plots treated with the highest acidity rain (pH 3.2) was 29% greater than in plots treated with rain having no strong acids (pH 5.4). A statistical comparison of biomass production indicates that timothy yield is significantly greater ($p = 0.04$) in the pH 3.2 plot compared with all other treatments in the LaHogue soil (Table 3.8).

Biomass from all harvests of timothy and clover over the two years of the study was combined for each species on each soil and analyzed for major nutrients. Treatment differences for nitrogen, phosphorus, potassium, and sulfur concentrations were not statistically significant in either species for the Alvin soil. Analysis of variance indicated a significant effect of simulated rain pH on the percent sulfur content of the clover harvested from the LaHogue soil and on total accumulation of phosphorus, potassium, and sulfur in timothy harvested from LaHogue.

Plant growth in the nutrient-deficient LaHogue soil, which was stimulated by the most acidic rain simulant in our study, may have benefited from the greater input of sulfur present in the highest acidity rain to both foliage and soil. The fact that the LaHogue soil had lower initial levels of nitrogen and sulfur than the Alvin plots and also had a greater yield response from the simulated rain is consistent with the explanation that the acidic rain treatments provided needed nutrients for plant growth. Elemental analysis of the plant tissue also supports this conclusion.

Our findings emphasize the importance of rain as a source of nutrients to vegetation in poorly managed ecosystems. However, it is unlikely that the growth stimulation observed in this study would have continued beyond many more harvests because some other plant nutrient, not provided by the acidic rain treatments, would have become limiting.

Table 3.7. Concentration of major plant nutrients in LaHogue and Alvin topsoil sampled in October 1982 (n = 21)

Soil	Concentration ($\mu\text{g g}^{-1} \pm \text{S.E.}$)			
	$\text{NO}_3\text{-N}$	$\text{PO}_4\text{-P}$	K	$\text{SO}_4\text{-S}$
LaHogue	4.7 ± 0.4	5.5 ± 0.6	200.5 ± 16.9	8.5 ± 0.5
Alvin	8.7 ± 0.3	42.5 ± 5.7	466.3 ± 36.8	12.6 ± 0.5

Table 3.8. Dry biomass (grams of above-ground growth) of timothy and clover in 3-m² plots of two soils exposed to simulated rain

Soil	Rain pH	1984		1983 + 1984	
		Timothy	Clover	Timothy	Clover
Alvin	5.4	2,266	163	3,148	471
	4.5	2,177	142	3,108	465
	4.2	2,425	93	3,453	462
	3.5	2,254	108	3,177	457
	3.2	2,523	128	3,480	585
LaHogue	5.4	979	30	1,105	125
	4.5	913	18	1,147	79
	4.2	800	13	909	135
	3.5	1,106	20	1,239	108
	3.2	1,250	16	1,425 ^a	106

^a T-test indicates this value is significantly higher (p = 0.04) than all others in its group combined.

3.4.3 Effect of Acidic Rain on Soil Acidity and Nitrification Rates in Two Plant/Soil Systems

P.M. Irving, W. Winston, and M.J. Sullivan**

Lack of information about the mechanisms of biochemical transformations of atmospheric pollutants has led to confusion and inconsistencies regarding the potential ecological impacts of acidic deposition. Although there has been much speculation regarding the possibility for harmful effects of acidic rain on the productivity of poorly buffered plant/soil systems, there have been few multidisciplinary studies to support this view. Studies to examine the interactions between the soil and plant communities in their response to a potential stress such as acidic rain are a necessary step in understanding total ecosystem response. Acidic rain is a source of potentially beneficial and potential toxic substances (nutrients and acidity, respectively). However, it is unknown what effects these substances may have on long-term nutrient cycling in poorly managed ecosystems. This report summarizes one aspect of the investigations of soil microbial activity performed in our Microcosm Facility (Irving et al. 1983a), which was designed to conduct process-oriented studies of plant/soil systems treated with controlled levels of acidic deposition.

After two years (1983 and 1984) of simulated rain treatments, the acidity of the surface soil (top 5 cm) was significantly ($p < 0.01$) affected by the rain treatments for both soils examined in the study (Table 3.9). The pH of Alvin soil appeared to be decreased in plots treated with the two highest levels of rainfall acidity (pH 3.5 and 3.2) while surface soil pH in the LaHogue soil decreased linearly with simulated rain pH. According to analysis of variance, total nitrate (NO_3^-) production in LaHogue soil amended with ammonium (potential nitrification) may have been affected by this increase in soil acidity (Table 3.9). Nitrification rate was less ($p = 0.07$) in the soil from plots treated with the pH 3.2 simulated rain compared with all other treatments (Figure 3.10). In comparison, the Alvin soil exhibited the greatest ($p = 0.003$) rate of nitrification in the soil from plots treated with the pH 4.2 simulated rain until week 5, when the rate began to decrease due to depletion of the ammonium source (Figure 3.10). These results are in contrast to those observed in 1983, when potential nitrification was inhibited in the pH 3.2 treated Alvin soils and stimulated in the pH 4.2 treated LaHogue soils (Irving et al. 1983b). As in 1983, rates of nitrification in water-amended soils were much lower than in the ammonia-amended soils (indicating they are substrate limited), and appeared to be unaffected by the pH of simulated rain (Table 3.9).

Since nitrification is, in itself, an acidifying process, the soil from LaHogue plots which had already been acidified by the pH 3.2 rain simulants may have been further acidified by the nitrification process to the extent

*Collaborator; affiliation is listed at the front of this chapter.

that the activity of nitrifying organisms was inhibited. In the unamended soils, the rate of nitrification was apparently too low for a deleterious buildup of hydrogen ions since no treatment differences were observed.

In unmanaged soils, ammonium levels would rarely be as high as those in the amended samples in our study, while with agricultural soils, addition of ammonium is routine. Based on these results, it appears unlikely that acidic rain will inhibit NO_3^- production in either managed or unmanaged soils because managed agricultural soils are routinely limed to prevent their acidification, and unmanaged soils do not normally have high ammonium levels.

Table 3.9. Surface soil pH (5-cm depth) and nitrification in two soil systems exposed to simulated acidic precipitation

Soil	pH		NO_3^- -N/g Soil ^b	
	Rain	Surface Soil ^a	NH_4 -Amended	H_2O -Amended
<u>Alvin</u>	5.4	6.09	77.7	23.1
	4.5	6.01	67.8	23.7
	4.2	6.11	95.6	25.4
	3.5	5.93	80.2	24.8
	3.2	5.60	77.2	24.8
ANOVA	R ²	0.93	0.67	0.27
	PR	0.0001	0.096	0.53
<u>LaHogue</u>	5.4	6.18	52.5	8.6
	4.5	6.02	44.2	11.6
	4.2	5.89	47.9	15.4
	3.5	5.86	49.0	6.6
	3.2	5.50	31.1	8.8
ANOVA	R ²	0.84	0.68	0.21
	PR	0.003	0.01	0.63

^a The top 5 cm of soil were sampled in October 1984 after 2 years of rainfall simulation.

^b Difference in NO_3^- -N concentration in top 5 cm of soil before and after 5 weeks of incubation.

Figure 3.10. Potential nitrification (rate of NO₃ accumulation) in ammonium-amended soils treated with simulated rain (n = 3).

3.4.4 Effect of Acidic Rain on Populations and Activities of Soil Microorganisms in Two Plant/Soil Systems

*P.M. Irving and K.H. Lavoie**

A very fine balance usually exists between vegetative and soil nutrient pools in poorly managed ecosystems where microbial transformations are essential components in the process of nutrient cycling. Acidic rain may affect both the pH and nutrient status (through sulfur and nitrogen input) of an ecosystem; thus, its overall impact may be quite complex. The sensitivity of microorganisms to changes in the pH and nutrient status of their environment justifies concern about the potential impacts of acidic rain on the productivity of unbuffered systems. This section summarizes another

*Collaborator; affiliation is listed at front of this chapter.

component of the below-ground studies in our multidisciplinary investigations of two plant/soil systems exposed to simulated acidic rain.

To quantify the net heterotrophic activity (bacterial, fungal, faunal, and root) of the soil, respiration was determined by measuring carbon dioxide (CO_2) evolution from the soil surface. These measurements were made on a weekly basis during the major period of vegetative productivity on a weekly basis in 1983 (Irving et al. 1984a) and 1984. Average soil respiration was highest in plots treated with pH 4.2 rain simulant for both 1983 and 1984 (Figure 3.11). The relationship between respiration and treatment acidity based on data from both years can be described by a quadratic function for both Alvin ($p = 0.12$) and LaHogue ($p = 0.03$) soils.

Figure 3.11. Soil respiration (rate of CO_2 release) in two soils treated with simulated rain (1983: $n = 18$; 1984: $n = 24$).

The effect of treatment acidity on surface soil pH (Irving et al. 1984b) prompted us to evaluate populations of soil microorganisms that may be important in the cycling of nutrients in our systems--specifically protozoa and mycorrhizal fungi. Protozoa, which are present at high numbers in the top 1 to 2 cm of most pastureland or grassland, increase mineralization of nutrients through predation of bacteria, thus increasing nutrient availability to plants. The infection of root tissue with vesicular arbuscular (VA) mycorrhizal fungi may benefit the host plant by enhancing nutrient uptake.

Population densities of protozoa and spores of VA mycorrhizal fungi in both soils during the 1984 growing season were greatest in the plots treated with pH 4.2 simulated rain compared with all other plots (Table 3.10). Analysis of variance of the data indicates that treatment differences were not statistically significant except for protozoa densities in the LaHogue soil

Table 3.10. Protozoa and VA mycorrhizal fungi in two soils as a function of simulated rain acidity

Rain pH	Protozoa (x 10 ³) Total ^a	Mycorrhizae ^b		
		Spores	cm of Root Colonized	Percentage of Root Colonized
<u>Alvin Soil</u>				
5.4	20.2	17.5 (1.6)	10.3	5.3
4.5	25.5	24.3 (3.0)	10.4	4.5
4.2	27.4	30.3 (7.7)	18.6	7.8
3.5	20.9	24.0 (2.8)	18.2	4.6
3.2	20.2	23.9 (6.4)	16.2	7.0
T ^c	1.45		-2.61	1.87
PR	0.15	n.s.	0.01	0.08
<u>LaHogue Soil</u>				
5.4	1.9	5.43 (0.9)	62.7	13.5
4.5	1.3	7.14 (1.5)	69.3	18.9
4.2	2.9	7.42 (2.1)	59.2	12.3
3.5	1.9	6.13 (0.8)	75.8	19.5
3.2	1.9	6.14 (1.3)	58.4	14.0
T	2.49			
PR	0.02	n.s.	n.s.	n.s.

^aActive ciliates, flagellates, and amoeba per g soil.

^bValues are per 50 g soil; value in parentheses is standard error.

^cT statistic comparing pH 4.2 to all other treatments except for cm root in Alvin soil where comparison is between pH $\geq$ 4.2, and pH $<$ 4.2.

($p = 0.02$). However, soil respiration in Alvin soil was highly correlated with spore numbers ($p = 0.01$) and marginally correlated with protozoa density ($p = 0.08$). The total length of roots colonized with indigenous mycorrhizal fungi was greatest ($p = 0.01$) from subsamples of root systems in Alvin plots treated with the pH 4.2, 3.5, and 3.2 simulated rain compared with the lower acidity treatments (Table 3.10). Alvin plots treated with pH 4.2 simulated rain had the highest percent colonization with VA mycorrhizal fungi. The overall differences in spore production and root infection between the two soils may have resulted in part from differences in the developmental stage of the vegetation at the time of sampling and/or from differences in soil nutrient content.

The results of these studies suggest that certain soil microorganisms in our systems function best at ambient levels of acids in rain and that

increases or decreases in the levels of acids will result in lower activity. In marginal, nutrient-limited systems such as those examined in this study (Section 3.4.2), the atmosphere can be a significant source of nutrients. In a system already at equilibrium with ambient conditions (such as in the soils used for these studies), removal of this source of nutrients (i.e., by reducing nitric and sulfuric acids in rain) may limit the growth of vegetative and soil biota, while increasing the input may stimulate growth (Section 3.4.2). The nutritional advantages of increased sulfur and nitrogen levels from higher concentrations of acids in rain, however, may be offset by increased acidification--hence, the quadratic response in some of our measures of microbial activity.

These data will be evaluated with other information collected during the two years of this study to assess the overall response of the two systems to the simulated rain treatments.

3.4.5 Effect of Temporal Variations in Rainfall Acidity on Field-Grown Soybeans

P.M. Irving, W. Prepejchal, R. Vogel, and H. Rosenbaum**

The normal variation in rainfall acidity from event to event may have important biological consequences. Thus, studies that utilize simulated rain with constant chemistry may be inadequate in assessing potential damage from acidic rain. A two-year (1983 and 1984) field study was initiated to determine the importance of event-to-event differences in the hydrogen ion concentration of rain in affecting the response of soybeans to acidic rain. This report summarizes results from the 1984 studies and presents conclusions based on the combined data from both years.

Field-grown soybeans (Glycine max cv. Amsoy 71) were exposed to simulated rain with one of four mean acidity levels and in two treatment groups: (1) temporal variations in acidity among events, and (2) no variation in acidity from event to event. Each treatment was replicated six times, resulting in a total of 48 experimental plots, each with 12 harvested plants. These and other characteristics duplicated the experiment performed in 1983 (Irving et al. 1984c).

Visual evaluations indicated that the soybean plants were (1) most sensitive to leaf injury, in the form of chlorosis and necrotic lesions, when the plants were in a vegetative growth stage; (2) less sensitive during flowering; and (3) least sensitive during the podfill period, when no injury was observed. Injury was positively correlated with the acidity of the simulated rain ($p < 0.001$). A quantitative determination of leaf injury during the vegetative stage (using an ethanol extraction technique to measure leaf chlorophyll content) indicated that plants in the pH 3.4 variable treatment group had lower ($p = 0.088$) chlorophyll than those in the pH constant acidity

*Collaborator; affiliation is listed at the front of this chapter.

group (Figure 3.12). There was no effect on the ratio of chlorophyll-a to chlorophyll-b.

Photosynthetic rates of one plant per plot were measured four times during August using a LiCor 6000 Analyzer that measures CO_2 exchange. These measurements were made on the middle leaflet of the third trifoliolate from the apex. Net photosynthesis was significantly affected by leaf temperature, relative humidity, and photosynthetically active radiation, but was unaffected by rain acidity and temporal variations in rain acidity. Treatment differences were not significant for any of the measurement dates, nor were there significant differences for the combined data.

Figure 3.12. Soybean leaf chlorophyll content (3rd node from apex) in plants exposed to rain with either constant or temporal variations in acidity ($n = 6$). Bars with a common letter are not significantly different ($p < 0.05$).

Chlorophyll content of the same leaves sampled for the photosynthesis measurements indicated no effect from temporal variations in rain acidity. However, in late August, when plants were undergoing senescence, leaves from plants in the highest acidity treatment (pH 3.4) had a significantly higher chlorophyll content than did plants treated with rain having no strong acids. These results suggest that plants that are injured by exposure to acidic rain may become more resistant to such stress later in their life cycle.

Analysis of variance indicated no significant ($p < 0.05$) effects from simulated rain acidity or temporal variations in rain acidity on seed weight per plant, pod weight per plant, and number of pods and seeds per plant. Neither were there obvious trends in the yield results. In analyzing the results from both years of the experiment, no treatment differences in yield were observed (Table 3.11).

Although there were differences in visible injury, it is difficult to assess the importance of temporal variations in the acidity of rain in affecting crop yield because we observed no acidity-related effects on the yield of soybeans. These results are in contrast to previous studies that reported negative effects on the yield of Amsoy soybeans from simulated acidic

Table 3.11. Seed weight per plant as a percent of control (mean for pH 5.6 constant and variable treatments) for 1983 and 1984 studies of acidic rain effects on soybeans

Treatment	pH	Seed Weight per Plant (% of control)		
		1983	1984	Average
Constant	5.6	100.1	109.4	104.7
	4.2	81.3	80.7	81.0
	3.7	102.9	99.0	100.9
	3.4	89.5	104.9	97.2
Variable	5.6	99.9	90.6	95.3
	4.2	108.8	98.7	103.7
	3.7	103.1	71.6	87.3
	3.4	116.4	97.3	106.9

rain (Evans et al. 1984), but are comparable to other acidic rain studies of Amsoy (Banwart 1985). The contrasting reports on the yield response of Amsoy soybeans to simulated acidic rain warrant further research to determine the conditions and mechanisms for which Amsoy soybean is sensitive to acidic deposition.

3.5 SOIL-PLANT PROCESSES PROGRAM

3.5.1 Summary

R.M. Miller

We have been investigating the role of mycorrhizae as part of a stress tolerance strategy in plants. In the past, we focused on determining the effects of disturbance on the vesicular-arbuscular (VA) mycorrhizal fungus community. This research required the identification of those factors, biotic and environmental, that influenced the occurrence of the mycorrhizal association. This approach, however, did not address the mechanisms by which plants may benefit from this symbiosis.

It currently is believed that the association between temperate grasses and mycorrhizal fungi is a facultative one. Also, other than through the ubiquitous nature of the occurrence of this fungus, little evidence exists that mycorrhizae are a necessary component of the grassland community. Considering that the majority of studies on the mycorrhizae of grasses have dealt with pasture grasses rather than with true grassland grasses, the apparent lack of necessity may be related to habitat. For example, when studies of growth response of grasses and mycorrhizae are grouped into the type of habitat where the grass occurs, it becomes apparent that the growth

strategy of the host is an important consideration in discussing the mycotrophic response. Similarly, in such studies the soils have had a narrow range of fertility where levels of nutrients were not limiting to host growth. When phosphorus (P) was added to the soil it typically was at levels higher than that occurring in grassland soils (Miller 1986).

The first three of the four investigations reported here represent a systematic approach to investigating how mycorrhizae can influence wild plants, in our case a grass of the mid-grass prairie (Sections 3.3.2 through 3.3.4). The final investigation reported is a new initiative that addresses how the soil-root interface may affect soil aggregation in a tallgrass prairie (Section 3.3.5). For these investigations to be carried out, it was important to establish biotypes of the mycorrhizal fungi for better control of genetic variability. It was also important to identify those attributes of a host that responded to the fungus. However, a significant problem to overcome was the lack of any quantitative methods for evaluating the mycorrhizal fungus aside from sand culture conditions. This required us to develop methods for measuring external fungus biomass in heavy soils. Similarly, a better understanding of the relationship between internal infection and fungus biomass was needed. Although not discussed in this report, a major accomplishment of this program has been the development of methods that enable us to characterize the different 'pools' of mycorrhizal fungi. This in turn has allowed us to initiate studies evaluating biomass allocation of the fungus and host along a resource gradient using a factorial design consisting of various combinations of nutrients and watering regimes. Also, through use of biotypes of both fungus and host, a genetic component was added to the model.

The investigation reported in Section 3.3.5 represents a new initiative to investigate the interrelationships between biotic factors and the processes of soil formation. We are using a restoration ecology approach to investigate the influence of the rhizosphere on soil aggregation in a restored tallgrass prairie. This project represents an attempt to learn how biotic processes are integrated with changes in physical and chemical characteristics of soil. We believe that a better understanding of the recovery process in soils and associated plant communities can be realized by such investigations. Future research will address the mechanisms of soil aggregation and the influences of biotic-mediated changes in soil structure on changes in hydraulic conductance and mineral ion uptake in the rhizosphere.

3.5.2 Mycorrhizal Fungus Isolate Development

A.-C. McGraw

The collection of strains of mycorrhizal fungi from a Red Desert, Wyoming, study site for use in disturbance experiments was detailed in a previous report (McGraw and Miller 1984). However, these strains were initiated as mass transfers of spores. The multinucleate status of the

spores, the most easily manipulated propagule, could contribute significantly to variability in plant response under controlled environmental conditions. The concern regarding variability is present as well in regard to the taxonomy of the mycorrhizal fungi. Identification to species is based almost exclusively on spore morphological criteria, in spite of the vague descriptive boundaries for each species. Additionally, future biotechnological endeavors to manipulate the mycorrhizal relationship must be based on an understanding of the genetic mechanisms of tolerance to edaphic and environmental variables. Thus, a study was initiated to ascertain the variability of morphological characters assumed to be stable.

Two species of vesicular-arbuscular mycorrhizal fungi, Glomus monosporum Gerd. & Trappe (GMN) and G. mosseae (Nicol. & Gerd.) Gerd. & Trappe (GMO), that are difficult to distinguish morphologically were inoculated as single spores or sporocarps (SP) (aggregates of 1-3 spores) on the roots of a grass hybrid. Plants were grown under controlled environmental conditions with adequate nutrient and moisture inputs, and mycorrhizal spore progeny were evaluated for size, shape, and color. For GMN, 70% of the colonizations were successful, while GMN-SP and GMO were both 40% successful. The spore diameters for GMN, GMN-SP, and GMO ranged from 163.0-178.6 μm , 139.7-194.6 μm , and 155.3-186.0 μm , respectively. The higher success rate of establishing colonization and the narrower variability in spore diameters of GMN compared with GMO could reflect a more active physiological status of the initial single spores. A gradient of aging spores, that is, spores that were past their prime in ability to germinate or colonize roots, may have been wider with GMO and GMN-SP. Thus, GMN may be an artifact of speciation through variable aging of spores of GMO.

Single-spore isolations currently provide the only means for understanding the genetics of VA mycorrhizal fungi. However, variation in associative parameters of progeny of single spores still can occur as a result of random segregation and independent migration of nuclei.

In spite of this, studies of lines obtained through single-spore isolation will aid in the verification of stability of parameters assumed to be independent of environmental factors. Significant contributions toward understanding mycorrhizae under field conditions could be made if mechanisms of tolerance to environmental variables were better understood.

3.5.3 Biomass Allocation of an *Agropyron smithii*-*Glomus* spp. Symbiosis

R.M. Miller

If the mycorrhizal association is to be of any evolutionary significance, it must have an effect on individual plants within a natural community, such that the fungus-mediated response of the host can affect survival, as well as increase the proportion of offspring a host contributes to the population. Thus, research that emphasizes mycorrhizal dependency based on biomass production alone measures only a component of host fitness. Similarly, the

use of host growth or production as a measure of mycorrhizal effectivity in the absence of measurements of mycorrhizal fungus biomass represents an oversimplification of the symbiosis, since only a part of the association has been characterized. The significance of this mutualism to the survival of a host can be evaluated only when the cost of possessing mycorrhizae is placed into the context of the benefits received.

Since a major means of propagation for many grasses of true grassland communities is clonal growth by rhizomes and tillers, an emphasis on the effects of mycorrhizae on biomass production may be misleading. Additionally, the relationship of mycorrhizal fungi to the host can be expected to change over a range of soil resource levels, especially in the allocation of fungus biomass. In previous studies, soil phosphorus has been found to vary from less than $2 \mu\text{g g}^{-1}$ to over $25 \mu\text{g g}^{-1}$ soil for samples collected within 24 m of each other in the shrub steppe of western North America (Miller 1984). Considering the paucity of information on mycorrhizae in wild plants, we conducted an experiment with a cool-season, C3, mid-prairie grass, Agropyron smithii Rybd., grown in a controlled environment where soil phosphorus level was manipulated to achieve a range of 2 to $20 \mu\text{g P g}^{-1}$ soil (other nutrients were supplied at rates not considered limiting). Soils were fumigated prior to inoculation with viable or sterilized spores of G. monosporum/mosseae. Ten weeks after the inoculation, we examined whether tillering and host biomass production, and, similarly, the mycorrhizal fungus could be affected by the position along the resource gradient.

We found that if growth of A. smithii had been evaluated by dry matter production alone, mycorrhizae would have been assumed to be of little importance for those plants grown at the high end ($20 \mu\text{g P g}^{-1}$) of the soil-phosphorus gradient, and would have been of more importance to those plants grown at levels of soil-phosphorus considered deficient ($2 \mu\text{g P g}^{-1}$). However, even at the highest soil-phosphorus level, a mycorrhizae-mediated effect on host biomass allocation still was evident, although the growth response was directed more toward the production of tillers than toward either biomass or changes in host stature.

Internal colonization of roots by the mycorrhizal fungus represents only a portion of total fungus biomass production. The measurement of internal and external fungus biomass allows for the estimation of the cost in carbon to the host, as well as for speculation on the function of the symbiosis across the resource gradient. The finding that the total amount of fungus biomass was not significantly ($p = 0.15$) different across the soil-phosphorus gradient, even though host biomass production was affected, suggests a relatively constant sink strength by the fungus. The allocation response of the fungus suggests either that a soil resource or the host influenced the mycorrhizal fungus. Also, when the cost to the host was highest (as expressed by the proportion of the root system occupied by fungus), the host also experienced its largest biomass increases (mycorrhiza dependency).

A good example of how a change in resource may affect the kind of influence the symbiosis exhibits is shown by both fungus and host biomass

allocation. It appears that at lower soil-phosphorus levels, the mycorrhizal association is directly related to survival of the host via nutrient acquisition, as shown by the increase in external fungus development. At higher soil-phosphorus levels, the mycorrhizal association influences the tillering capability of the plant, which is correlated with an increase in the amount of fungus produced within the cortex ($r = 0.73$, $p < 0.01$). When the tiller response of this host is expressed on a carbon cost per mg P concentration, it becomes evident that mycorrhizal plants are more efficient in carbon use (e.g., Figure 3.13). In an analysis of covariance of this data, with inoculation as the covariate, the slopes of the tiller response for mycorrhizal and nonmycorrhizal *A. smithii* did not differ significantly. The intercepts, however, did differ ($p < 0.005$), suggesting that mycorrhizal plants require a smaller shoot surface area to produce a tiller than do non-mycorrhizal plants. This increase in efficiency due to the mycorrhizal association appears to allow for a redirecting of carbon into tiller production rather than into increasing host stature or individual blade area. The reallocation response exhibited by this species in response to mycorrhizae is a partial measure of fitness.

Figure 3.13. The relationship of leaf surface area corrected for shoot phosphorus concentration and tiller production. The intercepts of inoculated (closed circles) vs. noninoculated (open circles) plants are significantly different ($p < 0.001$) from each other, and the slopes are parallel ($p < 0.001$).

3.5.4 Effects of Mineral Nutrition, and Water Stress on an *Agropyron smithii*/Glomus spp. Symbiosis

A.-C. McGraw and R.M. Miller

In arid ecosystems, scarce resources frequently are limiting factors for propagation and growth of vegetation. Disturbances such as those associated with energy extraction can exacerbate the problem of limiting resources and inhibit establishment and survival of vegetation. Plants have the potential to compensate for limiting conditions through several strategies, including slower growth, increased efficiency of acquiring and utilizing nutrient and water resources, and through symbiotic associations that can improve such efficiencies. It appears that plant/mycorrhizal fungus associations may be one such symbiotic relationship. Mycorrhizae are indeed ubiquitous, but functioning of the symbiosis under a range of edaphic and climatic conditions is poorly understood.

To simulate primary components of a natural semiarid ecosystem, we evaluated the interactive effects of varying plant nutrient (phosphorus [P] and nitrogen [N]) conditions, repeated drought, and different plant genotypes in a five-way analysis of variance. Two genotypes of *Agropyron smithii* were grown in fumigated soil from the Red Desert of Wyoming that had been inoculated with spores (0.7 g^{-1}) of the *Glomus monosporum*/*G. mosseae* complex obtained from the same site. Plants were harvested throughout the growing period, with final harvest at 16 weeks. Growth and morphological parameters of the host and growth of the fungus were measured at each harvest. At final harvest, measures of root absorptive surface area (based on root length, root hair numbers and lengths, and length of extramatrical hyphae) and of internal fungus infection were obtained. Also, stomatal resistance (a measure of the inverse potential for evapotranspirative water loss from plants through leaf stomates) and instantaneous photosynthesis were measured the week before final harvest.

In an analysis of variance of data collected at 16 weeks after inoculation, we found significant primary effects and several second- and third-order effects of the variables on plant biomass, biomass allocation, total absorptive root surface area, plant/water relations (stomatal resistance), and fungal productivity (intra- and extraradical biomass). A simplified example of some of the responses observed is presented in Table 3.12. In this case, data are presented for only one genotype grown.

The interactive effects of the independent variables, although not unexpected, emphasize the complexity of evaluating ecosystem functioning. Overall, nitrogen and drought affected the dependent variables more than did mycorrhizae and phosphorus. The altered root:shoot ratios and water relations in mycorrhizae-inoculated treatments compared to mycorrhizae-free treatments could mean that mycorrhizae affected plant growth and physiology indirectly by inducing hormone-nutrient interactions, rather than by having a direct effect on plant nutritional status. Tissue nutrient data, as yet unavailable, may

Table 3.12. Interactive effects of mycorrhizae, phosphorus, nitrogen, and water on growth and physiology of *A. smithii* (Barton) at 16 weeks of growth

Treatment ^a	Total Dry Weight (g)	Root: Shoot Ratio	No. of Tillers/ Plant	Stomatal Resistance (s m ⁻¹)	PSN ^b Rate
M ⁻ P ⁻ N ⁻ H ₂ O ⁻	1.646	1.64	3.6	4.61	0.352
M ⁻ P ⁻ N ⁻ H ₂ O ⁺	2.138	2.49	3.4	4.36	0.354
M ⁻ P ⁻ N ⁺ H ₂ O ⁻	1.832	1.68	3.4	4.82	0.558
M ⁻ P ⁻ N ⁺ H ₂ O ⁺	2.215	3.11	4.0	2.77	0.572
M ⁻ P ⁺ N ⁻ H ₂ O ⁻	1.607	1.46	3.6	4.33	0.357
M ⁻ P ⁺ N ⁻ H ₂ O ⁺	2.005	1.86	2.8	5.49	0.372
M ⁻ P ⁺ N ⁺ H ₂ O ⁻	2.024	1.60	4.5	4.35	0.406
M ⁻ P ⁺ N ⁺ H ₂ O ⁺	2.101	1.30	3.8	4.40	0.400
M ⁺ P ⁻ N ⁻ H ₂ O ⁻	1.684	2.77	2.6	3.67	0.535
M ⁺ P ⁻ N ⁻ H ₂ O ⁺	1.835	3.13	3.2	5.38	0.357
M ⁺ P ⁻ N ⁺ H ₂ O ⁻	1.804	1.87	4.6	3.99	0.465
M ⁺ P ⁻ N ⁺ H ₂ O ⁺	2.224	2.29	3.2	4.17	0.439
M ⁺ P ⁺ N ⁻ H ₂ O ⁻	1.883	1.79	3.0	5.06	0.343
M ⁺ P ⁺ N ⁻ H ₂ O ⁺	1.684	1.41	2.6	4.85	0.344
M ⁺ P ⁺ N ⁺ H ₂ O ⁻	2.630	2.44	3.2	3.67	0.467
M ⁺ P ⁺ N ⁺ H ₂ O ⁺	3.088	3.24	3.0	4.08	0.479

^a Components not added (-) or added (+), where M = mycorrhizae; P = phosphorus at 20 $\mu\text{g g}^{-1}$; N = nitrogen at 40 $\mu\text{g g}^{-1}$; and H₂O = moisture input.

^b PSN = photosynthesis; rate = $\text{mg CO}_2 \text{ m}^{-2} \text{ s}^{-1}$.

aid in interpreting the interactive effects. For example, an increase in stomatal resistance, indicating a lowering of evaporative water loss through closing of stomates, could be of value to a plant under low moisture conditions, or alternatively could inhibit uptake of adequate nutrients. Because these data were measured at a single point in time, caution should be exercised in making conclusions relative to the significance of altered water relations. Nondestructive physiological measurements taken serially in an experiment could contribute to an understanding of the functioning of mycorrhizae in natural ecosystems.

3.5.5 Aggregation Dynamics in Prairie Soils

J.D. Jastrow, R.M. Miller, and A.-C. McGraw

Investigators of plant/soil interactions have only recently begun to consider the importance of water-stable soil aggregates. The presence of soil physical conditions favorable for plant growth is largely dependent upon aggregate size distribution. Yet it also appears that plants play an intimate role in the development of water-stable aggregates, and thus, the plant/soil interface is located within and around the aggregates.

Previous studies have suggested that microaggregates (<0.2 mm diameter) are held together by relatively permanent inorganic means and by persistent organic binding agents. Macroaggregates (>0.2 mm diameter), however, are bound together largely by fine plant roots and fungal hyphae, particularly the hyphae of vesicular-arbuscular mycorrhizae (VAM). For soils where organic matter is the major binding agent, the water-stability of macroaggregates is affected by agricultural practices or other disturbances. In contrast, microaggregates are generally not disrupted by management practices.

It may be hypothesized that changes in the size distribution and degree of aggregation could be used as a measure of disturbance and as a method for following and evaluating the soil/plant system's recovery from disturbance. Furthermore, the interactions of water and nutrients within the soil/plant system are likely influenced by soil aggregation since the size distribution of aggregates will affect porosity, infiltration, hydraulic conductivity, and, thus, the availability and movement of water (and with it nutrients) through the soil and into the plant. However, if fine plant roots and associated VAM hyphae are major binding agents for macroaggregates, then plants (at least those, such as grasses, with a large proportion of fine roots) may be able to effect changes in the soil structure that improve moisture and nutrient relations.

To begin investigation of these hypotheses, we initiated field studies during 1985 to characterize plant development and soil physical and chemical properties for tallgrass prairie developing on previously cultivated soils. The study site included four plots at Fermi National Accelerator Laboratory (Fermilab) that were planted to tallgrass prairie in spring 1984, spring 1981, fall 1977, and spring 1975 (thus providing plots in their second, fifth, eighth, and eleventh growing seasons, respectively). For comparison, study plots were also established at Fermilab in a corn field and in an ungrazed pasture (planted with Eurasian grasses) in its seventeenth growing season, as well as in a virgin prairie remnant located about 6 km north of the Fermilab plots. All plots were established on similar soils, primarily Mundelein silt loam. Samples were obtained for determination of above- and below-ground plant biomass and nutrient content, plant species diversity, root lengths and percentage VAM infection, VAM hyphal lengths and biomass/biovolume, VAM spore populations, soil aggregate stability, size distribution of water-stable aggregates, organic carbon, and other soil physical and chemical properties.

Above-ground production of grasses and grass-like plants was surprisingly uniform for all plots except the 11-year restored prairie, which had an overabundance of grasses in comparison to other plots, and the corn field, which had very low above- and below-ground biomass due to the late June sampling time. Above-ground forb production was somewhat more variable. Root production to a depth of 20 cm, however, increased linearly with time since last cultivation in the restored prairie. Mean root dry weights in the virgin prairie fell between those of the 11-year and 8-year restored prairie, but were not significantly different ($p \leq 0.05$) from the means for either restored prairie. Similarly, mean root dry weights in the 17-year pasture fell between those determined for the 8-year and 5-year restored prairie. Preliminary analyses of VAM spore populations revealed increasing species abundance and diversity with time since cultivation.

A highly significant nonlinear relationship between the percentage of macroaggregates and the number of growing seasons since last cultivation was found for data from the corn field and restored prairie (Figure 3.14). Furthermore, the percentage of macroaggregation determined for soils in the 8-year and 11-year restored prairie and the 17-year pasture did not differ significantly ($p \leq 0.05$) from that of the virgin prairie. Overall, the percentages of macroaggregation for all plots were relatively high in

Figure 3.14. Relationship between macroaggregate development in prairie soil and time since disturbance (last cultivation). Samples taken to a depth of 10 cm; $n=10$ for each sampled plot--some values hidden.

comparison with values reported in the literature for other sites in other climates, suggesting that the Fermilab site offers optimal conditions for soil aggregate development. Initial comparisons of soil and biotic data indicated that the percentage of macroaggregates is positively correlated with root biomass and soil organic carbon (e.g., to a 10-cm depth: $r = 0.73$ and 0.47 , respectively; $p \leq 0.0001$).

These preliminary analyses suggest that, at least for grasslands, water-stable macroaggregation does increase as the soil/plant system recovers from disturbance. Additional analyses of samples and data obtained during 1985 are planned for 1986 in order to complete the initial characterization of the research site. Following the characterization phase, studies will be initiated to investigate the mechanisms of soil aggregation and the corresponding influences of aggregation on plant/soil interactions.

3.6. ENVIRONMENTAL CHEMISTRY

3.6.1 Summary

M.W. Findlay, Jr.

The numerous research projects included in the Environmental Effects Research Program require access to a broad range of analytical capabilities. This analytical work is conducted in the Environmental Chemistry Laboratories, which provide researchers with facilities for both sample analysis and methods development.

The environmental chemistry section does not exist as an entity separate from the other programs. It is integrated into all the programs, with each researcher providing input from his or her area of expertise. The areas of speciality in the group include soil and trace metal chemistry, biochemistry, organometal chemistry, inorganic and radiochemistry, and aquatic chemistry.

It is not the purpose of this section to delineate all of the analytical work done in the laboratories. Relevant chemistry and techniques are discussed in the research project sections, where appropriate. There is, however, a substantial level of work for studies that are not directly related to the major projects in the Environmental Effects Research Program. One of these efforts is discussed below (Section 3.6.2), and the remainder are discussed in Section 3.7. The mechanism by which the environmental chemistry section provides technical support for the research group is discussed in Section 3.6.3.

3.6.2 EPICOR II Resin Field Study

M.W. Findlay, Jr.

Ion-exchange media used in the cleanup of the damaged Unit 2 at the Three Mile Island Nuclear Station became highly loaded with radionuclides compared

with cleanup resins used in routine operations at operational reactors (McConnell 1983). This higher level of activity posed technical problems for long-term disposal, but also provided an opportunity to evaluate the effects of these high radiation levels upon the stability of the exchange resin and prefilter liners. The resins must be solidified and the radionuclides immobilized for at least 150 years because the principal nuclides, ^{90}Sr and ^{137}Cs , have half-lives of approximately 30 years.

Argonne National Laboratory is participating with Idaho National Engineering Laboratory (INEL) and Oak Ridge National Laboratory (ORNL) in the field-leaching phase of a multiphase study of the Three Mile Island resin liners. The entire project encompasses analyses of resin degradation due to ionizing radiation, liner integrity, and biodegradation of resins, as well as the field testing project to determine leachability of radionuclides from the solidified resins.

In 1984, meetings were held between Argonne staff and representatives from INEL to discuss Argonne's participation in the field test study. Initially, it was proposed that at least three field sites be established. However, the proposed arid site was dropped from consideration and studies were instituted at ORNL and ANL. The ORNL site provides a warm, wet climate with a sandy clay loam soil; the ANL site provides a temperate climate with cold winters and a clay soil. These sites should provide adequate conditions for studying weathering and degradation of the solidified resins, both by aqueous leaching and freeze/thaw cycling.

Test lysimeters were installed at both ANL and ORNL during the summer of 1985. Figure 3.15 shows the lysimeter dimensions as well as placement of the resin samples and instrumentation. The tanks were filled with soil and the solidified resin samples put in place at a depth of 111 cm. Probes were installed at several depths in each lysimeter to monitor soil temperature and moisture content, and porous cup tensiometers were placed around the resin samples to collect soil water samples. At ANL, the experiment was initiated in August 1985 when the covers were removed and the tanks exposed to ambient conditions. The soil water and any leachate reaching the collection chambers at the bottom of the lysimeter are to be sampled periodically and monitored for radioactivity. A control lysimeter filled with pure silica sand will provide data on the ability of the soil to bind the radionuclides should leaching ever occur.

The principal radionuclide present in the resin samples is ^{137}Cs . However, one resin type contains a substantial amount of ^{90}Sr --on the order of 25% of the total activity. Since the behavior of strontium in the soil is similar to calcium, it would be expected to be relatively mobile. In addition to total gamma-counting, therefore, it would be of interest to determine the composition of any leached radionuclides--at least the strontium/cesium ratio. At present, however, there are no plans for chemical separation and measurement of the strontium.

Figure 3.15. Schematic of a lysimeter used for field testing of solidified samples of EPICOR II resins (from McConnell 1984).

The proposed length of this leaching study is 20 years. Data gathered during that time will provide information on the effects of high radiation doses on the ion-exchange matrices, as well as the relative stability of the solidifiers under the two moisture and temperature regimes. Should radionuclides begin leaching from the resins, the experiment will also provide an opportunity to study the relative transport rates of the nuclides in the two different soil types.

