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RESEARCH

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THE COVER

A fuel-injector spray photographed with 10-keV x rays. The image, formed on standard x-ray film, has been color-enhanced by computer to show details of the spray pattern and density distribution. The spray is formed when liquid diesel fuel is forced at high pressures (10 MPa) through a small orifice (300- μ m diameter), producing many small droplets. Liquid fuel must be broken up into such droplets to burn effectively in combustion chambers.

Because of the importance of fuel injection in many combustors, we are studying the behavior of fuel sprays in detail. Both high-speed photographic techniques and numerical models of spray motion are being pursued as part of the combustion research program at LLL. This program is described in the article beginning on p. 1.

ABOUT THE JOURNAL

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April 1977

Energy and Technology Review

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BRIEFS

AUTOMATED PRINTED-CIRCUIT BOARD DESIGN

Each year, we design over 250 new printed-circuit (PC) board layouts and modify many existing designs. Not long ago the layout process, which consists of converting a schematic diagram into finished PC artwork and a hole-drilling tape, took from three to five weeks. Delays sometimes slowed the process even more. We recently completed the software development for an automated system that does the job in two to three days.

Previously, PC board layout was a manual task. First we applied decals representing components and their connector pads to two oversized transparent films, one for each board surface. We traced connections between the decals with strips of adhesive tape representing the copper-foil conductor paths. Then we mounted the completed layout films on a digitizing table to measure the exact locations of holes for component pins and through-the-board conduction paths. The digitizing process produced a computer-readable data file. That file enabled a computer program to punch onto a paper tape numerical instructions for an automated drill.

Our new computer system for producing PC boards saves time by eliminating the manual layout and digitizing operations. The layout requirements — including board-identification data, component types and their desired locations, and a specification of signal connections to each component — are written out on special coding sheets and entered directly into the computer.

When the program is run, it checks the PC board requirements for consistency and then does the board-layout calculations. It can also produce a layout checkprint before proceeding with the automatic production of the artwork masters and the drill-tape files. We can save the layout on punched cards or magnetic tape, or in the LLL computer network's photostore memory, for future retrieval and modification.

Our automated layout system accommodates both small boards (6 to 20 integrated-circuit chips) and the increasing number of larger layout problems (40 to 65 chips) being designed at LLL (see illustration). The system's current capacity is about 100 chips. Although the new system cannot produce better PC board layouts than those produced manually, its great speed reduces develop-

ment time from many weeks to a few days. By reducing the drudgery associated with PC board design, the new system gives circuit designers more time to think out better designs.

Superimposed artwork masters for both sides of a PC board. With our new computer system, it took about 20 s to calculate the layout for this medium-sized board (i.e., 40 integrated-circuit chips). The next step is to reduce the masters to the correct size for the PC board, sandwich a blank board between the two masters, and photographically transfer the layouts onto this blank. The board is then dipped in an acid bath, which etches away its copper-foil surfaces except where the conductor paths have been photographed. A drill run by the computer tape then puts in the holes.

CONSERVATION

Modeling Combustion Processes

We are developing computer codes to provide detailed numerical descriptions of combustion processes. The codes will be useful to designers of burners, furnaces, and internal combustion engines as they try to increase efficiency and reduce emissions.

Our computer model of the methane combustion reaction — including 20 chemical species and 54 reactions — agrees well with experimental results. Our one-dimensional computer model of the combustion of a stratified charge in an automobile engine indicates that this concept should reduce hydrocarbon emissions. We have completed a very fast two-dimensional hydrodynamic code that has calculated air flow patterns in our idealized engine. We are working to add

fuel-spray simulation and simplified chemical kinetics to it. We have begun the layout of a three-dimensional combustion code. To test the accuracy of our calculations, we have also devised a number of combustion and spray-injection experiments.

Oil, natural gas, and coal provide over 90% of the nation's energy. Because fossil fuels are in limited supply, it is important that the combustors in which they are burned be efficient. Improving combustor efficiency is a vital area in domestic conservation efforts. Also, to satisfy environmental concerns, the processes relied upon must be clean. Unfortunately, it has proved difficult to build combustors that are both clean and efficient. In fact, the two goals are often in conflict.

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Designers of internal combustion engines and other combustion devices are turning to numerical modeling for help in resolving this problem (see box below). Modeling combustion systems is difficult, but the cost is a small fraction of the economic and environmental costs of these systems. ERDA planning documents¹ suggest that in many cases,

combustion efficiency can be improved by 15 to 50%. Even smaller improvements would offer a significant payoff. Numerical modeling may make it possible for us to reach these goals.

We have modeling and experimental studies under way for a number of combustion processes. Progress in these studies is outlined in this article.

NUMERICAL MODELING

Numerical modeling with digital computers is being used more and more to study fluid dynamic systems. Weather systems, oceans, star interiors, oil reservoirs, chemical reactions, aerodynamic lift, and arterial blood flow have all been analyzed in this way. Numerical modeling involves dividing the system under study into numerous small cells, or zones, and calculating the transport of mass, momentum, energy, and chemical species between cells in a series of time snapshots. By changing the sizes and arrangement of the spatial zones, we can model systems with different sizes, shapes, boundary conditions, and initial conditions with the same computer program.

The equations governing a system can often be solved by the computer using numerical techniques with many fewer approximations than in the analytical case. Nonlinear terms can be included, and complicated dependencies of material properties on physical variables can be considered. The detail of the predictions is thus greatly increased. Space- and time-dependent values of the physical variables (which are difficult or impossible to measure in the real system) can be calculated. Moreover, results can be obtained quickly. Typically, only a few minutes of computer time are required.

There are two basic methods of zoning used in numerical modeling: Lagrangian and Eulerian. A Lagrangian mesh is patterned to conform to material boundaries. As the materials move, the mesh moves also, and the size and shape of the zones change to adjust to the changes in the materials. An Eulerian mesh is fixed in space, and materials are free to move through zone boundaries. Lagrangian meshes give the most accurate calculations for problems in which the zones do not become overly distorted. An Eulerian mesh eliminates the possibility of zone distortion because it is fixed in space.

