

Final Report

INTERACTIONS OF CO₂ WITH TEMPERATURE AND OTHER CLIMATE VARIABLES:
RESPONSE OF VEGETATION

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INTRODUCTION

The current project was initiated in 1991, and full details of the scope of the project are contained in the original proposal. That original proposal was reviewed and approved for three years funding. Progress made in 1991-92 and 1992-93 was described in annual Progress Reports and Statements of Work. This document summarizes progress made over the duration of the project, but with an emphasis on the final year's (1993-94) results. Several of the important experiments are ongoing, to the extent that alternative funding could be arranged, and analyses of data from several of the earlier completed experiments is continuing. Therefore, this Final Report is also intermediary in nature, and additional results from this project will be reported in the open literature in the future.

The overall objectives of the project were: 1) to examine experimentally, for major crop species, the interacting effects of CO₂ concentration, temperature, and water availability on plant growth and development, 2) to model these interactions, and 3) to continue developing physiologically-based mechanistic models for predicting crop response to increased CO₂ concentration and future global climate change.

To meet these objectives, controlled-environment studies were conducted on cotton, lemon, rice, and soybean and a long-term open-top chamber study was continued on orange. Much progress was made on development of plant growth models for cotton, wheat, rice, and soybean. In addition, there were two special modeling efforts which have the potential for contributing to all of the crop models. These efforts are concerned with modeling root growth and physical and chemical processes in soil and with modeling the effect of stomatal aperture on photosynthesis and transpiration rates as a function of CO₂ concentration, temperature, and vapor pressure deficit. The root growth and soil process modeling is important because it enables us to estimate the water available to the plant. The modeling of effects of stomatal aperture on photosynthesis and transpiration rates enables us to estimate dry weight gain and water use by the plant. These are both important components of the interaction of CO₂ concentration with temperature and water availability. The work on stomatal aperture, photosynthesis, and transpiration has the added benefit of allowing us to improve predictions of energy partitioning by the terrestrial biosphere. The lack of realistic energy partitioning is a serious deficiency of the present general circulation models which are used to predict how climate will change. An additional important aspect of the rice experiments is a study of methane emissions of paddy-grown (i.e., flooded) rice grown under two levels of CO₂ and three temperature regimes.

A. Controlled-environment studies

1. Cotton growth and "feedback inhibition" of photosynthesis.

a. Phoenix.

Cotton plants were grown in the first experiment in Phoenix at two levels of CO₂ concentration (ambient and 650 μmol mol⁻¹) and at two temperature regimes (40/32 and 32/22°C maximum/minimum following a typical diurnal pattern). Two refrigerated greenhouses were used with two smaller compartments (3 by 4 m) constructed within each using transparent plastic film to provide the necessary four compartments. The cotton was grown in 15-liter pots, with planting on 26 April and continuing until 21 July 1992.

Plant height increased significantly with increased air temperature and high CO₂. Fully expanded leaves were larger on the CO₂-enriched plants at each leaf position. The biomass production at high-CO₂, high-temperature increased significantly; however, production of squares and bolls per plant only increased with high CO₂ at the lower temperature. The relative growth rate (RGR) and net assimilation rate (NAR) increased significantly in the high temperature, high CO₂ environment during 30-60 days compared to low temperature, high CO₂ grown plants. The RGR and NAR increased in the low temperature, high CO₂ and low temperature, low CO₂ during 30-60 days growth interval followed by a decrease at 65-90 day growth period. The NAR gradually increased in low temperature, high CO₂ during 65 to 90 days corresponding with increased boll load compared to high temperature, low CO₂.

The mineral composition of leaves was considerably lower in plants grown in the high CO₂ atmospheres than from those grown at ambient CO₂ under either temperature regime.

b. Beltsville

Several controlled environmental studies were also conducted at Beltsville. Utilizing sunlit controlled-environment chambers (SPAR units), these experiments examined the effects of temperature and carbon dioxide concentration on physiological processes in cotton. The most significant findings are as follows:

Temperature effects on cotton fruit retention. Cotton plants grown from seedlings at 40°C for a 12 h day shed all their squares. Plants grown from seedlings in the natural environment, then exposed to daytime temperatures of 30, 35 or 40°C during the fruiting period accumulated 47, 5.7, and less than 1 percent, respectively, of their mass as bolls. The time of day when plants were exposed to high temperature did not influence percent boll retention. Number of bolls produced, bolls retained, and percent retention were progressively reduced as time per day at 40°C was increased. Three weeks of exposure to 40°C for 2 or 12 h per day resulted in 64 or zero percent bolls, respectively, retained on the plants.

Carbon dioxide and temperature effects on stem extension, node initiation and fruiting in cotton. Cotton plants were grown in plant growth chambers exposed to natural light levels with temperature and CO₂ as treatments. The average temperatures were 17.8, 18.7, 22.7, 26.6, and 30.6°C during a 70-d experimental period with CO₂ treatments of 350 and 700 μmol/mol at each temperature. Plant height and rate of stem elongation increased with increase in temperature and CO₂. The number of main stem nodes and fruiting branches increased with increase in temperature. However, no significant differences were observed in fruiting branch number due to doubling of CO₂ except at 30.6°C. The number of days from

emergence to first square was strongly influenced by temperature, but CO₂ had no effect on this process. The number of squares and bolls increased with increase in temperature, and the rate of increase was higher at 700 μmol/mol CO₂.

Carbon dioxide and temperature effects on cotton leaf growth and development. This experiment was conducted by growing cotton plants in plant growth chambers with temperature and carbon dioxide as controlled variables. The air temperatures in the growth chambers were maintained at 15/7, 20/12, 25/17, 30/22, and 35/27°C. The carbon dioxide concentrations were maintained at 350 and 700 μmol/mol for each temperature, utilizing 10 controlled-environment cabinets. Temperature and carbon dioxide had significant effect on growth and final size of the cotton leaves. Leaf initiation on the main stem was primarily temperature dependent and not limited by carbon supply in ambient CO₂ environment. Temperature had significant effect on the final sizes of the leaves, duration and rate of leaf growth, while CO₂ increased final leaf sizes and rate of leaf expansion. The rate of leaf expansion increased with temperature up to 26.6°C, and declined at higher temperature in both the CO₂ levels. Leaf expansion duration was not influenced by carbon supply, but strongly influenced by temperature. Carbon dioxide increased total leaf area due to small increases in individual leaf sizes and also due to the production of more nodes on fruiting and vegetative branches.

Carbon dioxide enrichment and temperature effects on cotton photosynthesis and respiration. A set of controlled environmental experiments were conducted to determine the effects of CO₂ enrichment and temperature on photosynthesis, respiration, and dry matter partitioning in cotton. Photosynthesis increased with increase in CO₂ from 350 to 900 μmol/mol, however the rate of increase was highest from 350 - 450 μmol/mol CO₂. Photosynthesis also increased with an increase in temperature, and the effect of increased levels of CO₂ was more pronounced at higher temperatures.

Effects of aerial carbon dioxide enrichment and temperature on root growth in cotton. Roots explored more of the soil profile as aerial temperature increased, and root distribution down the soil profile was more uniform in elevated CO₂.

2. Insect growth and development on host cotton grown at elevated CO₂ and varying temperature.

Due to the serious widespread outbreak of whitefly, the attention of entomologists was redirected to finding solutions to this immediate problem, and no global change experiments were conducted on insect growth and development.

3. Lemon tree growth and mycorrhizal activity.

The specific objective of this experiment was to determine the interactive effects of CO₂, temperature, and mycorrhizal species on the growth, photosynthesis and nutritional status of a tree species. Two glasshouses were controlled at maximum/minimum temperatures of 40.6/32.2 and 29.4/21.1°C programmed to approximate a normal diurnal temperature pattern. Inner chambers were at ambient and 650 μmol mol⁻¹ CO₂ to produce 4 CO₂ x temperature environments.

Small (approx. 30-cm tall) Eureka lemon trees from the same clone were grown in each of the 4 environments. The trees were potted into 27-liter black polyethylene "grow bags" filled with a 4-parts-autoclaved-sand:1-part-autoclaved-sandy-loam-soil (volume:volume) rooting medium. One third of the

trees in each environment were inoculated with a mycorrhiza isolate adapted to a high temperature environment (from low elevation). Another third were inoculated with a low-temperature-adapted isolate (from high elevation), and the remaining third were uninoculated controls. The mycorrhizal fungi were mixed into the top 1/3 of rooting medium at approximately 1500 spores per pot for the treated plants.

Thus, there were a total of 12 CO₂-temperature-mycorrhiza treatment combinations. Ten replicate trees received each treatment. Measurements were made of (1) macro- and micro-nutrients; (2) leaf chlorophyll contents; (3) photosynthesis and photorespiration; (4) whole tree gas exchange; (5) leaf A(c) curves; (6) carbon partitioning to shoots, roots, and fungal organisms; (7) water use efficiency; and (8) leaf spectral characteristics.

CO₂ enrichment increased total biomass gain by 21% when temperatures were near optimal and 87% when temperatures were supraoptimal. This amplification of CO₂ enhancement by supraoptimal temperatures may be best interpreted as a CO₂-induced alleviation of growth inhibition caused by high temperature. CO₂ enrichment did not affect carbon partitioning.

Supraoptimal temperatures suppressed shoot extension growth and leaf accumulation; however, this heat-induced growth suppression was alleviated by a near doubling of atmospheric CO₂. At near-optimal temperatures, shoot growth of CO₂-enriched trees and those grown under ambient CO₂ conditions was similar. Temperature was the sole factor affecting mycorrhizal colonization but increased arbuscular colonization relative to near-optimal temperatures. Shoot and root growth were also affected by an interaction of temperature and different ecotype populations of arbuscular mycorrhizal fungi. At near-optimal temperatures, lemon tree leaf area to root length ratio was not affected by mycorrhizal treatments, but at supraoptimal temperatures there was a 37% greater leaf area to root length ratio in trees inoculated with the plains grassland population of AM fungi compared with those trees inoculated with the Sonoran desertscrub population of AM fungi. These data suggest that benefits of the mycorrhizal symbiosis may not necessarily be based on growth enhancement of the host plant.

4. Rice photosynthesis, growth, and methane emissions, as affected by CO₂, temperature, and water stress.

The specific objectives of the rice experiments were:

- i. To quantify the effects and possible interactions of elevated [CO₂] and drought stress on rice (*Oryza sativa*, L.) phenological development, shoot and root biomass accumulation, tillering, seed yield and yield components as well as single leaf and whole canopy photosynthesis, dark respiration, and evapotranspiration.
- ii. To measure and compare seasonal trends in methane fluxes as affected by [CO₂] and water management treatments and further to determine diurnal time courses of methane efflux under constantly decreasing soil water availability in order to evaluate options of water management for reducing methane emissions while maintaining high productivity of rice.
- iii. To elucidate specific physical and physiological mechanisms by which season-long [CO₂] enrichment, through its effects on photosynthesis, tillering and root biomass production, influence seasonal trends in methane efflux.