3.6.3 Support Function for the Research Group

M.W. Findlay, Jr., and J.D. Taylor

The environmental chemistry facilities of the Environmental Effects Research Program consist of eight laboratories equipped to support a wide range of environmental analyses.

The radiochemical laboratories and counting facilities are used primarily by the transuranics research group. There are areas for sample preparation, chemical separation of the elements of interest, and final mounting of the isotopes for counting. Additionally, macro- and ultrafiltration of water samples is done in these laboratories. Due to the extremely low levels of radioactivity being measured, no other work is conducted in these laboratories.

Two laboratories contain all of the analytical instrumentation. Included is equipment for atomic adsorption, basic chromatographic separations, UV-visible spectroscopy, and other elemental analyses. In general, the facilities are user oriented, with the research staff doing the analytical portions of their own projects. Frequently, student assistants are assigned to the laboratories. Scheduling and maintenance of the analytical facilities, and training of students, is performed by the authors of this section. A small portion of the authors' efforts are spent on analytical work for others in the group when this is the most practical approach. One laboratory is used for preparation of soil samples prior to analysis. All physical analyses are done here, as well as extractions that may be required prior to chemical analysis. This area is a multiuser laboratory that is used extensively for the terrestrial and below-ground research projects.

The remaining laboratories are multipurpose laboratories, with bench space being used for various laboratory studies. The types of experiments performed include equilibration studies, leaching experiments, incubation, and mineralization studies of soils. Cooperation between researchers and advanced scheduling of experiments optimizes use of these laboratories, as well as their upkeep.

The access of the research staff to the facilities and technical support of the environmental chemistry section is a unique asset. Discussions on sampling and preservation techniques to maintain sample integrity during transport may improve data quality. Availability of equipment often reduces restrictions on the design of an experiment, providing the potential for

greater information yield. Also, the facilities allow researchers to do methods development work in areas where analytical methods are the limiting factors of an experiment.

3.7 SUPPORT TO OTHER PROGRAMS

3.7.1 Summary

J.P. Schubert

Members of the Environmental Effects Research Program commonly participate in joint projects with other divisions at Argonne. Currently, five staff members are conducting research on five different projects with the Energy and Environmental Systems Division. In a project for the U.S. Coast Guard, a light-weight, portable instrument is being developed, using innovative detection processes, that can quickly identify more than 25 different toxic gases. In a program funded by the Gas Research Institute, field studies are being conducted to evaluate the nature and magnitude of impacts caused by gas-pipeline construction on (1) agricultural soils and crop production in Oklahoma and (2) sediment transport and aquatic biota in streams being crossed by gas pipelines in Ohio and Michigan. Research being funded by the Corps of Engineers, Construction Engineering Research Laboratory (CERL), involves the optimization of land use and revegetation procedures to improve plant establishment and cover at Army training and maneuver ranges. The objectives of this research are to reduce erosion potential and improve long-term uses of these lands. In addition, laboratory experiments are being conducted for CERL to study the mobility, degradation, and volatilization of decontamination emulsions in different types of soils.

3.7.2 Universal Hazardous Gas Monitor

W.R. Penrose, J.R. Stetter, and S. Zaromb**

One of the many duties of the U.S. Coast Guard is inspection of marine shipping entering U.S. ports. During the course of this duty, Coast Guard personnel are exposed to chemical vapors whose nature is often unknown. In 1981, the Coast Guard formally identified a need for a small, portable instrument that could be used to determine the identity, concentration, and hazard level of chemicals in vapor form. In response to this need, we have developed a computer-operated device that successfully identifies more than 25 chemicals, including most industrial solvents, in the vapor phase.

The Chemical Parameter Spectrometer uses established technology in a novel way. Porous-electrode electrochemical cells are in wide use for the measurement of carbon monoxide, hydrogen sulfide, and other gases. Air

*Collaborator; affiliation is listed at the front of this chapter.

inducted into the instrument is passed through a reaction chamber containing two noble-metal filaments and then through an array of four electrochemical cells. Each of the four cells is adjusted to a different selectivity. In operation, filaments heated with an electric current cause the pyrolysis of chemicals passing over them. The pattern of outputs from the four cells is characteristic of the particular chemical. Moreover, compounds that are not normally electrochemically active, such as benzene or cyclohexane, give signals when converted into pyrolysis products.

Normally, an analysis is made by running the instrument in four modes. Four numbers are taken after running with the platinum filament on, then a rhodium filament is turned on and four more numbers taken. The temperature of the rhodium filament is increased and four more numbers taken. Finally, the filaments are switched off, and a final set of measurements is made. The 16 numbers so obtained yield a pattern vector that is distinctive. After normalizing to constant length, this vector is compared with a library compiled from measurements of known compounds, using a well-known pattern-matching algorithm. This operation yields not only the identity of the compound (if it is in the library), but also two independent measures of reliability. Once the compound is identified, a coefficient can be extracted from the library and combined with the original (unnormalized) data to obtain the concentration.

The instrument is highly reliable and sensitive in the analysis of electroactive gases and many toxic organic chemicals, such as benzene, carbon tetrachloride, and methyl isocyanate.

Several prototypes of the instrument have been built and are under evaluation by the Coast Guard's Research and Development Laboratory and by the National Oceanic and Atmospheric Administration under contract to the Coast Guard. Ruggedized versions are being built by Argonne's Electronics Division for clients in the Coast Guard, the Federal Railroad Administration, and the Canadian Environmental Protection Service.

3.7.3 Effects of Pipeline Installation on Stream Ecosystems

J.P. Schubert and W.S. Vinikour

During the construction of gas-transmission pipelines, streams and rivers often must be crossed. Federal regulations require that pipelines be buried below streambeds so that damage to pipelines by vandalism, falling trees, or debris traveling down the streams (especially during floods) can be avoided. When construction activities occur in a stream, disturbed streambed materials are suspended and transported in the flowing water. Federal and state regulatory agencies are often concerned about the ecological effects (especially on aquatic biota) in downstream reaches from suspended solids and streambed sedimentation. The objective of this project is to relate the nature and magnitude of these impacts to stream types, water velocity, substrate characteristics, and construction methods.

The first stream crossing investigation conducted as part of this study was on the Little Miami River in Glen Helen Nature Preserve near Yellow Springs, Ohio. Within the study area the gravel-bottomed stream is about 20 m wide and has a maximum depth of 1.1 m during low-flow conditions. A 2-m-deep trench was dug across the stream on October 17-18, 1983, with two backhoes. A 90-m-long, 51-cm-diameter pipe was placed in the trench on October 18. The trench was then backfilled and the riverbank restored during October 26-28, 1983. A sampling program was conducted to quantify the spatial and temporal variations in water quality, streambed composition, benthic invertebrates, and fish (Schubert et al. 1985).

More than 1,100 water samples were collected by automatic water samplers. Two samplers were located upstream and four were located at various distances downstream of the construction area. In the month preceding construction, suspended solids at all stations were generally below 20 mg L^{-1} (maximum concentration = 39 mg L^{-1}). During trenching operations, suspended solids increased significantly downstream. The maximum suspended-solids concentrations during this period were 1,461, 520, 359, and 250 mg L^{-1} at distances of 55, 95, 175, and 1,900 m downstream, respectively (see Figure 3.16). More than 50% of the suspended solids were redeposited on the streambed within 200 m of the construction site. Concentrations of suspended solids returned to ambient conditions ($<30 \text{ mg L}^{-1}$) by the morning following trenching. No impacts on water chemistry were observed.

Nearly 200 substrate samples were collected one time before and three times after construction at five different transects (one upstream, four downstream). Dry-sieving and hydrometer analysis of these riverbed samples showed a remarkable similarity of size composition (dominantly gravel), except for transects located within 100 m downstream of the pipeline that were sampled one month after construction. The samples collected from that area had considerably more clay, silt, and fine sand than occurred in the rest of the samples. High streamflows in late November 1983 through May 1984 washed away most of the fine sediments. The riverbed size composition returned to preconstruction conditions by June 1984.

Replicate quantitative samples of benthic macroinvertebrates were collected from three transects located upstream, at, and downstream of the pipeline. Samples were collected with a D-frame sampling net from sites with similar substrate composition and current velocities. Collections were made prior to pipeline construction and on six occasions following construction (ranging from less than 1 month to about 13 months following construction). Construction effects on macroinvertebrates were determined by spatial and temporal comparisons of species composition, densities, diversities, and community similarities. Fish were collected by seining at locations centralized around the macroinvertebrate sampling locations. Collections were made prior to construction and on three occasions (1, 8, and 12 months) following construction. The fish community was analyzed by means similar to those used for the macroinvertebrates. Additionally, size/age distributions and feeding habits were analyzed for silver shiners, the most prevalent fish species, for each date and sample site.

Figure 3.16. Concentrations of suspended solids during and two days following trenching operations, in the Little Miami River.

The study revealed that partial macroinvertebrate recolonization of the affected areas occurred within three weeks after disturbance. Species composition, density, and diversity were comparable to preconstruction conditions within 2 to 7 months of construction. Fish were reestablished within the affected areas within 1 month of construction; however, only young-of-the-year silver shiners were collected from these areas. Subsequent samples (8 and 12 months after construction) indicated that species composition and size/age distribution of silver shiners had returned to preconstruction conditions. Results of the study strongly imply that construction impacts to the Little Miami River biota were short-term and minimal.

Canada Creek in Presque Isle County, Michigan, was the second stream to be investigated. It is about 10 m wide and up to 2 m deep. The velocity of Canada Creek at the time of construction was about twice that measured in

Little Miami River. The streambed is composed primarily of medium to coarse sand, with logs and log debris scattered in pockets along the bottom. Construction began February 26, 1985, when a backhoe was used to clear brush from the stream and excavate ramps in the banks on both sides of the stream. On February 27, a 10-cm-diameter pipe was pulled through the streambed using an iron sled and deep ripper blade. This alternative construction technique supposedly creates less disturbance within a stream than does the more standard method of trenching with backhoes.

During the ramp construction, suspended solids rose to a maximum of 440 mg L^{-1} at a distance of 5 m downstream of the disturbance; concentrations dropped off quickly in a downstream direction due to sediments falling out of suspension. During the sled crossing the following day, which lasted about 20 minutes, only a slight rise of suspended-solids concentrations occurred. Background concentrations of suspended solids in the stream before and two days after construction were less than 20 mg L^{-1} . No impacts to water chemistry or size composition of the streambed materials were observed.

No apparent differences in fish composition were noted as a result of the construction. The mottled sculpin and American brook lamprey were the most abundant fish species in the study area. Comparable numbers of these species were collected before and after construction. Macroinvertebrate drift densities were observed to increase during periods of construction activity, particularly at the transects closer to the pipeline. The postconstruction benthic macroinvertebrate community composition was similar to preconstruction values.

A third stream crossing study is anticipated in 1987. That study will focus on a stream that contains contaminants in the streambed sediments. An attempt will be made to fit the data on transport of suspended solids in these streams into an existing model for sediment transport, thus developing some predictive capabilities for future stream crossings. Also, stream-crossing studies will be compared to published results of studies related to other types of instream construction (e.g., bridge building) or intensive watershed disturbances (e.g., surface mining, logging), so that a comparison can be made regarding the nature and magnitude of potential aquatic impacts.

3.7.4 Edaphic and Crop Production Changes Resulting from Pipeline Installation in Semiarid Agricultural Ecosystems

*J.D. Taylor and S.D. Zellmer**

Across the country, and particularly in the southern Great Plains, thousands of miles of small-diameter pipelines connect natural gas and oil wells to gathering stations before processing and transmission to markets in other regions of the country. Installation of these pipelines disturbs the soil profile and may cause temporary or permanent changes in soil productivity. Despite the extent of the pipeline gathering and transmission system,

*Collaborator; affiliation is listed at the front of this chapter.

only limited data are available on the effects of pipeline construction on soil properties, crop production, and agricultural ecosystems.

This study was initiated in the fall of 1983 to investigate the edaphic and crop-production changes that occurred following the installation of a pipeline in Beaver County, Oklahoma. The objectives of the study were (1) to determine the extent to which the physical and chemical characteristics of the soil are altered by a typical single-ditch** pipeline construction project, (2) to document crop production and the establishment of a pasture plant community on the right-of-way for several growing seasons, and (3) to relate crop production to edaphic changes caused by the pipeline installation.

In September 1983, a 20.3-cm pipe was laid in a 51-cm-wide ditch dug with a wheel trencher to a depth of about 1.3 m in order to maintain a minimum of 1.1 m of soil cover over the top of the pipe. The project route crossed native pasture land, as well as agricultural land where two major crops (wheat and grain sorghum) were grown and two different production methods (irrigated and dryland) were used.

The four study sites chosen for the Beaver County project represented four major land uses found in the area, i.e., dryland row crop, native pasture, dryland wheat, and irrigated cropland. Because of the linear nature of the pipe installation and the right-of-way, a systematic procedure was used to locate sampling sites. Three separate, parallel sampling transects were established. The first of these, the pipe ditch (P) sampling transect, was within the width of the ditch where maximum soil disturbance occurred. The second sampling transect, working side or intermediate (I), was in the area where construction traffic occurred but the soil was not removed and replaced. The third sampling transect, control (C), was at the edge of the right-of-way and was unaffected by construction activities.

At the native pasture site, six permanent 4-m plant data-collection lines were established on each of the three soil-sampling transects. During April, June, and November 1984 sampling trips, individual lengths of bare soil and plant cover were measured and recorded on each of the 18 separate lines. The line intercept method adopted from Cook and Bonham (1977) was used for this purpose. Plant cover was recorded on the basis of life form--grasses, leafy forbs, succulent forbs (cactus), and shrubs (sages).

The data on plant cover collected on the three transects during April, June, and November of 1984 indicates that less than 2% of the 96% to 98% total plant cover consisted of forbs or shrubs. The relatively low percentage ($8.2 \pm 4.7\%$) of bare soil on the working side transect in April indicates that the special efforts made to limit activities during construction resulted in only minor influence on plant cover by the pipeline installation. The percent bare soil on the working side transect decreased and by November was about the same as the control transect. The percent total plant cover on the pipe ditch

***In a single-ditching operation, no effort is made to separately remove or maintain the integrity of the topsoil or a horizon with respect to the subsoil or lower horizons during the trenching and backfilling operations.*

transect generally decreased during the first growth season: $20.8 \pm 18.4\%$ in April, $62.5 \pm 24.2\%$ in June, and $37.7 \pm 29.6\%$ in November. Forbs and species other than grasses accounted for less than 3% of the total cover on pipe ditch soil (Taylor and Zellmer 1984). The amount of plant cover (mainly grasses) on the pipe ditch was not equal to that in the rest of the pasture after one year. However, cover did increase from 0% at the time the pipeline was installed in October 1983 to about 37% in November 1984. If this trend continues, the pipe ditch cover could be expected to equal the cover on the other transects in less than three years.

The mean yields and standard deviations of ten individual samples of winter wheat, corrected to ideal conditions of 14% moisture and 773 g L^{-1} , collected from each of the three transects at the irrigated site were: control, 350.4 ± 60.3 ; working side, 329.4 ± 63.0 ; and pipe ditch, $525.0 \pm 75.7 \text{ g m}^{-2}$. The farm operator reported an average yield of 3.44 Mg ha^{-1} (344 g m^{-2}) (King 1984); thus, yields on the working side and control transects were representative of average field conditions. The wheat yield on the pipe ditch transect was significantly higher than on the other two transects, and no significant difference existed between control and working side yields. The significant yield increase on the pipe ditch transect can be attributed to higher theoretical moisture-retention capacity (Table 3.13) and lower bulk density of pipe ditch soil (Table 3.14).

The mean yields, their standard deviations, and extensions to Mg ha^{-1} of the ten grain sorghum samples collected in November 1984 from each of the three transects at the dryland row crop and irrigated sites are given in Table 3.15. The grain sorghum yields at both sites were somewhat below the long-term county averages of 1.90 Mg ha^{-1} on dryland fields and 4.85 Mg ha^{-1} on irrigated fields (Taylor and Zellmer 1984).

A review of the yield data for the dryland row crop site (Table 3.15) indicates that the mean yield of the control transect is significantly lower

Table 3.13. Theoretical moisture-retention capacity of Beaver County soils as altered by pipeline construction

Transect	Moisture-Retention Capacity ($\text{m}^3 \text{ m}^{-3}$)			
	Row Crop	Pasture	Dryland Wheat	Irrigated
Control	9.02 (0.710) ^a	9.76 (0.360)	4.99 (0.504)	9.55 (0.394)
Working side	8.89 (0.509)	9.83 (0.269)	4.96 (0.353)	9.43 (0.104)
Pipe ditch	10.51 ^b (1.058)	12.16 ^b (0.811)	5.47 (0.927)	10.15 ^b (0.322)

^a Mean and standard deviation, values $\times 10^2$, $n = 5$.

^b Indicates significance at the 0.05 level of probability for site.

Table 3.14. Effect of pipeline construction on surface-soil bulk densities at four sites and five observation dates in Beaver County

Site	Transect	Bulk Densities (Mg m ⁻³) ^a				
		October 1983	February 1984	April 1984	June 1984	November 1984
Row crop	Control	1.55 [*] (0.071) ^b	1.61 (0.032)	1.64 (0.055)	1.50 (0.032)	1.58 (0.063)
	Working side	1.62 [*] (0.032)	1.61 (0.032)	1.66 (0.045)	1.50 (0.000)	1.55 (0.089)
	Pipe ditch	1.35 [*] (0.045)	1.38 [*] (0.000)	1.37 [*] (0.032)	1.33 [*] (0.045)	1.34 [*] (0.063)
Pasture	Control	1.46 (0.032)	1.45 [*] (0.032)	1.47 [*] (0.032)	1.44 [*] (0.032)	1.46 (0.063)
	Working side	1.43 (0.055)	1.50 [*] (0.063)	1.52 [*] (0.032)	1.52 [*] (0.032)	1.48 (0.045)
	Pipe ditch	1.19 [*] (0.032)	1.24 [*] (0.045)	1.27 [*] (0.032)	1.34 [*] (0.032)	1.29 [*] (0.032)
Dryland Wheat	Control	1.52 (0.063)	1.54 (0.000)	1.56 [*] (0.000)	1.56 [*] (0.032)	1.53 [*] (0.032)
	Working side	1.51 (0.105)	1.62 (0.032)	1.60 [*] (0.000)	1.61 (0.045)	1.67 [*] (0.055)
	Pipe ditch	1.42 [*] (0.047)	1.61 [*] (0.000)	1.65 [*] (0.000)	1.64 (0.000)	1.59 [*] (0.032)
Irrigated	Control	1.60 (0.000)	1.61 (0.032)	1.58 (0.045)	1.46 [*] (0.055)	1.55 (0.032)
	Working side	1.59 (0.063)	1.59 (0.063)	1.58 (0.045)	1.51 [*] (0.045)	1.58 (0.063)
	Pipe ditch	1.41 [*] (0.055)	1.49 [*] (0.055)	1.51 [*] (0.045)	1.41 [*] (0.032)	1.40 [*] (0.109)

^a "*" indicates significance at the 0.05 level of probability for the same data and site.

^b Mean and standard deviation of 15-cm depth reading, n = 15.

Table 3.15. Influence of pipeline construction on the grain sorghum yields^a at two sites in Beaver County

Site	Transect	Mean Yield ^b (g m ⁻²)	Extended Yield (Mg ha ⁻¹)
Row crop	Control	124.9 ^c (47.3)	1.25
	Working side	185.1 (39.0)	1.85
	Pipe ditch	199.6 (24.7)	2.00
Irrigated	Control	115.1 (74.3)	1.15
	Working side	121.0 (47.7)	1.20
	Pipe ditch	127.8 (26.2)	1.28

^a Yields corrected to 14% moisture content.

^b Mean and standard deviation (n = 10).

^c Significance at the 0.05 level of probability.

than the yield of both the pipe ditch and working side transects. A possible explanation of the differences in yield between the transects at the dryland row crop site is differing availability of moisture.

The means of samples from the three transects at the irrigated site (Table 3.15) argue that no significant difference exists among yields. On the irrigated field, additional water was applied, and a yield response similar to that experienced with the wheat crop could have been expected. In 1984, however, climatic conditions prevented the late-planted sorghum from maturing and greatly decreased the overall yield.

This study will provide a better understanding of those factors associated with the reestablishment of a native pasture plant community following pipeline construction and related changes in edaphic conditions. This will lead to results that would be useful in determining the relative effects of single-ditching and double-ditching on crop production and soil properties in a more mesic agro-ecosystem.

3.7.5 U.S. Army Training Area Rehabilitation Project

R.R. Hinchman

The Department of the Army manages over 9 million acres of training and maneuver ranges, including significant semiarid and arid areas in the western United States. Training use of these western ranges by tanks and other tracked and wheeled vehicles has resulted in such ecosystem impacts as damage or destruction of existing plant communities and soil disturbance. These impacts result in increased susceptibility to erosion of the soil by wind and water. Other impacts include soil compaction and/or contamination, loss of wildlife habitat, and loss of training realism provided by diverse natural vegetation and topography. These impacts are particularly problematical in areas of low precipitation because of the relatively low percentages of natural, stabilizing vegetative cover; the long periods required for reestablishment of native, adapted plant communities; and the tendency of many western soils to be prone to erosion. The Corps of Engineers, Construction Engineering Research Laboratory (CERL), is responsible for the rehabilitation and maintenance of degraded training areas throughout the United States.

In cooperation with personnel from CERL and Fort Carson, Colorado, scientists from the Environmental Research Division and the Energy and Environmental Systems Division are conducting a program to develop and demonstrate ecologically effective and economically feasible soil rehabilitation and revegetation techniques at a highly disturbed tactical training area with rough terrain and steep slopes. The site is in the foothill pinyon-juniper vegetation type at Fort Carson, Colorado.

The research site is considerably varied in topography, vegetation, and levels of disturbance. As such, it is representative of many areas and conditions found at Fort Carson. Conditions include (1) steep, rocky slopes with thin soils and widely spaced clumps or individual trees of pinyon and juniper, (2) deep, sandy soils on moderate slopes with dense areas of pinyon-juniper separated by open areas, and (3) treeless, gently sloping or nearly flat shortgrass prairie areas. Levels of disturbance from training activities range from severe to none. Rehabilitation criteria based on future training use, other potential land uses (for example, wildlife habitat, grazing), as well as soil, vegetation, and climatic data from the site were used to develop a rehabilitation prescription and to select the revegetation species to be used. The rehabilitation prescription included specifications for fertilization, tillage (light ripping), seedbed preparation, seed mixture (80% native species), seeding methods, harrowing, cultural practices, and long-term management.

The research site (about 80 acres) was divided into eight treatment areas, representing all slope aspects. Four treatment areas totaling about 40 acres received the site-specific rehabilitation prescription in May 1984, and four were left untreated. The entire site has been excluded from training traffic by "no trespassing" signs around the perimeter. An adjacent site with

similar soil, vegetation, and disturbance characteristics, but receiving normal training use, is being used as a control.

The development and succession of the revegetation plant community is being evaluated using measurements of plant cover (by species), tree/shrub canopy cover, and ground cover (litter, rock, bare ground) on permanent transects. Vegetative cover and ground cover were chosen for measurement because they are parameters that are highly correlated with erosion rates and soil stability. Growth of volunteer native and weedy species is a natural and expected aspect of any revegetation effort. At present, such species comprise a significant part of the revegetation plant community.

Comparison of plant cover data from 1984 and 1985 shows that in 1985 there were increases in plant cover on virtually every transect on the site. The increases in cover on the tank trail transects were unusually large, ranging from 31% to 69%. These results indicate that excluding training traffic (disturbance) alone will result in the development of considerable plant cover. However, in most cases the plant cover on the untreated tank trails consists mostly of weedy species, while the cover on the treated tank trails contains a large component of planted and other native species. Some of the treated tank trails in the shortgrass prairie areas are already practically indistinguishable from the adjacent undisturbed areas. In other areas of the site, revegetation is progressing more slowly due to harsh environmental conditions. Monitoring of the transects will continue for several more growing seasons.

Adequate recovery of the treatment areas that received the rehabilitation prescription to a condition approximating that existing prior to training use will take both time and patience. It currently is estimated that the research site must be excluded from vehicular traffic and other tactical training uses for a minimum of six years for acceptable rehabilitation of all treated areas. Heavy training pressure on existing Fort Carson land resources may not permit exclusion of the research site for this length of time. However, significant increases in soil stabilization by new vegetation and in training realism have already occurred on the treated areas. The untreated areas of the research site are recovering much more slowly through processes of natural revegetation. In some steeply sloped portions of the untreated areas, erosion continues essentially unabated. Following rehabilitation, military training use should be controlled in terms of training intensity and season of use so that the level of damage and degradation sustained by the site remains considerably below that exhibited before initiation of rehabilitation work. The rehabilitation program, along with CERL-developed programs for rotational scheduling of land parcels for rehabilitation and environmental awareness, will be applied to other areas of Fort Carson and possibly to other military installations as well.

3.7.6 Environmental Fate of Army Decontamination Agents

R.R. Hinchman

Because federal regulations place considerable demands on actual or potential generators of environmental pollution, researchers in the Environmental Research Division and the Energy and Environmental Systems Division were requested to assist the Corps of Engineers, Construction Engineering Research Laboratory (CERL), in developing information on the environmental fate of Army decontamination agents that contain toxic substances. These agents are compounds or mixtures of chemicals that are designed to inactivate and/or facilitate the removal of contaminants resulting from chemical, biological, or nuclear warfare. In this project, a new decontaminant designated as C-8 and planned for use primarily on vehicles (such as tanks and armored personnel carriers) and other mobile tactical equipment is of primary interest. In use, C-8 is swabbed onto the contaminated vehicle and after about 30 minutes is flushed off with water. Testing and evaluation of C-8 is normally conducted over concrete sumps, permitting proper disposal of the wastewater. However, accidental release or spillage of C-8 or wastewater onto the ground creates the potential for environmental contamination because these materials percolate through the soil, and may, in some cases, reach groundwater.

Decontamination agent C-8 is a mixture of constituents in emulsion form that contains 15% tetrachloroethylene (perchloroethylene or PCE). The U.S. Environmental Protection Agency has classed PCE as a "priority" pollutant because it is a chlorinated organic solvent that is toxic to man and animals and is a suspected carcinogen. PCE is very persistent in soils (Wilson et al. 1981), but there is some evidence that PCE can be slowly degraded by certain bacteria found in soil and groundwater. However, C-8 also contains calcium hypochlorite, a source of free chlorine. Although the toxic effects of PCE on soil microorganisms is poorly known, the C-8 mixture, because it produces chlorine, is likely to be more toxic to soil organisms than PCE alone.

Initial experiments in this ongoing project have been designed to simulate, under laboratory conditions, the behavior of C-8 constituents in soils if washdown wastewater from Army vehicle decontamination testing and training procedures is accidentally spilled on the soil surface.

In these experiments we are attempting to determine the retardation (partitioning or sorption on soil constituents), migration, and vaporization of the PCE constituent of C-8 in soil microcosms. To realistically simulate field conditions, the soil microcosms were constructed using intact soil cores 10 cm in diameter and 61 cm long obtained with a hydraulic soil-coring machine. Locally obtained cores of sandy, loam, and clayey soils were used to span the range of soil types that are likely to be encountered at a variety of locations. Selected physical and chemical characteristics of each of the soil types used are being determined. The intact soil cores were inserted into glass microcosm columns of matching diameter and saturated with water to ensure good contact between the surface of the core and the column wall. The

C-8 emulsion was diluted with water to simulate the composition of the wastewater reaching the soil surface at a typical "nasty decon site" (Department of the Army 1983) used for military vehicle decontamination and washdown under integrated battlefield conditions. Following application of the simulated wastewater to the microcosm and collection of the effluents, each soil column was subjected to the leaching action of simulated rainwater added in four aliquots, each representing 2.5 cm of rainfall. These rainwater aliquots were allowed to drain through the column and were sampled before the next aliquot of rainwater was applied.

The PCE concentration in the microcosm column effluent after the wastewater application (if any) and after each simulated rainwater leach is being determined using gas chromatography (GC). To minimize vaporization losses from the microcosm effluent, these solutions were collected in gas-tight Teflon gas-sampling bags. The amount of PCE remaining in the microcosm soil after the rainwater leaching is being determined by solvent extraction of soil samples from the columns, followed by gas chromatography. Three replicate microcosms of each soil type were set up and run to ensure statistical validity of the results. A control column for each soil type, which received only simulated rainwater, was also run as a check and control for analytical procedures.

Data analysis, interpretation, and evaluation is currently underway. A final report will contain a description of methods, results, statistical analyses, and conclusions, as well as recommendations for additional experiments and potential methods to enhance the degradation of PCE in soils.

The ongoing studies will provide a basis for future investigations that could include (1) the development of criteria, based on soil characteristics, for the determination of the most acceptable locations for C-8 decontamination training sites at specific Army installations; (2) determination of the deleterious effects of C-8 on normal soil organisms; (3) the development of mitigative measures to reduce the adverse effects of C-8 on the soil environment; and (4) studies to develop and/or identify soil microorganisms adapted to degrade chloroethylenes.

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APPENDICES FOR CHAPTER 3
Environmental Effects Research Program

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APPENDIX 3-A. STAFF QUALIFICATIONS
Environmental Effects Research Program

Name	Position	Highest Degree	Major	Year Received	Institution
Findlay, Melvin W.	Assistant Soil Scientist	M.S.	Soil Science	1985	Northwestern University
Hinchman, Ray R.	Biologist	Ph.D.	Botany	1971	The University of Chicago
Irving, Patricia M.	Ecologist	Ph.D.	Botany	1979	University of Wisconsin
Jastrow, Julie D.	Environmental Scientist	M.S.	Agronomy	1979	University of Illinois
Kress, Lance W.	Ecologist	Ph.D.	Plant Pathology	1978	Virginia Polytechnic Institute and State University
McGraw, Anne-Cressey	Post Doctoral Appointee	Ph.D.	Plant Pathology	1983	University of Florida
Miller, R. Michael	Ecologist	Ph.D.	Botany and Microbiology	1975	Illinois State University
Nelson, Donald M.*	Chemist	B.A.	Chemistry	1964	Illinois Institute of Technology
Orlandini, Kenneth A.	Scientific Associate	B.S.	Chemistry	1957	University of Illinois
Penrose, William R.	Biochemist	Ph.D.	Biological Chemistry	1969	University of Michigan
Prepejchal, William	Scientific Assistant	B.S.	Electrical Engineering	1972	Illinois Institute of Technology
Schubert, Jeffrey P.	Hydrogeologist	M.S.	Geology	1978	The Pennsylvania State University
Smith, Harry J.	Scientific Assistant	M.S.	Plant Pathology	1976	Pennsylvania State University
Taylor, John D.	Environmental Scientist	B.S.	Environmental Studies	1973	California State University

*No longer a member of the Division

APPENDIX 3-B. OUTSTANDING PROFESSIONAL ACTIVITIES AND AWARDS
Environmental Effects Research Program

M.W. FINDLAY, JR.--Co-recipient of Research and Development Magazine's 1984 IR-100 Award for work on project developing the Chemical Parameter Spectrometer, or CP-100.

P.M. IRVING--Recipient of the Wolf Vishniac Memorial Award for Excellence at the Seventh International Symposium on Environmental Biogeochemistry, Rome, Italy, 1985.

APPENDIX 3-C. SPECIAL EVENTS ORGANIZED
Environmental Effects Research Program

P.M. IRVING and J.E. MILLER organized Watershed Proposal Workshop, National Laboratory Consortium, 9-11 May 1984, Countryside, IL.

P.M. IRVING organized Environmental Research Division Colloquium Series session (Speaker: J. Laurence Kulp, National Acid Precipitation Assessment Program; Title: current views on the National Acid Precipitation Assessment Program), 27 November 1985, Argonne National Laboratory.

L.W. KRESS conducted teach-in on diagnosis of abiotic plant stresses, 76th Annual Meeting, American Phytopathological Society, 12 August 1984, Guelph, Ontario, Canada.

APPENDIX 3-D. EDUCATIONAL PROGRAM PARTICIPANTS
Environmental Effects Research Program

- D. EATON. Fort Valley State College. Faculty Research Program. Conducted physiological measurements on plant water potential, leaf chlorophyll content, membrane permeability, plant growth, and crop yield. June 1985 - August 1985.
- B.J. FOX. Naperville Central High School. Faculty Research Program. Conducted research on aggregation dynamics in prairie soils. Summer 1985.
- L.G. HANSHAW. Alcorn State University. Faculty Research Program. Conducted photosynthetic measurements on soybeans and corn using a LiCor 6000 portable photosynthesis instrument. June 1985 - August 1985.
- K. LAVOIE. University of Michigan. Faculty Research Program. Conducted a study of the biota of two soils and their relationship to acidity in the Microcosm Facility, June - September 1984.
- P. OLEXIA. Kalamazoo College. Faculty Research Program. Conducted research on quantification of fungal biomass. Fall 1985.
- J. PILLAI. Hirxch High School. Faculty Research Program. Conducted research on quantification of fungal biomass. Summer 1985.
- H. ROSENBAUM. Von Steuben Metro Science Center. Faculty Research Program. Examined the effects of acidic rain on photosynthetic rate and chlorophyll concentration in soybeans. June - September 1984.
- M.V. MURCIA. Phillipines Atomic Energy Commission. IAEA Fellowship. Conducted research on measurement techniques for low levels of actinides in environmental samples. January - November 1985.
- R. ANDERSON. Illinois State University. Visiting Scientist. Research consultation-workshop (1 day). Fall 1985.
- N. JOHNSON. University of Wisconsin. Visiting Scientist. Master's thesis research-workshop (1 week). Fall 1984.
- A. LIBERTA. Illinois State University. Visiting Scientist. Research consultation-workshop (1 day). Fall 1985.

- J. LUSSENHOP. University of Chicago, Circle Campus. Visiting Scientist. Research consultation-workshop (1 day). Fall 1985.
- R. FRANSON. The University of Chicago. Graduate Research Program. Conducted research on plant-fungus-plant competition. 1984-1985.
- S. NAKAYAMA. Kyoto University, Kyoto, Japan. U.S.-Japan Graduate Student Summer Exchange Program. Conducted research on safety assessment of disposal of high-level radioactive waste and the behaviors of actinide elements in aquatic systems. August - October 1985.
- T. DRING. Eastern Illinois University. Post-Baccalaureate Research Program. Mycorrhizae in Natural Ecosystems. Winter 1984.
- A. JARSTFER. Friendly University. Post-Baccalaureate Research Program. Conducted research on mycorrhizae in natural ecosystems. Winter/Summer 1984.
- K. KUIPERS. Dordt College. Post-Baccalaureate Research Program. Conducted research on mycorrhizae in natural ecosystems. Winter 1985.
- D.K. BALDWIN. Pennsylvania State University. Undergraduate Research Program. Conducted field and laboratory research for Gas Research Institute stream crossing program. June - December 1984.
- R.C. CRONN. Drake University. Undergraduate Research Program. Conducted research on aggregation dynamics in prairie soils. Summer 1985.
- C. DAVIS. Carroll College. Undergraduate Research Program. Assisted in field studies to determine the effects of temporal variations in rainfall acidity on soybeans. September - December 1984.
- M. FINK. State University of New York-Binghamton. Undergraduate Research Program. Conducted research on aggregation dynamics in prairie soils. Fall 1985.
- T. GROTE. Briar Cliff College. Undergraduate Research Program. Conducted field research in ozone studies. June 1985 - August 1985.
- M. JAMES. Carroll College. Undergraduate Research Program. Conducted field research in ozone studies. June 1985 - August 1985.
- F. JANZEN. North Central College. Undergraduate Research Program. Conducted research on mycorrhizae in natural ecosystems. Spring/Summer 1985.
- C. JONES. Cornell University. Undergraduate Research Program. Conducted chemical analyses of soil samples for acid rain studies. June - August 1985.

- M. KIERSKI. St. Mary's College. Undergraduate Research Program. Conducted research on the effect of ozone on the photosynthetic rate of field-grown alfalfa. June - August 1984.
- K. KLEIN. Kalamazoo College. Undergraduate Research Program. Conducted field research in ozone studies. September - December 1985.
- K. KUIPERS. Dordt College. Undergraduate Research Program. Conducted research on the effect of ozone and sulfur dioxide on the below-ground ecosystem of field-grown alfalfa. September - December 1984.
- B. LIVINGSTON. Indiana University of Pennsylvania. Undergraduate Research Program. Conducted field research in ozone studies. September - December 1985.
- A. LUTTERMAN. Bemidji State University. Undergraduate Research Program. Conducted research on the behavior of actinide elements in natural waters. June - August 1985.
- S. MOCK. North Central College. Undergraduate Research Program. Conducted research on quantification of total root absorptive surface area/mycorrhizae in natural ecosystems. Fall 1985.
- C. NOLT. Lebanon Valley College. Undergraduate Research Program. Assisted in field studies on the effects of acidic rain on plant/soil systems. June - August 1984.
- F. SEAVEY. Suffolk University. Undergraduate Research Program. Conducted research on the effect of ozone on the photosynthetic rate of field-grown alfalfa. June - August 1984.
- B. SYMONS. Whitworth College. Undergraduate Research Program. Conducted field research in ozone studies. June 1985 - August 1985.
- R. VOGEL. Bradley University. Undergraduate Research Program. Assisted in field studies to determine the effects of temporal variations in rainfall acidity on soybeans. June - August 1984.
- W. WINFRED. Mississippi Valley State University. Undergraduate Research Program. Assisted in laboratory analyses to determine the effects of acidic rain on chemistry and microbial activity. June - December 1984.
- J.E. ZOLECKI. North Central College. Undergraduate Research Program. Conducted research on aggregation dynamics in prairie soils. Fall 1985.

- M. ALCANTAR. Wells High School. Post-High School Research Program. Research traineeship. Summer 1984.
- A. BEUSCHLEIN. Andrews High School. Post-High School Research Program. Research traineeship. Summer 1985.
- D. JUAREZ. Hinsdale Central High School. Post-High School Research Program. Research traineeship. Summer 1985.
- M. SULLIVAN. St. Charles High School. Post-High School Research Program. Assisted in field studies on the effects of acidic rain on plant/soil systems. June - August 1984.
- L. TORRES. Bremen High School. Post-High School Research Program. Research traineeship. Summer 1985.

APPENDIX 3-E. PUBLICATIONS AND ORAL PRESENTATIONS 1984-1985
Environmental Effects Research Program

1. Refereed Journal Articles*

1984

Heck, W.W., W.W. Cure, J.O. Rawlings, L.T. Zaragoza, A.S. Heagle, H.E. Heggestad, R.J. Kohut, L.W. Kress and P.J. Temple. Assessing impacts of ozone on agricultural crops: I. Overview. Air Pollution Control Association Journal 34:729-735 (1984). [EPA] **

Heck, W.W., W.W. Cure, J.O. Rawlings, L.J. Zaragoza, A.S. Heagle, H.E. Heggestad, R.J. Kohut, L.W. Kress and P.J. Temple. Assessing impacts of ozone on agricultural crops: II. Crop yield functions and alternative exposure statistics. Air Pollution Control Association Journal 34:810-817 (1984). [EPA]

Irving, P.M. and J.E. Miller. Synergistic effect on field-grown soybeans from combinations of sulfur dioxide and nitrogen dioxide. Canadian Journal of Botany 62:840-846 (1984). [EPA]

McGraw, A.-C. and J.W. Hendrix. Host and soil fumigation effects on spore population densities of species of endogonaceous mycorrhizal fungi. Mycologia 76:122-131 (1984).

Nelson, D.M., A.E. Carey and V.T. Bowen. Plutonium oxidation state distributions in the Pacific Ocean during 1980-1981. Earth and Planetary Science Letters 68:422-430 (1984). [DOE/OHER]

Toth, R. and R.M. Miller. Dynamics of arbuscule development and degeneration in a Zea mays mycorrhiza. American Journal of Botany 71:449-460 (1984). [DOE/OHER]

*For published material, the names of all Environmental Research Division authors are underlined. (Included are Division members who participated in a project but left the Division before the results were published.)