Without modern scientific computers, numerical modeling could not be done. Digital computers are now large enough (10^5 to 10^6 numbers can be stored) that we can construct a spatial model of a system, and fast enough (10^4 to 10^7 arithmetic operations per second) that we can follow the evolution of a system in time. On today's computers, however, full, three-dimensional models require large amounts of computer time. Thus we try to reduce the problem to one or two spatial dimensions and reserve the three-dimensional calculations for otherwise intractable problems.

Another limitation is that the basic physical data required are sometimes impossible to obtain. For example, the detailed reaction rates for complex hydrocarbons and data on the behavior of unsteady, compressible, reactive, turbulent flows are not presently available. Thus, approximations and estimates have to be built into a code. The approach is to use the best information available to make predictions.

Experimental data are an important check on the accuracy of a numerical model. One possible source of error is a lack of knowledge of certain fundamental equations and material properties (reaction rates, transport coefficients, etc.). In addition, we must determine whether the spatial zones and time steps used are small enough to resolve the details of the process being modeled.

The accompanying article reports on recent LLL numerical modeling and supporting experimental studies of combustion processes.

DETAILED KINETICS OF METHANE COMBUSTION

To calculate the rate of energy release in combustion, we need to consider in detail the chemistry of the particular reactions involved. We have concentrated initially on the chemistry of methane combustion because methane (natural gas) is the simplest hydrocarbon. This reaction is often written:

This expression correctly describes the atomic balance, but the kinetics of the reaction (i.e., the actual mechanisms involved) are much more complex.

The hydrogen atoms must be stripped off the carbon one at a time; the O_2 bond must be broken; and the oxygen atoms must be attached to the carbon atom one at a time. Highly reactive neutral atoms and radicals (fragments of molecules) are involved in each of these steps. If all of the radicals are considered, the reaction includes 15 to 20 chemical species participating in more than 50 elementary reactions, each with a particular rate constant.

We have constructed a numerical model of methane combustion with 20 chemical species in 54 reactions. From these reactions and rate constants, differential equations are derived and solved by a computer code to give detailed time histories of the species' concentrations. Although it is extremely difficult to test the validity of our model by measuring the concentrations of chemical species inside an operating combustion device, data from experiments with shock tubes, flames, and flow reactors are available.

In a flow reactor, the fuel and oxidizer are preheated and rapidly mixed in a fast flow. The fuel/oxidizer mixture flows downstream as it reacts; thus, the reaction's time history can be determined by sampling the chemical species at various points along the flow. To make accurate sampling possible, the flow velocity is adjusted so that the chemical

reaction is spaced out over a distance of tens of centimetres.

A comparison of calculated² and experimental flow reactor results³ is shown in Fig. 1. To get the agreement shown, we had to include HO_2 , H_2O_2 , C_2H_6 , C_2H_5 , C_2H_4 , and their reactions; in the past, they have often been ignored.

Our model provides information not readily available experimentally. For example, it gives the concentrations of a number of radical species not measured in the flow reactor. It also gives insight into the basic nature of the reaction.

Figure 2, which was constructed from model results, shows how the reaction branches in the induction period (when the concentration of radical species is increasing, but energy release is not yet significant). At the start of this period, a spark or heat source dissociates a little CH_4 to produce some H; these radicals multiply rapidly through a series of reactions. For example, in the reaction shown at the top of Fig. 2, one radical (H) undergoes a reaction ($\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$) that yields two radicals (OH , O) as products.

The widths of the arrows in Fig. 2 are proportional to the reaction rates. Thus during the induction period, the CH_3 radical is clearly being created faster than it is being consumed⁴, so we can expect an early buildup in the CH_3 concentration. Since radical concentrations are still very low, however, the reaction rates are too low to produce significant heat.

By analyzing the reactions shown in Fig. 2, we were able to develop a simple model involving only seven reactions. This model, which can be solved without a computer, predicts induction periods that agree with shock tube experiments.⁴

FLAME QUENCHING

In the cylinder of an automobile engine, a flame ignited by a spark propagates through an air/fuel mixture and along the cylinder walls toward the piston head. Since the walls are relatively cold, the

flame is extinguished as it approaches them; a thin layer of partly reacted fuel, called unburned hydrocarbons, is left behind. The phenomenon of flame quenching is of fundamental importance because it is a major source of hydrocarbons in the exhaust.

The thickness of the unburned fuel layer is affected by the air/fuel ratio, gas pressure, gas temperature, flame speed, wall temperature, and chemical concentrations. Because these parameters interact with one another, it is difficult to vary them independently and establish their individual effects experimentally. By means of numerical modeling, however, we may be able to establish rigorous relationships that will define flame quenching over a wide range of conditions. We are currently exploring the possibilities.

STRATIFIED CHARGE CONCEPT

One way to eliminate the layer of unburned hydrocarbons along the cylinder walls is to confine

the fuel to a subregion of the combustion chamber away from these walls. If this could be accomplished, the flame might consume all of the fuel before mixing and diffusion processes cause the fuel to reach the wall or reduce fuel concentration below the flammability limit. The result would be reduced hydrocarbon emissions.

It is difficult in practice to stratify the charge and analyze the resulting process, but with a computer model, we can do it easily. We have used a one-dimensional model³ for this purpose, composed of two submodels: one for fluid mechanics and one for chemical kinetics. The fluid mechanics submodel (i.e., the description of fluid motion in the chamber) uses a one dimensional, Eulerian difference scheme in which the equations of continuity, momentum, energy conservation, and chemical species transport are all fully coupled and solved simultaneously.

The chemical kinetics submodel assumes either a global (one-step) reaction rate mechanism or a detailed, multireaction, multispecies mechanism. We assume that methane is the fuel because the

Fig. 1. Comparison of model calculations (curves) and experimental data (symbols) on methane combustion in a flow reactor. The good agreement here between data and calculations is the result of having added HO_2 , H_2O_2 , C_2H_6 , C_2H_5 , C_2H_4 , and their reactions to our model. These species have often been ignored in the past.

detailed methane reaction mechanism is much better understood than that of other hydrocarbon fuels. The initial conditions assumed are those of an open-chamber, stratified charge engine.

In this one-dimensional code, we postulate a uniform, fuel-rich mixture in the left half of the cylinder and pure air in the right half. If a flame starts at the extreme left and burns through the fuel-rich region, hot gases will expand and push the fuel-air boundary to the right. At the same time, turbulent mixing will blur the boundary, and a fuel-lean region will develop to the right.