Rice (cv. IR-72) plants were planted on 15 July 1994 in eight naturally sunlit Soil-Plant-Atmosphere-Research (SPAR) chambers at ambient ($350 \mu\text{mol/mol}$, 4 chambers) and elevated ($700 \mu\text{mol/mol}$, 4 chambers). For each pair of chambers (one ambient and one elevated [CO_2]) the following water management-drought stress treatments were being imposed: 1) continuously flooded (fully irrigated controls), paddy flood water removed and drought stress imposed during 2) panicle initiation, 3) anthesis, and 4) both panicle initiation and anthesis. The soil was reflooded between these latter two drought timings. Air temperatures were controlled to $28/21^\circ\text{C}$ day/night. Based on our previous experiments, this temperature regime is near the optimum for growth and grain yield of the rice cultivar IR-30. Dewpoint is controlled to 18°C with a resulting daytime vapor pressure deficit of 1.7 kPa.

Quantifying Drought Stress: The degree of drought stress was quantified by several non-invasive techniques that allow the SPAR chambers to remain closed for continuous process measurements and which allow quick feedback on the degree of stress. During soil water draw-down and drought stress cycles, canopy photosynthesis, soil water content, measured with the soil potentiometers, and canopy foliage temperature, measured with infrared thermometers, were monitored continuously, in real time, and averaged over each 5 min. interval. We continuously measured canopy foliage temperature (T_c) with infrared thermometers mounted in each chamber. Additionally, individual leaf photosynthesis, leaf extension rates, final mainstem leaf size, and leaf water potential (pressure bomb techniques) were periodically measured.

Continuous Process Measurements: Season-long measurement of canopy photosynthesis, evapotranspiration, and nighttime respiration were being made at 5 min. intervals for each [CO_2] by water treatment combination.

Shoot Growth and Yield: Plants were sampled for above ground biomass accumulation, leaf area growth, and tillering at seven harvests during the growing season. At physiological maturity the last destructive plant sampling will include final grain yield and grain yield components.

Root Growth: Three cylindrical polyvinylchloride pots with a rooting depth of 0.5 m and a diameter of 0.2 m were filled with soil and placed in the center of three separate rows on the floor of the chamber lysimeters before filling the lysimeters with soil. Nine plants were grown in each pot in the same row orientation as the rest of the plants outside the pots. Except for the pot itself, cultural and environmental conditions were the same for plants inside and outside the pots. One pot was sampled from each chamber three times during the growing season. Growth attributes of the shoots of these plants was determined as previously described. Each sampled pot with the soil and roots intact was frozen solid to prevent the liquid paddy soil from flowing out of the pot. The soil and roots were thawed and separated and root biomass was measured after oven drying.

Phenology: Mainstem leaf appearance rates was measured on tagged plants. Timing of panicle initiation and gametogenesis was determined by plant dissections and visual observation of mainstem apical meristem, respectively. Anthesis dates were determined by periodically counting emerged and post flowering panicles on a canopy basis.

Methane: Whole canopy estimates of methane flux were measured continuously at 5 min. intervals throughout the growing season using automated sampling and in-line gas chromatograph. The technology for automated whole season canopy methane emission measurements was worked out in earlier experiments in 1992 and 1993. Air samples were pumped from each SPAR chamber and split streams analyzed for methane via a single gas chromatograph and for CO_2 via a set of infrared gas analyzers.

Of all of the methods to quantify the degree of drought that we used in this experiment, it was found that canopy photosynthesis rate measured at 5 min. intervals provided the best real-time estimate of the

progression of the drought and provided an easily measured and repeatable end-point for determining when to stop the drought stress treatment (eg. when mid-day canopy net photosynthesis drops to zero due to drought) and reflood the paddy. Shown in Fig. 1 are examples of canopy photosynthesis for the continuously flooded or irrigated control treatments and the drought stressed treatments at panicle initiation in both 350 and 700 $\mu\text{mol mol}^{-1}$ [CO_2] treatments. In this example, the paddies in both drought stress treatments were drained at 62 days after planting (16 September). By day 75 (Fig. 1) the 350 $\mu\text{mol mol}^{-1}$ had reached the end-point criterion (zero photosynthesis) and was reflooded on day 76. The 700 $\mu\text{mol mol}^{-1}$ [CO_2] treatment did not reach the end-point until day 77 and reflooded on day 78. Rather than impose durations of drought stress based on chronological time, our goal was to impose similar levels of physiological drought stress at specific growth stages.

With respect to drought stress effects and canopy photosynthesis our results to date can be summarized as follows:

- i) Due mainly to the antitranspirant effect of elevated [CO_2], the [CO_2] enriched chambers required on average 2 more days than ambient [CO_2] treatments to reach similar physiological levels of drought stress severity.
- ii) The drought stress imposed at panicle initiation delayed ontogeny and the beginning of panicle appearance and flowering by about three days compared with continuously flooded controls.

All other data are currently being analyzed.

Shown in Fig. 2 are seasonal trends in methane [CH_4] efflux for the continuously flooded controls for enriched and ambient [CO_2] treatments. Thus, far the [CH_4] efflux trends shows two seasonal peaks: the first is a comparatively small peak early in the season near 40 days after planting and a second, much larger peak, beginning near 80-90 days after planting. An example of the diurnal measurements for both the enriched and ambient continuously flooded treatments are shown in Fig. 3. The 'saw-tooth' pattern in [CH_4] during the night hours are the result of our chamber venting procedure at night to measure canopy dark respiration and [CH_4] efflux.

With respect to methane measurements our results to date can be summarized as follows:

- i) Carbon dioxide enrichment can result in a very large increase in methane efflux compared with ambient controls.
- ii) Draining the paddy for the drought stress treatments greatly reduced subsequent methane emissions following reflooding.

5. Controlled-Environment Experiments on Soybean

The specific objective of these experiments was to evaluate effects of elevated temperature in combination with elevated CO_2 upon photosynthesis and growth processes in soybean. The premise is that most past studies have evaluated effects of the cool-end of growth temperatures, but few studies have emphasized the high end of the temperature range.

Our first experiment was initiated 19 August 1993 on soybean cultivar 'Bragg' grown in sunlit, controlled-environment chambers at four temperatures (40/30, 36/26, 32/22, and 28/18°C daily maximum and daily minimum) and at two carbon dioxide levels (350 and 700 $\mu\text{mol/mol}$). Temperatures were programmed to progress through natural diurnal cycles. Canopy photosynthesis, night respiration, and

