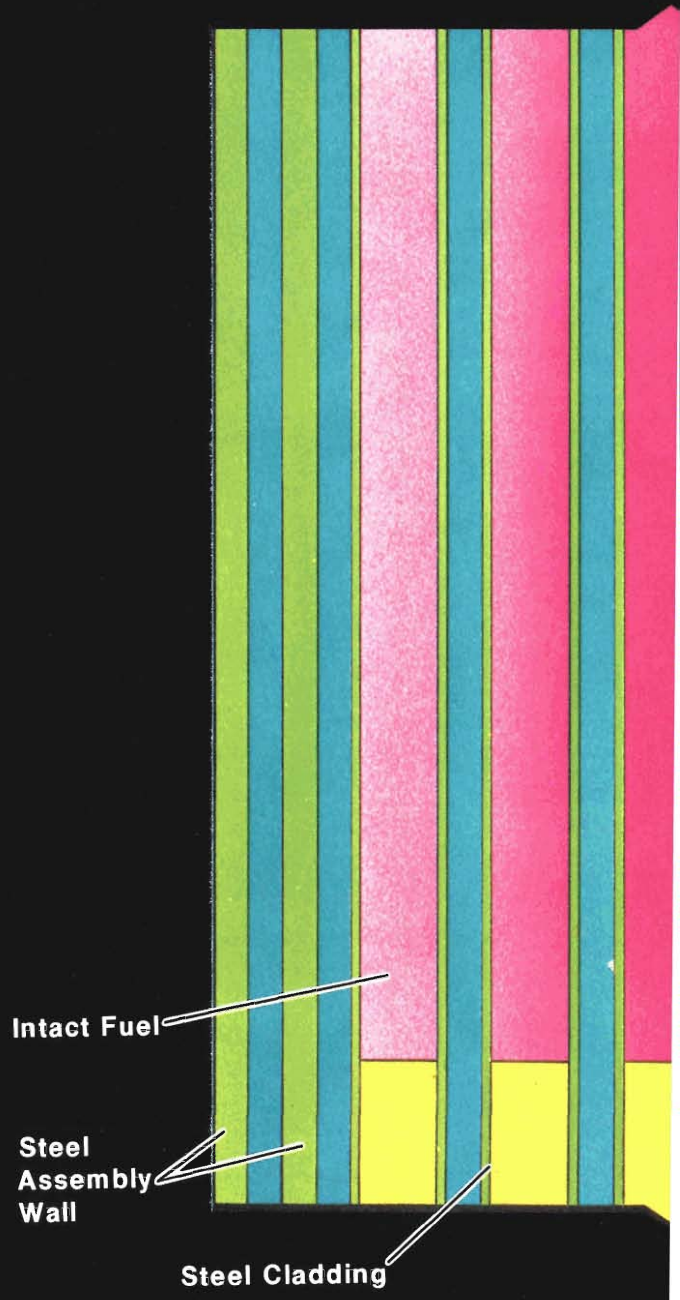
BREEDER REACTOR SAFETY: MODELING THE IMPOSSIBLE

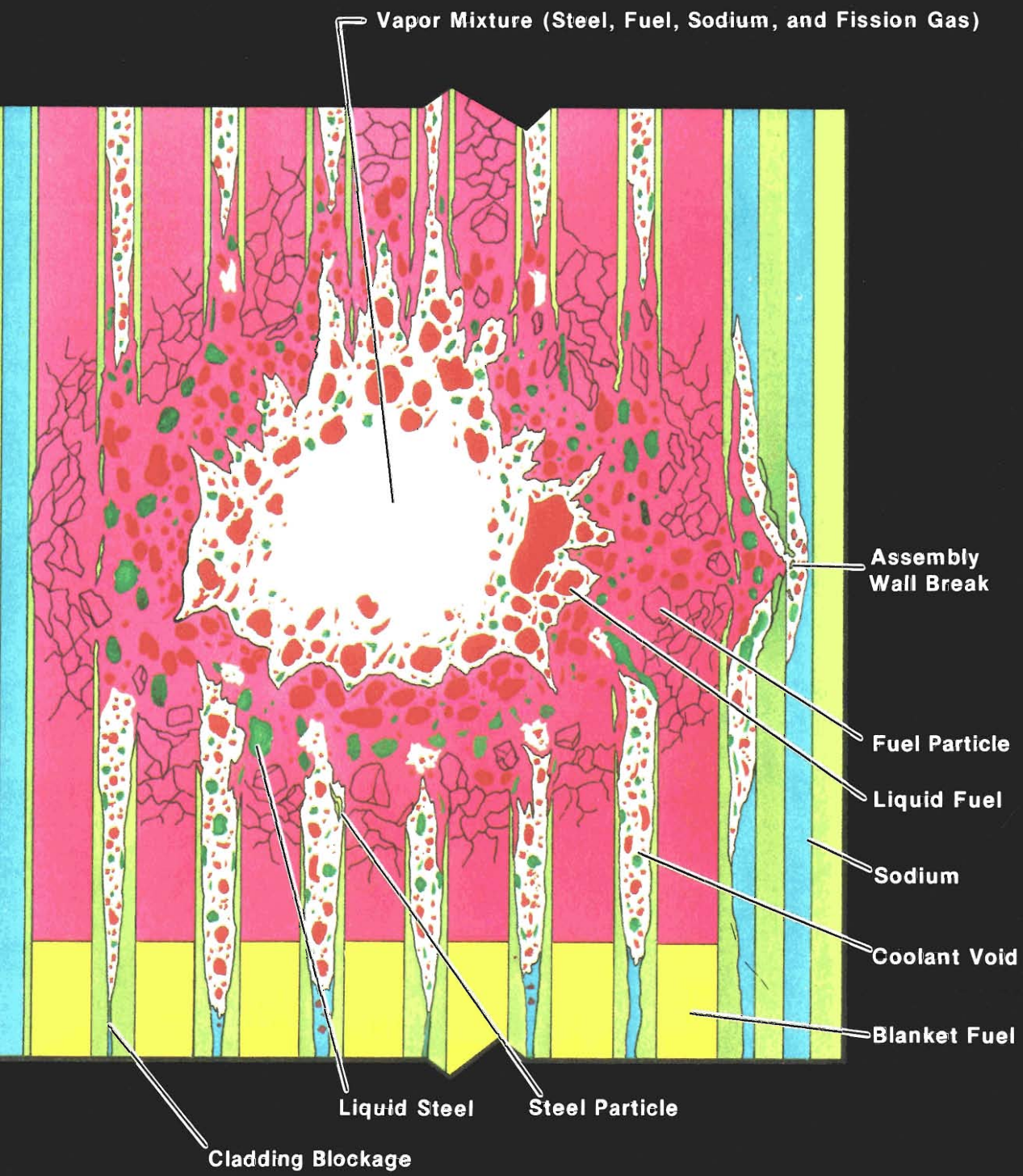
by Charles R. Bell

SIMMER, a computer code developed at Los Alamos National Laboratory, was designed to model an incredibly complex event—the disintegrating of the core of a liquid-metal fast breeder reactor during a hypothetical meltdown accident. Analyses with SIMMER are leading to a more realistic assessment of the safety of this type of reactor.



Is the breeder reactor an alchemist's dream come true? The ancient alchemists attempted to transform base metals of low value into noble metals of high value; the breeder transforms abundant isotopes of low value into rare but easily fissionable isotopes of high value. But the alchemists tried to achieve their transformations with chemical reactions. They were not aware that nuclear reactions, prompted by the collisions of neutrons and nuclei, could cause the hoped-for transformations.

All nuclear reactors depend on the generation of neutrons during the fission process to maintain a chain reaction, but a breeder is designed to produce an overabundance of neutrons. These excess



Artist's conception of disintegrating fuel pins in the fuel assembly of a liquid-metal fast breeder during a severe accident.

neutrons perform the alchemist's magic as they convert "fertile" fuel incapable of sustaining a chain reaction into "fissile" fuel at a rate faster than needed to replace the original fuel. Hence, in a breeder, not only is energy generated, but excess fuel is "bred."

But can the transformation process be adequately controlled? Physicists and engineers have long recognized that during certain hypothetical, low-probability accidents a burst of neutron production could generate a damaging surge of energy and pressure resulting in a potentially large radiation release to the environment.