Fig. 3. Location of fuel consumed in an internal combustion engine when the charge is homogeneous (A) and stratified (B). The right vertical axis represents the cylinder wall. The blue rectangle represents fuel distribution for the homogeneous charge, the yellow rectangle for the stratified charge. The charge is ignited on the left, and its flame front propagates toward the cylinder wall on the right. As the flame front moves, the burned gas expands and pushes the unburned fuel ahead of it. In case A, most of the fuel is burned near this far wall, leading to flame quenching and hydrocarbon formation. In case B, the fuel is burned away from the wall; this configuration should be inherently low in hydrocarbon emissions.

It is possible that the flame will go out somewhere in this lean region, leaving unburned hydrocarbons behind. It is also possible that, as the boundary is pushed to the right, some unburned fuel may reach the cold wall, where a reaction will be quenched. The purpose of the calculation is to determine whether either possibility will happen. If the flame consumes the fuel before reaching the wall, we can assume that the engine will be inherently low in hydrocarbon emissions. Such an engine could also be designed to give better fuel economy than current internal combustion engines.

In Fig. 3, we plot model-calculated fuel consumption as a function of position in the combustion chamber for a homogeneous charge (curve A) and a stratified charge (curve B). The initial boundaries of both charges are shown by color shading. A large fraction of the homogeneous charge is consumed near the chamber's outer wall (1.1 cm). As a result, flame quenching will probably result in a large amount of unburned fuel and a correspondingly high level of hydrocarbon emission. By contrast, most of the stratified charge is consumed in the chamber interior. Hydrocarbon emission due to wall quenching should thus be largely eliminated in a stratified charge engine.

Our calculations (Fig. 4) further indicate that, at an identical engine power level, exhaust from the stratified charge should contain much lower carbon monoxide and nitric oxide concentrations than that from the homogeneous charge. They also indicate that the flame in a stratified charge engine will not be extinguished before consuming all of the fuel. Thus, the model suggests that the stratified charge concept is worth pursuing.

TWO-DIMENSIONAL FLOW FIELDS

Combustion chambers in real engines are three-dimensional, but three-dimensional numerical models require a great deal of computer time. Consequently, experimental two-dimensional chambers have been built to provide data for two-dimensional models. These chambers are of two geometries: plane chambers thin enough so that one dimension

can be neglected, and axisymmetric chambers (i.e., chamber with cylindrical symmetry) with valves and spark plugs on the cylindrical axis.

We are developing a two-dimensional combustion code that will calculate combustion in either plane or axisymmetric geometries. It will also

calculate swirling combustible flows in axisymmetric geometries. The code has multifluid Eulerian hydrodynamics and can deal with either turbulent or molecular viscosity. In addition, the code can handle thermal conduction and turbulent mixing of materials. Chemical kinetics will be added to the

Fig. 4. Total calculated concentrations of CH₄ (methane) and NO, CO₂, and CO during combustion when the charge is homogeneous (A) and stratified (B). Since the stratified charge is inherently lean (contains excess air), fuel concentration on a ppm basis is lower. In this calculation, the stratified charge engine used 25% less fuel for the same power output as the internal combustion engine, and is more efficient. The stratified charge combustion was also lower in NO_x and CO formation.

code as soon as simplified schemes become available. We also plan to include two-phase flow (i.e., liquid droplets and gas).

Even in two dimensions, nonsteady-state combustion codes generally require a fair amount of computer time. However, improved algorithms for solving the basic hydrodynamic equations have made it possible for us to achieve speeds as high as $10 \mu\text{s}/\text{zone-cycle}$ on the CDC 7600 computer. Other codes of this type often require 500 to 1000 $\mu\text{s}/\text{zone-cycle}$.

We have applied our two-dimensional code to combustion in an axisymmetric motored engine (i.e., one that is driven externally and in which no combustion takes place). Figure 5 shows the experimental engine that we model at the beginning of the intake stroke, when the piston is at top dead center.

Our computational model places a fixed grid (Eulerian) in the blue area of Fig. 5 and in the gray area to the right of the piston face. The grid is 38 by 117 zones and has a spacing of 1 mm. In the figure,

Fig. 5. Initial configuration of an axisymmetric motored engine for which we have calculated the air flow. Since the engine is cylindrically symmetric, the motion in its top half is the same as in the bottom half. Our computational model places a fixed grid in the blue area and in the gray area to the right of the piston face. Initially, only the blue area is active; as the piston moves to the right, however, it exposes more grid which then becomes active. Figure 6 shows the gas dynamics of the expanding blue area.

Fig. 6. Individual frames from a computer-generated movie showing fluid motion during the intake stroke of an axisymmetric engine. The blue arrows show the magnitude and direction of the gas velocity; they are scaled to the problem's maximum velocity. The marker particles (yellow crosses) serve only as visual aids in the movie to show the gas flow's movement.

only the blue area is initially active. The head, valve, and piston faces are impenetrable boundaries. The valve and piston boundaries move across the grid with the velocity of the piston and valve in the experimental engine. As the piston moves it uncovers more grid, which then becomes active. The initial air pressure is 100 kPa (1 atm) at room temperature. The inlet boundary, which is 1 cm to the left of the boundary of the figure, is held at a constant pressure of 100 kPa.

The results of a calculation are shown in Fig. 6. This figure is a series of vector plots of the velocity field at 3-ms intervals (corresponding to 45° crank-angle increments at 2500 rpm). The velocity vectors are linearly scaled to the maximum gas velocity in each frame, which is approximately half the speed of sound. With a 1-mm grid spacing, this gives a Reynolds number for the zone of about 10^4 . At such a high Reynolds number, the effects of viscous forces are negligible, and turbulence effects become important. The turbulence is treated by conventional techniques: we introduce a turbulent viscosity obtained from a mixing-length turbulence model.

Although this model assumes two-dimensional symmetry and hence is not directly applicable to a real three-dimensional engine, it can yield information concerning the relative effects on the flow field of such parameters as valve size, swirl rates, head and piston geometries, and rpm's. These calculations are expected to be of use in engine research, and particularly in designing stratified charge engines.

THREE-DIMENSIONAL FLOW FIELDS

The fluid flows in three-dimensional combustors are often unstable; slight variations in initial and boundary conditions can result in substantial differences in flow. These detailed, asymmetrical, fluid flow patterns must eventually be understood if combustor efficiency and pollution control are to be improved.