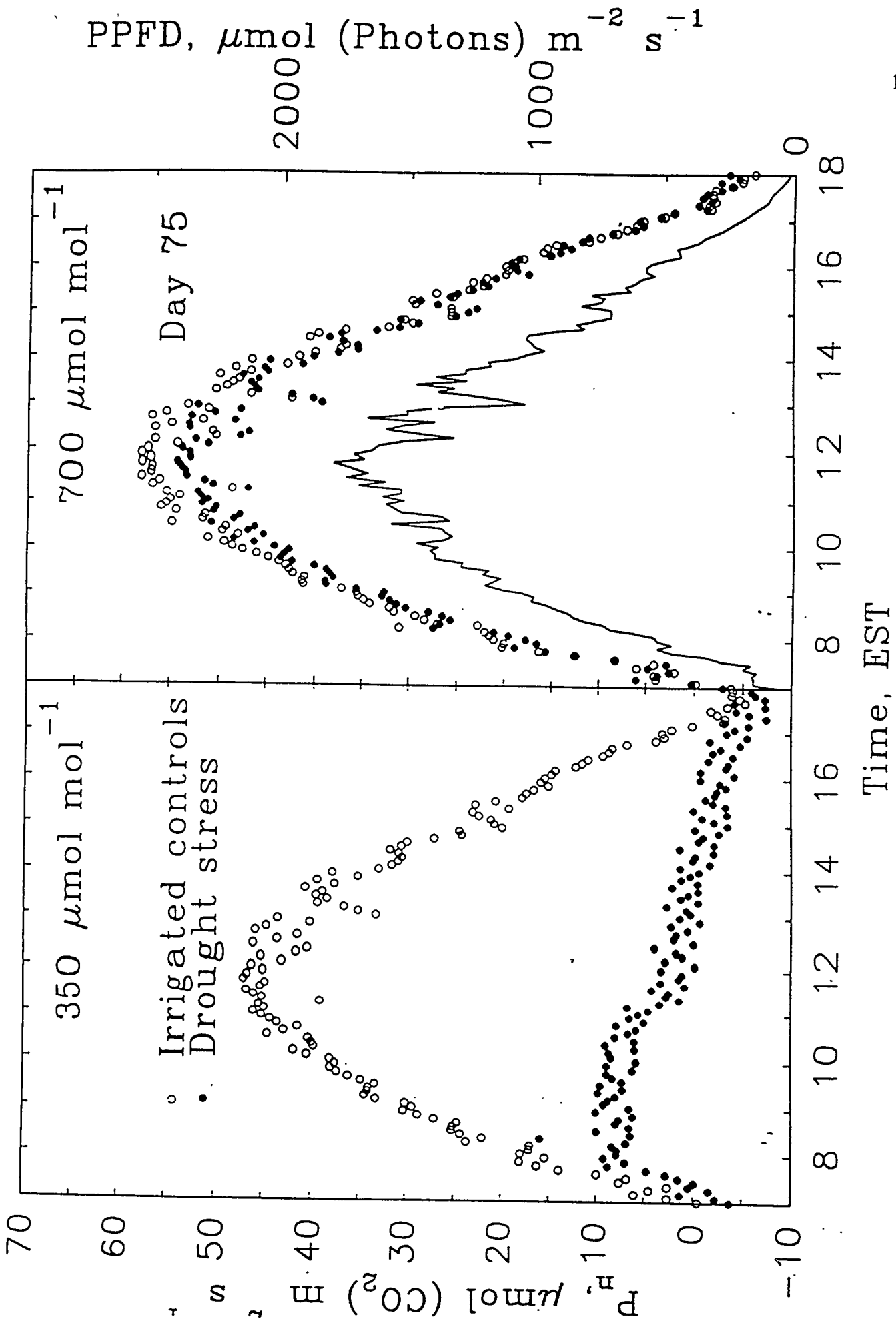


Figure 1

continuously flooded rice methane flux
1994 IR-72 rice experiment

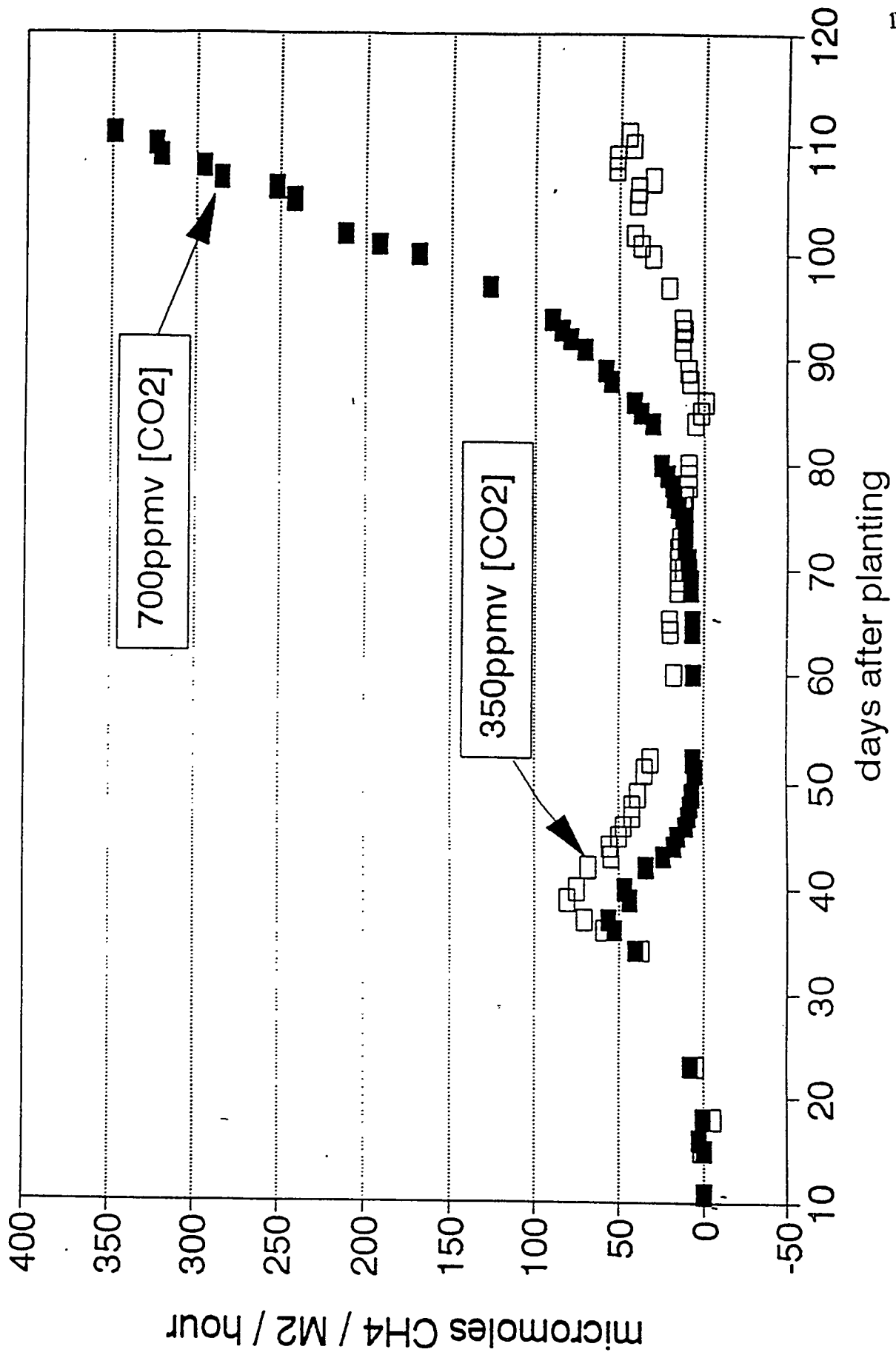


Figure 2

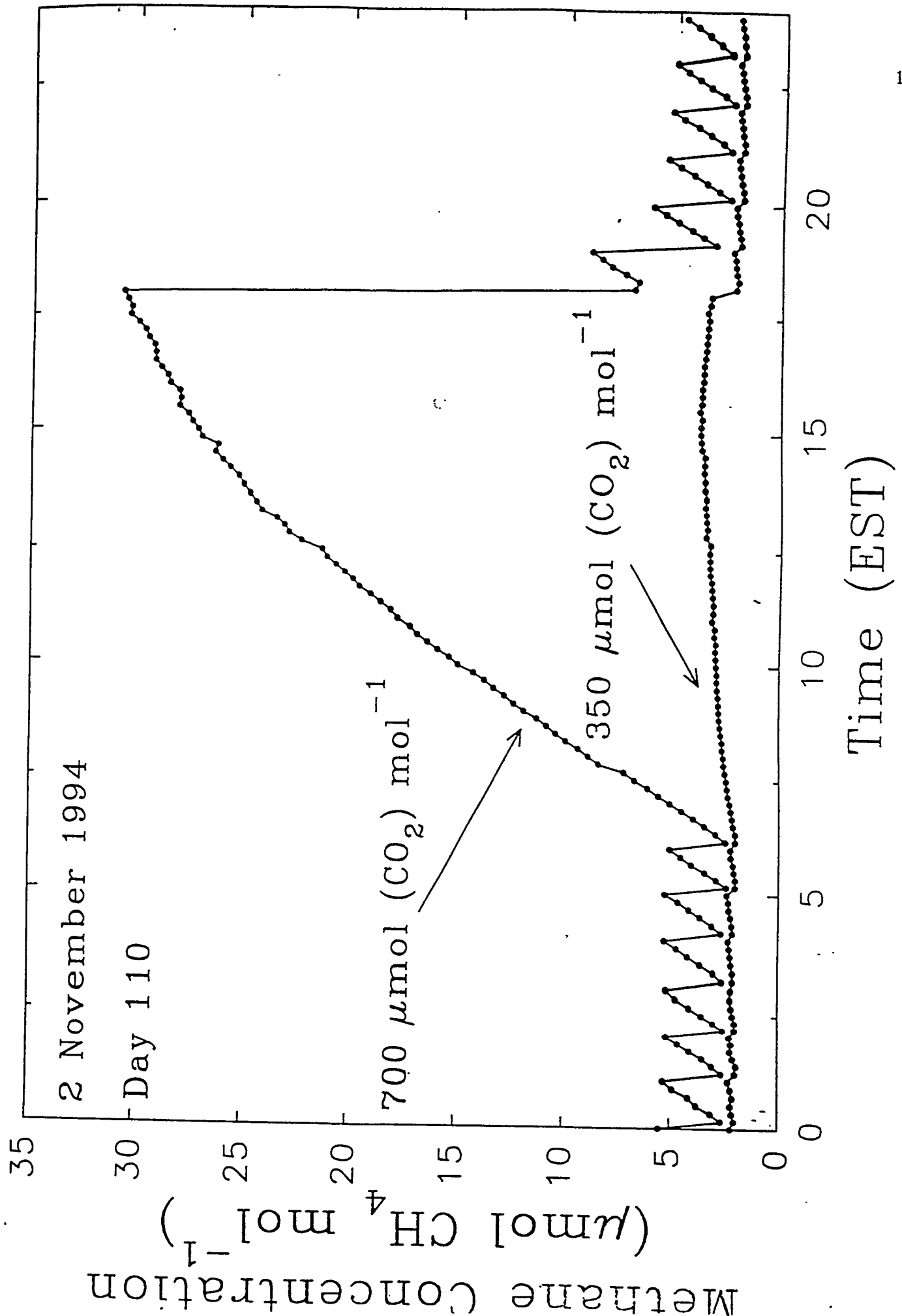


Figure 3

evapotranspiration (ET) were measured and summarized at 5-min intervals. High temperature treatments developed leaf area and nodes more rapidly, so that canopy photosynthesis and ET increased more rapidly. The 40/30°C treatment was not detrimental to vegetative growth, but it did produce more total main axis nodes and more vegetative branches. At the mature canopy stage, apparent canopy photosynthesis in high light at midday was similar across all temperature treatments, and was increased 40-50% by doubling of CO₂. Weekly measurements of leaf photosynthesis in high light at 30°C and 350 μmol/mol indicated no significant temperature treatment history effect. Under a short day environment, Bragg flowered at 30 days under the 36/26 and 32/22°C treatments, at 33 days in 28/18°C, and at 34 days in 40/30°C treatment. The 2-cm pod stage was achieved by 43 days in the 28/18 and 32/22°C treatments, and by 44 days in the 36/26 treatment. The 40/30°C treatment did not begin to set pods until after 47 days. Maturity was delayed for the highest temperature treatment, and leaves stayed green and did not senesce completely. Seed yield was increased about 33% by doubled-CO₂-enrichment, averaged across all treatments. Spider-mite infestations in two chambers prevented a good test of CO₂ by temperature interaction on final seed yield in the study. Seed yield was reduced at the 40/30°C treatment compared to the cooler treatments. Seed size and harvest index were reduced as temperature increased. Because we had not reached the critical thermal damage point for seed formation, we designed a follow-up study with much higher temperature treatments to determine the upper thresholds for vegetative and seed growth.

The second experiment on soybean was initiated 11 February 1994 on cultivar 'Bragg' grown in sunlit, controlled-environment chambers at six temperatures (48/38, 44/34, 40/30, 36/26, 32/22, and 28/18°C daily maximum and daily minimum, diurnal curve) at 700 μmol/mol CO₂. The 40/30 and 28/18°C treatments were also conducted at 350 μmol/mol CO₂. Neither this nor the previous experiment used artificial light for photoperiod extension because we wanted to avoid interaction effects of long photoperiods on the high temperature phenomenon. It was obvious after our study, that we saw some features previously attributed to long days in mid-summer that could, in fact, be caused by high temperatures in mid-summer.

Canopy photosynthesis, night respiration, and evapotranspiration were measured at 5-min intervals. Canopy photosynthesis was relatively unaffected in the range of daytime maximum air temperatures of 28 to 44°C. There was a broad optimum at 36 to 40°C, with slightly lower assimilation at cooler or warmer temperatures. These same temperatures were near the optimum for rate of total dry matter accumulation (highest at 36/26°C treatment), although there were only small differences across the entire range from 28/18 to 44/34°C. The 48/38°C treatment was not a legitimate comparison for canopy photosynthesis because many plants did not survive. Leaf photosynthesis was highest at 38°C leaf temperature occurring in the 40/30°C treatment).

One of the reasons for the apparent broad air temperature optimum for leaf and canopy photosynthesis is that the range for leaf temperature was much less than air temperature due to more evaporative cooling of the foliage as the treatment temperature increased. Range in foliage temperature was about 12°C at midday despite the 20°C range in air temperature, a feature we attribute to the larger vapor pressure deficit as temperature increased in our treatments. We propose that well-watered field-grown soybean has minimal sensitivity to relative humidity because there was little evidence of midday declines in leaf or canopy photosynthesis. Leaf assimilation rate showed faint evidence of acclimation because leaves grown at 700 μmol/mol CO₂ had about 10% lower rate than leaves grown at 350 μmol/mol, when exposed to the same 350 μmol/mol CO₂ level. Night respiration showed linear response to night time temperature within treatment for all treatments. Night time respiration was highest for the 36/26 and 40/30°C treatments, which had the highest photosynthesis and greatest biomass accumulation.