**Funding agency (abbreviations are spelled out at the end of this appendix). In cases where no funding agency is listed, the publication was not related to any specific funded project.

Vinikour, W.S. and R.V. Anderson. Macroinvertebrates and fishes of Trout Park Nature Preserve, Elgin, Illinois. Transactions of Illinois Academy of Science 77:95-102 (1984).

1985

Fried, S., A.M. Friedman, E. Callis, F. Schreiner, J. Hines, K. Orlandini, D. Nelson and E. Olsen. Enrichment of ^{235}U and concentrations of ^{239}Pu in volcanic samples. Nature 313:301-303 (1985). [DOE/OHER]

Irving, P.M. Modeling the response of greenhouse-grown radish plants to acid rain. Environmental and Experimental Botany 25(4):327-338 (1985). [EPA, EPRI]

Kress, L.W., J.E. Miller and H.J. Smith. Impact of ozone on winter wheat yield. Environmental and Experimental Botany 25(3):211-228 (1985). [EPA]

Kress, L.W. and J.E. Miller. Impact of ozone on field corn yield. Canadian Journal of Botany 63:2408-2415 (1985). [EPA]

Kress, L.W. and J.E. Miller. Impact of ozone on grain sorghum yield. Water, Air, and Soil Pollution 25:377-390 (1985). [EPA]

Miller, R.M. Overview: Mycorrhizae. Restoration & Management Notes 3(1):14-20 (1985). [Invited contribution] [DOE/OHER]

Miller, R.M., B.A. Carnes and T.B. Moorman. Factors influencing survival of vesicular-arbuscular mycorrhiza propagules during topsoil storage. Journal of Applied Ecology 22:259-266 (1985). [DOE/OHER]

Nelson, D.M., W.R. Penrose, J.O. Karttunen and P. Mehlhoff. Effects of dissolved organic carbon on the adsorption properties of plutonium in natural waters. Environmental Science and Technology 19:127-131 (1985). [DOE/OHER]

3. Reports

1984

Irving, P.M. Acid deposition effects study at Argonne National Laboratory. The Effects Division Environment Report, Journal of the Air Pollution Control Association, p. 600. 1984. [EPA, EPRI]

1985

Argonne National Laboratory et al. Ecological Studies of Disturbed Landscapes: A Compendium of the Results of Five Years of Research Aimed at the Restoration of Disturbed Ecosystems. DOE/NBM-5009372. U.S. Department of Energy, Washington, DC. Completed: September 1984; Issued: June 1985. [DOE/OHER]

Cowan, C.E., E.A. Jenne, D.M. Nelson and K.H. Abel. Transuranic Chemical Species in Groundwater: Final Report. PNL-5263. Pacific Northwest Laboratory, Richland, WA. 1985. [DOE/OHER]

Environmental Research Division, Annual Report. Environmental Effects Research. January - December 1983. ANL-83-100, Part III. Argonne National Laboratory. [DOE/OHER, EPA, EPRI]

Findlay, M. The Effects of Solution Acidity and Soluble Organic Compounds on Metal Mobilization in a Forest Soil. Masters Thesis, Northwestern University, Evanston, IL. 1985.

Schubert, J.S. Subsurface Leaching of Pyritic Coal Mine Spoils and Contaminant Migration. Open-File Report 10-85. U.S. Bureau of Mines. 1985. [Bureau of Mines]

4. Published Conference Papers

1984

Edgington, D.N. and D.M. Nelson. The chemical behavior of long-lived radionuclides in the marine environment. In: International Symposium on the Behavior of Long-Lived Radionuclides in the Marine Environment. Proceedings of a meeting jointly organized by the Commission of the European Communities and the ENEA, 28-30 September 1983, La Spezia, Italy. 1984. pp. 19-68. [DOE/OHER]

Irving, P.M. Acid rain research: A review and analysis of methodology. In: Trends in Electric Utility Research, C. Bullard and P. Womeldorff (eds.), proceedings of a conference organized by the Midwest Universities Energy Consortium, 3 April 1984, Chicago, IL. Pergamon Press. 1984. pp. 327-338. [EPA, EPRI]

1985

Franson, R. and R.M. Miller. The effect of endomycorrhizae on interactions between mycorrhizal and nonmycorrhizal plants. In: Proceedings of the Sixth North American Conference on Mycorrhizae, 25-29 June 1984, Bend, OR. Forest Research Laboratory, Corvallis, OR. 1985. p. 307. [DOE/OHER]

Jarstfer, A.G. and R.M. Miller. Effect of soil dilution on the growth and response of Agropyron smithii to mutualistic association with Glomus mosseae/monosporum. In: Proceedings of the Sixth North American Conference on Mycorrhizae, 25-29 June 1984, Bend, OR. Forest Research Laboratory, Corvallis, OR. 1985. p. 315. [DOE/OHER]

Jarstfer, A.G. and R.M. Miller. Progress in the development of a chitin assay technique for measuring extraradical soilborne mycelium of V-A mycorrhizal fungi. In: Proceedings of the Sixth North American Conference on Mycorrhizae, 25-29 June 1984, Bend, OR. Forest Research Laboratory, Corvallis, OR. 1985. p. 410. [DOE/OHER]

McGraw, A.-C. and R.M. Miller. Structure and function of mycorrhizal fungus communities of the Red Desert. In: Proceedings of the Sixth North American Conference on Mycorrhizae, 25-29 June 1984, Bend, OR. Forest Research Laboratory, Corvallis, OR. 1985. p. 314. [DOE/OHER]

Stetter, J.R., W.R. Penrose, S.Z. Zaromb, D. Christian, D.M. Hampton, M. Nolan, M.W. Billings, C. Steinke. Evaluating the effectiveness of chemical parameter spectrometry in analyzing vapors of industrial chemicals. In: Proceedings of the Technical Seminar on Oil Spills, 5-7 February 1985, Toronto, Canada. Environment Canada. pp. 332-343. 1985. [U.S. Coast Guard].

5. Published Abstracts, Notes, Reviews, Comments, and Letters

1984

Irving, P.M. Commentary. Journal of the Air Pollution Control Association, 34:1114-1115 (1984). [EPA, EPRI]

Irving, P.M. Parameters to consider when modeling plant response to acidic deposition (Abstract). NADP Technical Committee Meeting, 31 October - 2 November 1984, Asheville, NC, Abstracts of Papers. [EPA]

Nelson, D.M. The role of dissolved organic carbon in the partitioning of plutonium between water and sediments (Abstract). 1984 Ocean Science Meeting, American Geophysical Union, 23-27 January 1984, New Orleans, LA. [DOE/OHER]

1985

Findlay, M.W. and B.G. Lewis. Effects of input acidity and soluble organic compounds on the solubilization of metals in a forest soil (Abstract). In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 24. [DOE/OHER]

Irving, P.M. Factors relevant to extrapolation from specific sites to regional assessments. Response of soybeans to temporal variations in rainfall acidity (Abstract). In: Agricultural Effects Peer Review Abstracts and Summaries. National Acid Precipitation Assessment Program. February 1985. [EPA]

Irving, P.M. Letter to a journal: Statistical design controversy, Irving's reply. Journal of the Air Pollution Control Association 35:159 (1985). [EPA, EPRI]

Irving, P.M. Book Review of: "Direct and Indirect Effects of Acidic Deposition on Vegetation." Journal of Environmental Quality 14:458 (1985). [EPA]

Irving, P.M. Biogeochemical transformations in two plant/soil systems exposed to simulated acidic precipitation (Abstract). In: International Symposium on Environmental Biogeochemistry, September 1985, Rome, Italy, Book of Abstracts, p. 58. [EPA]

Irving, P.M. Comparison of effects of wet and dry deposition on crops (Abstract). In: Abstracts for Second U.S.-Dutch International Symposium: Aerosols. U.S. Environmental Protection Agency and Netherlands Ministry of Housing, Physical Planning and Environment, Williamsburg, VA, 19-24 May 1985, p. 60. [EPA]

Irving, P.M., J.C. Inman and K.H. Lavoie. Effects of acid rain on biogeochemical transformations in two forage systems (Abstract). In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 26. [EPRI]

Jastrow, J.D. and R.M. Miller. Effects of topsoil replacement method on revegetation of mined land in the Red Desert of Wyoming (Abstract). In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 27. [DOE/OHER]

Knight, M.J., J.D. Jastrow and L.A. Shannon. Plant growth on soil amended with spray-drying flue gas desulfurization waste (Abstract). In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 27. [DOE/OHER]

Kress, L.W. and J.E. Miller. Ozone-induced yield loss to important midwestern crop species (Abstract). In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 28. [DOE/OHER]

McGraw, A.-C., K. Kuipers, L.W. Kress and R.M. Miller. Effects of dosages of O_3 and SO_2 on indigenous mycorrhizae associated with field-grown alfalfa. In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 159. [DOE/OHER]

Miller, R.M. and A.J. Jarstfer. Mycorrhizal influences on growth and nutrient acquisition in Agropyron smithii (Abstract). In: Agronomy Abstracts (abstracts of papers to be presented at 1985 Annual Meeting of American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, 1-6 December 1985). p. 160. [DOE/OHER]

6. Oral Presentations*

1984

Franson, R.L. and R.M. Miller. The effect of endomycorrhizae on interactions between mycorrhizal and nonmycorrhizal plants. Poster presentation at Sixth North American Conference on Mycorrhiza, Oregon State University, 25-29 June 1984, Bend, OR. [Scientists]** [DOE/OHER]

*For oral presentations, the persons making the presentation are underlined.

**Audience for the presentation.

Hinchman, R.R. Rehabilitation and revegetation of disturbed ecosystems. Presented at meeting of the American Chemical Society, Joliet Chapter, 27 September 1984, Joliet, IL. [Chemists from industries and academic institutions] [DOE/OHER]

Irving, P.M. Effects of acid deposition on crops. Presented at National Acid Precipitation Assessment Program Annual Meeting, 31 January - 1 February 1984, Frederick, MD. [Scientists] [EPA]

Irving, P.M. Detailed description of acid deposition/agriculture project March 1984: Effects of acid precipitation on midwestern crop/soil systems. Presented at Peer Review Meeting--EPA Acid Precipitation/Agriculture Program, 6 March 1984, Champaign, IL. [Scientists] [EPRI]

Irving, P.M. Detailed description of acid deposition/agriculture project March 1984: Effects of temporal variations of rain on crop response to acidic deposition. Presented at Peer Review Meeting--EPA Acid Precipitation/Agriculture Program, 6 March 1984, Champaign, IL. [Scientists] [EPA]

Irving, P.M. Summary of acidic rain impacts on crops. Presented at Sixteenth Air Pollution Workshop, 1-3 May 1984, Banff, Alberta, Canada. [Scientists] [EPA, EPRI]

Irving, P.M. Parameters to consider when modeling plant response to acidic deposition. Presented at NADP Technical Committee Meeting, 31 October - 2 November 1984, Asheville, NC. [Scientists, program managers] [DOE/OHER]

Jarstfer, A.G. and R.M. Miller. Effect of soil dilution on the growth and response of Agropyron smithii to mutualistic association with Glomus mosseae/monosporum. Poster presentation at Sixth North American Conference on Mycorrhiza, Oregon State University, 25-29 June 1984, Bend, OR. [Scientists] [DOE/OHER]

Jarstfer, A.G. and R.M. Miller. Progress in the development of a chitin assay technique for measuring extraradical soilborne mycelium of V-A mycorrhizal fungi. Poster presentation at Sixth North American Conference on Mycorrhiza, Oregon State University, 25-29 June 1984, Bend, OR. [Scientists] [DOE/OHER]

Kress, L.W. NCLAN quality assurance program. Presented at Sixteenth Air Pollution Workshop, 1-3 May 1984, Banff, Alberta, Canada. [Scientists] [EPA, EPRI]

McGraw, A.-C. and R.M. Miller. Functional studies on V-A mycorrhizas from successional ecosystems of the Red Desert. Presented at Annual Meeting on Terrestrial Ecology in Arid and Semi-Arid Regions, U.S. Department of Energy, 5-6 June 1984, Rockville, MD. [Scientists, DOE program managers] [DOE/OHER]

McGraw, A.-C. and R.M. Miller. Structure and function of mycorrhizal fungus communities of the Red Desert. Poster presentation at Sixth North American Conference on Mycorrhiza, Oregon State University, 25-29 June 1984, Bend, OR. [Scientists] [DOE/OHER]

Miller, R.M. Factors influencing V-A mycorrhiza establishment during succession in the Red Desert. Presented at Annual Meeting on Terrestrial Ecology in Arid and Semi-Arid Regions, U.S. Department of Energy, 5-6 June 1984, Rockville, MD. [Scientists, DOE program managers] [DOE/OHER]

Nelson, D.M. The role of dissolved organic carbon in the partitioning of plutonium between water and sediments. Presented at 1984 Ocean Science Meeting, American Geophysical Union, 23-27 January 1984, New Orleans, LA. [Scientists] [DOE/OHER]

Nelson, D.M. Influence of organics on migration. Presented at Joint United States and Federal Republic of Germany Workshop on Geochemistry of Radionuclide Migration, 3-7 December 1984, Argonne National Laboratory and Oak Ridge National Laboratory. [Scientists] [DOE/OHER]

1985

Findlay, M. Effects of solution acidity and DOC on the leaching of iron, manganese, and aluminum from a forest soil. Presented at Environmental Research Division Ecology Seminar, 9 May 1985. [Division staff] [DOE/OHER]

Findlay, M. Effects of leachate acidity and soluble organic compounds on metal solubilization in a forest soil. Presented at Civil Engineering Department Seminar, Northwestern University, 15 May 1985, Evanston, IL. [Faculty, graduate students] [DOE/OHER]

Findlay, M.W., Jr. and B.G. Lewis. Effects of input acidity and soluble organic compounds on the solubilization of metals in a forest soil. Presented at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [DOE/OHER]

Hinchman, R.R. Land reclamation: re-creating healthy ecosystems on drastically disturbed landscapes. Presented to American Institute of Chemical Engineers, Joliet Section, 8 January 1985, Plainfield, IL. [Chemical engineers, chemists] [DOE/OHER]

Irving, P.M. Factors relevant to extrapolation from specific sites to regional assessments. Response of soybeans to temporal variations in rainfall acidity. Presented at Peer Review Meeting, National Acid Precipitation Assessment Program, 4-7 February 1985, Brookhaven National Laboratory, Upton, NY. [Scientists, program managers] [EPA]

Irving, P.M. Myths and facts about acid rain. Presented at Endangered Ecosystems Lecture Series, Chicago Academy of Sciences, 5 March 1985, Chicago, IL. [Scientists, general public, students] [DOE/OHER, EPA]

Irving, P.M. The contribution of acid rain to ecosystem stress: A comparison and assessment of research results. Presented at Division of Environmental Health Lecture Series, Lake County Health Department, 12 March 1985, Waukegan, IL. [Health professionals, scientists] [DOE/OHER, EPA]

Irving, P.M. Comparison of effects of wet and dry deposition on crops. Presented at Second U.S.-Dutch International Symposium: Aerosols, sponsored by U.S. Environmental Protection Agency and Netherlands Ministry of Housing, Physical Planning and Environment, 19-24 May 1985, Williamsburg, VA. [Scientists] [EPA]

Irving, P.M. Biogeochemical transformations in two plant/soil systems exposed to simulated acidic precipitation. Presented at Seventh International Symposium on Environmental Biogeochemistry, 8-13 September 1985, Rome, Italy. [International Scientists] [EPA]

Irving, P.M., J.C. Inman and K.H. Lavoie. Effects of acidic rain on biogeochemical transformations in two forage systems. Presented at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [EPRI]

Jastrow, J.D. and R.M. Miller. Effects of topsoil replacement method on revegetation of mined land in the Red Desert of Wyoming. Presented at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [DOE/OHER]

Knight, M.J., J.D. Jastrow and L.A. Shannon. Plant growth on soil amended with spray-drying flue gas desulfurization waste. Presented at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [DOE/OHER]

Kress, L.W. Sulfur dioxide effects on soybean yield. Presented at the Seventeenth Annual Air Pollution Workshop, North Carolina State University, 18 April 1985, Raleigh, NC. [Scientists] [EPA, EPRI]

Kress, L.W. Plant pathologist/ecologist. Presented at the First New Lenox Career Day Fair, Oster-Oakview Junior High School, 26 April 1985, New Lenox, IL. [Teachers, 7th and 8th graders] [EPA, EPRI]

Kress, L.W. and J.E. Miller. Ozone-induced yield loss to important midwestern crop species. Presented at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [EPA, EPRI]

McGraw, A.-C., K. Kuipers, L.W. Kress and R.M. Miller. 1985. Effects of dosages of O_3 and SO_2 on indigenous mycorrhizae associated with field-grown alfalfa. Presented at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [EPA, EPRI]

Miller, R.M. Stress-tolerance strategies in plants. Presented at the Terrestrial Ecology Section Review, Office of Health and Environmental Research, U.S. Department of Energy, 30 September 1985, Fort Worden, WA. [Scientists, program administrators] [DOE/OHER]

Miller, R.M. A fitness argument for mycorrhizae in grassland ecosystems. Presented to seminar at University of Illinois at Chicago, 17 October 1985, Chicago, IL. [Faculty, students] [DOE/OHER]

Miller, R.M. and A.G. Jarstfer. Mycorrhizal influences on growth and nutrient acquisition in Agropyron smithii. Poster presentation at American Society of Agronomy 77th Annual Meeting, 1-6 December 1985, Chicago, IL. [Scientists] [DOE/OHER]

Nelson, D.M. The role of natural dissolved organic compounds in determining the concentration of americium in natural waters. Presented at the Speciation-85 Seminar, Speciation of Fission and Activation Products in the Environment, the Commission of the European Communities and the National Radiological Protection Board, 16-19 April 1985, Christ Church, Oxford, UK. [Scientists] [DOE/OHER]

Nelson, D.M. Aquatic food chains. Presented at Workshop on Gastrointestinal Absorption of Actinides and Other Metals, Pacific Northwest Laboratory, 24-26 June 1985, Battelle, Seattle Research Center, Seattle, WA. [Scientists] [DOE/OHER]

Schubert, J.P. Pre-mine prediction of acid mine drainage. Presented at Technology Transfer Seminar on Acid Mine Drainage Control, 3-4 April 1985, Pittsburgh, PA. [Scientists] [U.S. Bureau of Mines]

Schubert, J.P. Environmental concerns and reclamation of gas pipeline construction sites. Presented at monthly meeting of the Association of Engineering Geologists (North-Central Section), 21 May 1985, Chicago, IL. [Civil, geological engineers] [GRI]

Schubert, J.P. Impacts of gas pipeline construction on streams. Presented at Ecology Seminar, Environmental Research Division, 20 June 1985, Argonne National Laboratory. [Division staff] [GRI]

CODES FOR FUNDING AGENCIES

DOE = U.S. Department of Energy

EPA = U.S. Environmental Protection Agency

EPRI = Electric Power Research Institute

GRI = Gas Research Institute

OTHER = Office of Health and Environmental Research (in DOE)

CHAPTER 4. ENVIRONMENTAL IMPACTS PROGRAM

4-3 / 4-4

CHAPTER 4. ENVIRONMENTAL IMPACTS PROGRAM

Program Staff

<u>Program Staff</u>	<u>Title</u>
R.D. OLSEN	Program Manager
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J.F. HOFFECKER	Archeologist
J.S. IRVING	Fisheries Biologist
R. KRUGER	Fisheries Biologist
K. LaGORY	Wildlife Ecologist
D.D. NESS	Terrestrial Ecologist
S.J. OLSHANSKY	Sociologist
T. O'NEIL	Wildlife Ecologist
B.A. PAYNE*	Sociologist
L.F. SOHOLT*	Ecologist
E.A. STULL	Aquatic Biologist
R.C. SUNDELL	Planner
R.L. TOBIN*	Operations Research Analyst
R.G. WILLIAMS	Sociologist
G.W. WITMER	Wildlife Ecologist
S. YIN	Hydrologist

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B. RUSSELL, Idaho National Engineering Laboratory, Idaho Falls, Idaho
M.A. SNIDER, Energy and Environmental Systems Division, Argonne National Laboratory

*No longer a member of the Division.

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4.1 PROGRAM OVERVIEW

R.D. Olsen

Work of the Environmental Impacts Program focuses on the prediction and evaluation of the effects of resource development on the human and natural environment. Most studies are conducted within the context of the National Environmental Policy Act (NEPA) of 1969 and subsequent environmental and regulatory legislation. Activities typically include analyzing existing environmental conditions, predicting changes in those conditions that could result from proposed activities or developments, and determining the significance of predicted changes. While the Program's primary role is assessing impacts, major emphasis also is placed on developing new assessment methods, proposing alternatives to proposed developments, and introducing new approaches to resource planning.

The staff of the Environmental Impacts Program possess diverse capability and experience in the areas of physical, ecological, and human aspects of the environmental sciences. Research projects are generally conducted by a multidisciplinary team that utilizes each member's expertise within the overall scope of the research effort. Specific areas of expertise range from terrestrial and aquatic ecology to sociological planning. Staff support capabilities include computer applications, modeling, and information management.

The most significant activity of the Environmental Impacts Program has been assisting the Federal Energy Regulatory Commission (FERC) Office of Hydropower Licensing relative to the NEPA and other pertinent environmental legislation. FERC is the federal agency responsible for issuing licenses for construction and operation of nonfederal hydroelectric developments. The assistance provided since 1978 by Argonne has involved comprehensive and multidisciplinary analysis of all aspects of hydropower development. These analyses have included both site-specific and generic impact assessments for construction and operation of hydropower facilities differing considerably in power capacity (1 to 1,620 MW), dam height (5 to 885 feet), and scope (power, irrigation, and water supply).

The number of pending license applications has increased in the past few years as a result of expanded private sector interest in development of hydroelectric projects. This interest is largely due to the federal tax incentives and power purchase stipulations in the Public Utility Regulatory Policies Act of 1978 (PURPA). FERC has received filings for thousands of preliminary permits for small hydroelectric projects since PURPA was implemented in 1980; more than 1,000 of the filings were for developments in the Pacific Northwest alone.

Prior to the "hydro-rush" stemming from PURPA, it was generally believed that smallscale hydroelectric projects were, for the most part, environmentally benign. Such projects often were recommended as alternatives to large hydropower projects and steam-electric plants in many parts of the country. However, as the magnitude of the potential development of small

hydro sites began to unfold over the past few years, a growing concern developed relative to environmental impacts of the construction and operation of large numbers of such projects in many river basins throughout the United States, particularly in the Pacific Northwest. Although most hydropower projects could be constructed and operated so that adverse impacts would be minimal, the combined impacts from several such projects could result in significant cumulative adverse effects. This concern is reinforced by the abundance of current filings before the FERC in many river basins.

As part of its FERC-supported work, Argonne completed one environmental assessment and two environmental impact statements for hydropower projects. Staff members also began two major evaluations of potential cumulative environmental impacts from hydropower development in northwestern river basins and a study of the impacts of a proposed hydropower/water supply project in Arkansas.

In related work, the Environmental Impacts Program is conducting a study for Bonneville Power Administration to develop cumulative effects methodologies for use in the Columbia River Basin. Other work for the U.S. Department of Energy includes preparation of an EIS for the importation of electrical power from Canada to New England and several reports documenting the development of a Freight Network Modeling System.

4.2 HYDROPOWER DEVELOPMENT IMPACT EVALUATION

4.2.1 Summary

R.D. Olsen

The principal projects involved in the Program's hydropower development impact assessment work are sponsored by the FERC. The analyses undertaken for FERC culminate in preparation of either an Environmental Impact Statement (EIS) or an Environmental Assessment (EA), depending on the potential for significant adverse impacts. To date, the majority of work for FERC has involved large or technically complicated projects, and the resulting documents have been full EISs. These documents ranged from about 100 pages up to 1,200 pages and required from six months to two years to complete.

During the two-year period covered by this report, work was undertaken on three single-project EISs. The Draft EIS for the mammoth Susitna Hydroelectric Project in Alaska was completed in May 1984; the Draft EIS for the much smaller Hamma Hamma Hydroelectric Project in the state of Washington was completed in April 1985; and an EIS for the Lee Creek Water Supply Project in Arkansas was initiated and then put on hold following the public scoping meetings until a water-quality issue was resolved. Additionally, one EA covering the installation of a generator at an existing lock and dam on the Mississippi River was also completed in 1984.

The major work in 1985 involved implementation of a procedure suggested by FERC for evaluation of cumulative environmental impacts of multiple

hydroelectric projects proposed for development within individual river basins. This is referred to as the Clustered Impact Assessment Procedure (CIAP). This work was a significant departure from all previous analytical strategies used for environmental evaluations. Argonne was responsible for developing the methodological details for use of the CIAP according to a basic matrix concept suggested by FERC. The CIAP projects undertaken for FERC parallel similar developmental work undertaken for the Northwest Power Planning Council through a contract from the Bonneville Power Administration. These and other individual projects mentioned above are detailed in the following sections.

4.2.2 Susitna Hydroelectric Project Environmental Impact Statement

R.D. Olsen, J.D. DePue, J.F. Hoffercker, J.D. Jastrow, D.D. Ness, B.A. Payne, A.J. Policastro, M.A. Snider,** L.F. Soholt, R.C. Sundell, R.G. Williams, M.C. Winters, and A.J. Zielen*

On March 1, 1983, the Alaska Power Authority (APA) filed a license application with FERC for construction and operation of a major hydroelectric development to be located on the Susitna River in southcentral Alaska (Figure 4.1). The APA proposed in its Susitna project application to construct two large dams--an 885-foot-high earthfill dam (Watana Dam) and a 645-foot-high concrete arch dam (Devil Canyon Dam). These dams would form two reservoirs with a combined length of nearly 75 miles and a surface area of nearly 50,000 acres. The proposed project would also include construction of about 300 miles of high-voltage transmission lines, over 50 miles of access roads, and a short rail spur to the construction area. Installed generating capacity would exceed 1600 MW, and the power output would meet about 80% of the needs of the populated portion of Alaska well into the next century. This was the largest development ever considered for licensing by FERC.

Because of the magnitude of the proposed development and its location in what is essentially a pristine wilderness area, the project was highly controversial within the state of Alaska and was opposed by federal land and resource management agencies and virtually all environmental groups in the state.

In the spring of 1983, FERC contracted with Argonne and Oak Ridge National Laboratory (ORNL) to prepare an EIS for the Susitna Project. Argonne was the lead laboratory for the environmental analysis and evaluated all terrestrial, socioeconomic and air quality issues. ORNL had the responsibility for analysis of all aquatic issues.

Following a comprehensive scoping process and technical analysis by the two Laboratories, during which all aspects of the project's environmental

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***Collaborator; affiliation is listed at the front of this chapter.*

Figure 4.1. Map showing location of the proposed Susitna Hydroelectric Project facilities in southcentral Alaska.

impacts, benefits, and alternatives were examined, FERC released the Draft EIS for public comment in May 1984 (Federal Energy Regulatory Commission 1984). The staff concluded in the document that the proposed project would result in largely unmitigable and significant adverse environmental impacts on fish, wildlife, and the human environment. Additionally, after comparing possible alternative power-production scenarios with the proposed project in terms of engineering feasibility, economic characteristics, and environmental impacts, it was concluded in the Draft EIS that a mixed thermal-based generation scenario, with selected non-Susitna hydropower projects added as needs dictated, appeared to be the most effective approach for meeting the projected generation requirements of the region.

As a result of the conclusions in the Draft EIS and its own ongoing studies of the project's engineering, economics, and environmental impacts, the APA undertook a major redesign of the project during 1984 and 1985. The APA is expected to file a substantially revised license application in early 1986 for reevaluation. It is likely that Argonne will be requested by the FERC to assume overall responsibility for reanalysis of the revised project design and for preparation of a supplement to the Draft EIS for release to the public during 1986. This would be followed by preparation in 1987 of a Final EIS that would contain the final recommendations for the Commission's consideration of issuance of a license for the proposed facility.

4.2.3 Hamma Hamma Hydroelectric Project Environmental Impact Statement

R.D. Olsen, J.D. DePue, J.F. Hoffecker, J.S. Irving, R.G. Williams, G.W. Witmer, and J.-Y. Yang*

The Public Utility District No. 1 of Mason County, Washington, proposed in a license application to FERC in August 1983 to construct and operate the 22-MW Hamma Hamma Hydroelectric Project to meet a portion of the projected electric power needs of its service area within the state of Washington. The project would be located on the lower Hamma Hamma River, which drains a portion of the eastern slope of the the Olympic Peninsula in northwestern Washington state. This river basin includes part of the Olympic National Forest and is near the Olympic National Park. The basin currently has no hydroelectric development and is considered an unspoiled environment by recreationists. The river supports runs of both salmon and steelhead trout and contributes to the commercially valuable Hood Canal salmon fishery.

The project would consist of a 37-foot-high, 255-foot-long dam on the river immediately above a natural 75-foot-high falls; a 28-acre impoundment; two small powerhouses; a 6,000-foot-long power tunnel, 10 feet in diameter; a 900-foot-long tramway downslope to the downstream powerhouse; and about a half-mile of new access road.

*Project leader.

FERC requested the assistance of Argonne in analyzing the probable environmental consequences of construction and operation of the facility and in preparing the EIS required for consideration of licensing by the Commission. The Draft EIS was prepared during early 1985 and released by FERC for public comment in April 1985 (Federal Energy Regulatory Commission 1985h). The analyses detailed in the Draft EIS included evaluation of the proposed project and two alternative configurations of that design, consideration of other power supply alternatives (including a capacity-proportional portion of a large coal-fired steam plant) and various nonstructural alternatives.

The staff's conclusions, as presented in the Draft EIS, were that the project as proposed could have significant adverse impacts on fishery resources of the Hama Hama River due to loss of spawning and rearing habitat in the reach of river bypassed by the power tunnel diversion and through sedimentation of habitat downstream of the project. It was further concluded that alternative project designs involving relocation of the powerhouses closer to the dam would greatly reduce, but not eliminate, potential impacts on salmon and steelhead trout habitat. The document also discussed the relative impacts of a large coal-fired powerplant and concluded that the plant location and design evaluated would have less impact on aquatic systems in general and salmonids in particular than would any of the hydroelectric alternatives considered.

Comments on the Draft EIS by federal and state resource managers suggested the potential for cumulative impacts from the Hama Hama Project in combination with other proposed hydropower developments in the upper part of the Hama Hama River Basin. As a result of these suggestions, FERC has requested that in 1986 Argonne evaluate the potential for such cumulative impacts and prepare a supplement to the Draft EIS if cumulative impact issues are deemed to be significant. Preparation of a Final EIS would follow, and depending on the findings of the cumulative impact investigation, might cover all project development proposed for the Hama Hama River Basin.

4.2.4 Lee Creek Water Supply/Hydroelectric Project Environmental Impact Statement

E.A. Stull, M.B. Bain, J.F. Hoffecker, K. LaGory, D.D. Ness,
S.J. Olshansky, A.J. Policastro, and S. Yin*

The City of Fort Smith, Arkansas, filed with FERC in November 1983 an application for a license to construct and operate a water supply and hydroelectric project on Lee Creek in Crawford County, Arkansas. The proposed project would be sited on the lower reaches of Lee Creek near its confluence with the Arkansas River. FERC contracted with Argonne in the spring of 1985 to assess the environmental impacts of the proposed project. The end product

*Project leader.

will be an EIS detailing the staff's evaluation of the impact issues and presenting their recommendations regarding licensing of the proposed project.

Argonne participated in initial scoping meetings and a public hearing on the project and submitted to FERC two reports outlining the issues that should be covered in detail in the EIS. Because the project is basically a municipal water supply development with a small turbine and generator added to provide power that would be used only to power water pumps, Argonne advised FERC that it would be necessary to evaluate in detail the water supply aspects of the project, including alternatives and the actual need for the water. The evaluation was also complicated by the existence of plans for a Phase II expansion of the project, which were not included in the license application. Speakers at the scoping meetings and public hearings contended that the Phase II plans should have been included in the license application or at least should be included in the comprehensive environmental evaluation to be performed by Argonne.

Because of uncertainty as to the proper approach to be taken in view of these complications, FERC placed the project on hold while the FERC Office of General Counsel evaluated the situation relative to requirements of the National Environmental Policy Act and other pertinent legislation. It has recently been determined by FERC that (1) it will be necessary to consider all water supply aspects of the project in detail within Argonne's environmental evaluation, and (2) to the extent the Phase II plans can be considered a reasonable foreseeable action, an evaluation of that aspect of the project must also be undertaken. Work by Argonne on the EIS has been reinitiated and completion is expected in late 1986.

4.2.5 Three-City Mississippi River Hydropower Project Environmental Assessment

E.A. Stull, J. DePue, J.S. Irving, R. Sundell, G. Williams, and G.W. Witmer*

The Three-City Mississippi River Hydropower Agency, consisting of the cities of Bellevue, Sabula, and Preston, Iowa, in 1983 filed an application with FERC for a license to construct and operate a hydroelectric facility at Lock and Dam No. 11 on the Mississippi River near Dubuque, Iowa. In 1984 Argonne was contracted to prepare an Environmental Assessment (EA) on the proposal and to make recommendations for conditions to the license relative to environmental matters.

The applicant proposed to develop the hydroelectric power potential of Mississippi River Lock and Dam No. 11 by installing a hydroelectric power-plant with a generating capacity of 18,400 kilowatts. Major features of the proposed project would include an intake channel, a powerhouse, a tailrace

*Project leader.

channel access and parking facilities, and a 3-mile-long transmission line to an existing substation in Dubuque. The plant would be located on the Wisconsin side of the Mississippi River in an earthen section of the existing dam (Figure 4.2).

Figure 4.2. Layout of the proposed Three-City Mississippi River Hydropower Project at Lock and Dam No. 11.

Argonne staff reviewed the environmental report for the project submitted by the applicant, as well as a Corps of Engineers EIS for alternative hydroelectric development options on the Mississippi River. During a visit to the site of the proposed project by Argonne staff, the Lockmaster was interviewed concerning operation of the lock and dam; local fishermen were interviewed with respect to the location and value of fisheries in the project area; and

natural resource management agencies in Iowa and Wisconsin were consulted regarding environmental issues.

Issues related to fish, wildlife, and recreation were emphasized in the environmental assessment. The project would change the pattern of river flow below the lock and dam, and, thus, the distribution of the fish resources would also change. However, it was not possible to confirm that fisheries productivity would be decreased. The construction of the powerhouse and raceway would eliminate fishing on the wings of the dam. However, a local park would be upgraded and additional fishing opportunities of a different kind would be produced. Impacts on wildlife would be localized to the immediate vicinity of the project. Resource agencies had expressed concern that the diversion of flow from the gates of the dam to the turbines in the powerhouse would reduce the overall ability of the lock and dam to reoxygenate the river's waters. Examination of the information on oxygen content of water upstream and downstream of the dam did not suggest any such oxygenation effect. Since the gates of the dam are raised, allowing water to flow under them (rather than lowered so water cascades over the top), Argonne staff concluded that aeration potential lost by construction of the power project would be minimal.

The project was concluded by submission of the draft environmental assessment and draft license conditions to FERC.

4.2.6 Cluster Impact Assessment Procedure Projects

4.2.6.1 Summary

R.D. Olsen

Recognizing the need for a more definitive and comprehensive approach to identification and evaluation of potential cumulative impacts from multiple project development in selected river basins, early in 1985 FERC formulated and published in the Federal Register for public comment a proposed strategy for assessment of cumulative impacts. The proposed methodology was termed the Cluster Impact Assessment Procedure (CIAP). Following a public comment period, FERC finalized the CIAP and prepared to implement the strategy. The CIAP will be employed to (1) identify river basins where there is a potential for cumulative adverse impacts on important resources (identified by resource managers, interested parties, project proponents, and the FERC staff) that could be caused by multiple project development; (2) determine the geographic extent of the important resources (termed target resources in the CIAP); (3) determine the interaction between target resources and proposed hydropower projects by identification of the impact zone for each project; (4) perform a cumulative impact analysis of the clustered projects; and (5) prepare the appropriate NEPA document (usually an environmental impact statement) describing the existing environment, detailing impacts, analyzing alternatives, discussing mitigation, and recommending the action to be taken by the Commission. The process is summarized in Figure 4.3.

Figure 4.3. Diagram of CIAP process as modified by Argonne for use on the Snohomish and Salmon River Basins.

The CIAP will be altered somewhat in application to each individual river basin in order to deal more specifically with the unique characteristics and problems of each situation. FERC has to date identified 19 river basins (most in the Northwest) that appear after preliminary evaluation to have significant potential for cumulative impacts due to the clustering of proposed hydro-electric developments.

On April 24, 1985, the FERC commissioners voted 4 to 0 to implement the CIAP in three river basins: the Owens River in California, the Snohomish River in Washington, and the Salmon River in Idaho. Following the Commission decision, FERC retained Argonne's Environmental Research Division to assist in application of the CIAP to the Snohomish and Salmon River Basins. The Division's responsibilities are to include all technical analyses required by the CIAP for the two basins and preparation of all reports and NEPA documents associated with the assessment. Work on these two basins will extend through 1986. Details of the CIAP method as it was applied to the Snohomish and Salmon River Basins have been discussed in various FERC reports (Federal Energy Regulatory Commission 1985a-g). Two important contributions to the general CIAP approach were developed by Argonne staff. Target resource distributions were mapped using digitized computer imagery and programs developed at Argonne. The maps could be printed at various scales, updated, modified, and used as needed for the CIAP and any subsequent work for FERC.

Additionally, a matrix approach with supporting software was developed for assessing potential cumulative impacts to target resources (summarized in Figure 4.4). This capability was needed because no methodologies existed that would serve staff needs. The maps and matrix methodology were explained at technical workshops during the fall and winter of 1985-1986.

Figure 4.4. Basic approach and formula for matrix-based cumulative impact model.

AN ABBREVIATED FORM OF THE BASIC FORMULA IS:

TOTAL IMPACT = SUM *adjusted by* INTERACTIONS

4.2.6.2 Salmon River Basin

J.S. Irving, R. Olsen, J. Hoffeecker, T. O'Neil, B. Young, D. Olsen,** R. Breckenridge,** and B. Russell***

In April 1985, the FERC authorized Argonne staff to begin work on the Salmon River CIAP. During June 1985, staff members visited project sites and held scoping meetings to solicit oral and written comments from state and federal resource agencies, Tribes, developers, and the general public. In an Environmental Analysis (FERC 1985b) released during the Geographic Scoping Phase of the CIAP, Argonne staff recommended as target resources (1) chinook salmon, (2) steelhead trout, (3) resident trout (rainbow, cutthroat, and bull), (4) mule deer, (5) elk, and (6) riparian habitat. The report recommended that the Warm Springs hydroelectric project be excluded from the CIAP because it did not have the potential for significant cumulative impacts to the target resources.

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Argonne staff collected information on the life cycle, distribution, and important habitats for each target resource. The Resource Sort Document (FERC 1985d) contains resource maps describing the distribution of target resources and the criteria and methodology used in assessing impact levels. (As an example, the winter and summer ranges and other important use areas for elk and deer are depicted in Figure 4.5). Input was solicited from interested parties, resource agencies, and Tribes to improve maps, criteria, and methodology. An Environmental Analysis (FERC 1985g) was released during the Resource Sort Phase of the CIAP reflecting changes to maps and impact criteria. The report recommended that the Goose Creek hydroelectric project be excluded from the CIAP because it did not have the potential for significant cumulative impacts to the target resources.

Argonne will prepare an EIS based on the results of the first two workshops and the potential for significant cumulative impacts from the 15 proposed hydroelectric projects. In addition to analyzing the 15 proposed projects, Argonne staff will evaluate the potential impacts of numerous alternative hydropower projects within and outside the basin. Other alternatives, such as a coal-fired powerplant, also will be analyzed. A Draft EIS will be completed in June 1986, and the Final EIS is scheduled for publication in December 1986.