Work has begun at LLL on a three-dimensional hydrodynamic code for combustion problems. A

number of physical considerations govern our approach:

- Flows containing small-scale turbulence cannot be modeled satisfactorily without special turbulence modeling techniques.
- Flows consisting of several reacting chemical species require highly accurate numerical solutions.
- The complexity of three-dimensional modeling problems is such that very high-speed numerical techniques and the highest speed computers are required. Our program will be designed to operate on the CDC STAR computers, although debugging will be done on the CDC 7600.

COMBUSTION EXPERIMENTS

As mentioned above, we need accurate experimental data to compare with model results. We will not have confidence in the predictive ability of our calculations until they agree reasonably well with experiments. The motion of fuel-injection sprays is one phenomenon currently under study in the laboratory. This is an important design area for stratified charge, diesel, and gas turbine engines. An experimental system for conducting Schlieren, flash x-ray, and shadowgraph photography of injector sprays and confined flames has been designed and installed.

Schlieren photography is based on the fact that in a transparent medium, light travels in a straight line unless it passes through a medium with a different refractive index. When it passes through such a medium, it will be refracted at an angle proportional to the gradient of the index perpendicular to the light path. Schlieren techniques are especially useful in obtaining information on the movements of transparent liquids or gases.

In our system, an argon laser provides a point source. The beam is collimated by one spherical mirror and then refocused by another. The spray in-

jector or confined flame is placed in the collimated beam. The gases or liquids in this beam refract the light, and this refracted light is therefore not focused by the second mirror. A Schlieren photograph is a film record of the refracted light, with light and dark bands corresponding to the density gradients in the gas or liquid medium.

The sensitivity of the Schlieren system depends on our ability to eliminate the focused beam entirely. To do this, we use a front surface mirror with a hole the size and shape of the focus spot. A camera placed to view the light reflected by this mirror will see only that part of the beam that was refracted by the gases or liquids under study. The degree of sensitivity and background lighting can be varied by changing the aperture at the focus spot.

In many cases, optical techniques cannot be used to study thick sprays because such sprays strongly scatter or refract the light. This problem can be overcome by using soft x rays as the probing medium. X rays can easily penetrate the most dense sprays and are not affected by thermal gradients. We can achieve exposure times under $1 \mu\text{s}$ with the LLL flash x-ray generator and thus "stop" the motion of high-velocity sprays.

A simple diagram of our x-ray apparatus is shown in Fig. 7. The diode tip of the x-ray source is shown at the left. A $25\text{-}\mu\text{m}$ -thick Mylar window separates the vacuum surrounding the x-ray diode from the experimental chamber. (The vacuum chamber is needed to minimize x-ray absorption.) The fuel nozzle injects into air at standard temperature and pressure, and a film cassette records the spray's image. The source-to-object distance is typically 790 mm, and the object-to-film distance 25 mm.

The radiograph can be analyzed by a scanning microdensitometer with a $50\text{-}\mu\text{m}$ -square collimated light beam. The film exposure density vs position is then digitized and processed by computer. The program used (TIXY) produces plots and data files

Fig. 7. Diagram of our x-ray apparatus for studying thick, high-speed sprays of fuel droplets. The diode emits a 50-ns pulse of low-energy x rays in a vacuum. When these x rays pass through the Mylar window separating the vacuum from the experimental chamber, some are absorbed by the fuel-injector spray and the remainder produce an image of the spray on film. This image can then be compared with model calculations of such sprays.

of the film density as a function of position. We can control the contour levels and the displayed area.

Each output scan is a close approximation of the original radiograph. If all the information in the original radiograph is not needed, the digitized data may be Fourier-analyzed to remove the high-frequency structure. The resulting data may then be processed with TIXY. Figure 8 is a plot made in this way, revealing contours of constant film density. Six equally spaced levels are shown in different colors.

The x-ray beam is absorbed by fuel in both the liquid and vapor states. Thus, regions of low film exposure correspond to thick spray regions. The exact film calibration is obtained by exposing droplets of known size to the x-ray beam. In this

way, we can relate film density to fuel density. For calibration purposes, we relate film density to the thickness of liquid fuel that would cause equivalent absorption. In Fig. 8, the red contour corresponds to an equivalent liquid-fuel thickness of 0.3 mm; the green contour corresponds to a thickness of 1.3 mm.

CONCLUSION

Numerical modeling has already yielded valuable insights into the physical and chemical processes involved in combustion, and codes currently being developed will greatly increase our capabilities. A great deal more work is required to realize the full potential of these tools, however, and even when

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they are fully developed, the task of applying them to combustor design remains. The dwindling fuel supply and mounting environmental concerns make this an urgent task.

Key Words: combustion; engines; internal combustion engines; methane — combustion; numerical analysis — computations; stratified charge engines.

The Magnetic-Quadrupole Spectrometer: Studying Neutron Reactions

We have developed a magnetic-quadrupole spectrometer to measure the charged particles from nuclear reactions induced by 14-MeV neutrons. A magnetic lens focuses the charged particles from the reaction site onto a distant detector. This protects the detector against neutron bombardment and greatly improves the signal-to-background ratio. We are using this spectrometer to assess potential radiation damage problems in fusion reactors of the future, to measure the energy deposited by neutron-induced reactions in biological systems, and to study the interaction between two neutrons. This same principle has been adapted to the measurement of fast charged particles from laser-induced fusion.

A serious obstacle to achieving economic electrical power from fusion reactors is the damage to reactor components that could be produced by the

high neutron flux. The 14-MeV neutrons from the $D + T \rightarrow n + \alpha$ reaction have much greater radiation-damage potential than the neutrons from present fission reactors; at comparable power, a fusion reactor will produce more neutrons, and they will have higher average energy. At these higher energies, nuclear reactions that deposit hydrogen and helium in structural materials are much more probable. Both gases can significantly weaken the materials. To assess the magnitude of this radiation damage, we must know the probabilities or cross sections of these nuclear transmutations.