Elevated temperature increased vegetative growth, leaf area, and total number of main stem nodes. The 27 to 31°C mean temperature was optimum for time to flowering, with later flowering at 23°C, and

progressively later flowering at mean temperatures of 35, 39 and 43°C. Although temperature treatments had a clear optimum of 31°C, the time to podset and maturity was shortest at the coolest temperature 28/18°C and delayed at higher temperatures. As temperature was increased, podset was delayed and flowering and pod formation prolonged, particularly above 36/26°C. Vegetative growth and photosynthesis were tolerant to high temperatures (up to 44/34°C), but temperatures above 36/26°C delayed reproductive stages, enhanced floral abortion, caused smaller, wrinkled seed, and reduced seed yield. Plants at 44/34°C produced very few pods. At 48/38°C, about 20% of the plants survived, flowered late, and produced no pods.

Seed size, individual seed growth rate, and harvest index was optimum at 28/18°C and declined progressively to zero as temperature increased to 48/38°C. The single seed growth rate curve had its optimum at 23°C mean temperature, and was quite similar to the seed growth response to temperature published by Egli and Wardlaw for soybean. Seed yield was highest for the 36/26°C treatment, but declined rapidly to less than 5% of maximum at 44/34°C, and zero at 48/38°C. Yield at the coolest treatments was somewhat less than optimum because these plants produced less total leaf area, fewer node numbers, and fewer pod numbers than the optimum treatments. Seed size was unaffected by CO₂ treatment. CO₂-enrichment increased yield and seed number 31%, and equally across all temperatures. There was no beneficial CO₂ by temperature interaction on seed yield, which contrasts with the beneficial CO₂ by temperature interaction often reported for vegetative growth.

Partitioning among vegetative tissues was computed and found to be primarily controlled by soybean life cycle progress. For example, the plants remained in a vegetative state when elevated temperature delayed podset and caused extended vegetative branch formation. There were minor effects of temperature; partitioning to leaf was minimum and that to stem was maximum at 31°C. At higher or lower temperature, partitioning to leaf was increased. This was closely paralleled by increase in SLW of soybean at the highest (44/34 and 48/38°C) or lowest temperature (28/18°C). Partitioning to reproductive tissue (pod mass increment divided by total crop growth increment, during the linear phase) was optimum at 27°C mean temperature and rapidly decreased above 31°C, reaching zero at about 40°C. Because seed growth rate was dramatically reduced as temperature increased, we propose that decreased partitioning must be attributed to failures within the seed (cell numbers, cell size, numbers of lipid and protein storing plastids). Samples of seeds have been preserved to analyze for these possibilities.

B. Long-term effects on orange trees

In July 1987, eight 30-cm-tall sour orange tree (*Citrus aurantium* L.) seedlings were planted directly into the ground at Phoenix, Arizona. Four identically-vented, open-top, clear-plastic-wall chambers were then constructed around the young trees, which were grouped in pairs. CO₂ enrichment--to 300 ppm above ambient-- was begun in November 1987 to two of these chambers and has continued unabated since that time. Except for this differential CO₂ enrichment of the chamber air, all of the trees have been treated identically, being irrigated at periods deemed appropriate for normal growth and fertilized as per standard procedure for young citrus trees.

Numerous measurements of a number of different plant parameters have been made on the trees, some monthly, some bi-monthly, and some annually. Results of our findings are summarized below, along with results of measurements made on some other plants grown in the four large chambers beneath the sour orange trees.

Idso et al. (1994) measured net photosynthetic rates of individual leaves of the large sour orange trees that had either been sprayed with methanol or left untreated. No effects of the methanol treatment were evident in any of the measurements. In the trees exposed to the extra 300 ppm of CO₂, however, the

upper-limiting leaf temperature for positive net photosynthesis was approximately 7°C higher than it was in the ambient-treatment trees. This phenomenon led to a 75% enhancement in the net photosynthesis of the CO₂-enriched trees at a leaf temperature of 31°C, a 100% enhancement at a leaf temperature of 35°C, and a 200% enhancement at 42°C.

Idso (1994) measured total biomass production in 12 different harvests of 3 plantings of a total of 424 *Agave vilmoriniana* plants that grew in the large CO₂ enrichment chambers beneath the sour orange trees over a period of 4 years. The growth enhancement produced by a 300 ppm increase in the air's CO₂ content was found to be a linear function of mean air temperature for this desert succulent, ranging from 28% at 19°C to 51% at 29°C.

Idso and Idso (1994) conducted a detailed analysis of several hundred plant carbon exchange rate and dry weight responses to atmospheric CO₂ enrichment that had been published in the scientific literature over the past ten years. They found that the percentage increase in plant growth produced by raising the air's CO₂ content was generally not reduced by less-than-optimal levels of light, water, or soil nutrients, nor by high temperatures, salinity, or gaseous air pollution. More often than not, in fact, the data showed the relative growth-enhancing effects of atmospheric CO₂ enrichment to be greatest when resource limitations and environmental stresses were most severe.

The major results have been summarized of six years and three months of continuous CO₂ enrichment of the four sour orange trees to 300 ppm above the nominal ambient concentration of 400 ppm at which four control trees are maintained. Fig. 4 shows that at the end of this period, the standing trunk plus branch volume of the CO₂-enriched trees was approximately twice that of the ambient-treatment trees, while the total fruit rind volume produced by the enriched trees over four consecutive harvests was about

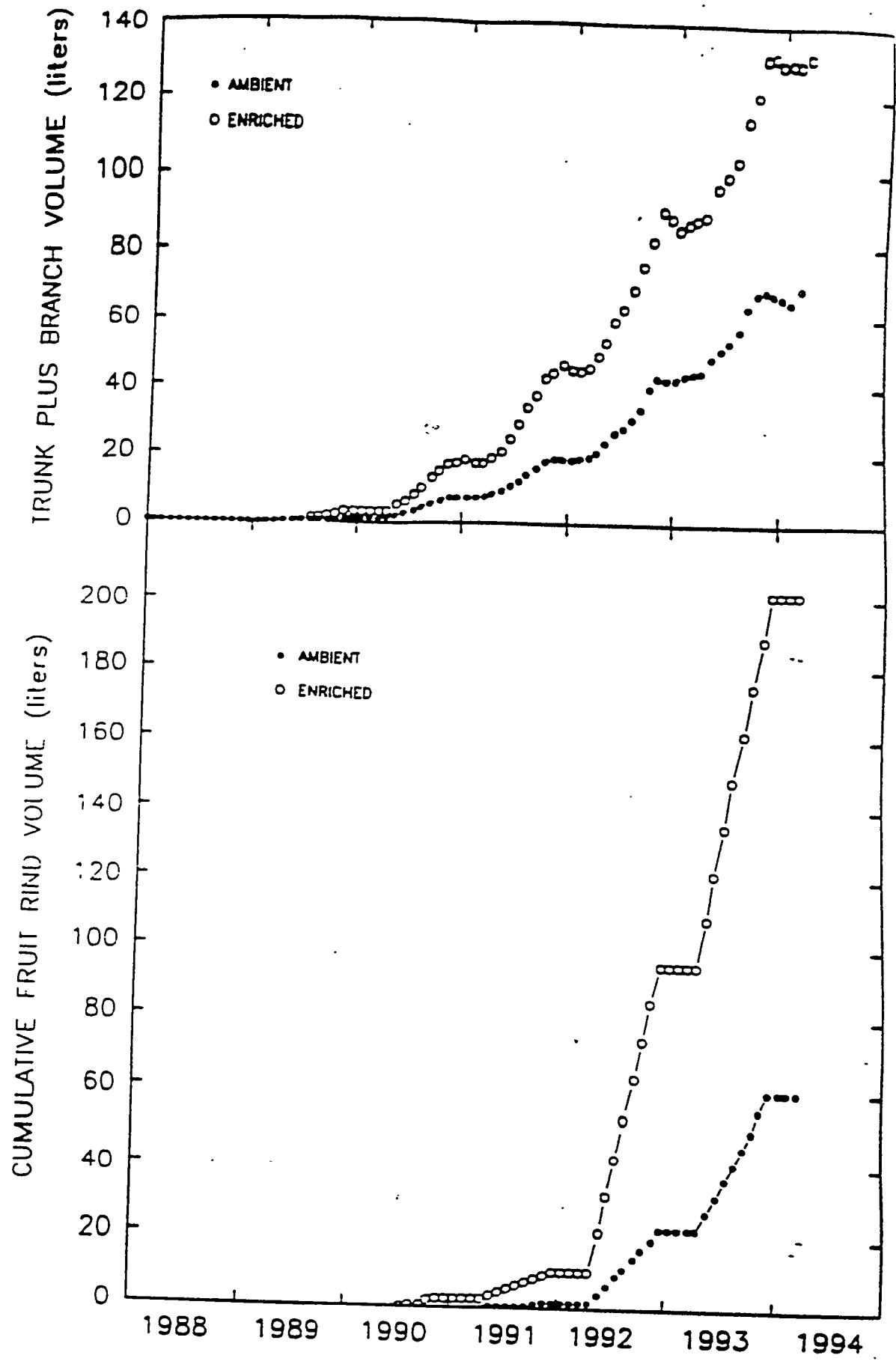


Figure 4. Six-plus years of trunk plus branch volume trends of the CO₂-enriched and ambient-treatment trees (upper panel) and four-year trends of their cumulative fruit rind volumes (lower panel).