4.2.6.3 Snohomish River Basin

G.W. Witmer, R. Breckenridge,** R. Kruger, C. LeBow, D. Olsen,** R. Olsen, B. Russell,** B. Young, and S. Zussman*

An interdisciplinary team of Argonne staff members and their subcontractor, the Idaho National Engineering Laboratory, began work on the CIAP for the Snohomish River Basin, Washington, in May 1985. The Snohomish Basin is noted for natural runs of salmon, recreational opportunities, forested slopes, and scenic rivers. Several reservoirs are present in the basin, and many sites have been identified for energy development--primarily small, run-of-the-river hydroelectric projects. After visiting the basin and receiving oral and written input from the public, Tribes, and several state and federal agencies, Argonne staff identified several target resources (anadromous and resident fish, black-tailed deer, and bald eagles) as warranting detailed analysis for the potential of cumulative impacts from the seven proposed hydroelectric projects in the basin. These initial findings were described in the Geographic Scoping Document (FERC 1985a). After additional evaluation, it was decided that none of the seven projects should be dropped from the next phase of the CIAP.

ANL staff members gathered information on the target resources and their distribution in the basin. Habitat or life cycle components important to each

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Figure 4.5. Example of computerized target resource distribution map showing wildlife features for deer and elk and proposed hydroelectric project locations (open circles) in the Salmon River Basin, Idaho.

target resource were identified for detailed analysis, and initial criteria were presented for assigning levels of impact. Components for anadromous and resident fish were spawning and incubation habitat, adult and juvenile rearing habitat, migration/movement, and sedimentation/bedload transport. For black-tailed deer, components were permanent habitat loss, winter range loss, loss of cover, and migration blockage. For bald eagles, components were salmon food supply, roost and nest sites, mature riparian forest loss, and a disturbance factor. Input was sought from interested parties to improve the maps and criteria developed. A Workshop Summary Report was produced, reflecting those changes and documenting information and references (FERC 1985e). Again, based on the target resource maps and the workshop findings, it was decided that no projects should be dropped from the next phase of the CIAP.

Based on the results of the first two workshops and the possibility of significant cumulative impacts, Argonne will prepare an EIS rather than a less detailed EA for the Snohomish Basin. A Matrix Technical Session was held in December 1985 to discuss preliminary impact levels and interaction coefficients assigned by Argonne staff and to consider agency-assigned impact thresholds based on agency management goals. Detailed aspects of the methodology and the impact criteria were also discussed. The technical session was followed by an EIS Scoping Meeting to seek input on the issues to be analyzed in the EIS as required by the National Environmental Policy Act.

The EIS for the Snohomish Basin will be a very lengthy, complex document. In addition to analyzing the seven proposed projects, Argonne staff will analyze the potential impacts of numerous alternative hydroelectric and nonhydroelectric projects within and outside the basin. A Draft EIS will be completed in the spring of 1986. After the public, Tribes, and resource agencies have had an opportunity to comment on that document, a Final EIS will be completed in the fall of 1986.

4.2.7 Columbia River Basin Cumulative Effects Assessment Methodology

E.A. Stull, M.B. Bain, K. Emery,** J.S. Irving, and G.W. Witmer*

In the fall of 1984, Argonne initiated a study to develop criteria and methods for assessing potential cumulative effects of hydroelectric development on fish and wildlife resources in the Columbia River Basin. The study is being funded and managed by the Bonneville Power Administration under the Columbia River Basin Fish and Wildlife Program of the Northwest Power Planning Council. Assistance on the scope of the work and review of task reports is being provided by the Hydropower Assessment Steering Committee of the Northwest Power Planning Council.

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**Collaborator; affiliation is listed at the front of this chapter.

The overall objective of the study was to recommend two alternative cumulative effects methodologies for use in the Columbia River Basin. This work was divided into the following seven tasks: (1) development of a list of key fish and wildlife species and habitats, (2) development of a list of hydropower effects on fish and wildlife that could potentially be cumulative, (3) identification of pathways and interactions of cumulative effects, (4) review of cumulative effects methodologies, (5) comparison of cumulative effects methodologies for application to the Columbia River Basin, (6) investigation of the possibility of using stock/recruitment concepts for cumulative assessment, and (7) recommendation of two methodologies for application to the Columbia River Basin.

The list of key fish and wildlife species and habitats was developed in consultation with resource management agencies and Indian Tribes. The final list included 40 species and 18 habitats. The management agencies and Tribes were unwilling to agree to any shortening of the list, arguing that although certain anadromous salmonid fish and certain big game species are highly impacted by hydroelectric development, a cumulative assessment methodology should be able to deal with a wide range of different species.

Hydroelectric development impacts were ranked according to their significance and importance in the Columbia River Basin. Again there was reluctance on the part of agencies and Tribes consulted to restrict the study to only the most important and significant impacts. The Argonne staff concluded that a desirable characteristic of a cumulative effects methodology should be its ability to synthesize impacts of diverse origins. Development of web and flow diagrams was impossible with the large number of species, habitats, and impacts. However, a matrix diagram was developed to illustrate that cumulative hydropower effects on fish and wildlife are highly interactive with other resource development activities in the Columbia River Basin. The matrix diagram developed for fish is shown in Figure 4.6. A similar diagram was developed for wildlife resources in the basin.

Eight common techniques used in environmental assessment and 11 potential cumulative effects assessment methodologies were reviewed and compared with the requirements for a Columbia River Basin methodology. The staff concluded that matrix, evaluative, and panel techniques were highly desirable for incorporation into the recommended methods. The Adaptive Environmental Assessment Methodology (AEAM) has many useful aspects for project scoping and study organization. Matrix techniques, such as in the Cumulative Impact Assessment Procedure (CIAP), were judged to be the most useful way to develop a framework for a cumulative effects assessment. This project will continue in 1986, when one or more methodologies will be recommended for hydropower assessment in the Columbia River Basin.

Figure 4.6. Diagram of interactions between hydroelectric development and nonhydro activities that contribute to cumulative impacts to fish in the Columbia River Basin.

4.3 NEW ENGLAND/HYDRO-QUEBEC TRANSMISSION LINE INTERCONNECTION PHASE II ENVIRONMENTAL IMPACT STATEMENT

R.R. Hinchman, J.D. DePue, J.F. Hoffecker, D.D. Ness, L.F. Soholt,
W.S. Vinikour, and J.-Y. Yang*

Energy production from hydroelectric generation is a long-proven technology. Hydroelectric facilities are both economical and reliable sources of power generation, often proving to be more feasible than equally sized traditional power sources (e.g., oil-, coal-, or nuclear-fueled generating plants). However, areas suitable for hydroelectric development are not always situated near a load center where the power is needed. Thus, utilities with an excess of available hydroelectric power could export electricity to other load centers by transmission line interconnections. One advantage for importing any electric energy is that the area receiving the power is not impacted by the construction and operation of the power source.

Impacts associated with the construction and operation of transmission lines for the importation of hydroelectric power would be similar in nature to transmission lines associated with a traditional powerplant. However, the extent of transmission lines and associated facilities (e.g., substation or converter terminals) is generally much greater for energy importation than for a local powerplant. Such importation across international borders is considered a major federal action, and as such requires the preparation of an Environmental Impact Statement (EIS).

In April 1984, the U.S. Department of Energy (DOE) issued Presidential Permit PP-76 granting permission for Vermont Electric Transmission Company to construct, connect, operate, and maintain a transmission line at the international border of the United States and Canada for the importation of hydroelectric power from Hydro-Quebec. This project involved the construction of a ± 450 kV direct current (DC) transmission line and a converter terminal at the southern terminus of the line in Monroe, New Hampshire. An EIS was published for this interconnection (U.S. Department of Energy 1984). Argonne had major responsibilities in preparing that document.

In order to import additional power from Hydro-Quebec, the applicant submitted an amendment in March 1985 to upgrade the authorized international interconnection. Several new facilities were proposed: (1) an extension of the ± 450 -kV DC line about 133 miles southward to a location between Groton and Ayer, Massachusetts, (2) a new 1800-MW converter terminal at the terminus of the DC line, and (3) two new 345-kV alternating current (AC) transmission lines eventually terminating at an existing AC substation in Medway, Massachusetts (Figure 4.7).

DOE assigned the Environmental Research Division at Argonne the major responsibility for preparation of the EIS related to the construction and

*Project leader.

Figure 4.7. Proposed transmission line extension to existing New England power transmission network.

operation of the facilities required for the extension of the transmission line interconnection.

Most activities required to prepare the EIS were conducted during 1985. These included (1) scoping the contents of the EIS, (2) assembling a multidisciplinary team, (3) identifying the significant issues to be analyzed in detail in the EIS, and (4) conducting review or consultation requirements with other agencies as required for preparation of the EIS. The preliminary Draft EIS is scheduled for completion in early 1986. Issues to be addressed include impacts to air, land, water, biological, visual, and cultural resources. Socioeconomic, health and safety, and radio and television interference concerns also will be considered. Included in the EIS will be descriptions of the proposed and alternative designs, routes, and energy sources; the potential impacts of the alternatives; and mitigative measures. Publication of the Draft EIS by DOE is scheduled for May or June 1986.

4.4 TRANSPORTATION MODEL DEVELOPMENT AND APPLICATIONS

A.J. Zielen and R.L. Tobin

Over the past five years, the Environmental Research Division has developed the Freight Network Modeling System (FNMS), which is a general and flexible freight transportation modeling system designed to have wide applicability to a variety of freight transportation analyses. It consists of predictive and optimizing freight transportation models, network data bases, data management software, report generators, and graphics output.

The network data bases include data on the rail, highway, and water systems in the United States. Study regions can be substate to national in scope. The major analytical tools are the Freight Network Equilibrium Model (FNEM) and the Shortest Path Analysis and Display (SPAD). FNEM is a predictive network model that takes into account congestion and competition for transportation facilities. It is unique in that it simulates decisions of both shippers and carriers. SPAD is a simpler model that optimizes routings. Through its interactive graphics capability, it is useful in analyzing transportation networks to determine optimal routings, alternative or contingency routings, critical links, and network capacity. A typical SPAD graphics output is illustrated in Figure 4.8.

The six-volume FNMS documentation package was completed in 1984 and 1985. The entire set (ANL/ER-TM-84-1) is listed below:

- Vol. I--FNEM Theory and Validation (April 1984)
- Vol. II--FNEM User's Guide and Programmer's Guide (April 1984)
- Vol. III--Preprocessors User's Guide (June 1984)
- Vol. IV--SPAD User's Guide (April 1985)
- Vol. V--Flexible Network Definition Software User's Guide (April 1984)
- Vol. VI--Rate Simulation Software User's Guide (April 1985).

A version of FNEM was also prepared for execution on a VAX-11/750 computer system. This version was installed at the Federal Emergency Management Agency in Washington, D.C., and a two-day training session was held in September 1985 for agency personnel.

A completely interactive and improved version of SPAD has been developed for freight studies in Southern Africa. A new African FNEM now being developed will feature color-coded graphics output to show commodity flow or flow/capacity for all network links. Thus, traffic patterns by commodity and congestion points will be readily visible. This work is a collaboration with the School of Engineering and Applied Science of The University of Pennsylvania and the Department of Geography of the University of Tennessee.

Figure 4.8. Typical SPAD graphics output showing route alternatives from Niagara Falls, New York, to Richland, Washington.

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- Federal Energy Regulatory Commission. 1985d. Resource Sort Workshop Document: Phase II of the Cluster Impact Assessment Procedure for the Salmon River Basin, Idaho. Docket No. EL-19-103. Office of Hydropower Licensing, Washington, DC.
- Federal Energy Regulatory Commission. 1985e. Resource Sort Workshop: Summary Report. Phase II of the Cluster Impact Assessment Procedure for the Snohomish River Basin. Docket No. EL-85-19-101. Office of Hydropower Licensing, Washington, DC.
- Federal Energy Regulatory Commission. 1985f. Matrix Technical Session Document: Phase III of the Cluster Impact Assessment Procedure for the Snohomish River Basin. Docket No. EL-85-19-101. Office of Hydropower Licensing, Washington, DC.
- Federal Energy Regulatory Commission. 1985g. Cluster Impact Assessment Procedure: Resource Sort Phase. Environmental Assessment for the Salmon River Basin. Docket No. EL-85-19-103. Office of Hydropower Licensing.
- Federal Energy Regulatory Commission. 1985h. Draft Environmental Impact Statement, Hamma Hamma Hydroelectric Project, FERC No. 3178 - Washington. Office of Hydropower Licensing, Washington, DC.
- U.S. Department of Energy. 1984. Environmental Impact Statement, New England/Hydro-Quebec ± 450-kV Direct Current Transmission Line Interconnection. DOE/EIS-0103. Washington, DC.

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APPENDICES FOR CHAPTER 4
Environmental Impacts Program

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APPENDIX 4-A. STAFF QUALIFICATIONS
Environmental Impacts Program

Name	Position	Highest Degree	Major	Year Received	Institution
Bain, Mark B.	Fisheries Biologist	Ph.D.	Fisheries Biology	1985	University of Massachusetts
Hoffecker, John F.	Archeologist	M.A.	Anthropology	1979	University of Alaska-Fairbanks
Irving, John S.	Fisheries Biologist	M.S.	Fisheries Biology	1979	University of Idaho
Kruger, Richard L.	Fisheries Biologist	M.S.	Aquatic Ecology	1972	University of California-Davis
LaGory, Kirk E.	Wildlife Ecologist	Ph.D.	Zoology	1984	Miami University
Ness, Darwin D.	Terrestrial Ecologist	Ph.D.	Forestry	1971	University of Minnesota
Olsen, Richard D.	Biologist	Ph.D.	Botany/Micro-biology	1974	Arizona State University
Olshansky, S. Jay	Sociologist	Ph.D.	Sociology	1984	University of Chicago
O'Neil, Thomas A.	Wildlife Ecologist	M.S.	Wildlife Biology	1981	University of Montana
Payne, Barbara A.*	Sociologist	Ph.D.	Sociology	1977	Stanford University
Soholt, Lars F.*	Ecologist	Ph.D.	Biology	1971	University of Southern California
Stull, Elisabeth A.	Aquatic Ecologist	Ph.D.	Zoology	1972	University of California-Davis
Sundell, Ronald C.	Planner	M.U.P.	Urban and Regional Planning	1978	University of Illinois
Tobin, Roger L.*	Operations Research Analyst	Ph.D.	Industrial Engineering	1973	University of Michigan
Williams, R. Gary	Sociologist	Ph.D.	Sociology	1981	Colorado State University
Witmer, Gary W.	Wildlife Ecologist	Ph.D.	Wildlife Sciences	1981	Oregon State University
Yin, Stephen	Hydrologist	M.S.	Hydrology/Water Resources	1970	University of Illinois

*No longer a member of the Division.

APPENDIX 4-B. OUTSTANDING PROFESSIONAL ACTIVITIES AND AWARDS
Environmental Impacts Program

MARK BAIN--received Honorable Mention recognition for a paper presented at the 46th Midwest Fish and Wildlife Conference (Effects of daily flow fluctuations on stream fish communities); received a Best Paper Award for a paper presented at the 1985 Annual Meeting of the Indiana Chapter of the American Fisheries Society (Quantitative field methods for stream habitat assessment and inventory).

APPENDIX 4-C. SPECIAL EVENTS ORGANIZED
Environmental Impacts Program

1984

R.L. TOBIN chaired session entitled "Spatial Price Equilibrium: Advances in Theory, Computation and Application I" at Thirty-first North American Meetings, Regional Science Association, 9-11 November 1984, Denver, CO.

1985

J.F. HOFFECKER co-organizer of ANL Social Sciences Luncheon Seminar series, 1985, Argonne National Laboratory.

J.S. IRVING organized Fisheries Technical Session of the Snohomish River Basin Resource Sort Workshop, 16-18 September 1985, Olympia, Washington.

J.S. IRVING organized Introductory and Fisheries Technical Sessions of the Salmon River Basin Resource Sort Workshop, 21-23 October 1985, Boise, Idaho.

J.S. IRVING organized Fisheries Technical Sessions of the Snohomish River Basin Matrix Technical Workshop, 3-5 December 1985, Olympia, Washington.

E.A. STULL organized Environmental Research Division Ecology Seminar (Speaker: J.P. Schubert, Argonne National Laboratory; Title: Impacts of gas pipeline construction on streams), 20 June 1985, Argonne National Laboratory.

E.A. STULL organized Environmental Research Division Ecology Seminar (Speaker: Chris Frenzen, Southern Methodist University; Title: A cell kinetics justification for the Gompertz equation), 13 June 1985, Argonne National Laboratory.

E.A. STULL organized Environmental Research Division Ecology Seminar (Speaker: John T. Finn, University of Massachusetts; Title: Use of Markov Chains in Land Use Analysis Trends), 23 July 1985, Argonne National Laboratory.

- G.W. WITMER organized Introductory and Wildlife Technical Sessions of the Snohomish River Basin Resource Sort Workshop, 16-18 September 1985, Olympia, Washington.
- G.W. WITMER organized Wildlife Technical Session of the Salmon River Basin Resource Sort Workshop, 21-23 October 1985, Boise, Idaho.
- G.W. WITMER organized Introductory and Wildlife Technical Sessions of the Snohomish River Basin Matrix Technical Workshop, 3-5 December 1985, Olympia, Washington.

APPENDIX 4-D. EDUCATIONAL PROGRAM PARTICIPANTS
Environmental Impacts Program

SUSAN E. GRESENS. University of Chicago. Thesis Parts Program. Conducted field research related to ecological community theory. June 1985 - Present.

JUDITH K. HASCHENBERGER. University of Southern Illinois and Arizona State University. Summer Research Participant. Developed geographic information systems for river basin planning. June - August 1984, June - August 1985.

LETICIA ARIAS. Joliet Junior College. Student Aide. Assisted with geographic information systems. June 1985 - Present.

MARK R. HOPF. Joliet Junior College. Student Aide. Assisted with geographic information systems. June 1985 - Present.

JOHN J. MIKLIC. Joliet Junior College. Student Aide. Assisted with geographic information systems. June 1985 - present.

JOHN M. PIRC. Lewis University. Student Aide. Assisted with geographic information systems. June 1985 - present.

APPENDIX 4-E. PUBLICATIONS AND ORAL PRESENTATIONS 1984-1985
Environmental Impacts Program

1. Refereed Journal Articles*

1984

Friesz, T.L., P.T. Harker and R.L. Tobin. Alternative algorithms for the general network spatial price equilibrium problem. Journal of Regional Science 24(4):475-507 (1984). [DOE/ERA]**

1985

Bain, M.B., J.T. Finn and H.E. Booke. A quantitative method for sampling riverine microhabitats by electrofishing. North American Journal of Fisheries Management 5:489-493 (1985).

Friesz, T.L., P.A. Viton and R.L. Tobin. Economic and computational aspects of freight network equilibrium models: a synthesis. Journal of Regional Science 25(1):29-49 (1985). [DOE/ERA]

Witmer, G.W. and D.S. de Calesta. Effects of forest roads on habitat use by Roosevelt Elk. Northwest Science 59:122-125 (1985).

2. Books, Book Chapters, and Collections of
Conference Proceedings

1984

Barchas, P.R., W.S. Jose, II, B.A. Payne and W.A. Harris. An attention-regulating function of social hierarchies: High status, attention, and the CNV brain wave. Chapter 7 In: Barchas, P.R. (ed.), Social Hierarchies. Essays Toward a Sociophysiological Perspective. Greenwood Press, Westport, CT. 1984. pp. 133-146.

*For published material, the names of all Environmental Research Division authors are underlined. (Included are Division members who participated in a project but left the Division before the results were published.)

**Funding agency (abbreviations are spelled out at the end of this appendix). In cases where no funding agency is listed, the publication was not related to any specific funded project.

1985

Witmer, G.W., M. Wisdom, E.P. Harshman, et al. 1985. Deer and elk. Chapter 11 In: Management of Wildlife and Fish Habitats in Forests of Western Oregon and Washington. Publication No. Rb-F&WL-192-183. U.S. Department of Agriculture, Forest Service, Pacific Northwest Region, Portland, OR. pp. 231-258.

3. Reports

1984

Draft Environmental Impact Statement, Susitna Hydroelectric Project, FERC No. 7114 - Alaska. FERC/DEIS-0038. Federal Energy Regulatory Commission, Office of Electric Power Regulation. 7 Vols. May 1984. [FERC/EPR]

Environmental Assessment, Three-City Mississippi River Hydropower Project, FERC No. 4154-001--Iowa/Wisconsin. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1984. [FERC/Hydropower Licensing]

Final Environmental Impact Statement, New England/Hydro-Quebec ±450-kV Direct Current Transmission Line Interconnection. DOE/FEIS-013. U.S. Department of Energy. 1984. [DOE/ERA]

Freight Network Modeling System. Vol. I: Freight Network Equilibrium Model -- Theory and Validation. Technical Memorandum ANL/ER-TM-84-1 (Vol. I). Environmental Research Division, Argonne National Laboratory. 1984. [DOE/ERA]

Freight Network Modeling System. Vol. II: Freight Network Equilibrium Model -- Version 4.1 User's Guide and Programmer's Guide. Technical Memorandum ANL/ER-TM-84-1 (Vol. II). Environmental Research Division, Argonne National Laboratory. 1984. [DOE/ERA]

Freight Network Modeling System. Vol. III: Freight Network Equilibrium Model--Version 4.1 Preprocessors User's Guide. Technical Memorandum ANL/ER-TM-84-1 (Vol. III). Environmental Research Division, Argonne National Laboratory. 1984. [DOE/ERA]

Freight Network Modeling System. Vol. V: Flexible Network Definition Software User's Guide. Technical Memorandum ANL/ER-TM-84-1 (Vol. V). Environmental Research Division, Argonne National Laboratory. 1984. [DOE/ERA]

1985

Cluster Impact Assessment Procedures: Geographic Scoping Document for the Snohomish River Basin. Docket No. EL 85-19-101. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

Cluster Impact Assessment Procedure, Geographic Scoping Phase: Environmental Assessment for the Salmon River Basin. Docket No. EL-85-19-103. Prepared for the Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

Cluster Impact Assessment Procedure, Resource Sort Phase. Environmental Assessment for the Salmon River Basin. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

Dettmann, E.H. and R.D. Olsen. Assessment of Existing Water Quality in the Tongue River, Wyoming, and Effects of Coal Mining. Technical Memorandum ANL/ER-TM-85-1. Environmental Research Division, Argonne National Laboratory. December 1985.

Freight Network Modeling System. Volume IV: Shortest-Path Analysis and Display User's Guide. Technical Memorandum ANL/ER-TM-84-1 (Vol. IV). Environmental Research Division, Argonne National Laboratory. 1985. [DOE/ERA]

Freight Network Modeling System. Volume VI: Rate Simulation Software User's Guide. Technical Memorandum ANL/ER-TM-84-1 (Vol. VI). Environmental Research Division, Argonne National Laboratory. 1985. [DOE/ERA]

Gilson, L.N., M. McCracken, J.G. Petot and E.A. Stull. Analysis of building site possibilities in the Gothic Township area. Special technical report submitted to Rocky Mountain Biological Laboratory, Gothic, CO. 1985.

Hamma Hamma Hydroelectric Project, FERC No. 3178, Washington, Draft Environmental Impact Statement. FERC/DEIS-0040. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

Hoffecker, J.F. The Moose Creek site. In: North Alaska Range Early Man Project. National Geographic Society Research Reports 19:33-48 (1985).

Hoffecker, J.F. Archeological research 1980. In: North Alaska Range Early Man Project. National Geographic Society Research Reports 19:48-59 (1985).

Lee Creek Water Power Project, FERC No. 5251, Scoping Document I. Prepared for Federal Energy Regulatory Commission, Washington, DC. 1985. [FERC]

Lee Creek Water Power Project, FERC No. 5251, Scoping Document II. Prepared for Federal Energy Regulatory Commission, Washington, DC. 1985. [FERC]

Matrix Technical Session Document: Phase III of the Cluster Impact Assessment Procedure for the Snohomish River Basin. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

New England Transmission Line Interconnection--Phase II: Implementation Plan for Environmental Impact Statement. Docket No. PP-76A. Prepared for U.S. Department of Energy, Washington, DC. 1985. [DOE/ERA]

Powers, W.R. and J.F. Hoffecker. Nenana Valley Cultural Resources Survey 1984. Final Report to Alaska Department of Natural Resources. 1985.

Resource Sort Workshop: Summary Report. Phase II of the Cluster Impact Assessment Procedure for the Snohomish River Basin. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, D.C. 1985. [FERC/Hydropower Licensing]

Resource Sort Workshop Document: Phase II of the Cluster Impact Assessment Procedure for the Salmon River Basin, Idaho. Prepared for Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

Resource Sort Workshop Document: Phase II of the Cluster Impact Assessment Procedure for the Snohomish River Basin. Prepared for the Federal Energy Regulatory Commission, Office of Hydropower Licensing, Washington, DC. 1985. [FERC/Hydropower Licensing]

4. Published Conference Papers

1984

Pomkamp, D.H., B.A. Payne and A.R. Valentino. Modification, adaptation, and prevention (MAP): A task of the DOE Carbon Dioxide Research Program. In: C.W. Bullard and P.J. Womeldorff (eds.), Trends in Electric Utility Research, proceedings of a conference organized by the Midwest Universities Energy Consortium, 3 April 1984, Chicago, IL. Pergamon Press, NY. pp. 421-428. [DOE]

Tobin, R.L. A network programming system for studying coal transportation. In: B. Lev, J.A. Bloom, F.H. Murphy and A.S. Gleit (eds.), Analytic Techniques for Energy Planning (Proceedings of the First Symposium, Operations Research Society of America, 7-8 June 1983, Washington, DC) (1984). pp. 21-32. [DOE/ERA]

1985

Paquet, P.J. and G.W. Witmer. Cumulative impacts of small hydropower developments: an overview of the issues. In: Proceedings of the Symposium on Small Hydropower and Fisheries (sponsored by the American Fisheries Society, 1-3 May 1985, Aurora, CO). 1985. pp. 343-345. [DOE/BPA, FERC]

Williams, G. Achieving aggressive mitigation through state regulation: a case of the Wyoming Industrial Development Information and Siting Act. In: Issues in Social Impact Analysis: Interagency Symposium Proceedings. Proceedings of a symposium held 22-25 August 1984, College Station, TX. U.S. Department of Agriculture, Forest Service. 1984. pp. 53-57.

5. Published Abstracts, Notes, Reviews, Comments, and Letters

1984

Hoffecker, J.F. Northeast Asian Upper Paleolithic chronology re-examined (Abstract). In: Preprint Volume, 11th Annual Meeting, Alaska Anthropological Association, 16-17 March 1984, Fairbanks, AK. p. 13. [FERC]

1985

Bain, M.B., J.T. Finn and H.E. Booke. Quantifying stream substrate for habitat analysis studies. In Management Briefs Section, North American Journal of Fisheries Management 5:499-506 (1985).

Hoffecker, J.F. Comment on Dolitskiy (Siberian Paleolithic Archaeology: Approaches and Analytic Methods). Current Anthropology 26(3):371 (1985).

Tobin, R.L. A solution method for competitive equilibrium freight network design (Abstract). Volume of Abstracts for papers presented at Joint National Meeting, The Institute of Management Sciences and the Operations Research Society of America, 29 April - 1 May 1985, Boston, MA. pp. 191-192. [DOE/ERA]

6. Oral Presentations*

1984

Bomkamp, D.H., B.A. Payne and A.R. Valentino. Modifications, adaptation, and prevention (MAP): A task of the DOE Carbon Dioxide Research Program. Presented at Conference on Trends in Electric Utility Research, Midwest Universities Energy Consortium, U.S. DOE, and EPRI, 3 April 1984, Chicago, IL. [Scientists]** [DOE]

Hoffecker, J.F. Northeast Asian Upper Paleolithic chronology re-examined. Presented at the 11th Annual Meeting of the Alaska Anthropological Association, 16-17 March 1984, Fairbanks, AK. [Professional anthropologists and students] [FERC]

*For oral presentations, the person who made the presentation is underlined.

**Audience for the presentation.

Tobin, R.L. A predictive freight transportation model for studying coal transportation. Presented at the General Engineering Design Seminar Series, April 1984, University of Illinois, Urbana, IL. [Faculty, graduate students] [DOE/ERA]

Tobin, R.L. Sensitivity analysis for variational inequalities. Presented at Joint TIMS/ORSA National Meeting, May 1984, San Francisco, CA. [Scientists] [DOE/ERA]

Tobin, R.L. and T.L. Friesz. Spatial competition facility location models: Definition, formulation and solution approach. Presented at ISOLDE III - International Symposium on Location Decisions, Boston University and Massachusetts Institute of Technology, 7-12 June 1984, Boston, MA. [Scientists, professionals] [DOE/ERA]

Tobin, R.L. The freight network equilibrium model revisited: the freight network modeling system. Presented at Coal Transportation Costing and Modeling Seminar, U.S. Department of Energy and Electric Power Research Institute, 15 October 1984, Kansas City, MO. [Utility transportation specialists] [DOE/ERA]

Tobin, R.L. Sensitivity analysis for spatial price equilibria. Presented at Thirty-first North American Meetings, Regional Science Association, 9-11 November 1984, Denver, CO. [Scientists] [DOE/ERA]

Tobin, R.L. Spatially competitive location models. Presented at Thirty-first North American Meetings, Regional Science Association, 9-11 November 1984, Denver, CO. [Scientists] [DOE/ERA]

Tobin, R.L. Impacts of utility coal conversions on the Northeast region. Presented at Joint National Meeting, The Institute of Management Sciences and the Operation Research Society of America, 26-28 November 1984, Dallas, TX. [Scientists] [DOE/ERA]

Williams, G. Achieving aggressive mitigation through state regulations: A case of the Wyoming Industrial Development Information and Siting Act. Presented at Annual Meeting of the Rural Sociological Society, 22-25 August 1984, College Station, TX. [Scientists]

1985

Bain, M.B. Fish communities in rivers with natural and modified daily flow regimes: Consequences of hydroelectric development. Presented at Environmental Research Division Seminar, 16 January 1985, Argonne National Laboratory. [Division staff]

Bain, M.B. A matrix analysis method for assessing cumulative impacts from multiple hydroelectric projects. Presented at Federal Energy Regulatory Commission meeting, 3 October 1985, Washington, DC. [Program administrators] [FERC/Hydropower Licensing]

- Bain, M.B. A matrix analysis method for assessing cumulative impacts from multiple hydroelectric projects. Presented at Salmon River Resource Workshop, 21 October 1985, Boise, ID. [Scientists, agency administrators] [FERC/Hydropower Licensing]
- Stull, E.A. Cumulative effects of hydropower development. Presented at Hydropower Conference, U.S. Environmental Protection Agency, 5 September 1985, Harper's Ferry, WV. [Scientists, Program Managers] [FERC, DOE/BPA]
- Stull, E.A. Cumulative effects of hydroelectric development. Presented at Small Hydro Workshop, U.S. Environmental Protection Agency, Region V, 7 October 1985, Chicago, IL. [Scientists, agency administrators] [DOE/BPA]
- Tobin, R.L. A predictive freight transportation model and extensions. Presented at Civil Engineering and Transportation Center Seminar, Northwestern University, 22 February 1985, Evanston, IL. [Faculty, students] [DOE/ERA]
- Tobin, R.L. A solution method for competitive equilibrium freight network design. Presented at Joint National Meeting, The Institute of Management Sciences and the Operation Research Society of America, 29 April-1 May 1985, Boston, MA. [Scientists] [DOE/ERA].
- Tobin, R.L. Assessment of regional impacts of increased freight transportation. Presented at Conference on Methods and Experiences in Impact Assessment, International Association for Impact Assessment, 27-28 June 1985, State University of Utrecht, Utrecht, The Netherlands. [Scientists] [DOE/ERA]
- Witmer, G.W. Assessing cumulative impacts of hydroelectric development. Presented at Second Biennial Symposium, Thorne Ecological Institute, 4-6 February 1985, Glenwood Springs, CO. [Scientists] [FERC]
- Witmer, G.W. Sympatric predators: bobcats and coyotes. Presented at Environmental Research Division Ecology Seminar, 16 May 1985, Argonne National Laboratory. [Division staff]
- Witmer, G.W. Assessing cumulative impacts to wetlands. Presented at National Wetland Assessment Symposium, 17-20 June 1985, Portland, ME. [Scientists, agency administrators] [DOE/BPA, FERC]
- Witmer, G.W. What are cumulative impacts all about? Presented at Conference on Managing Cumulative Effects in Florida Wetlands, University of Florida, 18-19 October 1985, Sarasota, FL. [Scientists, agency administrators] [DOE/BPA, FERC]

CODES FOR FUNDING AGENCIES

BPA = Bonneville Power Administration (in DOE)
 DOE = U.S. Department of Energy
 ERA = Economic Regulatory Administration (in DOE)
 FERC = Federal Energy Regulatory Commission

CHAPTER 5. FUNDAMENTAL MOLECULAR PHYSICS AND CHEMISTRY

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P.M. Dehmer

M.A. Dillon

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S.T. Pratt

D. Spence

Title

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Senior Physicist

Senior Chemist

Physicist

Physicist

Chemist

Physicist

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Boston, Massachusetts

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S.T. Manson, Department of Physics and Astronomy, Georgia State University,
Atlanta, Georgia

A.C. Parr, National Bureau of Standards, Gaithersburg, MD

J. Seger, Undergraduate Research Participant, Grinnell College, Grinnell, Iowa

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University of Science & Technology, Chengdu, Sichuan, People's Republic of
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5.1 PROGRAM OVERVIEW

Mitio Inokuti, Program Manager

The research of the Fundamental Molecular Physics and Chemistry Program deals with the properties of molecules related to their interactions with photons, electrons, and other charged particles. Specifically, we deal with photons ranging from the visible region to the far vacuum violet region, and with electrons of energies ranging from several electron volts to hundreds of electron volts. From this broad area of research we choose those topics of study that meet some of the needs of the agencies that support our work--primarily the Office of Health and Environmental Research (U.S. Department of Energy) and secondarily the Office of Naval Research (U.S. Department of Defense) and National Bureau of Standards (U.S. Department of Commerce).

A major thrust of our research is to provide certain fundamental data needed in radiation research. For example, we attempt to determine cross sections for the interactions of electrons and photons with molecules. Such data are indispensable as input to the microscopic analysis of the physical stage of radiation actions on any matter, including the biological cell and its constituents. The same data are also required in theoretical dosimetry. Another thrust of the Fundamental Molecular Physics and Chemistry Program is to develop methods for detecting and characterizing molecular species, including excited states, radicals, and other unstable species. To this end, resonance-enhanced multiphoton ionization spectroscopy is being developed to elucidate dynamics of electronic-excited states. This technique is important in advanced measurement science because of its high sensitivity and selectivity of the species analyzed.

The following reports on our research work are classified into four general areas: theoretical studies in radiation physics and chemistry (Section 5.2), electron collision studies (Section 5.3), photophysics studies in the vacuum ultraviolet (Section 5.4), and photophysics studies with multiphoton resonant absorption (Section 5.5).

5.2. THEORETICAL STUDIES IN RADIATION PHYSICS AND CHEMISTRY

5.2.1. Summary

We conduct theoretical studies on elementary processes that occur in molecular substances subjected to ionizing radiations. These studies concern two general areas: (1) the cross-sections data for collision processes, and (2) applications of these data to the analysis of the initial stage of radiation actions.

In the first area, one may deal with a large variety of collision processes involving a variety of incident particles. However, electrons are the most important because they appear abundantly as secondary particles in matter upon the incidence of any ionizing radiation. Photons in the far ultraviolet and soft x-ray regions are also important because they interact

most strongly with any matter and because there is a close relation between the photoabsorption and inelastic collisions of fast charged particles. Thus, our work on the cross-section data concerns electrons, other fast charged particles, and far-ultraviolet photons.

In the second area, we concentrate on the theory of the yields of initial molecular species such as ions and excited states under ionizing radiation. The work in this area starts with the knowledge of relevant cross-section data and involves an analysis of the consequences of many collision processes on both matter and all the electrons and other charged particles generated in matter.

In both of the areas, we have made considerable progress as seen in the following sections. Most of the reports represent summaries of articles scheduled for publication in the literature.

5.2.2. Theory of Initial Yields of Ions Generated by Electrons in Binary Mixtures

M. Inokuti and E. Eggarter

[Summary of a paper to appear in Journal of Chemical Physics]

When charged particles pass through matter, they interact with atoms and molecules in the medium. As a result of inelastic collisions, excited states, ions, and electrons appear. These are called initial products, and they lead to chemical and biological effects through a sequence of reactions. For practically all applications of interest to chemistry and biology, the matter consists of a mixture or chemically impure substance.

The analysis of the initial yield of ions generated by electrons is the most fundamental subject in radiation physics, because for any ionizing radiation much of the absorbed energy is delivered to molecules by energetic electrons. The analysis for pure substances has been carried out in many examples and from various angles, such as analytic treatments by use of the Fowler equation and the Spencer-Fano equation or Monte Carlo simulations (Inokuti 1983). The present work is the first rigorous and analytic study of ionization yield in a gas mixture over the complete range of composition. The purpose is to clarify the dependence of the yield upon composition and thus to contribute to the understanding of the general problem of radiation-energy partition among components of a mixture.

The total number $N(T)$ of ions generated in a mixture upon complete degradation of an electron of initial energy T and its all secondaries obeys a Fowler equation. The equation has coefficients that depend on electron-collision cross sections of component molecules A and B and on their number fractions C_A and C_B ($C_A + C_B = 1$). It is customary to express the result in terms of the average energy per ion pair $W(T) = T/N(T)$. It is also possible to write a Fowler equation for the number $N^A(T)$ of ions of component A , or for the number $N^B(T)$ of ions of component B (Inokuti 1983). Evidently, $N^A(T) + N^B(T) = N(T)$.

Numerical solutions of those Fowler equations were carried out specifically for the mixture of H_2 and Ar. This mixture was chosen for two reasons. First, a complete set of cross sections for each component is available from earlier work (Eggarter 1975; Gerhart 1975; Douthat 1979). Second, in this mixture there is apparently no appreciable energy transfer among initial products, and therefore it is justified to compare results of the $N(T)$ calculation with experiments (Bortner and Hurst 1954; Hurst and Strickler 1960; Strickler 1963). Figure 5.1 shows the comparison. The solid curve represents the $W(T)$ value as a function of the H_2 fraction, C , calculated for electrons of $T = 2000$ eV, which may be considered as effectively representing the high-energy limit. The crosses show experimental results with alpha particles (Hurst and Strickler 1960). In light of the qualifications that may be necessary because of different particles, the agreement is excellent.

Figure 5.2 shows the number N^{H_2} of H_2 ions (represented by the dotted curve), the number $N^{Ar}(T)$ of Ar ions (represented by the chained curve), and the total number $N(T)$ (represented by the solid curve), as functions of the H_2 fraction, C , calculated at $T = 2000$ eV.

It has been found that the results of Figure 5.2 show a remarkable regularity. That is to say, the ratio $r_N = N^{Ar}(T)/N^{H_2}(T)$ is closely linear to the concentration ratio $r_C = C^{Ar}/C^{H_2}$ over its complete range, as seen in Figure 5.3.

This finding can be interpreted in the following way (Eggarter and Inokuti unpublished data). Suppose that $y(T, T')dT'$ represents the Spencer-Fano degradation spectrum for electrons in a mixture resulting from the source electron flux of unit intensity and of initial energy T . Obviously, $y(T, T')dT'$ depends upon the mixture composition. We may write the number $N^A(T)$ of A ions as:

$$N^A(T) = n^A \int_0^T dT' y(T, T') \sigma_i^A(T'), \quad (5-1)$$

where n^A is the number density of A molecules and $\sigma_i^A(T')$ is the ionization cross section of an A molecule at electron energy T' . Similarly, we may write the number $N^B(T)$ of B ions as:

$$N^B(T) = n^B \int_0^T dT' y(T, T') \sigma_i^B(T'), \quad (5-2)$$

Figure 5.1. The dependence of $W(T)$ on the composition in the Ar - H_2 mixture. The symbol C represents the number fraction of H_2 .

Figure 5.2. Yields of individual ion species in the Ar - H_2 mixture at $T = 2000$ eV. The dotted curve shows $N^{H_2}(T)$, the chained curve $N^{Ar}(T)$, and the solid curve the sum $N(T)$.

Figure 5.3. The ratio of the ion yields plotted against the concentration ratio.

where n^B is the number density of B molecules and $\sigma_i^B(T')$ is the ionization cross section of a B molecule at electron energy T' . The lower limits of the integration are shown as zero for convenience; the integration extends down to the first ionization threshold, I^A or I^B .