In many cases, the best way to measure these cross sections is to detect the energetic nuclei of hydrogen (protons, deuterons, and tritons) and of helium (alpha particles and helium-3 ions) that result from the interaction of fast neutrons with materials. If the material is thin enough, i.e., a foil, then the charged particles lose little energy before they escape from it. A detector viewing the foil can count directly the numbers of hydrogen and helium nuclei formed. At the same time, an appropriately

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chosen detector can measure the ions' energy distributions, an important bit of diagnostic data. A typical, extensively used experimental setup is illustrated in Fig. 1a.

Previous measurements of this type have been beset by a low true counting rate and by large backgrounds. The true rate is small because conventional neutron sources produce only 10^9 or 10^{10} neutrons per second and because the target foils must be thin. The backgrounds are large because neutrons and gamma rays from the source interact

strongly with the detector itself. Shielding between the source and the detector helps, but there is seldom enough room in this geometry to shield the detector well.

Under the sponsorship of ERDA's Division of Physical Research, we have developed a magnetic-quadrupole spectrometer that focuses charged particles from the target foil onto the detector (Fig. 1b). Even though the detector is farther from the target foil, the focusing section of the magnetic lens significantly increases the detector's effective solid

Fig. 1. Experimental setups for measuring charged particles from neutron-induced reactions. (a) Former method, with the charged-particle detector close to the foil under neutron bombardment. The detector here receives all charged particles within its acceptance solid angle, but its proximity to the foil makes it hard to shield it adequately against background radiation such as neutrons and gamma rays. (b) Present technique, with a magnetic quadrupole lens focusing the charged particles onto the detector.

Fig. 2. Overall view of the quadrupole spectrometer, removed from the intense neutron source. The cylindrical target chamber at the right contains the foils to be bombarded with neutrons. Charged particles from the resulting reactions go down the long evacuated tube, through the triple quadrupole magnet array, and into the detector chamber (left).

Fig. 3. Working parts of the quadrupole spectrometer. In the front row, left to right, they are the target wheel with a selection of four different target foils, the first charged-particle collimator, internal shielding for the detector, a pair of collimating apertures, and the adjustable detector-telescope holder. Behind, the copper rod supported on thin wire legs is a shadow bar that is placed on axis to reduce the background of neutrons, gamma rays, and charged particles other than those of the selected energy.

angle. Neutrons and gamma rays, on the other hand, are unaffected by the lens. They disperse and become less troublesome as the square of the distance between the neutron source and the detector. Also, we can put much more shielding between the source and the detector to reduce the background still further. Even the material of the magnetic lens itself doubles as a neutron shield. These modifications improve the signal-to-background ratio by more than a factor of thirty.

The other key element in our experiments is the ILL rotating target neutron source (RTNS), the world's most intense continuous source of 13- to 15-MeV neutrons. This source produces 4×10^{12} neutrons per second, or perhaps 400 times more than sources typically used in such experiments. The quadrupole lens and selected shielding materials allow us to use this source at its full intensity without destroying the radiation-sensitive detectors.

Quadrupole magnets have been used before to focus nuclear-reaction products. What is new is applying them to studies of neutron-induced reactions. The combination of this spectrometer and the intense neutron source gives us a unique capability.

For the spectrometer's many advantages, we pay a small price. At any one setting of the quadrupole lens, only a part of the spectrum is focused onto the detector. We must change the magnetic field strength to observe different parts of the spectrum. In a sense, the lens acts as a band-pass filter with a fairly large band width. However, we can scan a complete charged-particle spectrum with only a few magnet settings.

The assembled spectrometer is shown in Fig. 2. In operation it is moved so that the target foil inside the cylindrical target chamber (right) is near the source. The charged particles travel in the evacuated tube through the quadrupole magnets and focus on detectors at the left end of the spectrometer. Typical target foils, silicon surface-barrier detectors, collimating apertures, and shielding materials from the inside of the spectrometer are shown in Fig. 3.

Figure 4 is one of our measured spectra: protons from aluminum bombarded with 15-MeV neutrons. We expected a continuous spectrum like this, but we

were surprised to find it extending clear down to 800 keV. It used to be very difficult to measure below 2.5 MeV, but this caused no concern because no one expected to find many protons there. Our data now show that, for aluminum, neglecting the protons below 2.5 MeV can lead to errors of 40% in the total hydrogen-production cross section.

Table 1 is a brief summary of some of our results at 15-MeV neutron energy. The correction to 14 MeV, the mean energy of fusion neutrons, is straightforward and small. Different fusion-reactor component materials yield widely differing amounts of hydrogen and helium by nuclear transmutation. Each material, of course, reacts differently to hydrogen or helium implantation, and these differences are being studied by metallurgists. Our cross-section data tell the metallurgists how much of these impurity gases to expect in fusion reactor components, giving them a sounder basis for assessing materials damage.

A second facet of radiation damage begins when one atom is knocked out of its lattice site. As it slows down in the material, it knocks other atoms out of their lattice sites, forming a track of displacement damage.

Such recoiling atoms have extremely short ranges, compared with hydrogen and helium ions, and almost none escapes from the foil. We can study them only by proxy, by measuring the energies and angular distributions of hydrogen and helium ions and calculating from these measurements what the recoiling-atom energy spectrum must be. Knowing the energy spectrum, we can calculate the displacement damage according to an approximate theory. Figure 5 is a spectrum of recoiling atoms from alpha-particle-producing reactions in stainless steel.

Our data deal only with primary recoil atoms from nuclear reactions that produce hydrogen or helium ions, of course, and this is only part of the total recoil-atom spectrum. It is an important part, however, because it includes all the reactions that produce helium ions. These recoils have the highest energy, so they individually cause the most displacement damage.

Fig. 4. Spectrum of protons from aluminum bombarded with 15-MeV neutrons, with the detector placed at 75° to the incident neutron direction. A few representative error bars are shown.

Beyond determining specific cross sections and recoil energy distributions, our measurements help to validate or refute nuclear-reaction model calculations. Correct calculations are essential to the fusion reactor program because we need much more nuclear data than could be produced by even a very ambitious measurement program. Only calculations can fill in the gaps between the measurements. Our cross sections and energy spectra have already been used to assess the validity of three different codes that calculate these reactions.

Another application of these measurements involves the heat released in a material by charged particles as they slow down. The charged particles' initial energy is important when calculating heating

Table 1. Summary of hydrogen and helium production cross sections at 15-MeV neutron energy.