Thus, a strong attack on these hypothetical accidents has been mounted, both to prevent them and to understand their consequences. An important analytical tool necessary for this understanding was developed over the last six years by the Energy and the Theoretical divisions at Los Alamos National Laboratory. The tool, SIMMER,* is a complex computer code that examines the dynamics of a typical breeder core when disrupted during hypothetical accidents. The core being studied is that of a liquid-metal fast breeder reactor, the breeder of primary focus in the United States since the 1960s. The code couples an accounting of neutron population and power generation with a fluid-dynamic calculation of the behavior of all core materials. Initially considered an almost impossible problem, the development of this code is leading to a more realistic assessment of the safety of liquid-metal fast breeders based on detailed knowledge concerning the temperatures, pressures, energies, and mass flows in a disrupted core.

The conclusions so far? The pressure and temperature surges expected in hypothetical accidents appear to be much less than previously estimated. As a result, management of this sophisticated alchemy

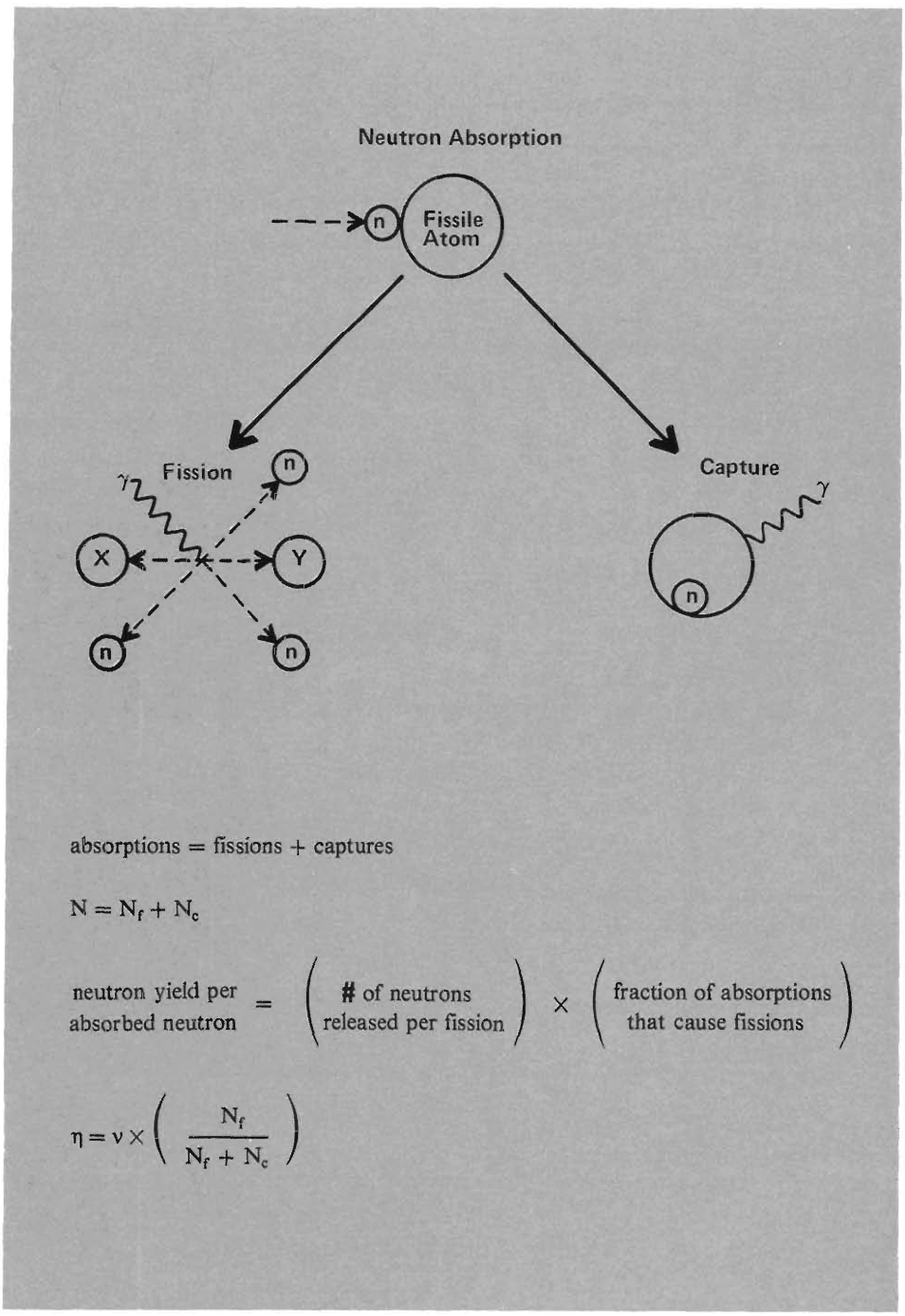


Fig. 1. When neutrons are absorbed by fissile atoms, a fraction of these cause fissions releasing other neutrons, but the remainder are captured. The neutron-yield parameter η accounts for this fraction as well as for the average number of neutrons released per fission event.