We take the ratio of Equations 5-1 and 5-2 and note that $n^A/n^B = c^A/c^B$. Then:

$$\frac{N^A(T)}{N^B(T)} = \frac{c^A}{c^B} \frac{\int_0^T dT' y(T, T') \sigma_i^A(T')}{\int_0^T dT' y(T, T') \sigma_i^B(T')} \quad (5-3)$$

According to the Cauchy's generalized mean value theorem (Hardy 1955), there is a value T_m of electron energy such that the ratio of the two integrals may be equated to the ratio of the integrands; then:

$$\frac{N^A(T)}{N^B(T)} = \frac{c^A}{c^B} \frac{\sigma_i^A(T_m)}{\sigma_i^B(T_m)} \quad (5-4)$$

The precise value of T_m is unknown unless one knows (T, T') . However, if $\sigma_i^A(T)/\sigma_i^B(T)$ is slowly varying over a wide range, one can evaluate Equation 5-4 without knowing the precise value of T_m . For the Ar - H₂ mixture, it turns out that the ratio of the ionization cross sections $\sigma_i^{Ar}(T)/\sigma_i^{H_2}(T)$ is indeed close to a constant. According to the data actually used in the Fowler equation calculation, the ratio starts with 3.2 at $T = 20$ eV, increases to 4.0 around $T = 100$ eV, and stays at 3.8-3.9 at higher energies. It is reasonable to expect that T_m should fall somewhere between a few hundred eV and 2000 eV, and therefore one is led to the estimate:

$$\frac{N^{Ar}(T)}{N^{H_2}(T)} = 3.8 \frac{c^{Ar}}{c^{H_2}}, \quad (5-5)$$

which is in excellent agreement with the result of Figure 5.3.

It turns out that the ratio of the ionization cross sections is especially slow-varying in electron energy for the Ar - H₂ case. For other combinations of other molecules, the ratio is often more strongly dependent on electron energy, and thus one expects that the linearity of the ratio of ion numbers in the concentration ratio may not be as close as in Figure 5.3. Nevertheless, some similarity to the linearity is to be found in general. Further study about this is in progress.

5.2.3. Analytic Representation of the Dipole Oscillator-Strength Distribution

M.A. Dillon and M. Inokuti

[Abstract of a paper published in Journal of Chemical Physics 82:4415-4425 (1985)]

In this study, we addressed the question of what analytic formula is the most suitable for fitting the dipole oscillator-strength distribution $df/d\epsilon$ over a wide range of the kinetic energy ϵ of an electron ejected from an atom or molecule. A suitable expression will enable one to interpolate or extrapolate data reliably and to use them readily in applications such as the modeling studies in radiation physics. It is useful to distinguish two factors that together constitute $df/d\epsilon$. The first factor is defined in terms of the dipole matrix element with respect to a final-state eigenfunction whose amplitude near the origin is independent of ϵ . As we showed earlier (Dillon and Inokuti 1981), this factor is analytic at all finite ϵ except at a singularity at $\epsilon = -I$, where I is the ionization threshold energy.

The other factor arises from the energy-scale normalization of the final-state eigenfunction, and is the object of the present discussion from several angles. First, we present a survey of numerical data for the s, p, and d states, with $0 \leq \epsilon \leq 5$ a.u. for all atoms with $Z \leq 38$, evaluated within the Hartree-Slater potential model. Next, we discuss analytic properties of the normalization factor, which include its relation to the phase shift, and its behavior near a resonance. We also elucidate the connection of the continuum normalization with the bound-state normalization. Finally, we illustrate the significance of our findings in the practical fitting of the $df/d\epsilon$ data in the presence of a resonance, taking the valence-shell ionization of Ar as an example.

5.2.4. Analytic Representation of the Generalized Oscillator Strength for Ionization

*M.A. Dillon, M. Inokuti, and Z.-W. Wang**

[Summary of a paper published in Radiation Research 102:151-164 (1985)]

The energy distribution of secondary electrons resulting from ionizing collisions of fast charged particles with an atom or molecule is an indispensable piece of input datum for the microscopic modeling of radiation actions. In the Bethe theory (Inokuti 1971), the energy distribution is determined from a more basic quantity, viz., the generalized oscillator strength for ionization.

We have examined analytic properties of the generalized oscillator strength $df(K, \epsilon)/d\epsilon$ for ionization from a fixed subshell as a function of the momentum transfer K and of the momentum k (or the kinetic energy $\epsilon = k^2/2$) of

*Collaborator; affiliation is listed at the front of this chapter.

an ejected electron, where all quantities are measured in atomic units. For fixed ϵ , $df(K, \epsilon)/d\epsilon$ is analytic on the complex K^2 plane at those points where

$$\Delta = [(K - k)^2 + 2I][(K + k)^2 + 2I] \quad (5-6)$$

vanishes, I being the ionization threshold energy of the subshell measured in atomic units.

On the basis of this observation and others, we show that a suitable expression for fitting the data is of the form:

$$df(k, \epsilon)/d\epsilon = \Delta^{-p} \sum_{n=0}^N A_n(\epsilon) K^{2n}, \quad (5-7)$$

where p is an integer or a half integer and $A_n(\epsilon)$ are coefficients that depend upon ϵ . The denominator power p is related to the degree N of the polynomial in K^2 so that the decline at large K^2 is consistent with the known asymptotic behavior, which depends upon the symmetry of the initial and final states involved. Through several examples we have demonstrated the use of Equation 5-7 in fitting data. Our expression applies both to atoms and molecules and provides a compact parametrization of data. This allows dependable interpolation and extrapolation and is useful for many applications, such as stopping-power evaluation and electron-degradation analysis in radiation physics. In particular, our results lead to an analytic representation of secondary-electron spectra.

5.2.5. Mean Excitation Energy for the Stopping Power of Metallic Aluminum

H. Bichsel, M. Inokuti, and D.Y. Smith**

[Abstract of a paper to appear in Physical Review A]

McGuire (1983a) suggested that the mean excitation energy I for the stopping power of metallic aluminum should be in the range of 145-150 eV, as opposed to the currently recommended value of about 166 eV (International Commission on Radiation Units and Measurements [ICRU] 1984). We have re-examined all pertinent information from two independent classes of data sources, i.e., the measurements of proton stopping power and the semi-empirical determination of the dielectric-response function over the entire spectral range (Shiles et al. 1980; Smith et al. 1985). Our conclusion is that the value of 116 eV is essentially correct. Moreover, we point out a number of deficiencies in McGuire's arguments. Some of our remarks concern the values of inner-shell corrections to the Bethe stopping-power formula as evaluated by McGuire (1983b).

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5.2.6. Cross Sections for Inelastic Collisions of Fast Charged Particles with Atoms and Molecules -- Data Needed in Radiotherapy and Radiobiology

M. Inokuti

[Summary of an invited paper presented at the International Atomic Energy Agency Advisory Group Meeting on Nuclear and Atomic Data for Radiotherapy and Radiobiology, Rijswijk, The Netherlands, 16-20 September 1985. Full text to appear in an IAEA Report.]

A large volume of data of the cross sections named in the title is required for solving problems of radiological physics and dosimetry, as well as for detailed analysis of the earliest stage of radiation actions on matter (including the biological cell and substances constituting it).

Despite the long history of research, the current experimental data of the cross sections are far from being complete or even satisfactory for tentative applications. Calculations from first principles are difficult in general and lead to reliable results only in exceptional situations. Thus, one practical approach to the cross-section determination is to test experimental data with general criteria. This is possible because cross sections for various processes are related among themselves and with many other properties of atoms and molecules. For example, the Bethe theory indicates a close connection between photoabsorption and energy absorption by glancing collisions, and puts many other useful constraints on the cross-section data.

Development and use of these data constraints, first put forth by Platzman, can now be demonstrated in many examples. More recent studies concern the determination of the analytic expression most suitable for fitting the data on the oscillator-strength distribution or the energy distribution of secondary electrons from ionizing collisions of charged particles. There are three areas to which major efforts should be directed. First, methods of absolute cross-section measurements both for electron and ionic collisions must be thoroughly reviewed so that sources of systematic errors may be identified and corrected. Second, efforts should be devoted to the understanding of the data systematics, viz., the trends of cross sections for a series of molecules. This is especially important because the variety of molecules relevant to radiological physics and radiation biology is so enormous that even the data presentation for each molecule will be impractical. Finally, electron and ionic collisions with molecules in condensed phases will be an important topic of study for years to come; initial reports on efforts toward this direction are encouraging.

5.2.7. VUV Absorption and Its Relation to the Effects of Ionizing Corpuscular Radiation

M. Inokuti

[Summary of an invited paper presented at the U.S.-Japan Joint Seminar on Ultraviolet Photobiology and Spectroscopy Using Synchrotron Radiation, Brookhaven National Laboratory, 2-5 October 1985]

There is a close relation between the photoabsorption (especially in the VUV region) and the energy transfer from glancing collisions of fast charged particles, first pointed out by Fermi (1924) and clarified in detail by Bethe (1930). This subject is fundamental for the understanding of the relation between photobiology and radiation biology. Among the key notions discussed there were oscillator-strength spectra, quantum yields for specific products, and action spectra. In particular, emphasis was placed on the importance of complete oscillator-strength spectra over the entire energy domain. A survey of relevant data was given, and areas of data deficiency were identified. These areas include quantum yields and action spectra for specific effects, such as the inactivation, single-strand breaks, double-strand breaks, or chemical alterations in a base or sugar in DNA. Significant advances in these areas were reported at the seminar by groups from Japan. Other topics of the lecture included special effects of inner-shell ionization leading to the Coulomb explosion and other violent consequences, as well as the role of soft x-rays in radiation biology. Finally, it was pointed out that current measurements of the action spectra of biomolecules probably need improvement in dosimetry; in particular, the spatial distribution of the energy absorption from photons should be fully taken into account.

5.2.8. X-Ray Scattering and Electron Mobility in the Liquid Isomers of Pentane

*J.A. Stephens**

[Abstract of a paper to appear in Journal of Chemical Physics]

Total coherent x-ray scattering cross sections were investigated for liquid neopentane, isopentane, and n-pentane at room temperature. An observed relative shift and broadening in the primary diffraction peak indicated substantially shorter-range intermolecular correlations in iso- and n-pentane than in neopentane. The possible implications of this result for relative variations of thermal electron mobilities in these liquids are discussed. A full report of the work is being published.

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5.2.9. Spectral and Electron-Collision Properties of Atomic Ions

C.E. Theodosiou, S.T. Manson,* and M. Inokuti*

[Abstract of a paper to appear in Physical Review A]

Threshold phase shifts (or equivalently, quantum defects at the series limits) are calculated within the framework of the Hartree-Slater central-field approximation for all positive atomic ions with nuclear charge $Z \leq 50$. The results are displayed in the isoelectronic picture (in which the number N of electron is kept constant), in the isonuclear picture (in which Z is kept constant), and in the isoionic picture (in which $Z - N$ is kept constant). The systematics of the threshold phase shifts are delineated, and the merits of each of these pictures has been clarified. We have also identified the possibilities and pitfalls of interpolation in generating new data. The present work is an initial report of a series of systematic studies of atomic-ion properties. Numerical data are to be published.

5.3. ELECTRON COLLISION STUDIES

5.3.1. Summary

The interaction of ionizing radiation with matter first generates secondary electrons. These secondary electrons degrade in energy through elastic and inelastic collisions and act as carriers of energy, subsequently producing a large variety of reactive species (often called initial products) which start a chain of chemical reactions that eventually lead to the net radiation effects, including biological changes. Thus, the measurement of the specific energy transferred per collision between electrons and molecules (or atoms), together with the probability of such energy transfer per collisions, is of prime importance for studies of the effects of energy deposition in matter by ionizing radiation.

The purpose of our research is the measurement of cross sections for inelastic scattering of electrons for characterization of those mechanisms important in energy-degradation processes. The resulting data can be used to estimate yields of irradiation products, to identify spectroscopically the energy levels of states initially excited in the target, and to test predictions or stimulate further development of electron scattering theory. The generalized oscillator strength derivable from the measured cross sections describes the response of the target to fast charged-particle impact and, in the limit of small momentum transfer, yields the optical oscillator strength. Moreover, measured generalized oscillator strengths can be used to calculate intermolecular energy transfer cross sections as well as singlet-triplet energy differences. Both topics are of fundamental importance in radiation chemistry and biology.

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One of the techniques we use to study such electron collision processes is called electron-energy-loss spectroscopy. Specifically, we shoot an electron of known energy at a target molecule and measure the intensity of the scattered electrons differential in both energy transfer and scattering angle. This technique, a form of spectroscopy, gives us the energy levels of the atom or molecule. By measuring how many electrons lose specific amounts of energy, we are able to determine the probability of each excitation event.

Electron collision studies are truly multidisciplinary. The data we obtain are often of immediate relevance to programs other than basic radiation research. For example, analogous processes occur in gas discharge lasers, plasma etching of microchips in the electronics industry, terrestrial and planetary atmospheres, and stellar atmospheres. Electron collision studies we have made recently have been directly applied to all of these fields.

In 1985 we expanded our experimental capabilities to enable us to examine photon emission from molecular systems that have been electronically excited by variable-energy, high-resolution electron beams. Because high resolution implies very small signal yield, no such studies have previously been attempted. The advantage of such measurements is that they allow a direct determination of the specific electronic state responsible for emission. Some of this new work is reported in this section.

In addition, we report here our measurements on progressively larger molecular systems, which we have made in order to understand possible systematic trends of electron excitation processes, with the near-term goal of understanding such processes in the heterocyclia DNA bases guanine, cytosine, adenine, thymine, and uracil.

5.3.2. Electron Impact Spectroscopy of Silane and Germane

M.A. Dillon, R.-G. Wang,* Z.-W. Wang,* and D. Spence

[Abstract of a paper published in Journal of Chemical Physics 82:2909-2917 (1985)]

Electron impact spectra of silane and germane have been recorded using electrons of 200 eV incidence at scattering angles of $\sim 2^\circ$ - 9° . The range of energy losses covers the entire region of single-electron excitation from the valence shell. In the bound state, spectrum evidence is presented supporting the existence of two valence transitions in addition to anticipated s, p, and d Rydberg transitions. The 9° spectra reveal much structural detail in the ~ 4 -eV energy range preceding the 2A_1 ion state. The most prominent band consists of a superposition of an optically allowed valence excitation and a symmetry forbidden Rydberg transition. The remaining peaks may be members of vibrational progressions belonging to either $[d(t_2), a_1]$, $[p, a_1] + (a_1)^2$ dipole allowed or $[d(e), a_1]$, $[s, a_1] + (a_1)^2$ dipole forbidden channels. Of these two possibilities, the evidence presented here favors the latter choice.

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5.3.3. VUV Emission Spectrum of Germane

*D. Spence, M.A. Dillon, and H. Tanaka**

A recent paper by Osmundsen et al. (1985) describes a technique whereby the ultraviolet spectrum of exotic radicals such as GeH may be obtained by multiphoton dissociation of GeH_4 . Our recent studies of GeH_4 and SiH_4 have demonstrated that electron impact excitations of valence transitions in these molecules are such that all those excited states are repulsive in nature, resulting in fragmentation of the parent molecule (Dillon et al. 1985). We have been prompted to study, therefore, whether emission spectra of exotic fragments may be obtained by the technique of electron impact in a manner similar to multiphoton dissociation. The results have been somewhat disappointing:

Where in the photon range 240-450 nm, Osmundsen et al. (1985) observed several new series arising from GeH in addition to many atomic lines from Ge, in the electron impact spectrum we merely observe many well-known Ge lines. In the far UV, 147-179 nm, we have obtained a somewhat more interesting spectrum, shown in Figure 5.4, although the origins of these bands are not known at present. Although many of the bands in Figure 5.4 result from

Figure 5.4. Fluorescence yield from GeH_4 between 147 and 182 nm following excitation by 30-eV electrons.

*Collaborator; affiliation is listed at the front of this chapter.

unresolved components, some of which may be of atomic origin, many are of a molecular nature, although it is not possible for us to distinguish at the moment whether these arise from GeH_4 or a fragment, or even which fragment.

5.3.4. Near-Threshold Electron Impact Excitation of HgBr_2

*D. Spence, M.A. Dillon, and J. Seger**

Some time ago, we published electron energy loss spectra of HgCl_2 and HgBr_2 obtained at 200-eV incident electron and scattering angles near the forward direction in the energy loss region 4 eV to 14 eV (Spence et al. 1982). This covered most of the energy region in which valence and Rydberg transitions occur. Because of the scattering conditions under which these experiments were performed, the energy loss spectra were "pseudo optical" in nature. These measurements located several intense energy loss features that had not previously been observed and also provided relative cross sections for use in modeling studies. Though these data were subsequently used as guidance to provide unified sets of cross section data for the modeling of mercuric bromide laser discharges (Nighan and Brown 1982; McGeoch et al. 1983), the question was raised as to whether it was appropriate to use relative cross sections obtained at high energies in modeling discharges in which the mean electron energy was much lower (Nighan and Brown 1982). Although we believed that this procedure was probably satisfactory, at the time we lacked experimental verification.

In order to resolve this question, we have obtained near-threshold electron impact spectra of HgBr_2 using a differential trapped electron technique (Spence 1975). We note that similar spectra have recently been obtained by Chantry and Chen (1983) using the usual trapped electron technique (Schulz 1958). This technique measures relative cross sections from threshold up to a chosen value of the well depth, which in the case of Chantry and Chen (1983) was about 0.5 eV. One disadvantage of the usual trapped electron technique is a superposition of cross sections if the spacing between various energy levels is less than the well depth. Additionally, the technique is sensitive to the presence of negative ions in that contributions to the measured signal from negative ions cannot, a priori, be distinguished from those contributions due to energy loss processes.

The differential technique we use (Spence 1975) is not sensitive to negative ions, and measures the true relative cross sections at an energy above threshold equal to the well depth above threshold, thus removing the complication in the spectra of overlapping cross sections.

A typical spectrum obtained at an energy of less than 0.1 eV above threshold is shown in Figure 5.5, where it is compared to our earlier spectrum

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Figure 5.5. Comparison of "pseudo optical" electron energy loss spectrum obtained for 200-eV incidence electron energy (upper curve) with a near-threshold spectrum obtained for electron energies only 0.1 eV above threshold. This comparison demonstrates that high-energy spectra may be of use for modeling cool discharges, at least so far as optical transitions are concerned.

obtained at an incident energy of 200 eV (Spence et al. 1982). The similarities between these two spectra obtained despite widely disparate excitation conditions are obvious. A comparison of the relative cross section of selected energy loss processes shown in these spectra with those chosen by Nighan and Brown (1982) and by McGeoch et al. (1983) is provided in Table 5.1. Although there are indeed differences in the relative cross sections obtained by the two electron impact techniques, the differences are probably not so severe as to preclude the use of pseudo-optical energy loss spectra in many modeling situations.

Indeed, the differences in relative cross sections obtained experimentally at threshold and 200 eV is not so great as the differences in the two sets of cross sections chosen for discharge analysis (Nighan and Brown 1982; McGeoch et al. 1983). Additional structures in the near-threshold spectrum, which do not appear in the 200-eV spectrum, are due to excitation of optically forbidden states, although identification of these states is not yet complete. Finally, we note that in other spectra we have obtained up to about 1.5 eV above threshold (not shown here). These forbidden processes never dominate the energy loss spectra.

Table 5.1. Relative magnitudes of near-threshold and pseudo-optical (200-eV) cross sections with model results inferred to explain HgBr₂ discharge conditions. Magnitudes arbitrarily normalized to 25.5 for the 1 ¹Σ_u state

State	Present Data		Nighan & Brown (Discharge analysis model)	McGeoch et al. (Discharge analysis model)
	Pseudo-optical (200-eV)	Near-threshold		
1 ¹ Π _u (5.3 eV)	9	11	5.1	6.4
1 ¹ Σ _u (6.3 eV)	25	25.5	25.5	25.5
Q _x (7.9 eV)	233	145	510	182

5.3.5. Studies of Fluorescence Radiation from F₂ by High Resolution Electron Impact with Reference to Molecular Halogen Lasing

D. Spence, M.A. Dillon, H. Tanaka, and K.E. Lanick**

For a number of years it has been assumed on the basis of rather indirect measurements (Woodworth and Rice 1978; Cooper et al. 1976) that the molecular transitions responsible for emission of the 7.95-eV laser photon in molecular fluorine were $f\ ^3\Pi_g \rightarrow a\ ^3\Pi_u$ (both forbidden from the F₂ ¹Σ_g ground state), although the locations of these two energy levels with reference to the ground state were not precisely known (Cartwright and Hay 1979; Nishimura et al. 1979).

In recent experiments (Wang et al. 1984), we resolved for the first time the vibrational levels of the F ¹Π_u state and determined the energy of the v = 0 level to be 11.702 eV and^g argued that the v = 0 level of the associated f ³Π_g state was probably lower in energy by about one vibrational quantum, i.e. ^g at about 11.57 eV. Recent low-energy electron scattering experiments (Hoshida et al. 1985) have indeed located the f ³Π_g state at 11.62 eV and the a ³Π_u state at 3.3 eV, the difference between these two being not quite equal to the laser photon energy of 7.95 eV.

We performed two experiments to resolve the questions concerning laser emission in F₂. Using a fixed electron energy of 100 eV, we first examined the yield of fluorescence radiation in F₂ as a function of wavelength in the VUV region under single collision conditions. The results of this experiment are shown in Figure 5.6, which shows the yield of fluorescence radiation vs. wavelength. This smoothly varying curve approximates the envelope of fluorescence yield from F₂/rare gas mixtures at high pressure irradiated by

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Figure 5.6. Yield of fluorescence radiation from F_2 following 100-eV electron impact excitation as a function of photon wavelength. Under lasing conditions, the energy of the laser photon is indicated at 157 nm.

high-energy (1.9-MeV) electrons. Note that we do not see the fine structures observed in previous experiments (Woodworth and Rice 1978), although our photon resolution is ~ 0.5 nm). This, however, may simply be a consequence of different states of relaxation of the target gas under the very different experimental conditions.

In the second experiment, by fixing the optical monochromator to pass only 7.95-eV photons, we measured the photon yield as a function of incident electron energy. Our electron beam was selected by a trochoidal monochromator and had a resolution of 0.1 eV. Our energy scale was established by simultaneously measuring the transmitted current through a mixture of He/ F_2 and calibrating against the well-known He resonance at 19.35 eV. In this way, our electron energy scale was established to within better than 0.1 eV. The results of this experiment are shown in Figure 5.7.

Surprisingly, the yield of 7.95-eV photons shows a sharp onset at 14.05 ± 0.10 eV. We observe no photon emission at the expected energy of 11.6 eV, even though we are definitely exciting the supposed upper laser level $f^3\Pi_g$ at this energy.

Ours and other experiments had previously shown only the $1^1\Sigma_u^+$ at an energy of about 14 eV, which cannot be responsible for lasing. However, the recent low-energy scattering spectra of Hoshiba et al. (1985) do show a new forbidden transition at about 14.05 eV, although those authors do not remark on this feature. Furthermore, these latter measurements (and those of Nishimura et al. 1979) show another forbidden transition at about 6.1 eV, the energy difference of these two states being 7.95 eV.

Figure 5.7. Yield of 157 nm (7.95 eV) photons from F_2 as a function of incident electron energy. Note the sharp onset at 14.05 ± 0.1 eV. The maximum photon signal corresponds to about 200 counts/channel. Below 14 eV, the count rate is 1 or 2 counts/channel and is purely statistical dark counts. No 157-nm photon signal is observed at the $f^3\Pi_g$ threshold at 11.5 eV.

Although our measurements at this stage must be considered preliminary and are undergoing refinement, we point out that in Figure 5.7 the maximum photon signal is about 200 counts/channel, whereas below the 14-eV threshold (with our dark count rate of only 1 or 2 counts/minute) the total number of counts is 1 or 2 counts/channel, i.e., statistical.

5.3.6. UV and VUV Emission Spectrum of XeF Produced by High-Resolution Electron-Impact Dissociative Excitation of XeF_2

D. Spence, K.E. Lanick, M.A. Dillon, and H. Tanaka**

The observation of fluorescence radiation from XeF in the near and far ultraviolet, made as part of the initial testing of a new apparatus, is reported here. This apparatus was designed to study photoemission from molecular systems upon irradiation by low energy (0-100 eV), high resolution (greater than 100 meV), well-controlled electron impact, and under single-collision conditions.

Although many fluorescence measurements have previously been made using unmonochromated electron beams (whose energy is often ill defined), the use of monochromatic electrons of well-defined (better than 0.1 eV) energy permits precise determination of which molecular levels of the target system are responsible for fluorescence (or fragmentation if that be the case) directly as transitions from the ground electronic state.

*Collaborator; affiliation is listed at the front of this chapter.

A difficulty in the use of monochromatic beams is the low incident electron beam current, which is typically 10^{-8} A, compared with 10^{-3} to 10^{-2} A for unmonochromated beams. This limitation results in very low fluorescence yields, especially under single-collision conditions where the target gas densities are of the order of 10^{-3} to 10^{-4} Torr, and requires extremely low dark count rates in the photon counting system. In our system, the dark count rate is typically one or two counts/minute.

In the present studies, no fluorescence radiation was identified as arising from electronic transitions within the XeF_2 manifold of electronic states. Rather, at least in the near UV, the fluorescence radiation arose solely from dissociative excitation of the XeF_2 π_u state centered at about 8.0 eV. This resulted in excited XeF fragments in various vibrational levels of the E state that decay by emission of a photon to the $\text{XeF}(X)$ state.

A typical fluorescence spectrum obtained at photon wavelengths between 325 and 360 nm is shown in Figure 5.8. This spectrum is similar to many previous emission studies of XeF^* , in which the XeF^* was produced in multifarious ways, usually in relatively high-pressure gas mixtures, such as $\text{Xe}/\text{F}_2/\text{buffer}$ gas. The spectrum of Figure 5.8, however, does show subtle differences from some previously published spectra (Brau and Ewing 1975; Rohni and Jacob 1982). For example, the intensities of individual $B(v') \rightarrow X(v'')$ vibrational transitions shown in Figure 5.8 seem to indicate the XeF^* produced in our experiments to be more vibrationally hot, i.e. unrelaxed, than in those experiments in which the XeF^* is prepared at high pressure.

Measurements of the photon yields shown in Figure 5.8, but at a fixed wavelength and as a function of incident energy (not shown here), show a sharp onset at an incident electron energy of ~ 8 eV, confirming that the XeF^* arises from dissociative excitation of the XeF_2 2π state at 8 eV.

Fluorescence measurements obtained in the VUV region are shown in Figure 5.9. The structure at 1468 Å is the Xe resonance transition, the Xe coming from surface decomposition of XeF_2 . Photon yields obtained as a function of incident electron energy indicate that the other structures have sharp onsets at incident electron energies somewhat above 10 eV, although their precise nature is as yet undetermined.

5.3.7. Electron Energy Loss Spectroscopy of XeF_2

M.A. Dillon, H. Tanaka, and D. Spence*

Electron impact spectra of xenon difluoride employing electrons of 200-eV incidence and recorded at three different scattering angles are shown in Figure 5.10. The energy-loss range includes the manifold of Rydberg levels for all single-electron excitation out of the first five molecular orbitals.

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Figure 5.8. Fluorescence yield from XeF^* produced by electron impact dissociative excitation of XeF_2 .

Figure 5.9. Fluorescence radiation from XeF_2/XeF in the VUV region. The small structure at 1468 Å is the Xe resonance line.

Figure 5.10. Electron impact spectra of xenon difluoride recorded with electrons of 200-eV incidence. The arrows mark the onsets of laser emission bands.

All of the peaks observed in the spectra are dipole-allowed transitions and have been previously reported in the optical spectrum (Nielsen and Schwarz 1976). The arrows indicate the onsets of the $B \rightarrow X$ and $C \rightarrow X$ emission bands at 6.1 eV and the $D \rightarrow X$ band at 7.3 eV.

The spectra reveal a feature of considerable interest. The intense valence transition at 7.8 eV falls off much more rapidly with scattering angle than the adjacent Rydberg bands. This difference in scattering angular distributions may prove helpful in distinguishing between Rydberg and valence transitions.

5.3.8. Collision Cross Sections and Electron Spectroscopy of Disilane

M.A. Dillon, H. Tanaka,* and D. Spence

The gas jet inlet system of an electron spectrometer was modified to accommodate an MKS capacitance manometer. This makes it possible to record electron impact spectra, as well as to determine differential cross sections by the relative flow method (Srivastava et al. 1975). In this work, a technique was developed in which the jet backing pressure, p , of the target gas is compared to the pressure, p_c , of a calibration gas. The differential cross section, σ , of the measured gas is related to that of the calibration gas by:

$$\sigma = R \frac{I}{I_c} \frac{p_c}{p} \sigma_c, \quad (5-8)$$

where I/I_c is the ratio of scattered electron intensities, and $R = 1$ when both transitions are discrete. However, if the measured intensity, I , corresponds to a continuous transition, then R is the ratio of peak height to the area of the elastic peak. An example of results from this method is displayed in Figure 5.11, which shows electron impact spectra of disilane obtained with

Figure 5.11. Electron impact spectra of disilane recorded with electrons of 200 eV incidence. The 0° spectrum has been corrected for the finite entrance aperture.

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electrons of 200 eV incidence and over an energy-loss range that includes all single-electron excitations from the valence shell.

The comparison peak and gas employed was the $1^1S + 2^1P$ transition in helium at 21.22 eV. Below an energy loss of 12 eV, the 0° spectrum reveals four well-defined peaks, as well as a shoulder at $W = 10$ eV. Examination of the 6° spectrum shows that the shoulder is in fact a separate peak. The corresponding photoelectron (PE) spectrum (Bock et al. 1976) consists of four diffuse bands indicative of ionization out of the highest four molecular orbitals. The qualitative angular distributions of the five bands deduced from a comparison of 0° and 6° spectra show that the first four bands fall off with scattering angle at roughly the same rate. Moreover, the peak positions fall in the same pattern as the bands present in the PE spectrum. Hence, we can conclude that the first four structures in Figure 5.11 represent Rydberg transitions terminating in the ionized orbitals observed in the PE spectrum. The large peak at $W \sim 10.8$ eV changes shape in the 6° spectrum, revealing an underlying band that falls off much more slowly with scattering angle than the first four peaks. This characteristic, along with the lack of Jahn-Teller splitting, makes it likely that the transition is optically forbidden and that the originating orbital is a_{1g} . In the energy loss range 13 - 15.5 eV, both spectra show some evidence of transitions from the a_{2u} valence orbital.

5.3.9. Discrete Structure in the Electronic Spectrum of Saturated Molecules

*M.A. Dillon, D. Spence, and H. Tanaka**

Electronic excitation from the valence shell of a saturated molecule involves the transition of an electron from a bonding orbital to a nonbonding or antibonding orbital. Such transitions, most of which are Rydberg in character, terminate either in a dissociative electronic state or above the dissociative limit of a bound state. For this reason, electronic spectra of saturated molecules often appear completely diffuse with little or no structural information (Robin 1974). In many cases, this behavior contrasts sharply with the corresponding photoelectron spectrum, which may contain discrete features such as vibrational progressions. To an approximation, molecular Rydberg states should mirror the positive ion states to which they converge. Thus, in saturated molecules with structured positive ion spectra, we should find some evidence of similar features in its electronic excitation spectrum.

In the past few years, weak structure has been reported in the electron impact spectrum of saturated molecules with tetrahedral symmetry (Dillon et al. 1984, 1985). The observed bands all consist of overlapping vibrational progressions converging to the second IP. More recent examples of this phenomenon are displayed in Figure 5.12.

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Figure 5.12. Electron impact spectra of ethane and neopentane obtained with electrons of 200-eV incidence at scattering angles of 3° and 9° . The amplitude of the structure in the 9° spectrum is about 2% of the continuum background.

Figure 5.12(a) shows electron impact spectra of ethane recorded at two different scattering angles. The 9° spectrum reveals at least one vibrational progression not found in the spectrum recorded at 3° . This new feature probably consists of overlapping members of a Rydberg series converging to the third IP at 20.13 eV. The emergence of a band system with increasing scattering angle is characteristic of an optically forbidden transition. Since the third IP corresponds to ionization out of the $2a_{2u}$ orbital, the terminating orbital is probably $3a_{2u}$ leading to the optically forbidden transition $1A_{1g} \rightarrow 1A_{1g}$.

A more complicated situation is depicted in the electron impact spectra of neopentane shown in Figure 5.12(b). The structure in the spectrum recorded at 3° consists of overlapping vibrational progressions from members of the optically allowed Rydberg series $2a_1 \rightarrow np$ ($n = 3, 4$). By 9° , this series has disappeared, as indicated by the angular trend of the lower energy bands in the near 15.5 eV. However, considerable structure either remains in the 9° spectrum or emerges by 9° . It is likely that these bands belong to the optically forbidden Rydberg series: $2a_1 \rightarrow ns$ or $nd(e)$.

5.4 PHOTOPHYSICS STUDIES IN THE VACUUM ULTRAVIOLET

5.4.1. Summary

Photophysics studies in the vacuum ultraviolet generally have two broad objectives. The first is to determine the spectroscopy of excited neutral states and ionic states. The second is to explore the dynamics of the photoionization processes. The work summarized below emphasizes basic studies of small molecules, including weakly bound van der Waals complexes. Various techniques are employed, including photoionization mass spectrometry using a Hopfield continuum light source (Sections 5.4.2. and 5.4.3), triply differential electron spectrometry using synchrotron radiation (Sections 5.4.4.-5.4.6), and theoretical calculations using the multiple scattering method (5.4.4., 5.4.7., and 5.4.8.).

Specific progress in the last year can be summarized briefly as follows: Sections 5.4.2. and 5.4.3. summarize new studies of the Rydberg structure and ionic state properties of the weakly bound systems ArCO_2 and KrCO_2 . Section 5.4.4. is an abstract of a major review article describing theoretical and experimental progress, over the last decade or so, in the study of shape and autoionizing resonances in molecular photoionization. Sections 5.4.8. and 5.4.5. represent, respectively, the theoretical prediction and experimental confirmation of a novel mechanism whereby shape resonant behavior is transferred to a nonresonant channel by continuum-continuum coupling. And, finally, Section 5.4.6. refers to the recent commissioning and calibration of a new high-resolution, high-sensitivity triply differential electron spectrometer system for use with synchrotron radiation.

5.4.2. Dissociation Energies of ArCO_2^+ and KrCO_2^+

P.M. Dehmer

The photoionization cross sections of both ArCO_2 and KrCO_2 show a very gradual onset at the ionization threshold. The dimer ion appearance potentials are 912.5 ± 2.5 Å (13.59 ± 0.04 eV) for ArCO_2 , 930.0 ± 3.0 Å (13.33 ± 0.04 eV) for KrCO_2 , and 931.0 ± 2.0 Å (13.32 ± 0.03 eV) for $(\text{CO}_2)_2$. Assuming that the appearance potential corresponds to the adiabatic ionization potential (I.P.) (which is true for the homonuclear rare gas van der Waals

dimers but may not be the case for other van der Waals molecules), the dissociation energy of a dimer ion ground state can be calculated from the relation:

$$D_0(X - CO_2^+) = I.P.(CO_2) + D_0(X - CO_2) - I.P.(X - CO_2). \quad (5-9)$$

Using values for the neutral ground state dissociation energies of 0.018 ± 0.010 eV for $ArCO_2$ (Parker et al. 1976; Loesch 1976), 0.023 ± 0.010 eV for $KrCO_2$ and 0.06 ± 0.02 eV for $(CO_2)_2$ (Brigot et al. 1977), and a value for the ionization potential of CO_2 of 13.773 ± 0.002 eV (McCulloh 1973), the following values were obtained for the lower limit to the dissociation energies of the dimer ion ground states: $D_0(ArCO_2^+) = 0.20 \pm 0.04$ eV; $D_0(KrCO_2^+) = 0.47 \pm 0.05$ eV; and $D_0(CO_2 - CO_2^+) = 0.51 \pm 0.05$ eV. (An estimate of the dissociation energy of the ground state of $KrCO_2$ was obtained by noting that the ratio of the dissociation energies for $Ar - X$ and $Kr - X$ [$X = Ar, Kr, Xe$] is constant and is approximately 0.8; see the compilation of rare gas dimer dissociation energies in Dehmer and Pratt 1985). Table 5.2 summarizes these values and includes the dissociation energies for all other pairs of Ar , Kr , and CO_2 dimer ions.

Table 5.2. Lower limit for ground state dissociation energies of homonuclear and heteronuclear dimer ions of Ar , Kr , and CO_2 (eV).

	Ar^a	Kr^a	CO_2
Ar	1.269 ± 0.017	0.528 ± 0.015	0.20 ± 0.04
Kr		1.150 ± 0.004	0.47 ± 0.05
CO_2			0.51 ± 0.05

^aFrom Dehmer and Pratt (1982).

The simple molecular orbital picture used to help explain the trends observed for the heteronuclear rare gas dimers is also useful in understanding the trends seen in Table 5.2. In this picture, the bond dissociation energy is given (Murrell et al. 1978) approximately by:

$$D_0 \approx \frac{H_{ab}^2}{H_{aa} - H_{bb}}. \quad (5-10)$$

Here, H_{ij} are the usual Hamiltonian integrals. The denominator of Equation 5-10 may be approximated by the difference in ionization potentials of the free partners in the van der Waals complex. This makes use of

Koopmans' theorem and also assumes that the effect on the energies of the free partners due to the presence of the other partner is small. The numerator of Equation 5-10 is called the "interaction energy" and is often taken as proportional to the overlap integral of the two partners. For the Ne-rare gas dimers, the values of $H_{aa} - H_{bb}$ are large and chemical effects are small; a large part of the binding is due to the ion-induced dipole interaction. However, for heteronuclear dimers containing CO_2 , this is not the case. In particular, the value of $H_a - H_{bb}$ is very small for KrCO_2 [I.P. (Kr) = 14.000 eV (Yoshino and Tanaka 1979) and I.P. (CO_2) = 13.773 eV (McCulloh 1973)], and chemical effects are expected to be substantial. Indeed, the ground state dissociation energy of the heteronuclear dimer ion KrCO_2^+ (0.47 ± 0.05 eV) is very close to that of the homonuclear dimer ion $(\text{CO}_2^+)_2$ (0.51 ± 0.05 eV), and both dissociation energies are significantly larger than the ion-induced dipole energies, which are ~ 0.1 eV.

These dissociation energies are significantly smaller than the dissociation energies of the homonuclear and heteronuclear rare gas dimers. We previously noted that the delocalized nature of the unfilled molecular orbital in CO_2^+ appears to reduce significantly the interaction energy and the bond energy of ArCO_2^+ compared to that of ArKr^+ (Pratt and Dehmer 1983). This is true even though the ionization potentials of CO_2 and Kr are comparable, as are their average polarizabilities. A similar effect was noted in the homonuclear dimers Kr_2^+ and $(\text{CO}_2)_2^+$; here, the dissociation energy of Kr_2^+ (1.150 ± 0.004 eV) is twice that of $(\text{CO}_2)_2^+$ (0.51 ± 0.05 eV), suggesting that charge delocalization also influences the bonding in $(\text{CO}_2)_2^+$. The substitution of Kr for CO_2 as the neutral partner in $(\text{CO}_2)_2^+$ has little effect on the dissociation energy. This is not unexpected, since the neutral partner influences the bond dissociation energy primarily through its polarizability and its ionization potential.

5.4.3. Rydberg States of ArCO_2 and KrCO_2

P.M. Dehmer

[Summary of a paper published in Journal of Chemical Physics 83:24 (1985)]

Photoionization cross sections were determined for ArCO_2 from 680 to 920 Å. Autoionizing Rydberg states based on both the $\text{Ar}^* + \text{CO}_2$ and $\text{Ar} + \text{CO}_2^*$ dissociation limits are observed in the photoionization cross section. For comparison, spectra of Ar_2 , ArKr , and ArXe were determined in the region of Ar^* transitions, and spectra of CO_2 , KrCO_2 , $(\text{CO}_2)_2$, and $(\text{CO}_2)_3$ were determined in the regions of CO_2^* transitions. The data are shown in Figures 5.13 through 5.16.