Material	Production cross section, fm ² (10 mbarn)	
	Hydrogen	Helium
Aluminum	42.4	12.1
Titanium	12.8	3.1
Vanadium	9.8	1.7
Stainless steel 316	26.0	4.8
Copper	25.1	3.4
Niobium	5.9	1.5

Fig. 5. An energy spectrum of atomic recoils from (n,α) reactions in stainless steel (SS-316) bombarded with 15-MeV neutrons.

rates in different regions of a fusion reactor. It is also important in weapons design and, on a microscopic scale, in understanding the biological and therapeutic effects of radiation.

As an example of the latter application, fast-neutron therapy has been successful in treating certain human tumors. Part of its success is attributed to a particular interaction of neutrons with carbon nuclei in the tissue, a reaction that disintegrates the carbon nucleus into three alpha particles. To understand the biological effect of the resulting energetic alpha particles, we must know the distribution of their initial energies. We are measuring this distribution directly with our spectrometer.

The spectrometer also improves the resolution of nuclear experiments, allowing fundamental new work in nuclear physics. In one such experiment, we measured the proton energy spectrum following the breakup of deuterons by 14-MeV neutrons. The reaction also gives off two neutrons, which go

Fig. 6. An energy spectrum of protons from the $D(n,p)2n$ reaction — deuterium bombarded with 14-MeV neutrons — compared with a theoretical calculation. The agreement is fairly good in general, but the departure near the peak of the smooth curve suggests that the theoretical treatment may be neglecting some significant factor.

undetected. Their interaction in the final state, however, strongly influences the shape of the proton spectrum. Measuring the shape of the spectrum, therefore, gives strong evidence of the neutron-neutron interaction.

Good resolution is essential in this measurement. The low background of our spectrometer allows us to use detectors of exceptional resolution. These detectors would be destroyed if they were not well shielded from the neutron source, and the quadrupole-spectrometer geometry makes this possible.

The resolution we obtained was 2.2 times better than any previous measurement. Figure 6 shows our data, superimposed on a theoretical calculation. The fine difference at the peak between our data and the theoretical curve indicates that modifications are necessary either in our conception of the neutron-neutron interaction or in the complex three-body theories used to calculate the final state interaction.

During the spectrometer's development, we realized that a similar technique could be used to focus the fast charged particles from laser-fusion experiments. This case presented the problem of overcoming a large background of γ rays and at the same time increasing the signal (alpha particles from the thermonuclear burn). Quadrupole lenses installed on the Argus experiments at LLL are successful in significantly increasing the signal-to-background ratios.

We are continuing to develop our spectrometer with the goals of increasing its effective solid angle and the width of its band pass, and of reducing the background. We began with a quadrupole doublet lens but found a triplet lens (Figs. 1 and 2) superior. We have made most of our measurements with silicon surface-barrier detectors. For certain experiments, however, proportional counters or scintillation detectors may be preferable. In collaboration with a group from the University of Wisconsin, we are developing these improved techniques that should yield cleaner data in an even shorter time. These new techniques will make possible many more experiments on charged particles from fast-neutron interactions.

Key Words: alpha particles; charged-particle detectors; deuterons; fast neutrons — cross sections; fusion reactors; materials — effects of radiation; protons; spectrometer — quadrupole

Tracking the Debris Cloud from a Chinese Nuclear Test

As the radioactive debris cloud from a Chinese nuclear test last Fall began drifting eastward, the Laboratory's computational facilities were pressed into service to predict the possible environmental effects. ERDA asked us to calculate cloud trajectories and to estimate the fallout dose. The FAA asked us to provide dose estimates both for commercial aircraft flights within the U.S. and for transatlantic flights of the Concorde SST. Our dose estimates — calculated with 2BPUFF, a large-cloud diffusion code — proved to be accurate predictions, correlating well with later observations. At FAA and ERDA request, we also worked with EG&G to measure cabin dose rates in some transatlantic SST and subsonic flights while the debris cloud moved out over the Atlantic Ocean.

On September 26, 1976, the Peoples Republic of China exploded an 840-TJ (200-kt) nuclear device over their test site at Lop Nor in northwestern

China. At this yield, over half of the debris cloud remains in the troposphere, where it is subject to precipitation scavenging (rainout).¹

On October 4, radiation monitors at the Peachbottom nuclear power plant near Philadelphia registered above-normal readings. Swipes from workers' cars also showed radioactivity well above background. Normal readouts in the reactor control room, along with nearly simultaneous reports of fission-product activity at other sites in New York and New Jersey, suggested that the Peachbottom reactor was not experiencing a safety problem but that the radioactivity was from a large-scale source, presumably the Chinese nuclear test. Many readings in Pennsylvania, New York, and New Jersey were the highest observed since the extensive Soviet and U.S. atmospheric tests in 1960-61.

Although no notice of the potential doses from rainout reached the general public, the September 26 debris cloud was tracked by Federal officials. Upon detection of another Chinese test on November 17, therefore, both ERDA and the Federal Aviation Administration (FAA) expressed concern

¹Contact Kendall R. Peterson (Ext. 8811) for further information on this article.

THE AIR AROUND US

Almost all weather happens in the troposphere, the lowest layer of air. This layer is about 9 km thick near the poles and 17 km near the equator. In the middle latitudes, its top fluctuates by season and even from day to day. The annual change can be from 9 to 17 km. Daily changes of 1 km or more are common, particularly in the winter and spring. These changes are like giant waves on the top surface of the troposphere; they take place with little mixing of tropospheric and stratospheric air.

In the troposphere, the air gets colder with height. Most particulates — smoke, dust, volcanic ash, radioactive debris — fall back from the troposphere in rain or snow within a month.

The stratosphere, which overlies the troposphere to a height of about 50 km, is a very stable region. Except for severe thunderstorms, whose tops occasionally climb above the troposphere in spring and summer, there are no storms here. Any particulate that gets into this region tends to stay a long time.

When a rare storm punches up into the stratosphere, it mixes with and drags down material that otherwise would have stayed up. There are also localized exchanges of tropospheric and stratospheric air above strong weather fronts. Thus pollutants placed in the stratosphere fall to earth in limited "spurts" over periods of months to years.

about surface doses in the U.S. and dose rates along commercial aircraft flight routes.