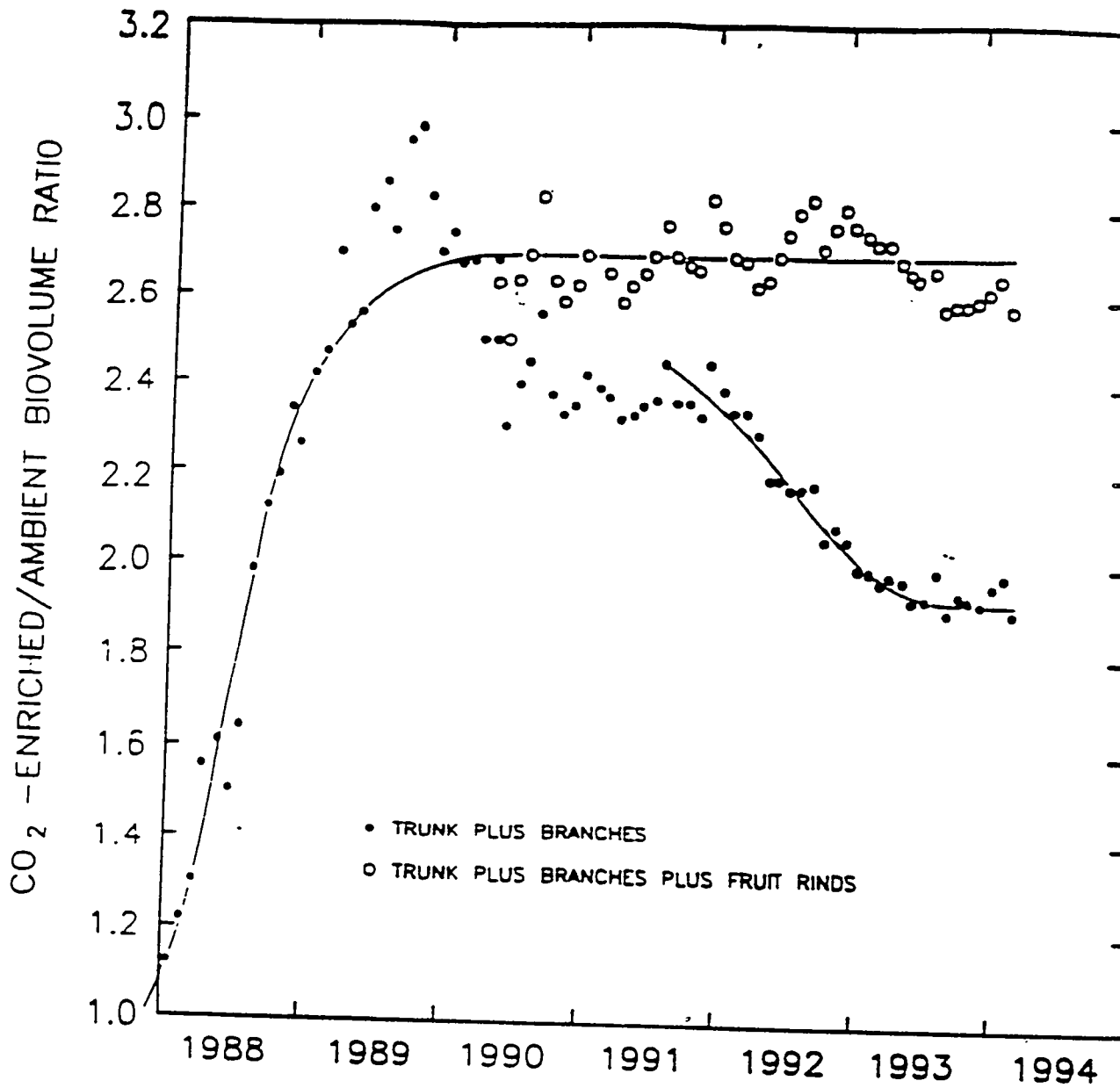


Figure 5. The long-term trend of the CO₂-enriched/ambient-treatment ratio of trunk plus branch volume and the long-term trend of the similar ratio of trunk plus branch plus cumulative fruit rind volume.

three-and-a-third times that produced by the ambient trees. Fig. 5 shows that it took almost two years for the maximum "aerial fertilization effect" of the elevated CO₂ to manifest itself and that it has maintained itself at a total biomass-enhancing factor of about 2.7 for over four years now.

The implications of our findings have a direct bearing on the current debate over anthropogenic CO₂ emissions. They demonstrate that CO₂ is an effective aerial fertilizer, enhancing plant growth under nearly all conditions.

C. Modeling

1. Cotton

a. Modeling cotton growth and phenology to temperature.

Most cotton simulation models were developed with data collected from a narrow temperature range, and hence have limited predictive capabilities under temperature extremes. Several studies of cotton growth under high CO₂ conditions examined the plants' response to a wide range of temperatures, including both high and low temperature extremes. A data set derived from these studies was used to construct a model of cotton growth and development. Plant height was modeled as a function of temperature, number of growing nodes, and duration of nodal expansion on the mainstem. The rates of approach to flower bud and fruit initiation were modeled as a function of temperature. The rates of pre-fruiting, sympodial, and monopodial leaf expansion were modeled as a function of temperature and existing area of the corresponding leaf structures. The daily increment for new node formation was a function of temperature and physiological stresses on the plant. The new model has been verified and is being validated over a range of conditions including temperature extremes.

b. Cotton Production Model -- Sigma+

Dr. V.R. Reddy developed a cotton growth and phenology model and worked with Dr. Hal Lemmon to integrate the phenology model into the Cotton Production Model, Sigma+. The Sigma+, written in C++ by Dr. Hal Lemmon, was developed using data collected from controlled-environment plant growth chambers at high carbon dioxide (700 μmol/mol) over a range of temperatures. This model is designed to simulate cotton growth and development over a range of climatic conditions. Dr. Reddy also collected over 50 comprehensive validation data sets from cotton scientists across the U.S. Cotton Belt to validate the Sigma+. These data sets include information on cotton growth, development, fruiting, and drymatter accumulation.

During this period, several improvements were made to Sigma+ model in the areas of vegetative branch development and leaf initiation and development. The cotton model has been validated with three data sets. The simulated plant parameters like dry weights of plant parts and plant height, number of main stem nodes, leaf area, and number of fruiting organs are found to be very close to the observed data in these three data sets.

c. COTCO₂

Dr. Jeffrey Amthor wrote an initial version of a cotton simulation model, COTCO₂, during his post-doctoral associate period (1989-1990). He employed a systems modeling approach to quantify alterations in physiological and biochemical response in cotton to global change, including the increasing atmospheric CO₂ concentration. In this model organs are initiated from meristems, plant organs "grow" at their own temperature, which may be several degrees different from air temperature, leaf photosynthesis and whole plant respiration processes alter the dynamics of carbohydrate pools so long term acclimation to high CO₂ and "feedback inhibition" of photosynthesis can be addressed. The model has variable time steps depending on the particular process being evaluated. Most processes are updated hourly, but some soil processes are calculated every minute, while variables such as phytomass accretion, leaf area index, canopy height, phenological development, and plant maps are output at the end of the daily loop.

In May 1991, Dr. Gerard Wall joined the project and began the process of documenting and validating the model, which contains over 5000 lines of FORTRAN code. Considerable progress was made in 1992 in documenting the model. Dr. Wall produced flow charts for the main body of the program and all the

subroutines or modules. He incorporated these into a manuscript describing the model which was recently published in a special issue of *Agriculture and Forest Meteorology* that will be devoted to papers describing the 1990 and 1991 free-air CO₂ enrichment (FACE) experiments on cotton at Maricopa, AZ. (Wall et al., 1994)

Additional detailed descriptions about the logic behind almost every line of code in COTCO2 were produced by Dr. Amthor in the form of 13 audio tapes (1 hr each). The flow of computer instructions in each of the ca. 60 routines in COTCO2 is discussed. Derivation of parameters and equations was discussed, and areas of the model needing additional development were highlighted. Variables thought to be especially important were identified for future sensitivity testing. Known errors in the model were corrected.

2. Soybean

Dr. Jonathan Haskett in collaboration with Dr. Yakov A. Pachepsky, have been successful simulating the response of soybeans to increases in atmospheric carbon dioxide concentrations and resulting climate change in Iowa. A preliminary stage of this work was accomplished when a validation study of the GLYCIM model demonstrated that it had the ability to realistically simulate the yield response of soybeans to increases in carbon dioxide concentrations within the range of interest, for both field and controlled environment conditions. Building on these findings simulations of soybean response to climate change between 1991-2051 were run using climate data and carbon dioxide increase estimates from the Goddard Institute for Space Studies (GISS) General Circulation Model (GCM). The results of these simulations indicate that where the predicted climate change is relatively small, that the primary influence on soybean yields would be the increase in atmospheric carbon dioxide.

Dr. Reddy and Dr. Basil Acock, in collaboration with dr. Tony Trent of the University of Idaho and Dr. Frank Whisler of Mississippi State University, are field testing GLYCIM in Mississippi. During the 1991 and 1992 crop years, the model was used in three farmers' fields and four experimental plots for crop management decision making. As a result of the on-farm use of GLYCIM, the areas of the model that need improvements were identified. Two studies during the summer of 1992 were also conducted to collect data on the effect of Benlate and plant density on soybean to incorporate into GLYCIM. To validate the model, they collected 20 data sets representing various soil types, cultivars, and management practices.

Dr. Reddy, Dr. Pachepsky and Dr. Acock identified several deficiencies in the soybean model GLYCIM and were corrected as follows: (1) To facilitate the farmer's setting up data files, running the model, and interpreting results, an interface, WINGLY, was written in the Windows environment. Through a series of menus and data entry screens, WINGLY helps the farmers to automatically download the weather data from a remote weather station, choose and modify data files, schedule runs of the model, and view the results as text or graphics. (2) The tendency of GLYCIM to rapidly explore the whole soil profile and to use the water profligately until growth stopped, was cured by reducing the potential root growth rate. (3) Large and sudden fluctuations in pod and seed numbers were stopped by keeping a record of the weight, actual growth, and potential growth of each pod and seed. These organs are now added when the carbon supply/potential growth ratio falls below 0.75. (4) An infiltration subroutine has replaced the previous model which wetted each layer to field capacity before instantaneously draining excess water to the next layer. The new infiltration subroutine enables the model to deal more realistically with flood and furrow irrigation, but is only an approximation since we know so little about soil surface seals. It was also became apparent that maturity group alone as input to represent cultivar differences was inadequate. Dr. Reddy developed cultivar dependent parameters for several cultivars belonging to maturity groups IV, V, and VI using field data collected from farmers' fields in Mississippi. The

observed data from farmers' fields include dryweights of plant parts and data on soybean plant morphology at weekly intervals. As a result of these parameter files the accuracy of the GLYCIM simulations vastly improved. Presently GLYCIM is being used as a "onfarm" management tool in six farms in Mississippi and one in each farms in states of Arkansas, Alabama, Louisiana, Missouri, and Tennessee. Many of these changes have been made in consultation with farmers, who were well pleased with the results.

Dr. Mary Acock conducted a series of experiments in controlled-environment chambers that revealed just how complicated soybean flowering is and why it has proved to be so difficult to model. Flowering in soybean is not dependent on photoperiod up to anthesis but only during specific phases. The lengths of the photoperiod-sensitive and -insensitive phases are functions of the photoperiod during the sensitive phase. Flowering times of soybean are difficult to predict under naturally changing environmental conditions because it is difficult to define when photosensitivity actually begins and ends for a specific meristem. Different meristems on the plant will have different photoperiod histories, depending on their age.