An examination of the $\text{Ar}^* \text{CO}_2$ bands in the region of the Ar^* 3d and 5s levels shows that the bands are blue shifted with respect to the corresponding $\text{Ar}^* \text{Kr}$ and $\text{Ar}^* \text{Xe}$ bands. The most probable interpretation is that the change in R_e between the ground and excited states of ArCO_2 is larger than the

Figure 5.13. Relative photoionization cross sections for ArCO_2 determined at a wavelength resolution of $0.24 \text{ \AA}$ and CO_2 , $(\text{CO}_2)_2$, and $(\text{CO}_2)_3$ determined at a wavelength resolution of $0.50 \text{ \AA}$.

Figure 5.14. Relative photoionization cross section for ArCO_2 , ArKr , and ArXe determined at a wavelength resolution of $0.24 \text{ \AA}$.

Figure 5.15. Relative photoionization cross section for ArCO_2 determined at a wavelength resolution of 0.24 Å and Ar_2 , ArKr , and ArXe determined at a wavelength resolution of 0.15 Å.

Figure 5.16. Relative photoionization cross sections for CO_2 determined at a wavelength resolution of 0.12 Å, for ArCO_2 determined at a wavelength resolution of 0.24 Å, and for KrCO_2 determined at a wavelength resolution of 0.4 Å.

corresponding change in either ArKr or ArXe; however, a complete interpretation of the complex band structure in this region requires a more sophisticated analysis that includes the effects of λ mixing on the molecular states associated with the various $\text{Ar}^*(3d, 5s) - \text{CO}_2$ dissociation limits.

Also observed are bands of the type ArCO_2^* and KrCO_2^* , which appear red shifted with respect to the corresponding CO_2^* bands of the Henning sharp and diffuse series. The binding energies as determined at R_e of the neutral dimer for the Rydberg states converging to $\text{Ar} = \text{CO}_2^+ B^2\Sigma_u^+$ are in good agreement with the calculated value of the ion-induced dipole energy. Using the ion-induced dipole approximation together with the observed binding energy of the high-lying Rydberg states in KrCO_2 and the known value of the polarizability of Kr, an estimate was obtained for R_e of KrCO_2 of 3.60 Å. The value of R_e for KrCO_2 is about 0.11 Å larger than that for ArCO_2 , which is similar to the difference in R_e for other pairs of Ar - X and Kr - X van der Waals complexes.

No structure was observed in the spectra of the van der Waals dimers that could be correlated with members of the Tanaka-Ogawa Rydberg series of CO_2 . Various experimental evidence appears to rule out both vibrational predissociation of the excited state of the neutral and vibrational predissociation of ion as the primary cause of this observation.

5.4.4. Resonances in Molecular Photoionization

J.L. Dehmer, A.C. Parr, and S.H. Southworth**

[Summary of a paper to appear In: G. V. Marr (ed.), Handbook on Synchrotron Radiation, Vol. II. North-Holland, Amsterdam, in press.]

Molecular photoionization is a rich source of information on fundamental intramolecular interactions. This is apparent when photoionization is viewed as a half-collision in which a collision complex, prepared by dipole excitation, decays by ejection of an electron from the field of the target. In the molecular case, the escaping electron must traverse the anisotropic molecular field and can undergo interactions with its nuclear modes. Hence, the photoelectron carries to the detector dynamical information on the two central aspects of molecular behavior--motion of an electron in a multicenter field and interplay among rovibronic modes.

Attention is invariably drawn to resonant photoionization mechanisms, such as shape resonances and autoionization. These resonant processes are important probes of photoionization for various reasons, the most obvious one being that they are usually displayed prominently against nonresonant behavior in such observables as the total photoionization cross section, photoionization branching ratios, and photoelectron angular distributions. More importantly, resonances temporarily trap the excited complex in a quasibound state, causing the excited electron to traverse the molecular core

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many times before its escape by tunneling or by exchange of energy with the core. In this way, resonances amplify the subtle dynamics of the electron-core interactions for more insightful analysis.

The last decade has witnessed remarkable progress in characterizing dynamical aspects of molecular photoionization. From among the great variety of successful streams of work, one can identify four broad classes that together have propelled the recent activities in this field.

In the first class, the extensive measurements of total photoabsorption/photoionization cross sections from the VUV to the x-ray range by a variety of means have continually provided fresh impetus to account for novel features displayed in molecular oscillator strength distributions.

Second, shape resonances have emerged as a major focal point in the study of molecular photoionization dynamics. Initially stimulated by observations of intense, broad peaks in inner-shell spectra, beginning in the late 1960s, the study of shape resonances in molecular photoionization has grown into a vigorous subfield. Benefitting greatly from the timely development of realistic, independent-electron models for treating molecular photoionization, studies in this area have not only accounted for the features in the total photoionization spectra of both inner and outer shells, but also have predicted and confirmed several manifestations in other physical observables.

Third, multichannel quantum defect theory (MQDT) was adapted to molecular photoionization, providing a framework for the quantitative and microscopic analysis of autoionization phenomena. This powerful theoretical framework has been successfully applied to a number of prototype diatomic molecules, yielding both insight into the detailed dynamics of resonant photoionization and some specific predictions for experimental testing by means discussed in the next item. Fourth, technical advances, especially the development of intense synchrotron radiation sources, have made it feasible to perform triply differential photoelectron measurements on gas-phase atoms and molecules. By this we mean photoelectron measurements are made as a function of three independent variables--incident photon wavelength, photoelectron energy, and photoelectron ejection angle. Variable wavelength permits the study of photoionization at and within spectral features of interest.

Photoelectron energy analysis permits separation and selection of individual (ro)vibronic ionization channels. Measurement of photoelectron angular distributions accesses dynamical information, i.e., relative phases of alternative degenerate ionization channels, that is not present in integrated cross sections. This level of experimental detail approaches that at which theoretical calculations are done and, hence, permits us to isolate and study dynamical details that are otherwise swamped in integrated or averaged quantities.

We emphasize that although the current trend is toward use of synchrotron radiation for variable wavelength studies, a variety of light sources have been successfully used to study photoionization dynamics. For example, in the shape-resonance literature, many of the pioneering measurements were carried

out with laboratory sources. Likewise, although most current measurements of vibrational branching ratios and angular distributions within autoionizing resonances employ synchrotron radiation, many early and ongoing studies with traditional light sources have made significant observations of the effects of autoionization on vibrational branching ratios and angular distributions.

In the chapter summarized here, we have reviewed recent progress in this field with emphasis on resonant mechanisms and on the interplay between experiment and theory. Sections 2 and 3 discuss elementary aspects of shape resonances and autoionization, respectively. Section 4 describes experimental aspects of triply differential photoelectron measurements which are currently the major source of new data in this field. Section 5 describes particular case studies of molecular photoionization, chosen to focus on a variety of basic resonant mechanisms that are both under active study currently and likely to form main themes in the future. Whereas these case studies draw heavily upon results of the authors' program at the National Bureau of Standards' SURF-II Facility, Section 6 surveys related work with a much broader perspective, stressing aspects which are often unique to other groups. Finally, Section 7 offers some thoughts about future directions of research within and beyond the present limitations of this field.

5.4.5. Channel-Coupling and Shape-Resonance Effects in the Photoelectron Angular Distributions of the $3\sigma_g^{-1}$ and $2\sigma_u^{-1}$ Channels of N_2

S.H. Southworth, A.C. Parr,* J.E. Hardis,* and J.L. Dehmer*
[Summary of a paper to appear in Physical Review A]

We have carried out measurements of photoelectron angular distributions for the $3\sigma_g^{-1}$ and $2\sigma_u^{-1}$ photoionization channels of N_2 from their thresholds up to 35 eV and 37.5 eV, respectively. The asymmetry parameter, β , for the $2\sigma_u^{-1}$ channel exhibits a broad dip in the range $h\nu \sim 27 - 32$ eV that was recently predicted theoretically to arise from shape-resonance-enhanced continuum-continuum coupling between the $3\sigma_g^{-1}$ and $2\sigma_u^{-1}$ ionization channels. The β parameter for the $3\sigma_g^{-1}$ channel exhibits a prominent feature at $h\nu \sim 23$ eV, which is tentatively attributed to the autoionization of a doubly excited valence-like state. Otherwise, the gross shape of the $3\sigma_g^{-1}$ β curve is in good agreement with independent-electron calculations, which realistically reflect the influence of the well-known σ_u shape resonance in this channel.

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5.4.6. Calibration of a Monochromator/Spectrometer System for Measurement of Photoelectron Angular Distributions and Branching Ratios

S.H. Southworth, A.C. Parr,* J.L. Dehmer, J.E. Hardis,* and D.M.P. Holland**

[Summary of a paper to appear in Nuclear Instrumentation Methods]

The measurement of wavelength-dependent photoelectron angular distributions, branching ratios, and partial cross sections is one of the important applications of synchrotron radiation in atomic and molecular physics. In combination with theoretical studies, photoelectron measurements reveal the structural and dynamical factors that underlie photoionization processes. For example, the tunable continuum property of synchrotron radiation has allowed the study of resonant processes such as those due to shape resonances and autoionization.

Quantitative photoelectron measurements using synchrotron radiation require knowledge of the wavelength-dependent intensity and polarization of the photon beam and of the transmission(s) of the electron analyzer(s) as a function of photoelectron kinetic energy and ejection angle. We have examined in detail the techniques used in calibration of a monochromator/spectrometer system for measurements of photoelectron angular distributions and branching ratios. The spectrometer was a second-generation instrument designed for high-resolution molecular studies. The monochromator was the high throughput, 2m, normal incidence instrument located at the Synchrotron Ultraviolet Radiation Facility at the National Bureau of Standards.

Ne, Ar, Kr, and Xe were used for calibration studies because their angular asymmetry parameters, β 's, and total cross sections are known fairly well. As discussed in the full article, some discrepancies occurred at certain energies in the calibration results based on the different rare gases. Our approach was to derive spectrometer calibration functions that were the most consistent among all of the rare gas data. We present the resulting self-consistent set of β 's for the Ne 2p, Ar 3p, Kr $4p_{3/2}$ and $4p_{1/2}$, and Xe $5p_{3/2}$ and $5p_{1/2}$ subshells and of the branching ratios Kr $4p_{3/2}:4p_{1/2}$ and Xe $5p_{3/2}:5p_{1/2}$.

5.4.7. Shape Resonances in the Photoionization of CF₄

J.A. Stephens, D. Dill,* and J. L. Dehmer*

[Abstract of an article to be published in Journal of Chemical Physics]

Calculations of photoionization cross sections and photoelectron angular distributions have been performed for all occupied orbitals of CF₄ using the multiple-scattering model. Results are compared with very recent experiments which employ synchrotron radiation to measure these quantities. The calculations predict intense shape resonances that are characterized by a_1 and

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t_2 final state symmetry, within 3 eV above the ionization threshold of each occupied orbital. Qualitative agreement is attained on comparing much of the theory with experiment, notably the five outer valence levels, which serves to establish a one-electron picture of the photoionization dynamics of CF_4 .

5.4.8. Shape Resonance Effects Mediated by Channel Interaction. Angular Distributions of N_2 $2\sigma_u$ Photoelectrons

J.A. Stephens, and D. Dill**

[Abstract of a paper published in Physical Review A 31:1968 (1985)]

We show that photoelectron angular distributions in the $2\sigma_u$ channel of N_2 are significantly distorted by continuum-continuum coupling with the f-wave ($l = 3$) shape resonance in the $3\sigma_g$ photoionization channel. This distortion is clearly seen in measured $2\sigma_u$ angular distributions. The effect is demonstrated using K matrix methods to couple the one-electron $2\sigma_u \epsilon \sigma_g$ and $3\sigma_g \epsilon \sigma_u$ $1\Sigma_u^+$ channels. Non-Franck-Condon $N_2^+ B^2\Sigma_u^+$ vibrational branching ratios and vibrationally dependent $2\sigma_u \epsilon \sigma_g$ photoelectron asymmetry parameters are predicted as additional effects.

5.5. PHOTOPHYSICS STUDIES WITH MULTIPHOTON RESONANT ABSORPTION

5.5.1. Summary

The purpose of this program is to develop and use resonantly enhanced multiphoton ionization (REMPI) with mass spectrometry (MS), photoelectron spectrometry (PES), and fluorescence spectrometry to study molecular photophysics and photochemistry at the quantum state specific level. The combination of the highly selective excitation technique and the variety of detection methods results in a powerful approach for the study of basic atomic and molecular physics and chemistry. In general, a tunable "pump" laser is used to excite a target molecule to a resonant intermediate level, and a second (or perhaps a second and a third) independently tunable "probe" laser is used to study the various physical and chemical transformations of the excited state. As an example, the probe laser may lead to ionization of the resonant intermediate state, and the products of the ionization event may be monitored by ion mass analysis or by electron kinetic energy analysis as a function of all pertinent parameters. Alternatively, a delayed probe laser can be used to examine the decay of a selected excited state at variable time intervals after the initial excitation, thus following the internal transformations or decay mechanisms as a function of time. It is also possible to use the probe laser to study the spectra and chemical reactions of fragments (such as free radicals) formed by the action of the pump laser on a

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radical precursor. Often, this is one of the most efficient ways of producing and studying the properties of free radicals.

During the past year, a variety of types of experiments have been performed. Such work includes (1) REMPI-MS studies of the spectroscopy of atomic and molecular excited states and quasibound states that cannot be accessed from the ground electronic state using single-photon excitation techniques; (2) REMPI-PES studies of the photoionization dynamics of excited states; (3) REMPI-MS and REMPI-PES studies of the decay mechanisms of excited states; (4) the production and study of photofragments (particularly fragments such as atomic carbon, sulfur, or iodine that are difficult to produce using conventional techniques) using both REMPI-MS and REMPI-PES; and (5) the production and study of loosely bound van der Waals clusters using both REMPI-MS and REMPI-PES.

5.5.2. Rydberg States of NeXe, ArXe, and KrXe Observed Using Resonantly Enhanced Multiphoton Ionization

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

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The two-photon resonant, three-photon (2+1) ionization spectra of NeXe, ArXe, and KrXe have been determined in the energy region containing the atomic Xe^{*} 5d and 6p states. The spectra display a number of extended molecular band systems that can be attributed to bound-bound and nominally bound-free transitions in the van der Waals molecule. All but two of these band groups occur in the vicinity of an excited atomic Xe state that is allowed via two-photon transitions from the atomic ground state. Thus, the empirical observation from single-photon absorption studies that the most intense van der Waals dimer transitions are to molecular states derived from dipole-allowed atomic dissociation limits also appears to apply to two-photon transitions.

As an example of these spectra, Figure 5.17 shows the (2+1) ionization spectrum of ArXe in the region of the atomic Xe^{*} 6p[1/2]₀ state. Although the spacings between the most intense bands in the ArXe progression in Figure 5.17 are somewhat irregular, these bands have been assigned as a vibrational progression of a single perturbed electronic state, rather than as two or more progressions associated with different electronic states. The irregular spacings can be rationalized if the perturbation is most intense between the $m + 3$ and $m + 4$ bands, pushing the $m + 3$ band to lower energy (making $\Delta G_{m+2}^{(m+2)} + 1/2$ smaller than expected) and pushing the $m + 4$ band to higher energy (making $\Delta G_{m+3}^{(m+3)} + 1/2$ larger than expected). A number of ArXe hot bands with $v'' = 1, 2$ are observed in Figure 5.17. The values for $\Delta G_{1/2}''$ and $\Delta G_{3/2}''$ should be compared with the theoretical values of 24.04 cm^{-1} and 20.72 cm^{-1} , respectively (Bobetic and Barker 1976). Although it is not possible to assign an absolute quantum number to the v' levels of ArXe or to conclusively assign

Figure 5.17. The $(2+1)$ ionization spectrum of ArXe in the region of the atomic Xe $6p[1/2]_0$ state.

the dissociation limit, the observed vibrational progression appears to converge to the $\text{Ar } ^1\text{S}_0 + \text{Xe}^* 6p[1/2]_0$ dissociation limit.

In the wavelength regions near the two-photon allowed atomic Xe transitions, the NeXe, ArXe, and KrXe spectra display a number of similarities, and the interpretation of these spectra is consistent with the prediction that the trend in the dissociation energies for the excited neutral dimer states will follow the trend in the dissociation energies of the corresponding dimer ion states, i.e., $D_0(\text{NeXe}^*) < D_0(\text{ArXe}^*) < D_0(\text{KrXe}^*)$.

5.5.3. Even-Parity Rydberg states of Xe_2 Observed Using Two-Photon Resonant, Three-Photon Ionization

P.M. Dehmer, S.T. Pratt, J.L. Dehmer

The two-photon resonant, three-photon $(2 + 1)$ ionization spectrum of Xe_2 was determined in the energy region containing the atomic Xe $5d$ and $6p$ states. Six prominent bands are observed in the wavelength region 2425–2630 Å. All of the bands correspond to bound-bound transitions. Bands are observed dissociating to each of three two-photon dipole allowed atomic limits; these atomic limits are the $6p[5/2]_2$ level at 78120.30 cm^{-1} , the

$6p[3/2]_2$ level at 79212.97 cm^{-1} , and the $6p[1/2]_0$ level at 80110.47 cm^{-1} . Molecular bands are also observed near the $5d[1/2]_1$ level at 79987.16 cm^{-1} , and the $5d[5/2]_2^0$ level at 81926.04 cm^{-1} . As an example of these bands, Figure 5.18 shows the spectrum of Xe_2 near the $\text{Xe } 6p[3/2]_2$ atomic level; the band positions are given in Table 5.3.

Figure 5.18. The (2+1) ionization spectrum of Xe_2 in the region of the atomic $\text{Xe } 6p[3/2]_2$ level.

Vibrational progressions are observed from both $v'' = 0$ and 1 in the wavelength region 2528–2539 Å. Because of the broad distribution of v' levels, the lowest observed v' level is assigned $v' = m$ and not $v' = 0$. The average value of $\Delta G'_{1/2}$ is 19.8 cm^{-1} . Values of $\Delta G'_{v+1/2}$ were determined for $v' = m$ to $m+7$. Assuming that this molecular state dissociates to $\text{Xe } ^1S_0 + \text{Xe } ^*6p[3/2]_2$, the dissociation energy of the $v' = m$ vibrational level is $D_m = 576.6 \text{ cm}^{-1}$. The average value of $\Delta G'_{v+1} = -2\omega_e x_e$ is -1.1 cm^{-1} ; thus, $\omega_e x_e = 0.6 \text{ cm}^{-1}$. Although neither ω_e nor R_e can be determined from the present data, it is apparent from both the magnitude of the dissociation energy and the broad vibrational distribution that R_e is substantially smaller than R_e of the ground state (4.362 Å).

Transitions to the molecular states of 0_g^+ , 1_g , and 2_g symmetry are derived from this limit and are two photon dipole allowed from the Xe_2 ground state; however, only one prominent band is observed in this energy region. The lower limit to the dissociation energy of 576.6 cm^{-1} suggests a Rydberg state converging to the $B \ ^2\Pi_{3/2g}$ state of the ion. The photoelectron spectra determined on the $(m+2,0)$ and $(m+3,0)$ bands show an intense peak corresponding to transitions that leave the ion in the $B \ ^2\Pi_{3/2g}$ state, with weaker peaks corresponding to the $A \ ^2\Sigma_{1/2u}^+$ and $C \ ^2\Pi_{3/2g}$ states of the ion. Thus, it is quite possible that this state has the $B \ ^2\Pi_{3/2g}$ ion core.

Table 5.3. Bands dissociating to $\text{Xe } ^1\text{S}_0 + \text{Xe}^* 6p[3/2]_2$

v''	v'	Laser Wavelength (Å)	Two Photon Energy (cm^{-1})	$\Delta G_{v''+1/2}$	$\Delta G_{v'+1/2}$				
0	m	2537.38	78821.5		37.9				
	m+1	2536.16	78859.4	19.3	39.2				
	m+2	2534.90	78898.6	19.3	39.3				
	m+3	2533.64	78937.9	20.4	38.3				
	m+4	2532.41	78976.2		35.8				
	m+5	2531.26	79012.0		33.7				
	m+6	2530.18	79045.7	19.9	31.9				
	m+7	2529.16	79077.6	20.0	30.1				
	m+8	2528.20	79107.7						
1	m+1	2536.78	78840.1		39.2				
	m+2	2535.52	78879.3		38.2				
	m+3	2534.29	78917.5						
	m+6	2530.82	79025.8		31.8				
	m+7	2529.80	79057.6						
Unidentified Line		2538.96	78772.4						

v'	=	m	m+1	m+2	m+3	m+4	m+5	m+6	m+7
$\Delta G_{v'+1/2}$	=	37.9	39.2	38.8	38.3	35.8	33.7	31.8	30.1

Dissociation Limit = $\text{Xe } ^1\text{S}_0 + \text{Xe}^* 6p[3/2]_2$									
$D_m = 576.6 \text{ cm}^{-1}$									

5.5.4. Predissociation and Ionization of Excited States of KrXe Observed Using Resonantly Enhanced Multiphoton Ionization -- Photoelectron Spectroscopy

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

[Abstract of a paper published in Chemical Physics Letters 116:245 (1985)]

The photoelectron spectrum of the heteronuclear rare gas dimer KrXe was determined using resonantly enhanced multiphoton ionization--photoelectron spectroscopy (REMPI-PES). The spectrum was obtained without interference from either atomic or homonuclear dimer photoelectron peaks by selectively ionizing KrXe via a resonant intermediate state. In addition to photoelectron peaks due to direct photoionization of the KrXe^* resonant intermediate state, the spectrum shows a number of peaks due to predissociation of the resonant intermediate state followed by photoionization of the excited atomic fragment, i.e., $\text{KrXe}^* \rightarrow \text{Kr} + \text{Xe}^* \rightarrow \text{Kr} + \text{Xe}^+ + e$.

The experiments were performed in two steps. First, the REMPI spectrum was recorded in the region of interest by monitoring the KrXe^+ ion signal as the wavelength of a frequency doubled dye laser was scanned. The laser wavelength was then tuned to the KrXe feature of interest and the KrXe photoelectron spectrum was determined.

The two-photon resonant, three-photon ionization spectrum of KrXe in the region of the atomic $\text{Xe}^* 6p[5/2]_2$ level at 78120.30 cm^{-1} is shown in Figure 5.19. Four intense vibrational bands are observed with (two-photon) energies of 77932.3 , 77963.2 , 77991.0 , and 78017.7 cm^{-1} . The rotational structure is very dense and is not resolved with the present wavelength resolution. The band at 77932.3 cm^{-1} ($2555.33 \text{ \AA}$) is the most intense and is assigned as the $v' = 0 + v'' = 0$ transition.

Figure 5.19. The two-photon resonant, three-photon ionization spectrum of KrXe obtained by monitoring the KrXe^+ ion signal. The peak at $2560.154 \text{ \AA}$ results from two-photon resonant, three-photon ionization of atomic Xe via the $6p[5/2]_2$ state. Ion signal appears at the mass of KrXe^+ as a result of tailing of the very intense Xe^+ mass peak, and is used to calibrate the spectrum.

The photoelectron spectrum shown in Figure 5.20, determined at the wavelength of the KrXe (0,0) band, displays five peaks between 0 and 3 eV. The most intense peak appears at a kinetic energy of 2.438 eV , which is greater than that expected for nonresonant photoionization of atomic Xe , indicating that the peak results from photoionization of KrXe^* to produce a bound state of KrXe^+ . This bound state corresponds to one of only two states

Figure 5.20. Photoelectron spectrum of KrXe following two-photon resonant, three-photon ionization at 2566.33 Å. The calculated positions of photoelectron peaks resulting from (three-photon) non-resonant ionization of ground state xenon atoms and from (single-photon) ionization of excited xenon atoms produced by predissociation of the KrXe* resonant intermediate level are indicated. The adiabatic ionization potential of KrXe, which corresponds to a photoelectron kinetic energy of 2.731 eV, is also indicated.

of KrXe⁺ that dissociates to Kr + Xe⁺ $2P_{3/2}^0$; these states are the A $2\Sigma_{1/2}^+$ ground state, which has a dissociation energy of 0.385 eV, and the B $2\Pi_{3/2}$ excited state, which is weakly bound, although no experimental value for the dissociation energy has been determined.

The four remaining peaks in the photoelectron spectrum result from predissociation of the KrXe* resonant intermediate level to form Kr + Xe* resonant intermediate level to form Kr + Xe*, followed by single-photon ionization of the excited xenon atom. There are only five excited states of Xe* that lie below the energy of the KrXe* resonant intermediate state. The kinetic energies of photoelectron peaks produced by a single-photon ionization of these states may be calculated using the relation $KE = h\nu + E(Xe^*) - IP(Xe^{2P_{3/2}^0})$, where $h\nu$ is the (single-) photon energy, $E(Xe^*)$ is the energy of the excited state of atomic Xe, and $IP(Xe^{2P_{3/2}^0})$ is the ionization potential of Xe. The calculated kinetic energies of these five peaks are indicated in Figure 5.19. The agreement between the calculated and the observed peak positions is excellent, indicating that predissociation of the resonant intermediate level is indeed the mechanism for production of the extra peaks in the photoelectron spectrum. Because the excited atomic fragments are ionized within the 5-ns laser pulse, which in most instances is shorter than both the fluorescence lifetime of the level and the mean collision time, the relative intensities of the photoelectron peaks provide information on the nascent branching ratios of the predissociation process. Qualitatively, the observation of photoelectron peaks following predissociation can be used to

determine the dissociation limits of the predissociating states. Although similar information has been obtained previously on a number of systems using dispersed fluorescence to determine the electronic state of the excited fragment, in some instances fluorescence may be extremely weak or forbidden. In these cases, REMPI-PES provides an alternative technique.

5.5.5. Photoelectron Spectrum of ArXe Obtained Using Resonantly Enhanced Multiphoton Ionization

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

[Abstract of a paper published in *Journal of Chemical Physics* 82:5758 (1985)]

The photoelectron spectrum of the heteronuclear rare gas dimer ArXe was determined using resonantly enhanced multiphoton ionization-photoelectron spectroscopy (REMPI-PES). As in the case of the KrXe photoelectron spectrum discussed in Section 5.5.4., this spectrum was obtained without interference from either atomic or homonuclear dimer photoelectron peaks by selectively ionizing ArXe via a resonant intermediate state. The two-photon resonant, three-photon ionization mass spectrum of ArXe in the region of the atomic Xe $6p[1/2]_0$ level displays a number of irregularly spaced vibronic bands that lie to the red of the atomic transition (Section 5.5.2.) The photoelectron spectrum shown in Figure 5.21 was obtained by exciting one of the most intense of these bands at 2501.88 Å. This band is well separated from all atomic Xe and Xe₂ structure, thus ensuring the selective ionization of ArXe. We assign the 2.776 and 2.864 eV photoelectron peaks to the ArXe⁺ B $2\Pi_{3/2}$ and A $2\Sigma^+_{1/2}$ electronic states, respectively. This results from photoionization of ArXe to

Figure 5.21. Photoelectron spectrum of ArXe following two-photon resonant, three-photon ionization at 2501.88 Å. The calculated positions of photoelectron peaks resulting from three-photon nonresonant ionization of ground state xenon atoms are indicated. The adiabatic ionization potential corresponds to a photoelectron kinetic energy of 2.899 eV. No photoelectrons were observed in the regions between 0.0-1.0 and 1.7-2.2 eV.

produce the $\text{ArXe}^+ \text{B } ^2\Pi_{1/2}$ state, which is the only ionic state that dissociates to $\text{Ar} + \text{Xe}^+ ^2\text{P}_{1/2}^0$ (Dehmer and Pratt 1982).

The kinetic energies of the photoelectron peaks can be used to determine lower limits to the dissociation energies of the $\text{A } ^2\Sigma_{1/2}^+$, $\text{B } ^2\Pi_{3/2}$, and $\text{B } ^2\Pi_{1/2}$ states of ArXe^+ from the relation $D_0(\text{ArXe}^+ ^2\Lambda_J) \geq \text{I.P.}(\text{Xe}^+) - \text{I.P.}(\text{ArXe}^+ ^2\Lambda_J) + D_0(\text{ArXe})$. Here, $\text{I.P.}(\text{Xe}^+)$ is the ionization potential of the appropriate electronic state of atomic Xe [$\text{I.P.}(\text{Xe}^+ ^2\text{P}_{3/2}^0) = 12.130$ eV, $\text{I.P.}(\text{Xe}^+ ^2\text{P}_{1/2}) = 13.436$ eV] (Moore 1949); $\text{I.P.}(\text{ArXe}^+ ^2\Lambda_J)$ is the ionization potential of the appropriate electronic state of ArXe , which is equal to the three-photon energy (14.867 eV) minus the kinetic energy of the photoelectron peak; and $D_0(\text{ArXe})$ is the dissociation energy of the neutral ArXe ground state (0.014 eV) (Bobetic and Barker 1976; Aziz and van Dalen 1983). Thus, $D_0(\text{ArXe}^+ \text{A } ^2\Sigma_{1/2}^+) \geq 0.141 \pm 0.010$ eV, $D_0(\text{ArXe}^+ \text{B } ^2\Pi_{3/2}) \geq 0.053 \pm 0.010$ eV, and $D_0(\text{ArXe}^+ \text{B } ^2\Pi_{1/2}) \geq 0.075 \pm 0.010$ eV.

The dissociation energy of the $\text{A } ^2\Sigma_{1/2}^+$ state has been obtained previously from the observation of the adiabatic ionization potential using (single-photon) photoionization mass spectrometry [$D_0(\text{ArXe}^+ \text{A } ^2\Sigma_{1/2}^+) = 0.176 \pm 0.012$ eV] (see Dehmer and Pratt 1982). It is not surprising that photoionization mass spectrometry yields a larger value for the dissociation energy for the $\text{A } ^2\Sigma_{1/2}^+$ state than does REMPI-PES, since autoionization and chemiionization provide mechanisms for the observation of the adiabatic ionization potential in the former case, whereas only the vertical transition from the resonant intermediate state is probed using REMPI-PES. The dissociation energy of the $\text{B } ^2\Pi_{1/2}$ state has been obtained previously from an extrapolation of a Rydberg series converging to the $\text{B } ^2\Pi_{1/2}$ ionic limit [$D_0(\text{ArXe}^+ \text{B } ^2\Pi_{1/2}) \geq 0.060 \pm 0.003$ eV] (Dehmer and Pratt 1982). The difference between that result and the present REMPI-PES result reflects the difference in the vertical transitions from the ArXe ground state and the ArXe^* resonant intermediate state. In this case, the REMPI-PES value is closer to the true dissociation energy. To our knowledge, the present measurement provides the only experimental information on $D_0(\text{ArXe}^+ \text{B } ^2\Pi_{3/2})$ to date. The remaining small peaks in the photoelectron spectrum result from predissociation of the ArXe^* level to $\text{Ar} + \text{Xe}^*$, followed by single-photon ionization of the excited Xe atom.

5.5.6. Resonantly Enhanced Multiphoton Ionization-Photoelectron Spectroscopy of the Xenon Dimer

P.M. Dehmer, S.T. Pratt, and J.L. Dehmer

Several years ago, photoelectron spectra of the homonuclear rare gas dimers Ar_2 , Kr_2 , and Xe_2 were determined using conventional HeI photoelectron spectroscopy. However, since the rare gas dimer is present in concentrations of only a few percent in the supersonic molecular beam, the HeI photoelectron

spectrum is dominated by photoelectrons from photoionization of the free atom. In the case of Xe_2 , these atomic photoelectron peaks completely or partially obscure three of the six molecular photoelectron bands.

We have recently determined the photoelectron spectrum of Xe_2 using resonantly enhanced multiphoton ionization--photoelectron spectroscopy (REMPI-PES). The spectrum was obtained without interference from atomic photoelectron peaks by selectively ionizing Xe_2 via a number of different resonant intermediate states. The resonant states were all in the region of the $\text{Xe}^* 5d$ and $6p$ excited states. Figure 5.22 shows an example of a HeI-PES and a REMPI-PES of Xe_2 in the region of the $\text{Xe}_2^+ 2P_{3/2}^0$ ionization threshold. This region of the photoelectron spectrum contains transitions to four molecular states. These are the $\text{Xe}_2^+ A^2\Sigma_u^+$, $B^2\Pi_{3/2g}$, $B^2\Pi_{1/2g}$, and $C^2\Pi_{3/2u}$ ionic states. The data of Figure 5.22 show that in the HeI-PES, only two of

Figure 5.22. HeI-PES of Xe and Xe_2 (lower frame) and REMPI-PES of Xe_2 (upper frame).

the molecular bands are clearly observed. In the REMPI-PES, however, all four molecular bands are seen, and there is no evidence of atomic photoelectron peaks. These data are now being analyzed to obtain information on the potential energy curves of the ionic states.

5.5.7. Two-Photon Spectroscopy of np and nf Rydberg States of Atomic Iodine

S.T. Pratt

[Summary of a paper published in Physical Review A 32:928 (1985)]

The two-photon resonant, three-photon ionization spectrum of atomic iodine in the $I^* 2P_{1/2}$ state is presented in the region of the first ionization potential ($I^+ 3P_2$). The $I^* 2P_{1/2}$ state is produced by photodissociation of methyl iodide, and the spectrum obtained between 2605 and 2665 Å is shown in Figure 5.23. An enlargement of the region near the $I^+ 3P_2$ threshold is shown in Figure 5.24.

Because of the large splittings among the I^+ ionic states and the large separation between the neutral $2P_{1/2}$ and $2P_{3/2}$ states, nearly all of the structure in Figures 5.23 and 5.24 can be assigned to two-photon transitions from the $2P_{1/2}$ state to Rydberg states converging to the $3P_2$ ionization limit. Exceptions occur at wavelengths longer than 2644 Å, where several transitions from the $2P_{3/2}$ state to the $(3P_2)7p$ states and from the $2P_{1/2}$

Figure 5.23. Two-photon resonant, three-photon ionization spectrum of atomic iodine between 2605 and 2665 Å. Atomic iodine was produced by the photodissociation of methyl iodide. Note that the top frame has been expanded by a factor of 5.

Figure 5.24. $I^+ 3P_2$ threshold region accessed by two-photon resonant, three-photon ionization of atomic iodine. All of the observed transitions are from the $I^+ 2P_{1/2}$ state to $(3P_2)np$ and $(3P_2)nf$ Rydberg states.

state to the $(3P_1)7p$ states are observed. The only other exception is the peak at 2625.26 Å, which is assigned to the $2P_{1/2} \rightarrow (3P_0)4f[3]_{5/2}$ transition. The $(3P_0)4f[3]_{5/2}$ level is seen to perturb the $(3P_0)nf[3]_{5/2}$ Rydberg series. This effect is further discussed in Section 5.5.14.

In conclusion, two-photon resonant, three-photon ionization of atomic iodine has allowed the first observation of the single-photon forbidden np and nf Rydberg series for $n \approx 15 - 35$.

5.5.8. Autoionizing Rydberg States in Atomic Iodine Using Two-Color Multiphoton Ionization

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

The development of high-power, tunable dye lasers has led to a dramatic increase in the study of high Rydberg states of atoms through the use of multiphoton and multistep excitation. Although the alkali and alkaline earth atoms have been explored in great detail using these techniques, other groups (such as the halogens) remain relatively unstudied. For this reason we have recently performed experiments using two-color resonantly enhanced multiphoton ionization to study the autoionizing Rydberg states of atomic iodine. In these experiments, the first laser was used to produce atomic iodine and to pump it via two-photon transitions to low-lying np Rydberg states. The second

laser was then used to probe transitions from these low-lying states to high-lying states, even parity Rydberg states converging to the excited states of I^+ . These high-lying Rydberg states will autoionize and the transitions are detected by monitoring the I^+ ion signal. For example, by pumping the two photon $2P_{1/2} + (1D_2) 6p[3]_{5/2}$ transition, and then probing single photon transitions from the $(1D_2) 6p[3]_{5/2}$ level to the region surrounding the $I^+ 1D_2$ threshold, we observed $(1D_2)$ ns and nd Rydberg series up to $n > 30$. Although these Rydberg states did autoionize, the line widths were quite small and the peaks were symmetric, indicating a weak coupling to the continuum. By pumping the $(3P_2) 8p[1]_{1/2}$ transition and probing in the same region, one accesses a different set of $(1D_2)$ ns and nd states, due to the angular momentum selection rules. In this case, one of the series was quite broad and asymmetric, while others were again quite sharp. In some cases, the same final states can be accessed from two different pumped states, and in these instances, one expects to observe that the Beutler-Fano lineshape parameter, q , depends on the excitation pathway (Ganz et al. 1984).

5.5.9. Observation of Spin-Forbidden Autoionization in Atomic Sulfur Using Two-Color Multiphoton Ionization

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

We have performed two-color REMPI studies on atomic sulfur. In these experiments, the first laser was used to produce atomic sulfur in the excited $1D_2$ state by photodissociation of carbon disulfide (CS_2) and to pump these excited atoms to the $4p 1F_3$ state via a two photon transition. The second laser was then employed to probe transitions from the $1F_3$ level to the previously unobserved singlet Rydberg states converging to the $2D$ excited state of S^+ . Although these Rydberg states are above the $4S$ ground state of S^+ , they are forbidden to autoionize in an LS coupling scheme. Therefore, the widths and profiles of the observed autoionizing peaks provided new information on the effects of spin-orbit coupling as manifested by the breakdown of LS coupling in open shell atoms. These experiments are of particular interest as they probe relativistic and many-body effects in a theoretically tractable atom.

5.5.10. Two-Photon Spectroscopy of Autoionizing Rydberg States of NO

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

The two-photon ionization spectrum of rotationally cooled nitric oxide (NO) was determined at high resolution in the region between the $NO^+ X 1\Sigma, v^+ = 0$ and two thresholds (2500-2680 Å). The present two-photon ionization

spectrum is completely different than the corresponding single-photon ionization spectrum because of the difference in selection rules for one- and two-photon absorption. In particular, the $n = 7 - 11$ members of two Rydberg series converging to the $\text{NO}^+ X^1\Sigma^+$, $v^+ = 1$ and 2 thresholds were observed and were assigned as previously unobserved members of the nd series. In addition, the $5d v = 2$ band was observed at somewhat lower energy. All of the ne bands showed sharp rotational structure, which is currently being analyzed. Several other bands also were observed, but have not yet been assigned. Thus, two-photon spectroscopy of autoionizing states of NO is shown to provide complementary information to the conventional single-photon studies.

5.5.11. Three-Color Multiphoton Ionization Studies of N_2

S.T. Pratt, P.M. Dehmer, and J.L. Dehmer

We have performed three-color multiphoton ionization studies on N_2 to gain information on the gerade manifold of discrete and autoionizing Rydberg series. In one example of this work, the first laser was used to excite a single rotational level of the $a^1\Pi_g$, $v = 1$ level, via a two-photon transition. The second laser was used to pump the N_2 molecules from this first resonant intermediate level into a single rotational level of the $c'^1\Sigma_g^+$, $v = 0$ level. Finally, the third laser was used to excite autoionizing levels that lie above the first ionization threshold from the second resonant intermediate level. Because the overall process involved four photons, the final state was of gerade (g) symmetry, i.e., the opposite of that reached by single-photon excitation. The third laser was then scanned through a region of the ionization threshold. Because the second laser prepared a single rotational level, scanning the third laser provided information on the autoionizing levels with unprecedented detail. Preliminary data have been taken and show the feasibility of this work. Finally, by varying the second intermediate level ($b^1\Pi_u$, $c^1\Pi_u$, $o^1\Pi_u$, or $c'^1\Sigma_u^+$) we can control the relative intensities of the observed autoionizing level. This work is currently being pursued.