*SIMMER is an acronym for S_n, implicit, multifield, multicomponent, Eulerian, recriticality.

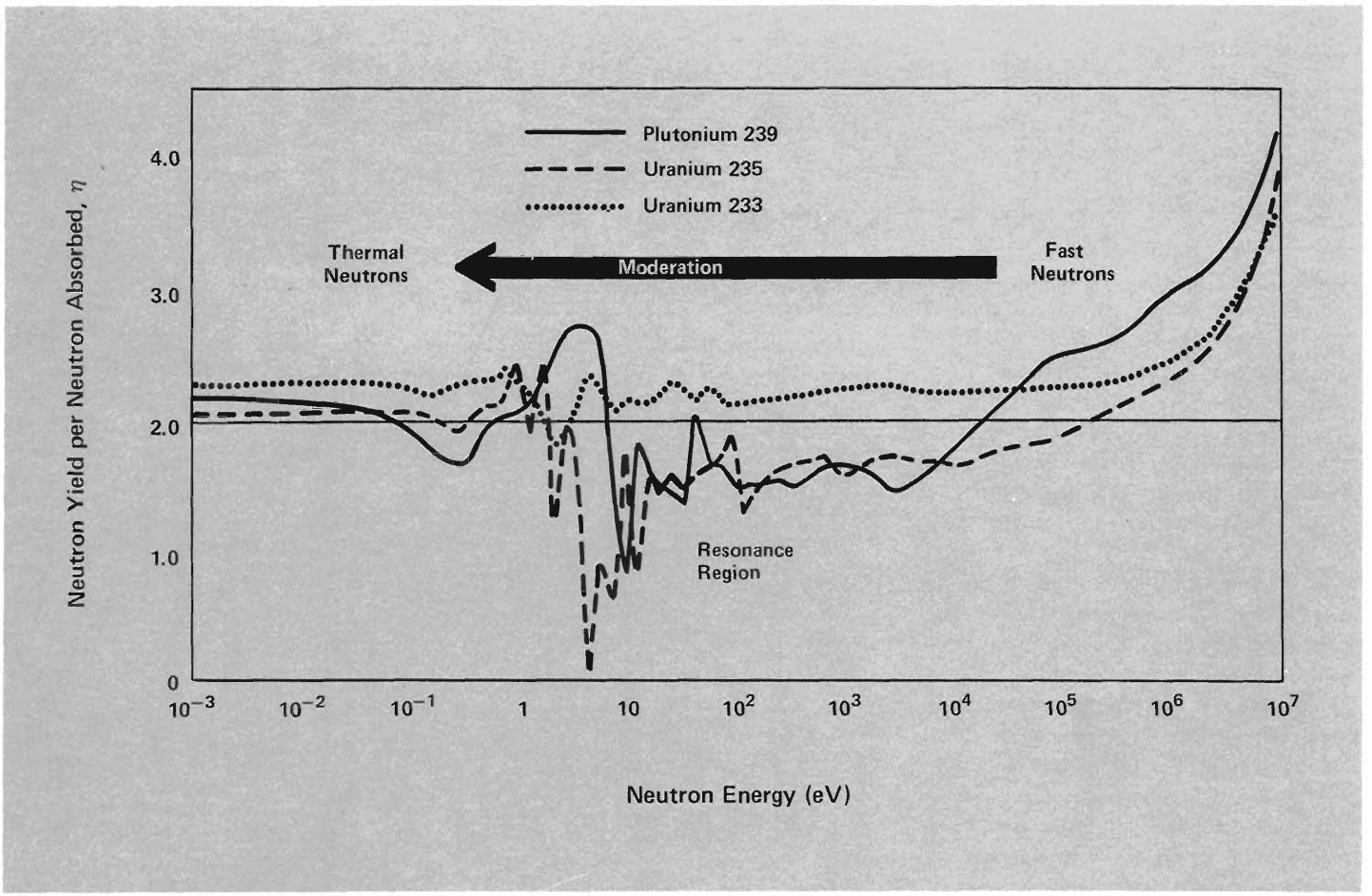


Fig. 2. The neutron yield per neutron absorbed, η, as a function of neutron energy. Fast neutrons have an η large enough to achieve breeding: that is, η is significantly larger than the "break-even" value of 2. Plutonium-239 has the highest η for fast neutrons, but uranium-233, the fissile isotope in the thorium-uranium breeding cycle, has η larger than 2 over most of the neutron energy range. (Figure adapted from ERDA-1541, Vol. 1, p. II-77, June 1976.)

may be safer than imagined.