Dr. Mary Acock analyzed and interpreted data from a series of experiments in controlled-environment chambers on flowering in soybean. She founds that the lengths of both the photoperiod-sensitive and photoperiod-insensitive phases of flower development could be described as two lines which intersected at a critical photoperiod (CP). When photoperiod (P) was $< CP$, the length of the phase was not changed. For $P > CP$, the length of the phase was a positive linear function of $P > CP$. The appearance of a clearly distinguishable floral primordium in the soybean apex marked the end of the photoperiod-sensitive phase and the irreversible commitment to flower. The length of the photoperiod-insensitive phase of flower development was strongly correlated with the length of the photoperiod-sensitive phase. This understanding of flower development makes it possible to predict flowering time in field-grown soybeans without relying on different response curves for increasing and decreasing daylengths as currently done in the crop simulator, GLYCIM. Knowledge of three parameters are required for each phase: (a) minimum length of phase, (b) CP, and (c) the rate of increase in length of phase for $P > CP$. Further study will determine whether the length of the photoperiod-insensitive phase can reliably some of the parameter values are constant for all cultivars.

3. Wheat

a. WHEAT

Dr. Jeffrey Amthor, author of the COTCO2 model described above, has written a wheat growth model called WHEAT. Started while on a post-doctoral appointment at University of California, Davis, he has continued the work at new positions at Woods Hole Research Center and Lawrence Livermore National Laboratory. A working version of WHEAT is now complete and validation has commenced.

Like COTCO2, WHEAT was conceived at the outset to have the capability to account for effects of increasing CO₂ and changing climate on the growth of the crop. WHEAT uses a biochemically based model of photosynthesis and photorespiration. It has an hourly time step and is able to account for changing carbohydrate-pools throughout the plant. The model responds-strongly to CO₂ and temperature in a number of ways and is consistent with results of the few previous CO₂ enrichment experiments conducted with wheat.

4. Simple models of energy partitioning by the terrestrial biosphere.

Dr. Ludmila Pachepsky in collaboration with Dr. Basil Acock, Dr. Jim Bunce, Dr. Vangimalla Reddy, and Dr. Jonathan Haskett studied the process of photosynthesis at a several levels of organization

(biochemistry, cell, leaf, and canopy) using both empirical and mechanistic models whichever was better for the particular problem. The "principle of the reasonable sufficiency" was considered "the best guide for developing the model".

Many models of photosynthesis are known but there have been no attempts to compare them and determine their adequacy. Three of the most popular models of leaf photosynthesis were compared on the basis of the experimental data for tomato plants. The methodology for statistical assessment and comparison was formulated which was so much needed in the agricultural research. The series of two publications were accepted by the journal "Agricultural Systems".

The hyperbolic model of leaf photosynthesis proved to be adequate quantitatively and it can be used in models of productivity for predictive calculations. It is not necessary to introduce a more complicated model with a greater number of parameters. The two interpretations of Farquhar's model (his own and Harley's) were quantitatively and qualitatively adequate, and can be used for research purposes.

Statistical analysis of the parameter values for the hyperbolic model allowed to find their dependencies on environmental factors. Light utilization efficiency proved to be constant at ambient and elevated CO_2 . Leaf conductance for CO_2 transfer depended on temperature as well as on CO_2 concentration. Simple model, the combination of linear and exponential functions, was proposed and proved to perform well for a wide range of the environmental conditions.

The methodology of model development, validation and parameterization was applied to analyze the data on cotton canopy CO_2 exchange in day-lit chambers with controlled air temperature and CO_2 . The empirical model consisting of 4 equations contained 7 parameters which have been determined with the data. The dependencies of parameters for canopy on temperature and CO_2 concentration were compared with the analogous dependencies for leaf parameters that allowed to explain the scaling up from the leaf to the canopy level in modeling photosynthesis. The results were published in the journal "HortScience".

In further development of these studies a four-step process for building a canopy photosynthesis model was proposed on the basis of the cotton experimental data. The first step in modeling was to validate the hyperbolic model of canopy photosynthesis light response curves for each combination of temperature and CO_2 concentration. The second step included selecting formulae that would describe the main features of the dependencies of the parameters of the hyperbolic model on temperature and CO_2 concentration. The third step was to combine these formulae with the hyperbolic model into a composite model. Then the coefficients in the formulae were recalculated fitting the composite model to the entire data set. This fourth step proved to be essential for the good model accuracy. The resulting composite model was shown to be qualitatively and quantitatively adequate to describe the effects of light, temperature, and CO_2 concentration in predicting cotton productivity in a changing environment. This methodology is published in the journal "Biotronics".

The new model of photosynthesis and transpiration, 2DLEAF, the two dimensional model of leaf gas exchange accounting for leaf anatomy was developed. The model presents a combination of (i) two-dimensional CO_2 , O_2 , and water vapor diffusion in intercellular space schematized according to the leaf anatomy, (ii) CO_2 assimilation on cell surfaces as described by Farquhar's biochemical model, and (iii) stomatal movements. Parameters describing the leaf cross-section and gas diffusion properties replace the empirical parameters of earlier models. The model was tested for soybean and tomato and performed well in representing light, CO_2 , and temperature response curves as well as the dependence of transpiration on temperature and water vapor deficit. The model allows the calculation of the steady state distribution of CO_2 and water vapor concentrations in the intercellular space and the boundary layer. The direct calculation of diffusion in leaves showed that stomatal aperture effectively regulates the transpiration rate but usually has much less significant effects on the rate of transpiration. The paper has been presented

at the GCTE conference in Woods Hole and was accepted for publication by the journal "The Global Ecology and Biogeographic Letters".

Parameterization and validation of the model 2DLEAF were performed also with the data on tomato leaf photosynthesis and transpiration. On the basis of the tomato leaf anatomy the series of numerical experiments have been performed with the model 2DLEAF to test several hypothesis which are important for predictions of photosynthesis and transpiration in both current ambient and future changed climate conditions. The 2DLEAF demonstrated the powerful abilities for testing various hypothesis.

Will stomatal density change in future elevated CO₂ atmosphere? This question is the source of contradictions in the current literature. The calculations were performed for tomato leaf with (a) normal, (b) 25% increased and (c) 25% decreased stomatal density for the same internal leaf structure with the appropriate changes for substomatal cavities. Simulations were performed in three replicates. Calculations unexpectedly showed that both a decrease and increase of stomatal density causes a decrease of the photosynthesis rate at both current ambient and doubled CO₂ concentration. The water utilization efficiency increased for elevated CO₂ concentration and all stomatal densities. Consequently the above hypothesis is not confirmed by this numerical experiment at least for tomato leaf or for species with a similar leaf anatomy.

Direct measurements of stomatal aperture are extremely rare in current publications, all of them are replaced by "measurements" of conductance that a really calculations of conductance from transpiration data by a very approximate empirical model. At the same time the stomatal conductance very often if not always is equated to the stomatal aperture. The calculations of stomatal aperture were performed with 2DLEAF for a measured light response curves for tomato. Stomatal conductances have been calculated for these data too. The relationship between these two variables, very different in their nature, is very close but essentially nonlinear one. So it's not correct to replace one characteristic with the other one.

2DLEAF being more mechanistic model than those based on the resistance (conductance) analogy allows to test the accuracy of the calculations of the internal CO₂ concentration C_i routinely accepted. The difference depends on light intensity and varies from 7 to 18% of the maximum. Consequently if the precise value of C_i is needed it's better to use 2DLEAF for it's calculations. These very recent results are in the process of the preparation for publications.

5. Soil process model

The Beltsville-based group (Drs. Ya.Pachepsky, D.Timlin, B.Acock, H.Lemmon, and A.Trent) developed 2DSOIL - a new two-dimensional modular simulator of soil and root processes for interfacing with plant and micrometeorological models.

The environmental effects of many agricultural management practices depend on the interplay between the horizontal and vertical movement of water and solute in soils. There has been a need to enhance crop models by developing a soil simulator that is able to model these interactions and can be easily interfaced with crop models.

We developed the comprehensive two-dimensional soil and root simulator 2DSOIL and designed the simulator to be modular to allow it to encompass a range of management practices and to be easily interfaced with plant models. The simulator has been interfaced with comprehensive models of potato and cotton to realistically simulate root water uptake, surface shading, and stemflow among other processes. It is now ready to be used as a tool to evaluate and compare water and fertilizer management practices, especially for row crops, intercropping, and crops on sloping land.

a. General description of soil process model development project

It is desirable that comprehensive crop models be able to provide a reliable way of testing various management scenarios to assess their potential for polluting water in addition to predicting yield. The soil component of these models has to simulate soil processes in at least two dimensions since both vertical and horizontal movement of water has been shown to affect solute leaching in row crops, intercrops, and crops on sloping land. The objective of the project was to develop the first comprehensive soil simulator of this kind.

There are a number of crop/soil models that have been developed specifically to simulate the effects of management practices on chemical transport. These models, however, contain only simple representations of plant processes. To make the simulator suitable for incorporation into crop models, we developed a generic, modular simulator using a novel design. To achieve the goal of building a comprehensive two-dimensional description of soil processes, we had to develop new modules. These modules were based on the most recent mathematical descriptions of solute transport in porous media, multicomponent chemical interactions, and demand/supply-based plant root activity.

The model, called 2DSOIL which is coded in FORTRAN, has been developed and the second version has been released. A user interface has also been developed to allow easy data entry and graphical depiction of the simulation results as the program runs.

A general description of the 2DSOIL design together with some examples is given in papers by Timlin et al. (1995a,b). 2DSOIL is thoroughly documented in the two reports (Pachepsky et al., 1992, 1993c).

b. Design of the 2DSOIL Simulator

2DSOIL includes a number of independent modules, each for a specific soil or root process. Table 1 summarizes the functions and output of the process modules included in 2DSOIL. Each module inputs its own data. Each module contains specific information (data) and knows how to perform certain operations (functions). This design makes the modules highly independent.

Several control modules supervise interactions. In order to share data among process modules, the data must be represented consistently in all the modules. Soil processes in the soil-plant-atmosphere system are characterized by the volumetric contents of substances (e.g., water content, bulk density, oxygen concentration, adsorbed ammonium, etc.). Potentials of physical fields and related physical values are also used (e.g., pressure head, temperature, etc). These contents of substances, potentials, and related physical values are state variables of the soil system, and are known for specific locations within the soil profile.

Because values of the state variables are known at specific spatial locations, the coordinate systems for all process modules must coincide. The coordinate system is represented by a spatial grid which is a polygonal geometric structure representing a vertical and horizontal cross-section of soil. The spatial locations where the values of the state variables are known are called nodes. The nodes provide a spatial reference for the interactions between soil and root processes.

To facilitate sharing of information among modules and creation of independent program units we used the concept of encapsulation of information which is a characteristic of object-oriented programming. Encapsulation is the grouping, into a single module, both data and operations that affect the data (Wirfs-Brock et al., 1990). The data and operations, encapsulated in a single module, can be hidden from other program units. For example, each process module in 2DSOIL reads its own input file. This eliminates the need to use an input module and the ensuing problem of moving data from the input module to the

module containing the operations that use that data. Selected variables, however, such as the coordinate locations of the nodes, can be made accessible to other program units. This will be discussed later.