5.5.12. Photoionization of Excited Molecular States Using Multiphoton Excitation Techniques

P.M. Dehmer, S.T. Pratt, and J.L. Dehmer

[Summary of a paper published in Multiphoton Processes, P. Lambropoulos and S. J. Smith (eds.), Springer-Verlag, Berlin (1984)]

Rapid advances in laser and detector technologies have made it possible to investigate molecular photophysics and photochemistry in powerful new ways. For example, resonantly enhanced multiphoton ionization (REMPI) measurements, in which the total (or the mass selected) ion current is monitored as a function of laser wavelength, have yielded extensive and often novel information on the spectroscopy of the resonant intermediate states. With the

addition of photoelectron spectrometry (PES) to analyze the kinetic energy of the ejected electrons, it is possible to determine the branching ratios into different electronic, vibrational, and rotational levels of the product ion and to focus directly on both the dynamics of the multiphoton ionization process and the photoionization of excited state species. Several recent REMPI/PES studies of H_2 (Pratt et al. 1983, 1984a) and N_2 (Pratt et al. 1984b, 1984c) reflect both the spectroscopy and the dynamics of photoionization of excited molecular states. The results are discussed in terms of the selection rules for photoionization and the relative probabilities of photoionization from Rydberg and valence states. In some cases, in accordance with the Franck-Condon principle, the results demonstrate that resonant multiphoton ionization through Rydberg states may be a powerful technique for the production of electronic, vibrational, and rotational state selected ions. However, in other cases, systematic departures from Franck-Condon behavior are observed, which reflect the more subtle dynamics of excited state photoionization.

5.5.13. Testing a New "Magnetic Bottle" Electron Spectrometer

J.L. Dehmer, P.M. Dehmer, and S.T. Pratt

The magnetic bottle electron spectrometer, shown schematically in Figure 5.25, is a high-resolution, high-collection efficiency spectrometer, originally designed by Kruit and Read (1983) at the FOM Institute in Amsterdam. We have acquired a copy of the original prototype instrument for use in multiphoton ionization studies at Argonne. The spectrometer consists of an ionization region, a magnetic lens that parallelizes electrons with different ejection angles, a 50-cm flight tube, and a channel-plate detector. Any electron produced in the ionization region with a finite velocity component in the direction of the detector is transported down the spectrometer axis. Because of the magnetic parallelization of the electron paths, the transit time to the detector is independent of the forward velocity component to an accuracy of better than 1% for a 10-eV electron. Hence, the instrument combines extremely high acceptance (~ 50%) with the high resolution of a time-of-flight device. Another salient aspect of this approach is that the acceleration/deceleration of electrons in the weak magnetic field in the flight tube introduces no lens effect, such as that occurring in purely electrostatic lenses. Accordingly, electrostatic retardation can be used to lengthen flight times, thereby improving energy resolution without altering the constant 50% transmission of the device. At FOM, a constant energy resolution of 15 meV was obtained for electron energies in the range 0-10 eV. The main limiting factor was believed to be electrical noise on the cylindrical retarding electrode in the flight tube. We believe this can be effectively eliminated, resulting in ultrahigh energy resolution in the few meV range--even for electron kinetic energies as high as 10 eV. This combination of resolving power, collection efficiency, kinetic energy range, and constant transmission makes this a very important instrumental approach, capable of extending the scope of the field.

Figure 5.25. Schematic diagram of the magnetic bottle electron spectrometer showing: (1) ionization region; (2) laser beam; (3) water-cooled energizing coil; (4) drift tube; (5) retarding grid; (6) channel plate electron detector; and (7) flange for mounting in vacuum chamber.

Use of the magnetic bottle electron spectrometer will result in a data collection rate for high-resolution electron spectra that will be approximately three orders of magnitude greater than that of our current instrument. This means that it will be possible to rapidly obtain high-resolution (15 meV or better) photoelectron spectra as a function of wavelength, which then permits a number of new types of studies that are not possible with the current slow data acquisition rates. In particular, it will be possible to obtain photoelectron branching ratios as a function of the rotational level of the resonant intermediate level, thus permitting detailed observation of perturbations of the resonant level. It should also be possible to obtain

photoelectron spectra as a function of laser wavelength within autoionizing resonances in the ionization continuum, thus permitting detailed tests of theory and greater insight into autoionization phenomena. We envision this instrument as a powerful, high-resolution, general purpose tool. Assembly and initial testing of the new instrument are now complete.

5.5.14. Photoelectron Spectroscopy of Rydberg States of Atomic Iodine

S.T. Pratt

[Summary of an article published in Physical Review A 33:1718 (1986)]

Some of our recent studies using resonantly enhanced multiphoton ionization-photoelectron spectroscopy (REMPI-PES) have shown that ionization into a structureless continuum via an unperturbed Rydberg state usually proceeds by the ejection of the Rydberg electron without a change in the electronic or vibrational state of the ion core. Thus, in many instances REMPI can be used as a source of state-selected ions. However, the results can be quite different if the resonant intermediate level is perturbed, because the character of the unperturbed level will then be mixed with that of the perturbing level. If the two interacting levels have different ion cores, the perturbation is revealed in the photoelectron branching ratios following REMPI. In this work, REMPI-PES is used to study a perturbation in the odd parity Rydberg series of atomic iodine and to determine the feasibility of producing state-selected I^+ ions using REMPI. It is shown that while state-selected ions can be produced in some cases, the state-selecting capability of REMPI is dramatically reduced for perturbed levels. For example, in Figure 5.26 the photoelectron spectra obtained via the $(^3P_2)nf[3]_{5/2}$ levels show the effect of a perturbation by the $(^3P_2)4f[3]_{5/2}$ level, as both $I^+ ^3P_2$ and 3P_0 are observed. As a general principle, it is worth remembering that most of the oscillator strength into the ionization continuum is concentrated near threshold in an energy region corresponding to a few multiples of the binding energy of the ionized level. Thus, in general, for high Rydberg levels, the ionization cross section with an ultraviolet photon will be quite small, and perturbations by a low-lying Rydberg level converging to a higher ionization potential (i.e., a level with a larger binding energy) can have dramatic effects on the photoelectron branching ratios.

As a consequence of the small ionization cross sections of the Rydberg levels in the present experiments, two processes are observed that compete with REMPI. The first involves fluorescence of the resonant intermediate level to a lower-lying level, which is then ionized with greater efficiency, and the second involves energy transfer (either collisional or radiative) between $I^* ^2P_{1/2}$ atoms and the Rydberg atoms. Although these two processes would be indistinguishable from direct REMPI using mass spectrometric techniques alone, the use of REMPI-PES allows the separation of the contributions of these different mechanisms and provides a more complete understanding of the overall process.

Figure 5.26. The photo-electron spectra of atomic iodine obtained following two-photon resonant, three-photon ionization via the $(^3P_0)4f[3]_{5/2}$, $(^3P_2)15f[3]_{5/2}$, $(^3P_2)14f[3]_{5/2}$, and $(^3P_2)11f[3]_{5/2}$ levels.

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APPENDICES FOR CHAPTER 5
Fundamental Molecular Physics and Chemistry

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APPENDIX 5-A. STAFF QUALIFICATIONS
Fundamental Molecular Physics and Chemistry Program

Name	Position	Highest Degree	Major	Year Received	Institution
Dehmer, Joseph L.	Senior Physicist	Ph.D.	Chemical Physics	1971	University of Chicago
Dehmer, Patricia M.	Senior Chemist	Ph.D.	Chemical Physics	1972	University of Chicago
Dillon, Michael A.	Physicist	Ph.D.	Physical Chemistry	1965	University of Notre Dame
Inokuti, Mitio	Senior Physicist	Ph.D.	Applied Physics	1962	University of Tokyo
Pratt, Stephen T.	Chemist	Ph.D.	Chemistry	1982	Yale University
Spence, David	Physicist	Ph.D.	Physics	1967	University of Newcastle-Upon-Tyne

APPENDIX 5-B. OUTSTANDING PROFESSIONAL ACTIVITIES AND AWARDS

- J.L. DEHMER--Member, Editorial Board, The Journal of Chemical Physics, 1983-1985; Member, National Research Council Committee on Atomic and Molecular Sciences, 1983-1986; Member (1984), Chairman (1985), Department of Energy Review Committee, Department of Chemistry, Brookhaven National Laboratory; Member, Nominating Committee, Division of Electron and Atomic Physics, American Physical Society, 1984; Vice-Chairman (1983-1984), Chairman (1985-1986) Gordon Research Conference on Electron Spectroscopy.
- P.M. DEHMER--Member, Executive Committee, American Physical Society Division of Electron and Atomic Physics, 1979, 1981-1984; Member, Program Committee, American Physical Society Division of Electron and Atomic Physics, 1980, 1982-1984; Secretary-Treasurer, American Physical Society Division of Electron and Atomic Physics, 1981-1984; Chairperson, Committee on Bylaws, American Physical Society Division of Electron and Atomic Physics, 1984; Member, American Physical Society Committee on Opportunities in Physics, 1984-1986; Member, Program Committee, International Laser Science Conference, 1985; Member, Editorial Board, Review of Scientific Instruments, 1985-1987; Member, Subcommittee for Presidential Young Investigator, Physics Division, National Science Foundation, 1985; selected one of the 100 Most Outstanding Young Scientists in the United States by Science Digest Magazine, 1984; Vice-Chairman (1983-1984), Chairman (1985-1986), Gordon Research Conference on Multiphoton Processes; Organizer, Symposium on Multiphoton Ionization and Dissociation, International Laser Science Conference, 1985; elected Fellow of the American Physical Society, 1984.
- M. INOKUTI--Member of the International Commission of Radiation Units and Measurements (ICRU), 1985-1989; Member of the Science and Technical Talent Pool, Committee on Interagency Radiation Research and Policy Coordination (CIRRPC), 1985; Associate Member, Local Organizing Committee for the Tenth International Conference on Atomic Physics, August 1986, Tokyo, Japan.
- S.T. PRATT--awarded the Argonne National Laboratory Pacesetter Award in July 1985.

APPENDIX 5-C. SPECIAL EVENTS ORGANIZED

P.M. DEHMER, program organizer, Fifteenth Meeting of the Division of Electron and Atomic Physics, the American Physical Society, 30 May - 1 June 1984, Storrs, CT.

M. INOKUTI--organized DOE Radiological Physics Contractors' Meetings, 18-21 June 1984, Argonne National Laboratory.

APPENDIX 5-D. EDUCATIONAL PROGRAM PARTICIPANTS

DAVID DeMILLE. University of Chicago. Undergraduate Research Program. Conducted research in electron-collision physics. June 1984 - August 1984.

JANET SEGER. Grinnell College. Undergraduate Research Program. Conducted research in electron-collision physics. June 1984 - August 1984.

KENNETH LANIK. Bates College. Undergraduate Research Program. Conducted research in electron-collision physics. June 1985 - August 1985.

HIROSHI TANAKA. Visiting Foreign Scholar, Departments of General Sciences and Physics, Faculty of Science and Technology, Sophia University, Tokyo, Japan

R.-G. WANG. Visiting Foreign Scholar, Department of Physics, Chengdu University of Science and Technology, Chengdu, Sichuan, People's Republic of China

Z.-W. WANG. Visiting Foreign Scholar, Institute of Atomic and Molecular Physics, Jilin University, Changchun, People's Republic of China.

APPENDIX 5-E. PUBLICATIONS AND ORAL PRESENTATIONS
Fundamental Molecular Physics and Chemistry Program

1. Refereed Journal Articles*

1984

Dehmer, J.L., A.C. Parr, S.H. Southworth and D.M.P. Holland. Angle-resolved photoelectron study of the valence levels of BF_3 in the range $17 \leq h\nu \leq 28$ eV. *Physical Review A* 30:1783-1790 (1984). [DOE/OHER, DOD/ONR]**

Dehmer, P.M. Photoionization of OH in the region 750-950Å. *Chemical Physics Letters* 110(1):79-84 (1984). [DOE/OHER, DOD/ONR]

Dehmer, P.M., P.J. Miller and W.A. Chupka. Photoionization of $\text{N}_2 \text{ X } ^1\Sigma_g^+$, $v'' = 0$ and 1 near threshold. Preionization of the Worley-Jenkins Rydberg series. *Journal of Chemical Physics* 80:1030-1038 (1984). [DOE/OHER]

Dillon, M.A., R.-G. Wang and David Spence. Electron impact spectroscopy of methane and methane- d_4 . *Journal of Chemical Physics* 80:5581-5588 (1984). [DOE/OHER]

Holland, D.M.P., A.C. Parr and J.L. Dehmer. Photoelectron branching ratios and asymmetry parameters for the two outermost molecular orbitals of hydrogen cyanide. *Journal of Physics B* 17:1343-1352 (1984). [DOE/OHER, DOD/ONR]

Holland, D.M.P., A.C. Parr and J.L. Dehmer. Photoelectron branching ratios and asymmetry parameters of the two outermost molecular orbitals of methyl cyanide. *Journal of Electron Spectroscopy and Related Phenomena* 34:87-96 (1984). [DOE/OHER, DOD/ONR]

*For published material, the names of all Environmental Research Division authors are underlined. [Included are Division members who participated in a project but left the Division before the results were published.]

**Funding agency (abbreviations are spelled out at the end of this appendix). In cases where no funding agency is listed, the publication was not related to any specific funded project.

Inokuti, M. Series of articles entitled "Lectures on the oral presentation of physics papers" in Kotai Butsuri (Solid State Physics), a Japanese journal: I: Vol. 18, pp. 240-241 (April 1983); II: Vol. 18, pp. 357-358 (June 1983); III: Vol. 18, pp. 421-422 (July 1983); IV: Vol. 18, pp. 481-482 (August 1983); V: Vol. 18, pp. 550-551 (September 1983); VI: Vol. 18, pp. 779-780 (December 1983); VII: Vol. 19, pp. 45-47 (January 1984); VIII: Vol. 19, pp. 361-363 (June 1984); IX: Vol. 19, pp. 427-428 (July 1984); X: Vol. 19, pp. 548-549 (September 1984).

Parr, A.C., S.H. Southworth, J.L. Dehmer and D.M.P. Holland. High-resolution angle-resolved photoelectron spectrometer system. Nuclear Instruments and Methods 222:221-229 (1984). [DOE/OHER, DOD/ONR]

Poliakoff, E.D., J.L. Dehmer, A.C. Parr and G.E. Leroi. Fluorescence excitation studies of molecular photoionization in external electric fields. Chemical Physics Letters 111:128-132 (1984). [DOE/OHER, DOD/ONR]

Pratt, S.T., P.M. Dehmer and J.L. Dehmer. State selection by resonant multiphoton ionization: $N_2^+ A^2\Pi_u, v^+$. Journal of Chemical Physics 80:1706-1708 (1984). [DOE/OHER, DOD/ONR]

Pratt, S.T., P.M. Dehmer and J.L. Dehmer. Photoionization of excited molecular states $H_2C^1\Pi_u$. Chemical Physics Letters 105(1):28-33 (1984). [DOE/OHER, DOD/ONR]

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Spence, David, R.H. Huebner, H. Tanaka, M.A. Dillon and R.-G. Wang. Electronic structure of Cl_2 from 5 to 15 eV by electron energy loss spectroscopy. Journal of Chemical Physics 80:2989-2996 (1984). [DOE/OHER]

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Kosman, W.M. and S. Wallace. Complete dipole oscillator strength distribution and its moments for N_2 . Journal of Chemical Physics 82:1385-1395 (1985). [DOE/OHER]

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Wang, Z.-W. and K.T. Lu. Eigenchannel quantum-defect theory of open-shell atoms. II. Calculation of $3p^4(^3P)ns$ Rydberg spectra of the chlorine atom. Physical Review A 31:1521-1528 (1985). [DOE/OHER]

2. Books, Book Chapters, and Collections of Conference Proceedings

1984

Berger, M.J., H.H. Anderson, H. Bichsel, J.A. Dennis, M. Inokuti, D. Powers, S.M. Seltzer and J.E. Turner. Stopping Powers for Electrons and Positrons. Report 37. International Commission on Radiation Units and Measurements, Washington, DC. October 1984. 271 pp. [DOE/OHER]

Dehmer, J.L. Shape resonances in molecular fields. In: Resonances in Electron-Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics. ACS Symposium Series, Vol. 263. D.G. Truhlar, ed., American Chemical Society, Washington, D.C.; 1984. pp. 139-163. [DOE/OHER, DOD/ONR]

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1984

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5. Published Abstracts, Notes, Reviews, Comments, and Letters

1984

Dehmer, J.L., P.M. Dehmer and S.T. Pratt. Photoelectron studies of excited molecular states. H_2 $C^1\Pi_u$ and N_2 $o_3^1\Pi_u$ (Abstract). In: Advance Program, XIII International Conference on Quantum Electronics, 18-21 June 1984, Anaheim, CA. p. 44. [DOE/OHER, DOD/ONR]

Dehmer, J.L. Resonant processes in molecular photoionization (Abstract). VIII Conference on the Applications of Accelerators in Research and Industry, 12-14 November 1984, Denton, TX, Bulletin of the American Physical Society 29:1089 (1984). [DOE/OHER, DOD/ONR]

Dehmer, J.L. Shape resonances in molecular fields (Abstract). National Meeting of American Chemical Society, 8-13 April 1984, St. Louis, MO, Book of Abstracts, Phys.-2 (1984). [DOE/OHER, DOD/ONR]

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- Eggarter, E. and M. Inokuti. Book Review of: Absorption of Ionizing Radiation, by David W. Anderson (University Park Press, Baltimore, MD, 1984). Radiation Research 102:148-150 (1985). [DOE/OHER]
- Inokuti, M. Platzman. A man of culture and thought. Hoshasen Kaguka (Radiation Chemistry) (in Japanese) 40:2-4 (1985). [DOE/OHER]
- Inokuti, M. Book review of: Modern Quantum Mechanics, by J.J. Sakurai, edited by S.F. Tuan (Benjamin/Cummings, Menlo Park, California, 1985), Butsuri (Bulletin of the Physical Society of Japan 40:812-813 [1985]). [DOE/OHER]
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Spence, D., R.-G. Wang and M.A. Dillon. Electron impact spectroscopy of silane and germane (Abstract). In: Fourteenth International Conference on the Physics of Electronic and Atomic Collisions, Palo Alto, CA, 24-30 July 1985, Palo Alto, CA, Book of Abstracts, p. 85. [DOE/OHER]

6. Oral Presentations*

1984

Dehmer, J.L. Photoionization dynamics of selectively excited molecular states. Presented at Chemical Physics Seminar, California Institute of Technology, 14 February 1984, Pasadena, CA. [Faculty and students]** [DOE/OHER, DOD/ONR]

Dehmer, J.L. Photoionization dynamics of selectively excited molecular states. Presented at Chemical Physics Seminar, University of Southern California, 16 February 1984, Los Angeles, CA. [Faculty and students] [DOE/OHER, DOD/ONR]

Dehmer, J.L. Shape resonances in molecular fields. Presented Symposium on Resonances in Electron-Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics, National American Chemical Society Meeting, 8-13 April 1984, St. Louis, MO. [Scientists] [DOE/OHER, DOD/ONR]

Dehmer J.L. Advanced techniques for electron energy analysis and ion mass analysis following resonantly enhanced multiphoton ionization. Presented at DOE/OHER Workshop on Chemical Measurement Needs in Energy-Related Health and Environmental Research, 16 May 1984, Battelle Seattle Research Center, Seattle, Washington. [DOE contractors] [DOE/OHER]

Dehmer, J.L., P.M. Dehmer, and S.T. Pratt. Resonantly enhanced multiphoton ionization of molecules. Presented at DOE/OHER, BES contractor's meeting on Advanced Laser Technology for Chemical Measurements, 23-25 October 1984, Brookhaven National Laboratory, Long Island, NY. [DOE contractors] [DOE/OHER]

*For oral presentations, the person who made the presentation is underlined.
**Audience for the presentation.

- Dehmer, J.L. Triply differential photoelectron studies of resonant processes in molecular photoionization. Presented at VIII Conference on the Applications of Accelerators in Research and Industry, 12-14 November 1984, Denton, TX. [Scientists] [DOE/OHER, DOD/ONR]
- Dehmer, J.L. Molecular photoionization dynamics - progress and prospects. Presented at Physics Colloquium, University of Oregon, 29 November 1984, Eugene, OR. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]
- Dehmer, P.M., S.T. Pratt, and J.L. Dehmer. Photoionization of excited molecular states using multiphoton excitation techniques. Presented at Second Topical Meeting on Laser Techniques in the Extreme Ultraviolet, Air Force Office of Scientific Research and Optical Society of America, 5-7 March 1984, Boulder, CO. [Scientists] [DOE/OHER, DOD/ONR]
- Dehmer, P.M., P.J. Miller and W.A. Chupka. Photoionization of vibrationally excited N_2 . Presented at Fifteenth Meeting of the Division of Electron and Atomic Physics, the American Physical Society, 30 May - 1 June 1984, Storrs, CT. [Scientists] [DOE/OHER, DOD/ONR]
- Dehmer, P.M. Photoionization of the hydroxyl radical. Presented at Fifteenth Meeting of the Division of Electron and Atomic Physics, the American Physical Society, 30 May - 1 June 1984, Storrs, CT. [Scientists] [DOE/OHER, DOD/ONR]
- Dehmer, P.M. Multiphoton ionization as a probe of electronic structure of small molecules. Presented at Gordon Research Conference on Visible/UV Multiphoton Ionization and Dissociation, Colby-Sawyer College, 15 June 1984, New London, NH. [Scientists] [DOE/OHER, DOD/ONR]
- Dehmer, P.M. Photoionization of excited molecular states. Presented at Third International Conference on Multiphoton Processes, 5 September 1984, Iraklion, Crete (Greece). [Scientists] [DOE/OHER, DOD/ONR]
- Dehmer, P.M. Interaction of discrete and continuum states. Presented at Physical Chemistry Seminar, 25 October 1984, Indiana University, Bloomington, Indiana. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]
- Dehmer, P.M. Interaction of discrete and continuum states. Presented at the Chemical Physics Institute Seminar, University of Oregon, 30 November 1984, Eugene, OR. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]
- Dillon, M.A., R.-G. Wang and David Spence. Electron impact spectroscopy of methane and methane- d_4 . Presented at Fifteenth Meeting of the Division of Electron and Atomic Physics, the American Physical Society, 30 May - 1 June, 1984, Storrs, CT. [Scientists] [DOE/OHER]

Dillon, M.A., Z.-W. Wang and M. Inokuti. Analytic representation of the generalized oscillator strength for ionization. Presented at the National Conference on Atomic and Molecular Physics, 23-26 October 1984, Fudan University, Shanghai, China. [Scientists, faculty, students] [DOE/OHER]

Inokuti, M. Formulation of a variational principle for a given quantity. Presented at Technological Institute, Northwestern University, 5 April 1984, Evanston, IL. [Graduate students] [DOE/OHER]

Inokuti, M. What formulas are good for representing dipole and generalized oscillator-strength spectra? Seminar presented at Oak Ridge National Laboratory, 9 August 1984, Oak Ridge, TN. [Scientists] [DOE/OHER]

Inokuti, M. and M.A. Dillon. What formulas are good for representing dipole and generalized oscillator spectra? Presented at the XIIth Yugoslav Summer School and International Symposium on Physics of Ionized Gases, 3-7 September 1984, Sibenik, Yugoslavia. [Scientists] [DOE/OHER]

Inokuti, M. Presented a series of lectures in China with the following titles: (1) Distribution of the oscillator strength over the entire range of excitation energy for atoms, molecules, and solids, (2) The Bethe theory of inelastic collisions of fast charged particles with atoms and molecules, and (3) Topics from radiation physics. These lectures were presented at the following places and times: (1) Institute of Physics, Chinese Academy of Sciences, Beijing, 11 October 1984; Chengdu University of Science and Technology, Chengdu, 17-19 October 1984; and Chinese Academy of Sciences, Institute of Nuclear Research, Shanghai, 25 October. (2) Institute of Physics, Chinese Academy of Sciences, Beijing, 12 October 1984, and Chengdu University of Science and Technology, Chengdu, 20, 22 October. (3) Graduate School of Physics, Chinese Academy of Sciences, Beijing, 10 October 1984; Department of Physics, Beijing University, Beijing, 12 October 1984; Chengdu University of Science and Technology, Chengdu, 23 October 1984; and Chinese Academy of Sciences, Institute of Nuclear Research, Shanghai, 26 October 1984. [Scientists, faculty, and students] [DOE/OHER]

Inokuti, M. What formulas are good for representing dipole and generalized oscillator-strength spectra? Presented at the National Conference on Atomic and Molecular Physics, 23-26 October 1984, Fudan University, Shanghai, China. [Scientists, faculty, students] [DOE/OHER]

Naleway, C.A., M. Inokuti and M.C. Sauer, Jr. A theoretical study of excited-state formation due to sub-excitation electrons in rare-gas-nitrogen mixtures. Presented at 32nd Annual Meeting, Radiation Research Society, 26-29 March 1984, Orlando, FL. [Scientists] [DOE/OHER]

Pratt, S.T., P.M. Dehmer and J.L. Dehmer. Photoelectron studies of resonant multiphoton ionization of H_2 and N_2 . Presented at Fifteenth Meeting of the Division of Electron and Atomic Physics, The American Physical Society, 30 May - 1 June 1984, Storrs, CT. [Scientists] [DOE/OHER, DOD/ONR]

Pratt, S.T. Multiphoton ionization as a probe of excited state photoionization Dynamics. Presented at Chemistry Department Seminar, University of Nevada, 13 January 1984, Reno, NV. [Scientists] [DOE/OHER]

Pratt, S.T. Survey of recent multiphoton ionization studies using electron spectroscopy. Presented at Gordon Research Conference on Electron Spectroscopy, 16 July 1984, Wolfeboro, NH. [Scientists] [DOE/OHER, DOD/ONR]

Southworth, S.H., A.C. Parr, J.L. Dehmer and D.M.P. Holland. Angle-resolved photoelectron study of the valence levels of BF_3 . Presented at Fifteenth Meeting of the Division of Electron and Atomic Physics, the American Physical Society, 30 May - 1 June, 1984, Storrs, CT. [Scientists] [DOE/OHER, DOD/ONR]

Spence, David, R.-G. Wang and M.A. Dillon. Rydberg structure of mercuric halides by electron impact. Presented at Fifteenth Meeting of the Division of Electron and Atomic Physics, the American Physical Society, 30 May - 1 June 1984, Storrs, CT. [Scientists] [DOE/OHER]

1985

Dehmer, J.L., P.M. Dehmer and S.T. Pratt. Photoelectron spectra of Xe_2 using resonantly enhanced multiphoton ionization. Presented at the Sixteenth Meeting of the Division of Electron and Atomic Physics, 29-31 May 1985, Norman, OK. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]

Dehmer, J.L. Dynamics of photoelectron escape from molecular fields. Presented at Physics Colloquium, Los Alamos National Laboratory, 6 June 1985, Los Alamos, NM. [Scientists] [DOE/OHER, DOD/ONR]

Dehmer, J.L. Dynamics of photoelectron escape from molecular fields. Presented at Chemical Physics Seminar, Institute for Physical Science and Technology, University of Maryland, 25 June 1985, University Park, MD. [Scientists, graduate students] [DOE/OHER, DOD/ONR]

Dehmer, P.M. Spectroscopy and dynamics of excited molecular states using multiphoton techniques. Presented at the Sixteenth Meeting of the Division of Electron and Atomic Physics, 29-31 May 1985, Norman, OK. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]

Dehmer, P.M., J.L. Dehmer and S.T. Pratt. Electronic spectra of NeXe, ArXe, and KrXe using resonantly enhanced multiphoton ionization. Presented at the Sixteenth Meeting of the Division of Electron and Atomic Physics, 29-31 May 1985, Norman, OK. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]

Dehmer, P.M., J.L. Dehmer and S.T. Pratt. Resonantly enhanced multiphoton ionization and photoelectron spectroscopy of NeXe, ArXe, KrXe, and Xe₂. Presented at Fourteenth International Conference on the Physics of Electronic and Atomic Collisions, 24-30 July 1985, Palo Alto, CA. [Scientists] [DOE/OHER]

Dehmer, P.M., J.L. Dehmer and S.T. Pratt. Two photon spectroscopy of autoionizing levels of nitric oxide. Presented at the First International Laser Science Conference, American Physical Society, 18-22 November 1985, Dallas, TX. [Scientists] [DOE/OHER, DOD/ONR]

Dillon, M.A., M. Inokuti and Z.-W. Wang. Analytic representation of the generalized oscillator strength for ionization. Presented at Thirty-third Annual Scientific Meeting, Radiation Research Society, 5-9 May 1985, Los Angeles, CA. [Scientists] [DOE/OHER]

Dillon, M.A., H. Tanaka and D. Spence. Energy loss spectroscopy of xenon difluoride. Presented at the Thirty-eighth Annual Gaseous Electronics Conference, Naval Postgraduate School, 15-18 October 1985, Monterey, CA. [Scientists] [DOE/OHER]

Eggarter, E. and M. Inokuti. Theory of initial yields of ionization in binary mixtures. Presented at Thirty-third Annual Scientific Meeting, Radiation Research Society, 5-9 May 1985, Los Angeles, CA. [Scientists] [DOE/OHER]

Eggarter, E. Theory of initial yields of ionization in binary mixtures. Presented at Radiation and Photochemistry Seminar, Argonne National Laboratory, 6 August 1985, Argonne, IL. [Scientists] [DOE/OHER]

Inokuti, M. Distribution of oscillator strengths over the entire range of excitation energy for atoms, molecules, and solids. Presented at Special Chemical Physics Seminar, Department of Chemistry, University of British Columbia, 28 January 1985, Vancouver, British Columbia. [Students, faculty, scientists] [DOE/OHER]

Inokuti, M. What formulae are good for representing the oscillator-strength distribution and related quantities? Presented at Special Chemical Physics Seminar, Department of Chemistry, University of British Columbia, 29 January 1985, Vancouver, British Columbia. [Students, faculty, scientists] [DOE/OHER]

- Inokuti, M. Analysis of initial processes in radiation physics and chemistry. Presented at Department of Physics Seminar, Atlanta University, 13 February 1985, Atlanta, GA. [Faculty, students, scientists] [DOE/OHER]
- Inokuti, M. Physics of electron slowing-down processes. Presented at The Miller Conference, 15-19 April 1985, Bowness-on-Windermere, Cumbria, England. [Scientists] [DOE/OHER]
- Inokuti, M. Topics in the physics of the energy absorption from ionizing radiation to complex media. Invited lecture presented at the Gordon Research Conference on Radiation Chemistry of Macromolecules, 12-16 August 1985, Plymouth, NH. [Scientists] [DOE/OHER]
- Inokuti, M. Analysis of energy deposition on matter by ionizing radiation. Seminar presented to Medical Research Council Group of Radiation Science, Faculty of Medicine, University of Sherbrooke, 19 August 1985, Sherbrooke, Quebec, Canada. [Faculty] [DOE/OHER]
- Inokuti, M. Cross sections for inelastic collisions of fast charged particles with atoms and molecules. Presented at the IAEA Advisory Group Meeting on Nuclear and Atomic Data for Radiotherapy and Radiobiology, 16-20 September 1985, Rijswijk, The Netherlands. [Scientists] [DOE/OHER]
- Inokuti, M. VUV absorption and its relation to the effects of ionizing corpuscular radiation. Presented at U.S.-Japan Joint Seminar on Ultraviolet Photobiology and Spectroscopy Using Synchrotron Radiation, Brookhaven National Laboratory, 2-5 October 1985, Upton, Long Island, NY. [Scientists] [DOE/OHER]
- Inokuti, M. Proposal for a general science course. Colloquium talk presented at Department of General Science, Sophia University, 28 November 1985, Tokyo, Japan. [Faculty members] [DOE/OHER]
- Inokuti, M. Cross-section data needed in radiation therapy and biology. Seminar presented at the Tokyo Office, Japan Atomic Energy Research Institute, 26 December 1985, Tokyo, Japan. [Scientists] [DOE/OHER]
- Pratt, S.T., P.M. Dehmer and J.L. Dehmer. Multiphoton studies of highly excited states of atomic iodine. Presented at Fourteenth International Conference on the Physics of Electronic and Atomic Collisions, 24-30 July 1985, Palo Alto, CA. [Scientists] [DOE/OHER]
- Pratt, S.T., P.M. Dehmer and J.L. Dehmer. Photoionization and predissociation of excited states of NeXe, ArXe, KrXe, and Xe₂. Presented at the First International Laser Science Conference, American Physical Society, 18-22 November 1985, Dallas, TX. [Scientists] [DOE/OHER, DOD/ONR]

Southworth, S.H., J.L. Dehmer, A.C. Parr and J.E. Hardis. Channel-coupling and shape-resonance effects in the photoelectron dynamics of N_2 and NO. Presented at the Sixteenth Meeting of the Division of Electron and Atomic Physics, 29-31 May 1985, Norman, OK. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]

Southworth, S.H., A.C. Parr, J.L. Dehmer, J.E. Hardis and D.M.P. Holland. Calibration of a monochromator/spectrometer system for the measurement of photoelectron angular distributions and branching ratios. Presented at the Synchrotron Radiation Instrumentation Conference, 2 August 1985, Stanford University. [Scientists, faculty, students] [DOE/OHER, DOD/ONR]

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DOD = U.S. Department of Defense
ONR = Office of Naval Research
U of C = University of Chicago
OFE = Office of Fossil Energy (in DOE)

CHAPTER 5. FUNDAMENTAL MOLECULAR PHYSICS AND CHEMISTRY

CHAPTER 6. WASTE MANAGEMENT PROGRAM

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5.1 PROGRAM OVERVIEW

P. Merry-Libby (Acting Program Manager)

The mission of the Waste Management Program is to conduct programmatic, generic, and site-specific analyses of systems for management of radioactive and hazardous wastes. The program's scientists and engineers are experienced in analyzing environmental impacts from production facilities (such as uranium mills), storage of fuel and wastes, waste treatment, transport, and disposal. They are knowledgeable about current waste management practices and regulatory requirements, as well as alternative technologies. Staff input to decision makers includes assessment of the technical, environmental, risk, economic, and sociological aspects of waste management systems.

During 1984-1985, the Waste Management Program continued to provide support to the U.S. Department of Energy (DOE), U.S. Army, and U.S. Nuclear Regulatory Commission (NRC). Major funding continues to come from two of DOE's remedial action activities: the Formerly Utilized Sites Remedial Action Program (FUSRAP) and the Surplus Facilities Management Program (SFMP). Efforts continue in two major areas: (1) site-specific assessments of cleanup, storage, and disposal alternatives and (2) development of state-of-the-art procedures for deriving cleanup guidelines from site-specific pathway analysis. Two major sites for which Environmental Impact Statements (EISs) are being prepared are the Niagara Falls Storage Site near Buffalo, New York, and the Weldon Spring site near St. Louis, Missouri.

Other DOE work during 1984-1985 included preparation of a handbook for DOE's Low-Level Waste Management Program (LLWMP) on greater confinement disposal for low-level radioactive wastes that may need confinement by means other than standard shallow land burial. In addition, a Draft EIS was prepared on a new Central Waste Disposal Facility for DOE's Oak Ridge Reservation.

Work was completed in 1985 on the evaluation of alternatives for restoring groundwater that has been contaminated as a result of past operations at the Army's Cornhusker Army Ammunition Plant near Grand Island, Nebraska. Study of a new site, the Joliet Arsenal, began in 1985.

Assistance to the NRC on the Kerr-McGee West Chicago project continued in 1985. Work began on a supplement to the Final Environmental Statement on NRC's proposed licensing of the decontaminating and decommissioning of the West Chicago site. It is expected that the supplement will be issued in late 1986 or early 1987.

A major new initiative that began in October 1985 provides assistance to the DOE's Office of Civilian Radioactive Waste Management, Siting Division, relative to National Environmental Policy Act (NEPA) compliance and related environmental analyses for the high-level waste repository program. Additional work for the repository program in 1985 included an analysis of barge transport of spent nuclear fuel.

Several staff members in the Waste Management Program contributed to a new Laboratory initiative in the area of hazardous materials management. A "white paper" was prepared on the current status of hazardous materials management in the United States, a proposed national research and development program, and suggested institutional mechanisms for implementing such a program.

6.2 FACILITY AND SITE DECOMMISSIONING PROJECTS

6.2.1 Summary

P. Merry-Libby

Two DOE remedial action activities continue to provide funding to the Waste Management Program: the Formerly Utilized Sites Remedial Action Program (FUSRAP) and the Surplus Facilities Management Program (SFMP). Site-specific work is funded through DOE-Oak Ridge Operations, and work on the development of cleanup criteria is funded through DOE-Headquarters. New sites continue to be added to these programs and environmental assessment activities are planned for several years.

The sites that the Waste Management staff deal with are contaminated primarily with radionuclides of the uranium and thorium transformation series. The bulk of the wastes are slightly contaminated soils, although some sites have concentrated processing residues that have both radiological and nonradiological chemical contaminants. Typical property-cleanup/interim-storage activities at FUSRAP sites are shown in Figure 6.1. In addition to conducting site-specific analyses, the staff analyze and compare alternative systems for remedial action and waste management, including transport of wastes to alternative sites. New efforts began in October 1985 to support DOE's search for central disposal sites for FUSRAP wastes in the states of New Jersey, New York, and Missouri.

An ongoing effort is the preparation of a manual detailing methods for site-specific pathways analyses for deriving cleanup guidelines. The first test of the manual methods is currently being done for cleanup of various vicinity properties near DOE's Weldon Spring site in Missouri.

6.2.2 Weldon Spring Environmental Impact Statement

L. Trevorrow, P.A. Benioff, S.A. Curtis, C. Luner, N.K. Meshkov, B.A. Payne,* J. Peterson,* A.J. Policastro, L. Sohlt, R.L. Tobin, S. Tsai, W.S. Vinikour, J. Wang, R.G. Williams, M.C.B. Winters, D.J. Wyman, J. Yang and Y. Yuan*

In 1984-1985, the staff began preparation of a Draft Environmental Impact Statement (Draft EIS) on several alternatives for the long-term management of

*Project leader.

Excavation Using Backhoe.

Unloading Dump Truck at Storage Pad.

Storage Pad in Final Form with Cover and Drain System.

Figure 6.1. Typical property cleanup/interim storage activities at FUSRAP sites.

existing radioactive and other waste materials in the vicinity of Weldon Spring, Missouri, located about 40 miles west of St. Louis (Figure 6.2). These wastes resulted from the production of TNT and the processing of concentrates from uranium and thorium ores. The Weldon Spring site consists of four raffinate (residue) pits, a quarry, a chemical plant, and vicinity properties. It is estimated that about 690,000 yd³ of contaminated materials are present at these areas.

Figure 6.2. The Weldon Spring site.

The Argonne team assisted DOE in developing an EIS Implementation Plan that provided guidelines for the scope of the EIS and alternatives to be considered. The team was also involved in negotiations with EPA Region VII, the board of St. Charles County, Missouri, and the Missouri State Department of Natural Resources. The EPA is a cooperating agency because part of DOE's proposed action involves cleanup of contaminated wastes from a quarry that is on EPA's Superfund list under the Comprehensive Emergency Response, Compensation, and Liability Act (CERCLA). Negotiations with EPA focused on defining EPA's future role in reviewing the EIS and their Remedial Action/Feasibility Study process under CERCLA. The team also interacted with local citizens, including the St. Charles Countians Against Hazardous Waste.

The first preliminary Draft EIS was completed in September 1985, and a second draft was completed in December 1985. The EIS will present the results of assessments of environmental impacts from continuance of existing

conditions (no action) and several alternative remedial actions. Based on input from local citizens, the team developed an alternative design for a new above-grade containment system for the wastes at the present site. Other alternatives analyzed include use of the existing raffinate pits, improved containment in a new clay-lined facility, long-term management at an arid DOE-owned site, long-term management at a new site in Missouri, and reprocessing of the raffinates at another site.

Modeling efforts are being carried out to predict potential transport of radioactive and nonradioactive contaminants in air, soil, and water. In some instances, these calculations require the adaptation of mathematical models for the site-specific situation. Of particular interest is the modeling of groundwater flow and potential transport of contaminants from the quarry to a nearby county well field.

The potential environmental impacts of each alternative are being assessed in terms of two time frames: action period and long term. Impacts incurred during the action period are those related to construction, waste removal, transportation, waste emplacement, and closure of the containment facility. This period is assumed to last 10 years. Impacts incurred during the long term (time period extending beyond 10 years) are those related to the long-term integrity of the waste containment system, possible migration of contaminants from the site, land commitment, and need for continued controls. For the purpose of analysis, the long term was assumed to be 1,000 years.