The yield of this second device was estimated at 17 PJ (4 Mt). The energy from such a petajoule-range yield pushes more than 99% of the debris cloud into the stratosphere, from which it gradually reenters the troposphere over a period of years¹ (see box above). During this time, atmospheric diffusion spreads the debris over the entire globe. The maximum surface deposition would occur in the middle latitudes of the hemisphere where the explosion occurred.

After this second Chinese test, LLL was asked to conduct several studies. For ERDA, we provided trajectory and dose estimates as the debris cloud crossed the United States. For the FAA, we prepared dose estimates for commercial aircraft flights in the U.S. and for transatlantic flights of the Anglo-French Concorde. All dose estimates were calculated with our large-cloud diffusion code, 2BPUFF. In conjunction with EG&G, we also measured cabin dose rates on transatlantic military and Concorde flights as the debris cloud moved out over the Atlantic.

ERDA DOSE ESTIMATES

Our preliminary trajectories for the tropospheric portion of the debris cloud (9 km) and for the cloud center (20 km) are shown in Fig. 1. We felt that dry deposition (fallout) would amount to 1% or less of the radioactivity, assuming a 50% fission yield, and would present no problem, but that areas of wet deposition (rainout) deserved close attention.

Weather forecasts indicated that rain or snow would be falling in the Pacific Northwest, the Great Lakes, and the Southeast as the tropospheric debris cloud passed overhead. Surface and upper air charts showed, however, that the only precipitation tops likely to extend more than a few kilometres above ground, and thus be able to scavenge debris of any consequence, would occur in the Southeast (Fig. 1). We calculated potential doses from such scavenging with 2BPUFF, our large-cloud diffusion code.² Although originally developed to estimate concentrations and doses from Plowshare nuclear cratering tests, this code is also applicable to airbursts.

With conservative input assumptions, the results from 2BPUFF showed potential doses from rainout in the Southeastern U.S. to be much less than one

millirem for all pathways to man. (The average, natural background radiation in the U.S. is 100 mrem/yr.) Even if the storm clouds extended to the top of the troposphere (10 to 11 km) — an unlikely occurrence for the forecast storm system — the maximum dose predicted was 200 mrem from

whole-body exposure and 300 mrem to an infant's thyroid from iodine-131 via the forage-cow-milk pathway. (These dose estimates are not additive.)

The 2BPUFF predictions were updated periodically, with no significant change, until the tropospheric debris cloud left the East Coast. To

Fig. 1. Estimated trajectories for the tropospheric portion of the debris cloud (9 km) and for the cloud center (20 km). Numbers along the trajectories are day and position at noon Greenwich Mean Time (GMT); the intermediate dots are for mid-night GMT positions.

our knowledge, neither the Environmental Protection Agency's monitoring network nor other ERDA or university monitoring efforts detected fresh nuclear debris in excess of 1 mrem in surface air, rainwater, or cow's milk.

FAA DOSE ESTIMATES

Shortly after ERDA's request for trajectory and

dose predictions, the FAA expressed concern over the dose rates that might be encountered on commercial aircraft flights within the U.S. We predicted that, for flights entirely within the troposphere, dose rates would be far less than natural dose rates from cosmic-ray activity (about 0.2 mrem/hr). Those flights that were partly within the lower stratosphere (the flight ceiling for most commercial jet aircraft) would experience somewhat higher dose

Fig. 2. Predicted (curves) and observed (data points) air concentrations and dose rates for the debris cloud from the November 17 Chinese nuclear test. The yellow band represents typical flight levels for the Concorde SST.

rates, but still less than or, at most, equivalent to cosmic-ray dose rates.

Our predictions were again based on 2BPUFF calculations, in which we assumed that 1% of the radioactivity would be in the troposphere. Also, in the lower stratosphere, the aircraft would be about 8 km below the debris cloud center, and if the vertical distribution of radioactivity approximated a Gaussian curve — as is usually the case — dose levels at this altitude would be reduced by several orders of magnitude from cloud-center dose rates.

After flying beneath the projected cloud center, many commercial aircraft were examined by Federal officials for radioactive contamination. A few aircraft showed low levels of gross beta and gamma activity on parts of the planes that normally become oily. However, no similar checks were made during passage of the September debris cloud. Since commercial aircraft are washed down infrequently, we suspect that the radioactivity detected in late November came, at least in part, from the September test, which had a larger debris fraction in the troposphere. To our knowledge, no analyses were made of individual isotopes in the aircraft contamination that would have permitted dating the debris.

While the November debris cloud center was over Canada, the FAA also asked us to prepare dose estimates for transatlantic flights of the Anglo-French Concorde SST. Typically the Concorde climbs quickly to about 15 km and then, as fuel is consumed, maintains a slow climb to about 18 km shortly before descent for landing. At these flight levels, the SST would be much closer to the debris cloud center than U.S. civil aircraft.

We ran the 2BPUFF code for the stratospheric portion of the cloud. By this time several aircraft measurements had been made near the cloud center at 20 km. These observations helped us select horizontal and vertical diffusion parameters. Over the eastern U.S. and Atlantic Ocean, values selected for both the vertical diffusion coefficient (which determines the rate of vertical mixing of debris-cloud air with clean air above and below the cloud) and the horizontal diffusion coefficient (which

determines the rate of horizontal mixing) were a factor of 3 to 10 lower than previously observed values.³ Apparently, the lower stratosphere was in a quiescent state during this time.

Based on these new parameters, our calculations showed that if the Concorde's flight path intersected the debris cloud, dose rates would be between 1 and 100 mrem/hr. We conservatively chose 10 mrem/hr as the most likely dose rate. Later stratospheric measurements verified these calculations.

Figure 2 shows predicted and measured concentrations and dose rates for various altitudes from the November 17 airburst. A measurement below the curve for a given height suggests that the observation was made outside the cloud center. The cosmic-ray contribution, measured at 0.6 mrem/hr, has been removed from the SST observations.

Based on these dose-rate predictions, the FAA further requested, through ERDA, that we work with EG&G to measure cabin dose rates on transatlantic flights as the debris cloud moved over the ocean. Because of projected cloud heights, we focused on monitoring supersonic flights with their higher altitudes. The British Airways and Air France Concorde flights listed in Table 1 were monitored from November 25 through December 1, 1976. A few subsonic flights during this time were also monitored.