Subroutines that calculate transport, transformation or equilibrium parameters needed in process modules are also encapsulated within the process modules. For example, the water movement requires hydraulic conductivity and water content as a function of metric potential. The subroutine containing the equations for these calculations is hidden in the water mover, other process modules have no need to call it or know of its existence. It reads its own data file with parameters and calculates water content and hydraulic conductivity to be passed to the water mover. The water mover module only requires hydraulic conductivity, it does not know how those conductivities are determined. This facilitates the replacement

Table 1. The functions and output variables of process modules in 2DSOIL.

Group of modules	Content and results of calculations
Transport modules	Distributions of substances and energy in soil as affected by intrasoil gradients, boundary fluxes and sources and sinks in soils
Soil-atmosphere	Fluxes of substances and energy through the soil surface boundary modules as affected by state of the atmosphere (radiation, precipitation, temperature, wind, etc.), presence of plants (shadowing, stem flows, canopy penetrability, etc.) and state of the soil surface.
Boundary modules	Fluxes of substances and energy through soil boundaries that are assumed to be not controlled by atmosphere status; those may include drains, heat pipes, etc., and also boundaries of soils in controllable experiments where surface conditions are maintained artificially at prescribed levels.
Root activity	Sources and sinks of substances in soil caused by root modules uptake, root exudation and root respiration
Interphase	Equilibrium and/or nonequilibrium distributions of exchange modules substances between soil solution, mineral phases, ion exchange phases, and gas phases; these modules produce sources and sinks for the transport modules
Biotransformation	Sources and sinks of substances in soil caused by modules microbial/biochemical transformation of compounds
Management	Changes in either contents of substances, or in soil modules media distribution, or in material fluxes through soil boundary, following technological operations.

of equations that describe soil hydraulic properties (van Genuchten, Brook-Corey, Campbell, etc.). If a different method is desired, one creates a new subroutine and data file, no other changes to the model or other input files are required.

In order to implement encapsulation of data in FORTRAN, variables are subdivided into two fields: public and private. The public field can be global, e.g., available to all process modules (these variables are not encapsulated), or locally, e.g. available to the process module and a subroutine within it. Process modules share information with each other only through the global field. The global field includes soil state variables, coordinates of grid nodes, nodal soil material numbers, updated boundary fluxes and/or state variables, updated root uptake rates, sources, sinks, time stepping parameters, and updated numbers of iterations in modules with iterations. The process module communicates with submodules via variables that are locally public (shared between the two of them only). The private field includes information needed only within the module such as values of state variables from previous time steps and parameters to calculate moisture capacity or nitrification rate, and variables needed for the numerical calculations such as convergence criteria.

Global variables in upper level process modules are passed in COMMON BLOCKS; no arguments are passed in CALL statements in process level modules. The use of an INCLUDE statement, with a list of common blocks, that is inserted into each of the process module files, simplifies management of the code. If a global variable is updated or added, only one file (the INCLUDE file) needs to be changed. Locally public variables (i.e., between process modules and subroutines) are passed in CALL statements. The number of global variables that need to be passed in COMMON BLOCKS is reduced by having each module input it's own data from an individual data file. This data, then, does not have to be passed from an input module to the program unit in which it is used. In fact, it is good practice to use the minimum number of global variables possible.

COMMON BLOCKS are also used to store private information within a module. This provides a method to save the values of any private variables between subroutine calls. Any particular COMMON BLOCK, that contains private information, is present only in the module containing the variables. Because there is no reference to them in other program units they remain hidden in a particular module.

The modules in 2DSOIL share information through the public information field. When plant and atmosphere models are interfaced with 2DSOIL or new soil process modules added, the public data field will also need to include public variables of the plant and atmosphere models.

For coupling of modules, 2DSOIL uses a sequential iteration approach (Yeh and Tripathi, 1991) in which the transport equations, chemical and biochemical transformation transport equations, and root growth and water uptake equations are in separate subsystems. The processes are decoupled from each other and execute sequentially. It is assumed that the values of all sources and sinks of transport processes are available at the beginning of the time step.

In 2DSOIL, each process module may have its own time step because the required time intervals among modules may vary greatly. For example, the time interval between two applications of fertilizers can be two months, the atmospheric boundary can be modified hourly, and calculation of infiltration may require time steps on the order of several seconds. Combining modules, which work with different time steps, into one simulator is referred as asynchronous coupling (ten Berge et al., 1992).

In general, a process module may require a time increment which depends on convergence of the solution of nonlinear system of equations. This may occur in highly nonlinear models of soil processes like water movement or microbial transformation when the conditions change drastically, for example, when

infiltration into dry soil begins. Such modules require an algorithm to calculate a suitable time step. For now, such a case is anticipated only for the water movement module.

The control module 'Synchronizer' calculates the actual time step that the model uses during a simulation. It is invoked at the end of every time step. The selected time step is the optimum increment that allows for convergence of non-linear equations and enables the model to input or output data at specific times.

If there are no modules with time step requirements, 2DSOIL will gradually increase the time step until it reaches a prescribed maximum value. 2DSOIL can also work with a constant time step.

2DSOIL is designed to accept five types of boundary conditions for water, solute, heat, and gas transport:

- i. the state variable (pressure head, solute concentration, temperature, or gas content) is constant for all values of time or depends on time;
- ii. the gradient of a state variable is equal to zero ("an impermeable boundary");
- iii. the flux of water, solute, heat, or gas depends linearly on the surface value of the pressure head, solute concentration, temperature, or gas content, respectively. Coefficients of the linear dependencies must be constant or input as a function of time;
- iv. the fluxes may have a complex dependence both on surface soil status and on variables external to the system (atmosphere and plant canopy);
- v. an interior boundary, which may be either a point boundary or a two-dimensional boundary as in a buried cavity.

These five types of boundaries include all common formulations used in modeling soils. Each boundary node is assigned a code which defines the type of boundary. We adopted a coding system which is traditional for finite element transport models in hydrogeology (Neuman, 1972).

The generic, modular structure of 2DSOIL offers many advantages for the development and maintenance of agricultural management models.

- i. Computer code can be easily modified and evaluated. This simplifies the process of incorporating ideas, derived from experimentation, into models.
- ii. Submodels, which are components of a larger model, can easily be tested and validated in more than one model. For example, nitrogen cycle models must be evaluated in crop growth and water transport models. The evaluation would not be limited to one particular model.
- iii. Users can add management practices as modules to build models for specific tasks from program units developed by researchers.
- iv. Because the developer of a particular process module does not need to know the details of the other modules, each developer gains access to a wide range of code in areas outside her or his field of expertise.

c. Modules of the 2DSOIL Simulator

In 2DSOIL, modules correspond to soil processes. We built an example simulator using the following groups of processes:

- transport processes: water movement, transport of solutes, heat movement, transport of gases; finite element models are used;

- soil-atmosphere interaction processes: surface gas and heat exchange influenced by shading, evaporation, sealing;
- soil-plant interaction processes: root water and solute uptake, root respiration;
- mass exchange through defined boundaries within soil: subsoil irrigation, drainage;
- chemical interactions: reversible Ca-Mg-Na exchange, dissolution precipitation of sparingly soluble salts, speciation of ions in the solution, dissociation of water and H_2CO_3 ;
- biotransformation processes relevant to nitrogen cycling and transformation in soils: mineralization, immobilization, nitrification, denitrification;
- management processes: tillage, application of nitrogen fertilizers.

A brief description of each module follows including (1) development and/or adaptation, (2) parameter determination and/or data acquisition, and (3) validation and/or use in research.

i. Water movement modules

Development and/or adaptation. At present, we have 3 modules to describe water movement in soils: 2D finite element module, 1D finite difference module, and a hybrid 1D module with Green-Ampt-like infiltration and the finite difference redistribution component.

The 2D finite element module has been adopted from the report of US Salinity Lab (Simunek et al., 1992). It uses Galerkin-type linear triangular finite elements and numerically solves Richards' equation for saturated-unsaturated water flow.

The 1D finite element module has been developed by us using approximation of the Richards equation based on the Taylor expansion of the water retention function (Pachepsky et al. 1986). This method demonstrated an excellent mass balance accuracy and applicability in soils with strongly nonlinear hydraulic functions.

2D module can be also used to model 1D problems, but the use of triangular elements introduces an artificial asymmetry in results.

Even the 1D algorithm was too time-consuming when multiple runs of a crop models were carried out. It happened mainly because the time step became very small during infiltration. To avoid this we developed a hybrid 1D algorithm that used Green-Ampt-like infiltration and a finite difference redistribution component (Pachepsky and Timlin, 1995b). This algorithm uses a new Green-Ampt-like method to simulate infiltration into layered soil through the surface crust.

Parameter determination and/or data acquisition. To use data on properties of soil in the water movement models, some formula is usually fitted to data and then used in the model. The statistical error of the second type is introduced by this procedure, and the induced error can be high. To prevent this, we developed a technique of interpolation of soil hydraulic properties with piece-wise polynomials (Pachepsky and Timlin, 1995c). This technique preserves shapes of the experimental curves and diminishes errors of the derivative calculations. The corresponding routine is incorporated into 2DSOIL.

Techniques are needed to estimate variability of soil hydraulic properties and to incorporate this variability into models. We carried out data analysis to assess an applicability of the geostatistics to data on water retention of gray forest soil (Gummatov et al., 1992). Our results were in agreement with results of other authors who showed earlier that high nugget effect prevents using results of kriging to describe and map field variability of soil water retention. Therefore the scaling of water retention as a scale-independent property seems to be a legitimate procedure. We developed a technique of fractal scaling of soil water retention which is based on the fractal model of soil pore space (Pachepsky et al., 1995c). This technique use the variance of pore radii distribution as a single scaling parameter in the wide

range of soil water potentials from 1 kPa to 160 000 kPa. The technique is incorporated into a stand-alone program which can be obtained together with 2DSOIL.

Soil hydraulic properties demonstrate temporal variability. It is caused by both management operations and plant development. We developed a submodule which simulates changes in soil hydraulic properties due to soil subsidence after tillage. This module is incorporated in 2DSOIL. To assess the influence of plant development on soil hydraulic properties we made the data analysis of the water retention data collected under developing crops (Gummatov and Pachepsky, 1994). Results show that hydraulic properties of the root zone do change during the vegetative period, and this problem seems to be overlooked in the modern models of the water movement in soils.

Field measurements of the hydraulic conductivity of soils usually do not distinguish between conductivities of macropores and micropores. However, the difference between these conductivities is important for the simulation of preferential movement of solutes in soils. We evaluated techniques to measure macropore conductivities and recommended the technique giving the most stable results (Timlin et al., 1993).