Preliminary results indicate that implementation of any of the action alternatives would expose workers to a very small radiological health risk. Transport of the waste to other sites would expose workers and the general public to a potentially significant risk associated with transportation accidents.

The radiological health impacts to the general public for the long term are predicted to be greatest for the no-action alternative. Of the action alternatives, the greatest long-term risk would be for burial of the wastes at an arid DOE site. The risk would be due primarily to the increased emission of radioactive gases in the arid environment. Based on conservative modeling assumptions, preliminary results indicate that even after the wastes are removed from the quarry, low concentrations of some contaminants may eventually appear in the groundwater between the quarry and the county well field. This is primarily because the wastes were placed in the quarry several years ago, and the more mobile contaminants have already migrated from the quarry.

It is expected that the Draft EIS will be issued in the summer of 1986, and the Final EIS will be issued in early 1987.

6.2.3 Weldon Spring Historical Dose Estimate

N.K. Meshkov, P.A. Benioff, Y. Yuan, J. Wang, D. Wyman, and A. Zielen*

This study is being conducted to estimate radiation doses to individuals in several critical groups as a consequence of past activities at the Weldon Spring uranium and thorium processing plant. The study is retrospective, covering the period 1957 through 1982, and encompasses plant operation (1957-1966) and closure and postclosure activities (1966-1982).

There has been some concern that the radioactivity released during and after the period of plant operation may pose a health hazard to the surrounding population. This study was undertaken to provide a documented basis for an epidemiological study being conducted by the Missouri Department of Health. The Missouri study is intended to assess whether any radiation-induced health effects could have been caused by the radioactivity released from Weldon Spring. The Argonne study will provide dose estimates (including bounds and uncertainties) for individuals in several critical population groups. The geographic extent of the study encompasses all offsite areas likely to have exposures significantly above background. Exposures include external exposure to radiation and internal exposure from inhalation and ingestion of radionuclides. For each critical population group the exposure is being estimated for a typical individual and for a maximally exposed individual. The variation of exposure with location is also being estimated, i.e., the maximum exposure and the manner in which exposure decreases with increasing distance from the source are being considered. The first draft of the study was completed in November 1985. Revisions are currently underway to incorporate new information on past activities at the site and the results of a recent DOE materials balance report on the former operations at the site.

6.2.4 Niagara Falls Storage Site Environmental Impact Statement

P. Merry-Libby, J.K. Alexander,** P.A. Benioff, J.E. Bogner,** P.C. Chee, S.A. Curtis,** R.R. Hinchman, M.J. Knight, S.J. Olshansky, J.M. Peterson, W.E. Pfanenstiel, E.A. Stull, R.C. Sundell, R.L. Tobin, S.Y.H. Tsai, W.S. Vinikour, S. Vogler,** W.S. White, M.C.B. Winters, D.J. Wyman, and Y. Yuan*

The Waste Management staff continued preparation of the Draft EIS (U.S. Department of Energy 1984a) and the Final EIS on long-term stabilization and control of existing radioactive wastes and residues at DOE's Niagara Falls Storage Site near Buffalo, New York. DOE published the Final EIS in April 1986, and Record of Decision is expected in the summer of 1986.

About 250,000 yd³ of wastes and residues contaminated with radium-226 are stored in a large mound at the site. The Waste Management staff has assessed and compared several alternatives for long-term management and control of the

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***Collaborator; affiliation is listed at the front of this chapter.*

radioactive wastes and residues, including: (1) no action (continued interim storage within a diked and capped containment area), (2) long-term management at the existing site (improved containment, with or without modified form of the residues), (3) long-term management at other DOE sites (Hanford, Washington, or Oak Ridge, Tennessee), and (4) offsite management of the residues at Hanford or Oak Ridge and either leaving the wastes at NFSS or removing them for disposal in the ocean. Alternative 2 is DOE's preferred alternative. Conceptual designs for the containment systems at the three alternative sites are shown in Figure 6.3. In addition to analyzing the four major alternatives in depth, the staff also considered several options, including other modifications of residue form, modification of the basic conceptual designs, other containment design options, transportation routes, and transportation modes.

The radiological health effects (primarily increased risk of cancer) associated with long-term management of the wastes and residues are expected to be much smaller than the nonradiological risks of occupational and transportation-related injuries and deaths. The greatest radiological risk for workers would occur if all the wastes and residues were removed to Hanford. The greatest radiological risks for the general public would occur if the wastes were removed to the ocean through the densely populated New York metropolitan area and the residues were removed to Hanford.

For all alternatives, DOE plans provide for institutional control of the waste containment areas and restriction of site access. It is predicted that if controls were partially lost (e.g., the containment area was not maintained), containment would still be effective for the design life (at least 200 years and, to the extent reasonably achievable, for 1000 years). At all sites, releases of radioactive radon gas to the air through the earthen covers of the containment system are predicted to result in no significant adverse health effects. Also, no offsite contamination of groundwater is predicted for any of the sites for the 1000-year design life. If all controls ceased, there would be risk of human intrusion into the contaminated materials. A 3-foot layer of riprap (rock) in the earthen cover for the preferred alternative is intended to discourage such intrusion. An additional intruder barrier over the more radioactive residues, such as a slab of reinforced concrete, is also being considered.

Concurrent with the EIS effort, Waste Management Program members are providing general environmental support to DOE relative to ongoing interim remedial actions at the site. A report prepared in 1985 (Wang and Merry-Libby 1985) presents the staff's analysis of radiological data on an offsite portion of the central drainage ditch relative to DOE's cleanup guidelines to determine what, if any, material needed to be excavated.

NIAGARA FALLS

HANFORD

OAK RIDGE

Figure 6.3. Conceptual designs of containment systems for three alternative sites for storage of radioactive wastes and residues from the Niagara Falls storage site (source: U.S. Department of Energy 1984a).

6.2.5 New Jersey Sites

C. Luner,* P.A. Benioff, P. Chee, S.A. Curtis,** P. Merry-Libby,*
J.M. Peterson, W.S. Vinikour, S. Vogler,** J.H.C. Wang, D.J. Wyman, and
C. Yu

Three FUSRAP sites in New Jersey are undergoing interim remedial actions: Wayne, Middlesex, and Maywood (Figure 6.4). Previous operations at these sites involved the processing of thorium ores and storage of resulting wastes. Radioactive wastes were stored at these sites, and a number of properties in the vicinity of the sites were contaminated and required cleanup. Until a permanent disposal site can be found in New Jersey, wastes are being stored on an interim basis in large mounds at each of the sites.

During 1984, analyses of impacts of some proposed remedial actions at the three sites were completed. A major public concern was the potential radiological impact to the population and workers during cleanup operations. At all sites, assuming mitigative measures are implemented, the doses to the population and to nearby individuals were predicted to be negligible. Doses to workers could readily be controlled and limited to less than those

Figure 6.4. Locations of the Wayne, Middlesex, and Maywood, New Jersey, sites.

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specified by DOE regulations. Implementation of the remedial actions was predicted to have only minimal effect on biota in the project area. Other issues analyzed included runoff, sedimentation, and potential groundwater contamination. These impacts differed from site to site, but were predicted to be minimal because of the limited extent and the short duration of the remedial actions and interim storage. It is expected that contaminated materials from all three sites will eventually be disposed at a central New Jersey disposal site or perhaps in the ocean.

6.2.6 St. Louis Airport Site

G. Williams, P. Benioff, J. Yang, Y. Yuan, C. Yu, and S.K. Zussman*

The St. Louis Airport Site (SLAPS) is one of four sites in the state of Missouri under the Department of Energy's FUSRAP/SFMP programs. This site is problematic in that it is located in an industrial area adjacent to the St. Louis airport and has a complicated surface and subsurface hydrologic system. Surface water (a creek) flows along one side of the site, and there is a perched, shallow aquifer in which some of the existing wastes are buried. The wastes are residues, soils, and rubble contaminated with naturally occurring radionuclides in the uranium transformation series. Because of the population density and geohydrological conditions in the site vicinity, the presence of the contaminated materials and the proposed use of the site for permanent disposal has generated much controversy.

Three reports relating to the SLAPS project were prepared for DOE in 1985: a public participation plan, an analysis of potential environmental issues associated with DOE emergency maintenance at the site (construction of a gabion wall along the creek), and description of existing environmental conditions at the site (unreleased). Work planned for 1986 includes assessing the potential environmental impacts associated with site characterization efforts, development of site-specific cleanup criteria, and preliminary work for an EIS on use of the site for permanent disposal of wastes.

6.2.7 Cleanup Criteria and Pathways Analysis Manual

T.L. Gilbert, K.F. Eckerman,** W.R. Hansen,** J.W. Healy,**
W.E. Kennedy,** B.A. Napier,** J.K. Soldat,** and D.J. Wyman*

A critical part of the DOE remedial action programs is development of guidelines for residual radioactivity. These guidelines establish the level of decontamination required at a site and provide criteria for certifying completion of the remedial action. The development of generic guidelines was initiated in 1982 and culminated in July 1985 with the release of a document

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(U.S. Department of Energy 1985) that sets basic dose limits, generic residual radioactivity criteria, and requirements for control of residual radioactivity for all FUSRAP and remote SFMP sites. The Waste Management Program has the lead role in developing these guidelines.

A workshop on the guidelines was organized by Argonne for DOE in February 1984 and was attended by representatives from DOE field offices, FUSRAP contractors, DOE laboratories, and representatives from the U.S. Environmental Protection Agency and U.S. Nuclear Regulatory Commission. It was agreed that soil concentration guidelines should be derived from a basic radiation dose limit by means of site-specific pathway analyses, and that a manual presenting standard state-of-the-art procedures should be prepared. It was also agreed that the manual should be prepared jointly by experts from several DOE laboratories (Argonne National Laboratory, Oak Ridge National Laboratory, and Battelle Pacific Northwest Laboratory), with Argonne taking the lead role.

A draft manual for implementing the residual radioactivity guidelines was completed in September 1985. This manual incorporated a new approach for structuring the pathway analysis in a modular form that permits incorporation of different models for different pathway segments in a systematic manner using concentration-independent source-to-dose (D/S) conversion factors. The most difficult and complicated pathway is the groundwater pathway, for which a new approach was developed. A generalized diagram of the groundwater pathway is shown in Figure 6.5.

Figure 6.5. Diagram of transport process involved in the groundwater exposure pathway.

The manual's approach enables independent updating of models and data for individual pathway segments and facilitates critical review of the scenarios, models, assumptions, and data used to calculate the D/S factors for the different pathways and radionuclides. In addition to the new approach for structuring the analysis, a new screening model for the groundwater pathway and a new approach to the problem of taking into account inhomogeneities in the radionuclide concentrations were developed. A natural analogue method, also developed at Argonne in earlier work for FUSRAP, was used to verify the expectation that the exposure estimates were conservative.

This work is being extended in 1986 by incorporating procedures presented in the manual into a computer code that will permit sensitivity analyses to identify critical parameters and estimate uncertainties, in addition to reducing the labor of applying the procedures.

6.3 GREATER CONFINEMENT DISPOSAL

T.L. Gilbert, C. Luner, N. Meshkov, J. Schubert, L. Trevorow,
S. Tsai, and D.J. Wyman*

Low-level radioactive waste (LLW) generated at hospitals, research laboratories, industry, nuclear power plants, and defense activities in the United States is primarily disposed of by conventional shallow-land burial (SLB), typically in trenches about 8 m deep with a 1- to 2-m earthen cap. Most of this waste consists of radionuclides with relatively short half-lives (30 years or less) at low concentrations (averaging about 6 Ci/m^3). A small volume-fraction (less than 1%) is waste that contains radionuclides with half-lives of thousands to millions of years or radionuclides in concentrations that may be as high as several thousand Ci/m^3 . This waste may require disposal by means that provide greater confinement than a typical SLB disposal facility.

To provide a convenient reference source of information for government officials and contractors responsible for disposing of LLW, the Department of Energy sponsored a project to conduct a generic analysis and evaluation of the alternatives for Greater-Confinement Disposal (GCD). During 1984-1985, the Waste Management Program prepared a draft document that presents procedures for selecting a preferred disposal alternative based on cost and risk and presents technical information on alternative GCD technologies. The analysis and evaluation involved five tasks: (1) identifying the major alternatives; (2) estimating the projected volumes and radionuclide concentrations of GCD waste for a 20-year period; (3) developing a benefit-cost-risk approach for comparison of costs and risks of GCD alternatives, taking into account the large uncertainties in predicting long-term performance (confinement up to 10,000 years and beyond); (4) evaluating and comparing costs and risks for the alternatives; and (5) drawing conclusions based on the analysis and results.

*Project leader.

The selection procedure is based on risk and cost. The risk to members of the public and the work force must be less than applicable standards established by DOE, EPA, and NRC regardless of cost. Beyond that, the risk must be reduced to levels that are as low as reasonably achievable, taking into account cost and other socioeconomic factors. Procedures for carrying out a comparative site-specific assessment of risks for different low-level waste streams are given, and the problem of determining the relationship between different design attributes and the risks of occupational and public exposure is addressed. Descriptions and technical information are given for six major categories of GCD: deep trenches, augered shafts, engineered structures, hydrofracture (injection of waste-containing grout into deep fractured layers of bedded shale), improved waste form, and high-integrity containers.

The GCD technologies analyzed span a cost and health risk spectrum between a SLB facility and a high-level waste repository. A separate discount rate was introduced to take into account long-term uncertainties. Other topics covered in the document include regulatory requirements, determination of need, waste characterization, waste-acceptance criteria, and performance objectives.

A peer review of the draft was conducted in July 1985, and the report of the peer review committee was issued in August 1985. A major recommendation of the committee report was to reorganize the working draft of the document into two volumes. Volume 1 will be a short summary volume to provide an overview for administrators and project managers; Volume 2 will contain detailed information. The scope of the document has also been extended to include mined cavities. Revisions are in progress, and a final report is expected in 1986.

6.4 GROUNDWATER RESTORATION PROJECTS

6.4.1 Cornhusker Army Ammunition Plant

S.Y. Tsai, P.A. Benioff, M. Davis,** D.J. Wyman, and A. Zielen*

The objective of this study was to evaluate a remedial action program for restoring groundwater that has been contaminated with explosive compounds such as 2, 4, 6--trinitrotoluene (2, 4, 6-TNT) and cyclotrimethylenetrinitramine (RDX) as a result of past operations at the Cornhusker Army Ammunition Plant near Grand Island, Nebraska. The study was conducted for the U.S. Army Toxic and Hazardous Materials Agency from November 1984 through May 1985. Seven alternative schemes for extracting contaminated groundwater and disposing of it were analyzed. Groundwater flow and contaminant transport models were used

**Project leader.*

***Collaborator; affiliation is listed at the front of this chapter.*

to evaluate the effectiveness of each dewatering scheme in controlling contaminant migration. The capital and operating costs for each alternative also were estimated.

The study indicated that (1) if no remedial action were taken, existing RDX contamination would continue to migrate at the rate of about 0.07 miles per year toward the northern part of the city of Grand Island (Figure 6.6), and it would take about 30 years for the maximum plume concentration to decrease from its current value of 200 parts per billion (ppb) to 35 ppb (the criterion established by the Army for protection of human health), (2) the pumping alternatives considered could remove the contaminated groundwater within a maximum of 2 to 5 years, (3) the total volume of water pumped over the decontamination period would range from 4 to 26 billion gallons for the various pumping schemes, (4) disposal of the contaminated water in local streams or on farmland would have minimal impacts on the quality and use of receiving waters, and (5) the approximate costs for construction of wells and transmission pipelines would range from \$1.3 to \$12 million. A report documenting the study results was published in May 1985 (Tsai et al. 1985).

Figure 6.6. Migration of contaminant (RDX) at the Cornhusker Army Ammunition Plant (Source: Tsai et al. 1985).

6.4.2 Joliet Army Ammunition Plant

S.Y. Tsai, A. Anderson,** A. Zielen*

The objective of this ongoing project is to develop an approach to resolve the groundwater contamination problems at the Joliet Army Ammunition

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***Collaborator; affiliation is listed at the front of this chapter.*

Plant south of Joliet, Illinois. These problems have resulted from past production and storage of munitions at the site. Information to be used in developing the technical approach will include (1) history of the site, focusing on materials that were produced there, as well as production practices which were followed, (2) a site visit to examine facilities and terrain, (3) surface water information, (4) geologic setting (from both a surface and subsurface perspective, with particular focus on any fractured formations which would necessarily affect groundwater flow), and (5) information on groundwater aquifers in terms of their physical attributes and any potential domestic or agricultural uses.

A technical approach focusing on an accurate groundwater flow model based on available data will be developed in consultation with USATHAMA staff. The model will be used to evaluate groundwater flow direction (gradients), flow rates, and the hydrologic cycle. The modeling effort will include proper documentation of the relationships and assumptions between theoretical calculations and the site-specific hydrological and geological characteristics. A draft report is expected to be completed in the spring of 1986.

6.5 KERR-McGEE PROJECT

S.Y. Tsai, P.A. Benioff, J.F. Hofferger, N.K. Meshkov, S.J. Olshansky, J.P. Schubert, J. Sheih, R.C. Sundell, L. Trevorow, W.S. Vinikour, J. Wang, R.G. Williams, D.J. Wyman, C. Yu, and Y. Yuan*

In 1978 the Kerr-McGee Chemical Corporation proposed to decommission its inactive thorium facility located in West Chicago, Illinois. In response to Kerr-McGee's proposal and under the requirements of the National Environmental Policy Act, the U.S. Nuclear Regulatory Commission (NRC) contracted with the Waste Management Program to prepare an environmental impact statement on Kerr-McGee's decommissioning plan and reasonable alternatives to that plan. In 1983, the Final Environmental Statement (FES) prepared by the Waste Management Program was issued by the NRC (U.S. Nuclear Regulatory Commission 1983).

Following the issuance of the FES, the U.S. Environmental Protection Agency (EPA) promulgated new standards governing the stabilization and control of uranium and thorium mill tailings and residues (40 CFR 192). To evaluate the compliance of the Kerr-McGee decommissioning plan with the new EPA standards and to extend the alternative site study, NRC requested that Argonne prepare a supplement to the FES. This ongoing study will analyze the environmental, social, and economic impacts associated with the permanent disposal of waste materials at the West Chicago site or at alternative sites (Figure 6.7). The principal issues that are to be evaluated include

*Project leader.

Figure 6.7. Kerr-McGee West Chicago site and alternative waste disposal sites within the state of Illinois.

alternative site screening, long-term groundwater contamination, containment system durability/stability, near-term and long-term radiological impacts, land-use and socioeconomic impacts, and implementation and maintenance/monitoring costs. A summary comparison of the results of the evaluations will be presented in a cost-benefit analysis. A draft Supplemental FES is expected to be completed in 1986.

6.6 OAK RIDGE CENTRAL WASTE DISPOSAL FACILITY ENVIRONMENTAL IMPACT STATEMENT

C. Luner, J.D. DePue, T.L. Gilbert, A.J. Policastro, S.Y.H. Tsai, L.E. Trevorrow, W.S. Vinikour, R.G. Williams, M.C.B. Winters, D.J. Wyman, and J.-Y. Yang*

A Draft Environmental Impact Statement was prepared for the U.S. Department of Energy to assess the potential environmental impacts associated with the proposed construction and operation of a Central Waste

*Project leader.

Disposal Facility (CWDF) for low-level radioactive waste (LLW) at the DOE's Oak Ridge Reservation, located in Oak Ridge, Tennessee (U.S. Department of Energy 1984b). The CWDF would be used for the disposal of LLW and by-product material generated by activities at three DOE facilities on the Oak Ridge Reservation--Oak Ridge National Laboratory, Y-12 Production Plant, and Oak Ridge Gaseous Diffusion Plant.

Waste Management staff assisted DOE in conducting a scoping process to determine the alternatives and significant issues to be analyzed in depth in the EIS. A range of alternatives was developed, including the four alternatives previously identified (no action, other sites within the Oak Ridge Reservation, an above-ground disposal facility, and disposal at other DOE sites); three reasonable site alternatives (West Chestnut Ridge, Central Chestnut Ridge, and East Chestnut Ridge); and two design alternatives (below-grade engineered trenches and above-grade tumuli). From these, DOE identified its preferred alternative: construction of below-grade trenches on West Chestnut Ridge.

The most significant impacts identified in the assessment were (1) potential radiological impacts to individuals who might occupy the site if there was unrestricted use of the site in the future and to the people who depend on the Clinch River for drinking water; and (2) the commitment of land to use for radioactive waste disposal for an extended period of time until it is safe to release the site for unrestricted use.

The health effects over the long term were estimated based on a pathway analysis for a case in which institutional controls cease 100 years after closure. The pathway analysis represents a worst-case situation applicable to failure of all trench or tumulus design features and construction of a residence on the site immediately after assumed cessation of institutional controls in 100 years. The radiological dose that an individual might incur from residential use of the site would exceed current radiation protection standards. The dose corresponded to a maximum annual risk of fatal cancer of 0.0002/year. Prior to actual release of the site for unrestricted use, a reassessment of potential impacts, based on monitoring information and other data, would be necessary to ensure that the risk to an onsite resident would be within acceptable limits.

Comparison of the maximum individual doses indicated that the dose would be slightly greater for tumuli than for trenches. However, within the range of uncertainty in the radiological impact estimates, the two design alternatives are essentially equivalent. The only significant difference is the more rapid erosion that would occur on the edges of the tumuli where the slope of the cover was greatest. The trench covers, being at ground level, would be subject to much slower erosion.

Implementation of either design alternative would expose workers and the public to a very small risk of injury (0.8 injuries) and death (0.5 deaths) from transportation of the wastes within the Reservation during the 40-year operation of the CWDF. The cumulative radiological health effects to workers during operation, closure, and institutional care correspond to a probability

of 0.005 that a single worker in the entire work force involved would die of cancer as a consequence of exposure to radioactivity from the waste. The health effects for the general population during this period would be negligible.

The long-term health effects for the general public would be from release of radionuclides into the Clinch River, which serves as a drinking water supply for many communities. A bounding estimate of the resulting lifetime risk of fatal cancer for an individual in the exposed population is 2×10^{-8} for below-grade trenches, which may be compared with a lifetime risk of 0.16 that this individual will die of cancer from other causes. This level of risk would continue for a few hundred years and then decrease. The long-term health effects associated with the above-grade tumuli are estimated to be slightly greater, but are considered comparable when the uncertainty in the estimates is taken into account.

DOE has put the CWDF project on hold and issuance of a Final EIS has not been scheduled.

6.7 HIGH-LEVEL WASTE REPOSITORY PROGRAM

6.7.1 Barge Transport Analysis

Y. Yuan, N. Meshkov, R. Tobin,* A. Zielen, and S.K. Zussman*

Use of barges in conjunction with trains is a viable option for shipping spent fuel and other nuclear waste from nuclear reactors that either are not served by railroads or are served by railroads but also are near good ports. In 1985, DOE sponsored a study of barge transport to support the environmental assessment of potential candidate high-level waste repository sites. The purpose of the study was to analyze the costs and risks associated with transporting spent fuel by barge. The barge movements would be made in combination with rail movements to transport spent fuel from nuclear plants to a repository. For the purposes of this analysis, three candidate repository sites were analyzed: Yucca Mountain (Nevada), Deaf Smith (Texas), and Hanford (Washington).

Shipments were considered for which a large portion of the shipping distance could be by barge or for which direct access to water makes barging convenient. For these shipments, an integrated railcar/cask would be used with roll-on/roll-off (RORO) loading to transfer between rail and barge. The differences in costs and risks brought about by using lift-on/lift-off (LOLO) instead of RORO were also analyzed. The only nuclear power plants considered in the study were those in operation at the beginning of 1985 that were located east of the Mississippi River. The list was further limited to those plants having direct access to navigable water and those having rail access that are within 300 miles of an Atlantic port. Shipments from the plants with

*Project leader.

water access would travel by barge to a transshipment location on the Gulf of Mexico or on the Mississippi River, where they would be transferred to rail for delivery to the candidate repository. Shipments from plants with rail access only would travel by rail to an Atlantic port and from there by barge to the transshipment location on the Gulf, where they would be transferred to rail for delivery to the repository. Analysis of routes showed that the ports of Baltimore, Norfolk, and Charleston were convenient for most of the shipments originating on rail. The transshipment locations were assumed to be Houston on the Gulf and Memphis on the Mississippi. In general, shipments from plants on the Atlantic coast or on the Gulf coast or shipments that travel by rail to an Atlantic port were assumed to travel by water to Houston. Shipments from plants on inland waterways or on the Great Lakes were assumed to travel by water to Memphis.

Distances for both rail and water travel and travel times for water were determined using Shortest Path Analysis and Display (SPAD), a routing model that is part of the Freight Network Modeling System developed at Argonne. The travel times for rail were calculated using the values of average speed as a function of distance.

The transportation costs developed were subdivided into capital and maintenance costs for the railcar/cask system and shipping costs. The costs for moving the spent fuel from the nuclear plants to the transshipment locations of Houston and Memphis totaled \$738 million--\$54 million for maintenance, \$375 million for capital, and \$309 million for shipping. This is an average cost of \$146,000 per shipment, or \$22 per kilogram of spent fuel. Depending on repository site, the total costs for moving the spent fuel from Houston and Memphis to the repository ranged between \$42 and \$57 million for maintenance, \$299 and \$410 million for capital, and \$193 and \$356 million for shipping--a total between \$533 and \$825 million. The average cost would be between \$105,000 and \$163,000 per shipment, or \$16-\$25 per kilogram of spent fuel. If LOTO were used instead of RORO, approximately \$3,000 per shipment in crane charges would be incurred for loading and unloading the casks, or an additional cost of \$15 million. This amounts to \$0.47 per kilogram of spent fuel, or a cost increase of 2.1%.

The nonradiological risks for the water portion of the shipments considered in this analysis amounted to 1.7 deaths and 4.4 injuries. For rail transport between plants and ports, the risks were predicted to be 0.056 deaths and 2.1 injuries. For rail transport from Houston or Memphis to the repository site the predicted risks are between 1.1 and 3.5 deaths and between 43 and 130 injuries, respectively.

Radiological risks were calculated assuming that external radiation is at the limit allowed by regulations. The calculations were conservative and the risk estimates can be considered maximal. These risks are for normal transportation only and include both occupational and nonoccupational exposure. Only gamma radiation was considered for this assessment. Analysis of accident scenarios has been proposed for future work.

The total radiation dose due to all shipments from nuclear power plants to the transshipment locations at Houston and Memphis was estimated to be 1,000 person-rem for workers involved in the transport and 490 person-rem for the general population. This translates to an estimated 0.10 latent cancer fatalities for workers and 0.049 latent cancer fatalities for the general population. The total radiation dose due to all shipments from Houston and Memphis to the candidate repository sites ranged between 390 and 560 person-rem for transportation workers and between 100 and 180 person-rem for the general population. The resulting latent cancer fatality estimates ranged between 0.039 and 0.056 for workers and 0.010 and 0.018 for the general population. Using LOLO instead of RORO decreases both the worker and general population risk during loading and unloading. The reduction in worker risk is due to reduced crew and greater distances from casks. The general population dose is reduced because of the slightly shorter time required for LOLO. The total reduction in worker dose for all shipments is 100 person-rem, or a decrease of 10%. The total reduction for the general population for all shipments is 10 person-rem, or a decrease of 2%. A maximally exposed individual would receive a dose on the order of 10 millirem, which translates to a cancer death risk of 10^{-6} .

6.7.2 NEPA and Other Environmental Assistance

E.D. Pentecost, A.P. Campbell,** J.D. DePue, J.D. Ditmars,**
D.E. Edgar,** L.J. Habegger,** J.F. Hoffecker, K. LaGory, G. Marmer,
D.L. McCown,** P. Merry-Libby, M.R. Monarch,** J.P. Peerenboom,**
A.J. Policastro, R.C. Sundell, W.S. Vinikour, R.G. Williams,* Y. Yuan*

In October 1985, the Waste Management staff, with assistance from several members of the Energy and Environmental Systems Division, began providing assistance to the Site Evaluation Branch, Office of Geologic Repositories, in DOE's Office of Civilian Radioactive Waste Management (OCRWM) in matters relating to environmental evaluations of proposed alternative sites for the high-level waste (HLW) repository. Several tasks have been designated for FY86, including:

- 1) Preparing guidance documents for the DOE Project Offices on the preparation, organization, scope and detail of Environmental Monitoring and Mitigation Plans (EMMPs) for the site characterization efforts at the potential repository sites (including review of the actual EMMPs prepared by the Program Offices);
- 2) Assisting in National Environmental Policy Act (NEPA) compliance, such as scheduling activities for the scoping process, drafting a Notice of Intent, providing guidance in organizing scoping meetings,

**Project leader.*

***Collaborator; affiliation is listed at the front of this chapter.*

preparing a presentation on the applicability of the NEPA process under the Nuclear Waste Policy Act, preparing other materials for presentation at public scoping meetings, reviewing and summarizing the results of the scoping meetings, developing a systems approach to construct a matrix of alternatives and issues hierarchy (to clarify the alternatives, scope and depth of analyses in the Environmental Impact Statement), and drafting of an EIS outline and Implementation Plan;

- 3) Providing other environmental support, including preparation of technical reports on specific environmental issues that can serve as reference documents to support the EIS; and
- 4) Assisting on the second (crystalline) repository program, including providing guidance on the preparation, structure, scope and detail of the Area Phase Regulatory Compliance and Environmental Field Studies Plan; reviewing applicable environmental standards and regulations; and providing general guidance to ensure consistency between the first and second repository programs with respect to environmental matters.

Although DOE expects to hire a commercial contractor to prepare the EIS, it is expected that the Siting Branch will continue to require assistance from Argonne in the above-mentioned matters. A goal of the Waste Management Program staff is to clarify and expand support on the third task (preparation of reference documents on specific environmental issues).

Draft guidance on the Environmental Monitoring and Mitigation Plan has been prepared and is currently undergoing revisions based on comments from the DOE Project Offices. It is expected that the guidance document will be presented to the states for review in early 1986.

Two subtasks are underway with respect to scheduling and scoping the EIS. A complete schedule of all major activities, such as preparation of planning and support documents, reviews, concurrences and revisions, is being developed using a computerized project management system. It is expected that this will be a major management tool during the several years of preparation of the Draft and Final EIS and the Record of Decision.

Another area of importance is the management of information to be gathered during the scoping process. Management of comments will be a complex job and thousands of pages of transcripts can be very difficult to analyze without a management system. The Waste Management Program is in the process of developing a data management system that will use microcomputers. This approach will require that the scoping meetings be transcribed directly into a data management software package. Once all comments are entered, content analysis will be used to identify primary and secondary concerns and other matters. Frequency distributions can then be provided as well as basic statistics and tests of significance to compare the comments from different meetings and sites. A questionnaire is being developed for use in scoping

meetings as a way to summarize positions, values, and concerns and, at the same time, provide basic demographic information on the participants.

This data management system will provide an efficient method for managing and reducing information, a defensible and reproducible summary of comments, a data base for content analysis, and statistical bases for comparison of meetings. It is expected that such an approach will be widely adopted in large EIS scoping proceedings in the future.

6.8. OTTAWA LUMINOUS PROCESSES FACILITY

R.C. Sundell, J.D. DePue, N. Meshkov, R. Tobin, W. Vinikour, J. Wang, and R.G. Williams*

In 1984 the Illinois Legislature appropriated \$2 million for the cleanup, removal, and disposal of the radioactively contaminated materials at the Luminous Processes Facility located in Ottawa, Illinois. The responsibility for the cleanup was assigned to the Illinois Department of Nuclear Safety (IDNS). The IDNS contracted with the Waste Management Program to assess the environmental impacts of decontamination and decommissioning of the Ottawa facility, including segregation of the radioactive and nonradioactive materials, disposal of uncontaminated materials, and transport and disposal of the contaminated materials at a licensed radioactive waste burial site.

The major source of contamination at the site was ^{226}Ra and its transformation products. The radium had been mixed with luminous paints that were used at the facility. Radiological impacts of the cleanup included the potential health risks to workers and members of the general public from exposure to radioactive materials at the Ottawa site and along the transportation route to the radioactive waste disposal facility. It was estimated that the accumulated radiation doses to workers and the general public would be small and that no short-term or long-term impacts to the local urban environment would occur.

Nonradiological impacts included various socioeconomic impacts that might result from the temporary closure of or traffic restrictions on streets surrounding the plant site. Continued interaction between the IDNS, city officials, and the general public is planned to keep the local community informed of activities and to address problems that might arise.

*Project leader.

6.9 HAZARDOUS MATERIALS MANAGEMENT

P. Benioff, T. Gilbert, P. Gustafson, P. Merry-Libby, N. Meshkov, B. Payne, L. Soholt, R. Sundell, L. Trevorrow, G. Williams, and C. Yu

Several staff members in the Waste Management Program contributed to a major new Argonne initiative in the area of hazardous materials management. A "white paper" was prepared on the current status of hazardous materials management in the United States, a proposed national research and development program, and suggested institutional mechanisms for implementing such a program. This paper served as a basis for discussion at a national workshop that was held at Argonne in August 1985. Followup efforts have focused on building support for this initiative among universities, industry, and government.

Members of the Waste Management Program continue to explore avenues for expanding the initiative into integrated systems analysis of the risks, socioeconomic issues, engineering aspects, and other tradeoffs between waste management systems from generation to transport to storage and disposal of wastes. It is expected that DOE's waste management problems will continue to become more complicated as more wastes are identified as being co-contaminated with radioactive and nonradioactive materials. It becomes more and more apparent that a total systems approach is needed in order to make rational, long-term decisions.

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Waste Management Program

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CHAPTER 6. WASTE MANAGEMENT PROGRAM

APPENDIX 6-A. STAFF QUALIFICATIONS
Waste Management Program

Name	Position	Highest Degree	Major	Year Received	Institution
Benioff, Paul	Chemist	Ph.D.	Nuclear Chemistry	1959	University of California-Berkeley
Chee, Ping*	Radiological Engineer	Ph.D.	Health Physics	1976	Purdue University
Gilbert, Thomas	Physicist	Ph.D.	Theoretical Physics	1956	Illinois Institute of Technology
Luner, Charles*	Chemist	Ph.D.	Physical Chemistry	1952	McGill University
Marmer, Gary	Physicist	Ph.D.	Physics	1968	Ohio State University
Meshkov, Natalia	Scientist	Ph.D.	Physics	1961	University of Pennsylvania
Merry-Libby, Pamela	Environmental Scientist	B.S.	Biology	1971	Michigan State University
Pentecost, Edward	Ecologist	Ph.D.	Zoology	1972	University of Illinois
Peterson, John*	Nuclear Engineer	M.S.	Nuclear Engineering	1977	University of California
Trevorrow, Laverne	Chemist	Ph.D.	Inorganic-Physical Chemistry	1955	University of Wisconsin-Madison
Tsai, Steve	Hydrologist	Ph.D.	Civil Engineering	1978	University of Illinois
Vinikour, William	Environmental Scientist	M.S.	Biology	1977	Northern Illinois University
Vocke, Robert*	Aquatic Ecologist	Ph.D.	Water Resources/ Botany	1978	Iowa State University

APPENDIX 6-A. Continued

Name	Position	Highest Degree	Major	Year Received	Institution
Wang, John	Health Physicist	Ph.D.	Health Physics	1984	Northwestern University
Winters, Margery	Geologist	M.S.	Physical Geography	1979	Queen's University
Yang, Jing	Hydrologist	Ph.D.	Environmental Engineering	1973	Cornell University
Yu, Charley	Assistant Environmental Scientist	Ph.D.	Nuclear Engineer	1984	The Pennsylvania State University

*No longer a member of the Division

**APPENDIX 6-B. OUTSTANDING PROFESSIONAL ACTIVITIES AND AWARDS
Waste Management Program**

T.L. GILBERT--Nominated to the Radiation Protection Advisory Council of the Illinois Department of Nuclear Safety.

APPENDIX 6-C. SPECIAL EVENTS ORGANIZED
Waste Management Program

- T.L. GILBERT and R.W. VOCKE organized Workshop on Remedial Action Criteria - I for U.S. Department of Energy, 22-24 February 1984, Gaithersburg, MD.
- T.L. GILBERT and R.W. VOCKE organized Workshop on Remedial Action Criteria - II for U.S. Department of Energy, 26-27 June 1984, Argonne National Laboratory.
- T.L. GILBERT organized Workshop on Remedial Action Criteria III for U.S. Department of Energy, 30-31 May 1985, Argonne National Laboratory.
- T.L. GILBERT organized and hosted peer review committee meeting for "Planning for Greater-Confinement Disposal," 9-10 July 1985, Argonne National Laboratory.
- P.F. GUSTAFSON organized Integrated National Hazardous Materials Research Workshop 7-8 August 1985, Argonne National Laboratory.
- N.K. MESHKOV organized Summer Institute on Risk Analysis, July 1985, Argonne National Laboratory.
- N.K. MESHKOV organized Environmental Research Division Risk and Systems Analysis Seminar (Speaker: Edmund Crouch, Harvard University; Title: The Uses and Abuses of Risk Assessments and Other Turkeys), 25 November 1985, Argonne National Laboratory.
- N.K. MESHKOV organized Environmental Research Division Risk and Systems Analysis Seminar 16 December 1985 (Speaker: Loren Habegger, Energy and Environmental Systems Division, ANL; Title: Comparative Health and Safety Assessments of Future Electrical Generation Options").
- B.A. PAYNE and R.G. WILLIAMS organized session entitled "Social Effects of Hazardous Waste Management on Rural Communities" at Rural Sociological Society Meetings, 22-24 August 1985, Blacksburg, VA.

APPENDIX 6-D. EDUCATIONAL PROGRAM PARTICIPANTS
Waste Management Program

DONALD LIBBY. University of Wisconsin-Madison. Graduate Research Program.
Conducted study on affect of waste storage facility siting on local
property values. June - August 1984.

ANN M. CLARK. Western Michigan University. Undergraduate Research Program.
Conducted preliminary alternative site screening study for the
decommissioning of Kerr-McGee's Rare Earths Facility in West Chicago,
Illinois. June-August 1985.

MARY JEAN WALTER. University of Dayton. Undergraduate Research Program.
Developed computer simulation for predicting soil erosion by water.
June-August 1985.

APPENDIX 6-E. PUBLICATIONS AND ORAL PRESENTATIONS 1984-1985
Waste Management Program

1. Refereed Journal Articles*

1985

Yu, C., W.A. Jester and A.R. Jarrett. Hydrogeologic parameter identification from nuclear tracer breakthrough curve data for waste disposal in porous media. International Journal of Radioactive Waste Management and the Nuclear Fuel Cycle 7(1):15-34 (1985). [DOE/ORO]**

2. Books, Book Chapters and Collections of Conference Proceedings

1985

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1984

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*For published material, the names of all Environmental Research Division authors are underlined. (Included are Division members who participated in a project but left the Division before the results were published.)

**Funding agency (abbreviations are spelled out at the end of this appendix). In cases where no funding agency is listed, the publication was not related to any specific funded project.

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White, W.S. Directory and Profile of Licensed Uranium-Recovery Facilities. NUREG/CR-2869, ANL/ES-128, Revision 1. Prepared for Office of State Programs, U.S. Nuclear Regulatory Commission. 1984. [NRC/State Programs]

1985

Job Control Language and FORTRAN Unit Changes, IBM to VAX/VMS, for FNEM4 Programs. Addendum to ANL/ER-TM-84-1 (Vols. II and III). Prepared for U.S. Department of Transportation and Federal Emergency Management Agency. 1985. [DOT/FEMA]

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DOT = U.S. Department of Transportation
FEMA = Federal Emergency Management Agency
FUSRAP = Formerly Utilized Sites Remedial Action Program (in DOE)
IDNS = Illinois Department of Nuclear Safety
LLWMP = Low-Level Waste Management Program (in DOE)
NMSS = Office of Nuclear Material Safety and Safeguards (in NRC)
NRC = U.S. Nuclear Regulatory Commission
NRR = Office of Nuclear Reactor Regulation (in NRC)
OHER = Office of Health and Environmental Research (in DOE)
ORO = Oak Ridge Operations (in DOE)
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