In-Flight Measurements. Radiation levels aboard the aircraft were measured in several ways: Geiger counter, proportional chamber, passive dosimeters, air sampling, and scintillation detectors. A portable Geiger counter was carried on board to detect small variations in radiation background during flight. Readings were tabulated periodically throughout the flight. The gas proportional unit was packaged in a suitcase with a self-contained strip-chart recorder. It was started before takeoff and provided a log of activity seen during the flight. The passive dosimetry (LiF thermoluminescent dosimeters) and air samples furnished an integrated assessment of radiation exposure for the total flight.

The primary tool for identifying increases in radiation due to debris-cloud contact rather than to

Table 1. In-flight radiation-dose measurements for transatlantic flights.

Aircraft	Departure date	Route	Fission-product signal (above background), min	Maximum dose rate, ^a mrem/hr
SST	11/25	Dulles-Paris		0.6
SST	11/26	Paris-Dulles	14	1.3
SST	11/26	Dulles-Shannon		0.6
SST	11/27	Shannon-Dulles	10	0.7
SST	11/27	Dulles-Paris		0.6
C141	11/27	Dover (Maine)-Frankfort		0.2
707	11/28	JFK-London		0.2
C141	11/28	Frankfort-Pease AFB		0.2
SST	11/28	Paris-Dulles	40	0.9
SST	11/28	Dulles-London	20	0.3
SST	11/29	Dulles-Paris		0.6
SST	11/30	London-Dulles		0.6
707	11/30	London-JFK		0.2
SST	12/1	Paris-Dulles		0.6

^aReading includes background: 0.6 mR/hr for SST flights, 0.2 mR/hr for all others.

cosmic background variations was a portable gamma spectrometer that we designed and built (Fig. 3). The unit is fully self-contained, with power supply, detector, controls, and logic circuits in one case. Data can be stored in any one of four 256-channel memories, gamma peaks are identified by movable markers, and peak integrals are performed by operating push buttons on the unit's face.

Before each flight, we also performed energy calibrations with standard isotope sources. Gain settings viewed the full range of expected gamma energies. The data were recorded primarily by photographing the display panel. Some data were also recorded on cassette tape for further analysis.

In addition to the special monitoring instruments carried aboard the aircraft, the Concorde has as part of its flight instrumentation three Geiger-Müller tubes that provide an integrated reading for each flight. These tubes warn of extreme solar flare activity, which may cause the cosmic background to vary an order of magnitude or more.

Only by studying the gamma spectra can one determine the source of an exposure-rate increase under the conditions of these flights. Figure 4 shows: (top) normal ground-level background, (middle) normal cosmic-radiation background at flight altitude (18 km), and (bottom) fallout activity during one of the SST flights. The principal gamma photopeak in Fig. 4 (middle) is at 0.51 MeV, annihilation radiation typical of high altitudes; in Fig. 4 (bottom), the peak is due to the fission product lanthanum-140 at about 1.6 MeV.

Postflight Measurements. The postflight measurements consisted of standard radiation survey swipes taken from the exterior surface of the aircraft at locations marked in Fig. 5. Sample positions were chosen from representative leading edges most likely to have contamination debris embedded on their surfaces.

Gamma-ray spectra were taken outside the aircraft at the conclusion of return flights to the U.S. With EG&G assistance, we acquired data directly

under the aircraft fuselage to aid in identifying possible surface contamination.

Study Results. Table 1 summarizes the data acquired on the transatlantic flights. The largest reading, 1.3 mrem/hr, is about a factor of two greater than natural background in the lower stratosphere. Although no debris cloud signal was found on the subsonic flights, the portable analyzer detected a depleted-uranium counterweight in the tail of one aircraft and identified radiation from a previously undetected shipment spillage in another. Background-subtracted spectra failed to detect any activity due to manmade radiation, but did record radiation analyzed by EG&G as beryllium-7 formed by natural cosmic-ray spallation.

Surface contamination swipes taken postflight showed a maximum beta activity of 3800 Bq/m^2 ($2300 \text{ dpm}/100 \text{ cm}^2$) of swipe area and a maximum

alpha activity of 33 Bq/m^2 ($20 \text{ dpm}/100 \text{ cm}^2$). Postflight analysis of the passive dosimeters and of air samples taken on board indicated no elevated bomb-produced radiation.

Of the flights monitored, only four SST flights (shaded data in Table 1) showed dose rates above cosmic-ray background (about 0.6 mrem/hr). For the November 26 flight from Paris to Dulles International Airport, the dose rate was a factor of 2 above background; the three other flights showed smaller increases.

As shown in Fig. 2, three of the SST measurements — taken more than 200 hours after the detonation — were very close to the 18-km calculations of 2BPUFF made three to five days earlier. Based on our calculations, it appears that these three flights passed near the 18-km center of the debris cloud.

CONCLUSIONS

Our dose predictions for both ERDA and the FAA helped to alleviate public fears of gross contamination from the November 17 Chinese nuclear test. Our predictions for the FAA (i.e., curves in Fig. 2) were within a factor of two or three of actual cloud-center observations in the upper troposphere and lower stratosphere. Both agencies have requested our assistance in the event of future foreign nuclear testing. In the case of another Chinese test, the FAA will need early-time dose rate estimates for U.S. aircraft over the Pacific Ocean.

Our portable pulse-height analyzer proved an extremely valuable tool in identifying nuclear cloud debris. Its sensitivity and operating range are great enough to detect and identify radiation at levels far below those posing a personnel hazard. Postflight aircraft-swipe surveys and later laboratory analyses proved the most effective means of detecting contamination due to debris-cloud passage.

Key Words: Chinese nuclear tests; fallout — computations; fallout — deposition; fallout — distribution; fission products; nuclear explosions — fallout; radiation detectors; radiation — measurements; radioactive debris; radioactive fallout; rainout; 2BPUFF.

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PAST TITLES

Articles in the *Energy and Technology Review* have been organized into subject areas approximately corresponding to the Assistant Administrators' areas of responsibility in the Energy Research and Development Administration. These subject areas are listed below with references to some recent articles in each category. (A semiannual index appears in the June and December issues.)

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- National MFE Computer Center: 1976 Update (*December 1976*)
- LLL Magnetic Fusion Energy Program: An Overview (*June 1976*)

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