To validate 2DSOIL using data on soil water regimes in crops, we developed a technique of continuous soil moisture data acquisition based on time domain reflectometry (TDR). A system consists of the TDR equipment set up to collect data from different depths, data logger, laptop computer, and solar batteries. This system was tested during two growing seasons under soybean crop, and demonstrated high reliability and good data quality. Soil water content was measured each hour during 4 months both in 1993 and 1994. The data show that during infiltration and drainage, the water dynamics are very different in the row and interrow positions. There is greater infiltration and more rapid rates of drainage in the row positions than in the interrow positions. Patterns of water uptake in the two regions, however, are similar. This data will be used for the validation of 2DSOIL.

Validation and/or use in research. 2DSOIL with 1D water movement module was used to evaluate the relative importance of the evaporation and transpiration in desert plant communities (Kemp et al., 1995). Predictions of 2DSOIL had shown that earlier estimates based on the rough estimates of the soil water balance gave a distorted picture of the transpiration/evaporation interplay in these ecosystems.

2DSOIL with 2D water movement module was used to simulate the below ground competition in intercrops (Caldwell et al., 1994).

2DSOIL with 2D water movement module was used to simulate the differences in water and nitrogen transport between alternate and regular furrow irrigation (Pachepsky et al., 1993). We found that when alternate furrow irrigation is used instead of regular furrow irrigation, the root distribution is concentrated near the irrigated furrow; this creates favorable conditions for nutrient uptake and will limit leaching of fertilizers if they are placed in the ridge, near the plant.

1D water movement module was used to evaluate the influence of the water transport regime on the pesticide movement in sandy soils (Galiulin et al., 1993). It was found that the soil layering can be an important factor in the formation of the final pattern of the 2,4-D distribution over the soil profile.

ii. Solute movement modules

Development and/or adaptation. At present, we have 2 modules to describe solute movement in soils: 2D finite element module and 1D finite difference module.

The 2D finite element module has been adopted from the report of the U.S. Salinity Laboratory (Simunek et al., 1992). It uses Galerkin-type linear triangular finite elements and numerically solves convective dispersive equation. We modified this module to exclude error accumulation related to the use of the flow velocities (Pachepsky et al., 1993c).

The 1D finite element module has been developed by us using approximation of the convective-dispersive equation (Pinski and Pachepsky, 1994).

Parameter determination and/or data acquisition. We demonstrated the need in two dimensional simulations of the solute transfer in soil, studying solute leaching in crop row vs. interrow zones (Timlin et al., 1992). We also used conjugated data on solute movement in soil cores and in the field to demonstrate the necessity to use field solute transport data to determine parameters of the solute transport in clay loams (Shein et al., 1994).

Validation and/or use in research. 2DSOIL with 2D solute movement module was used to simulate the differences in solute movement between row and interrow positions in the soybean crop. We found that when the subirrigation is in effect or the beginning of the growing season is very dry, wide row spacings may cause the leaching of chemicals into deep soil layers (Pachepsky et al., 1993c)

1D solute movement module was used to evaluate the influence of the shape of the adsorption isotherm on cadmium transport in soils (Pinski and Pachepsky, 1994).

1D solute movement module was used to evaluate the influence of the water transport regime on the pesticide movement in sandy soils (Galiulin et al., 1993). It was found that the CDE equation in general does not predict solute movement in studied soils even though the water movement can be predicted satisfactorily.

1D solute movement module was used to investigate reasons of the bimodality that occurs in breakthrough curves of adsorbing solutes in soils. Differences in rates between adsorption and desorption were found to be a probable reason.

iii. Heat movement module

Development and/or adaptation. The 2D finite element module has been written by us using as a base source the report of US Salinity Lab (Simunek et al., 1992). It uses Galerkin-type linear triangular finite elements and numerically solves heat transport equation.

Parameter determination and/or data acquisition. We did not carry out any research in this field.

Validation and/or use in research. 2DSOIL with the heat movement module was used to simulate the differences in soil environment of plants resulting from the development of surface shading. We found that the shading reduces evaporation in the interrow zone and causes soil temperature and moisture differences between row and interrow zones can reverse the ratio of the nitrogen transformation rates in these zones (Timlin et al., 1995b).

2DSOIL has been interfaced with SIMPOTATO, a potato simulation model developed by Dr. Thomas Hodges of the USDA/ARS in Prosser WA. It is being used to study possible temperature regimes of soils, since the potato tuber development is extremely sensitive to this variable.

iv. Gas movement module

Development and/or adaptation. The 2D finite element module has been written by us using as a base source the report of U.S. Salinity Laboratory (Simunek et al., 1992). It uses Galerkin-type linear triangular finite elements and numerically solves diffusion equation.

Parameter determination and/or data acquisition. We collected a data base on the dependence of the gas diffusion coefficients on air-filled soil porosity as related to soil properties (Pachepsky et al., 1993).

Validation and/or use in research was not performed.

v. Soil-atmosphere boundary module

Development and/or adaptation. We adapted the module developed by B. Acock and used in the soybean crop simulator GLYCIM (Acock and Trent, 1991). This module uses meteorological information on a daily basis. It transforms these data to hourly updated soil surface boundary input for water movement, solute movement, heat movement, and gas movement calculations within the soil domain. Several parameters of the crop canopy are used to distinguish between evaporation from bare soil and from covered soil. Equations of celestial mechanics, solar radiation attenuation and irradiance distribution, geometry of a canopy, and Penman equation together with semi-empirical correction factors are used to obtain boundary fluxes.

Parameter determination and/or data acquisition. A proper selection of the water vapor adsorption isotherm equation can be crucial for the ability of the model to predict surface evaporation properly. We carried out studies based on the theory of gas adsorption on heterogeneous surfaces and found that the bimodal distribution of adsorption energy seems to be feasible approximation to calculate adsorption isotherms (Ponizovsky et al, 1993; Pachepsky et al. 1995b).

Validation and/or use in research. This module has been used in all applications of 2DSOIL described above: simulation of the below ground competition in intercrops (Caldwell et al., 1994), simulation the differences in water and nitrogen transport between alternate and regular furrow irrigation (Pachepsky et al., 1993), evaluation of the relative importance of the evaporation and transpiration in desert plant communities (Kemp et al., 1995), solute movement between row and interrow positions in the soybean crop (Pachepsky et al., 1993), simulation of differences in soil environment of plants resulting from the development of surface shading (Timlin et al., 1995b), and many other that were not documented.

iv. Root development and water uptake module

Development and/or adaptation. We adapted the module developed by B. Acock and used in the soybean crop simulator GLYCIM (Acock, Trent, 1991). This module generates the relationship between the potential transpiration rate and leaf water potential. The concept of trade of the shoot carbon for the root water is a driving hypothesis in the model. Osmoregulation of leaf potentials, root activity dependence on soil environment, and differences in the activity of young and mature roots are taken into account.

Parameter determination and/or data acquisition. Estimation of root water uptake in crops often involves two assumptions: (1) that a critical soil water potential exists which is constant for a given combination of soil and crop and which does not depend on root length density, and (2) that the local root water uptake at given soil water potential is proportional to root length density. We observed a linear dependency of a critical soil water potential on the logarithm of root length density for all plants studied.

Soil texture modified the critical water potential values, but not the linearity of the relationship (Shein and Pachepsky, 1995).

Validation and/or use in research. This module has been used in several applications of 2DSOIL described above: simulation of the below ground competition in intercrops (Caldwell et al., 1994), simulation the differences in water and nitrogen transport between alternate and regular furrow irrigation (Pachepsky et al., 1993), evaluation of the relative importance of the evaporation and transpiration in desert plant communities (Kemp et al., 1995), solute movement between row and interrow positions in the soybean crop (Pachepsky et al., 1993c), simulation of differences in soil environment of plants resulting from the development of surface shading (Timlin et al., 1995b), and some other that were not documented.

vii. Chemical interactions module

Development and/or adaptation. We adapted the module developed by Ya. Pachepsky and used in the simulator LIBRA (Pachepsky, 1990). Macroelement equilibria chemistry module in the 2DSOIL model describes a system of interphase chemical interactions: dissolution-precipitation of gypsum and calcite, Ca-Mg-Na cation exchange, formation of ion pairs in solution, and dissolution of gaseous CO₂. Besides, the adsorption is treated as separate process.

Parameter determination and/or data acquisition. Adsorption of anions can be of particular interest in the regions with acid soils, since it can diminish an environmental hazard of the nitrate migration in soils below the root zone. We studied the adsorption of nitrate-ions in such a soils and found that the average velocity of nitrate movement can be an order of magnitude less than that of water (Pachepsky et al., 1993b). We had shown also that the acidification can modify cation exchange equilibria in soils depending on soil clay mineralogy (Ivanova et al., 1992).

Validation and/or use in research. This module has been used to evaluate an effect of irrigation on exchangeable cation composition and selectivity of ion exchange in solonets soils (Tolpesta et al., 1993).

d. Incorporation of 2DSOIL in crop models.

2DSOIL has been interfaced with SIMPOTATO, a potato simulation model developed by Dr. Thomas Hodges of the USDA/ARS in Prosser WA. It is being used to study possible temperature regimes of soils, since the potato tuber development is extremely sensitive to this variable.

2DSOIL simulator has been interfaced with comprehensive models of cotton.

e. Technology Transfer

The code and documentation have been released to 40+ potential users in the USA. We have also received requests and released the current version of the model to users in Canada, Israel, Germany, Finland, Russia, and the Netherlands. 2DSOIL has been incorporated into a cotton model and a potato model which are now being used by the USDA to study the fate of nitrogen fertilizer for several management practices in California and Washington. At the moment there are few mechanisms to collect information on the use of model by those to whom it was released. We would estimate that about half the users apply 2DSOIL or its components in projects related to crop productivity and water quality problems.

The most recent version of 2DSOIL with code and documentation is available on the Internet at the Anonymous FTP site ASRR.ARSUSDA.GOV. Login as userid 'anonymous' and use your e-mail address as password.

f. Publications and Presentations

We published results of the development and use of 2DSOIL in 32 technical paper and reports.

The development and use of 2DSOIL has been presented and discussed at the Conference on Agricultural Research to Protect Water Quality, Minneapolis, MN, 21-24 February, 1993, at the '93 ASA meeting, the '94 Cotton Beltway Conference, the '93 and '94 Annual Crop Workshop Simulation, and the '94 Conference of The International Society for Ecological Modeling.

We presented and demonstrated 2DSOIL at the American Society of Agronomy meetings in Seattle, WA, November, 1994, and at the at The Workshop on Computer Applications in Water Management, May 25, 1995 in Ft. Collins, CO.

The use of 2DSOIL in the intercrop model for the simulation of two competing root systems was presented at the "Workshop on Nitrogen Dynamics of Intercropping Systems in the Semi-arid Tropics", 21 to 25 November, 1994, Sponsored by ICRISAT.

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ATTACHMENT # 1.

INTERAGENCY AGREEMENT DE-AI02-93ER61720

Number of students trained = 1.

Number of Postdocs who worked on the Project = 4.