The Liquid-Metal Fast Breeder

NEUTRONICS. The key to a breeder is the neutron. The generation of energy, the control of the reactor, the breeding of new fuel, and particular safety problems unique to breeders are all related to the reactor's neutronics. For example, the pioneers in nuclear physics early recognized the potential for breeding from the fact that each nuclear fission releases two or three neutrons. Since one of these neutrons is necessary to continue the chain reaction, then one or two "byproduct" neutrons remain. Some of these byproduct neutrons can be utilized through transmutation processes to produce fissile isotopes from fertile isotopes. [The two main processes contemplated for breeders are the "uranium-plutonium cycle" ($^{238}U + n \xrightarrow{\gamma} {}^{239}U \xrightarrow{\beta} {}^{239}Np \xrightarrow{\beta} {}^{239}Pu$) and the "thorium-uranium cycle" ($^{232}Th + n \xrightarrow{\gamma} {}^{233}Th \xrightarrow{\beta} {}^{233}Pa \xrightarrow{\beta} {}^{233}U$). In both cycles the first isotope is fertile, the last is fissile.] If, on the average, one byproduct neutron per fission is used to provide replacement fuel, the remaining neutrons are free to breed excess fuel.

Of course, there are a variety of fates possible for a neutron wandering free in a reactor core. Some neutrons are lost to other processes: for example, absorption by nonfuel constituents or leakage from the core. Other neutrons are captured by the fissile-fuel atoms, but are only absorbed; there is no fissioning and no further release of neutrons. As a result, efficient breeder design, like efficient financing, attempts to maximize the return yield for each investment, that is, attempts to maximize the number of neutrons liberated for each absorbed neutron. This concept and the parameter η representing the neutron yield per absorbed neutron are illustrated in Fig. 1. For a nonbreeder reactor if η is enough larger than 1 to account for neutron losses, a chain reaction can be maintained. However, for a breeder η should be significantly larger than 2.

Figure 2 is a plot of η versus neutron energy for three fissile isotopes and shows the most promising region for breeding to be that of "fast" or high-energy neutrons. The parameter η rises here because the ratio of fissions to captures for absorbed neutrons is rising with neutron energy; the more energy the neutron brings to the interaction, the more likely the fission event. The figure also

shows that, with respect to neutron yield, plutonium-239 is the preferred choice for breeder fuel.

Neutrons released in the fission process are already fast. Commercial light-water reactors reduce these energies, with the water acting as moderator, to the thermal region where there is high total absorption of neutrons by the fuel. But to take advantage of a large η, the neutrons must remain fast, so breeders are purposefully designed with little moderation.

How is this population of neutrons and the ensuing chain reaction controlled? The neutrons resulting directly from the fission process are called "prompt" neutrons (Fig. 3). In liquid-metal fast breeders, the prompt neutrons have an average "lifetime" of about 10^{-7} second between their birth and their death due to absorption or escape from the core. Since neutron population growth is exponential, a slight overpopulation of prompt neutrons will grow very rapidly to a new, larger population. For example, a neutron population only 0.1 per cent in excess of the stable, "critical" population will take slightly longer than 10^{-4} second to triple. This is much too fast for realistic control of the reactor.*

Fortunately, "delayed" neutrons are also part of the total neutron population. These neutrons are released in the decay of some of the unstable nuclei produced by the original fission event and are thus born on the order of seconds after that event. If the neutron population is always kept underpopulated, or subcritical, with respect to prompt neutrons, delayed neutrons can be used either to complete a stable, balanced population or to provide the slight imbalance needed to alter the population. The growth to a new stable population will then be slowed considerably and mechanical control of the process becomes feasible.

The Clementine reactor, designed and built in 1945 at Los Alamos, successfully demonstrated the feasibility of delayed neutron control of a fast-neutron system. This

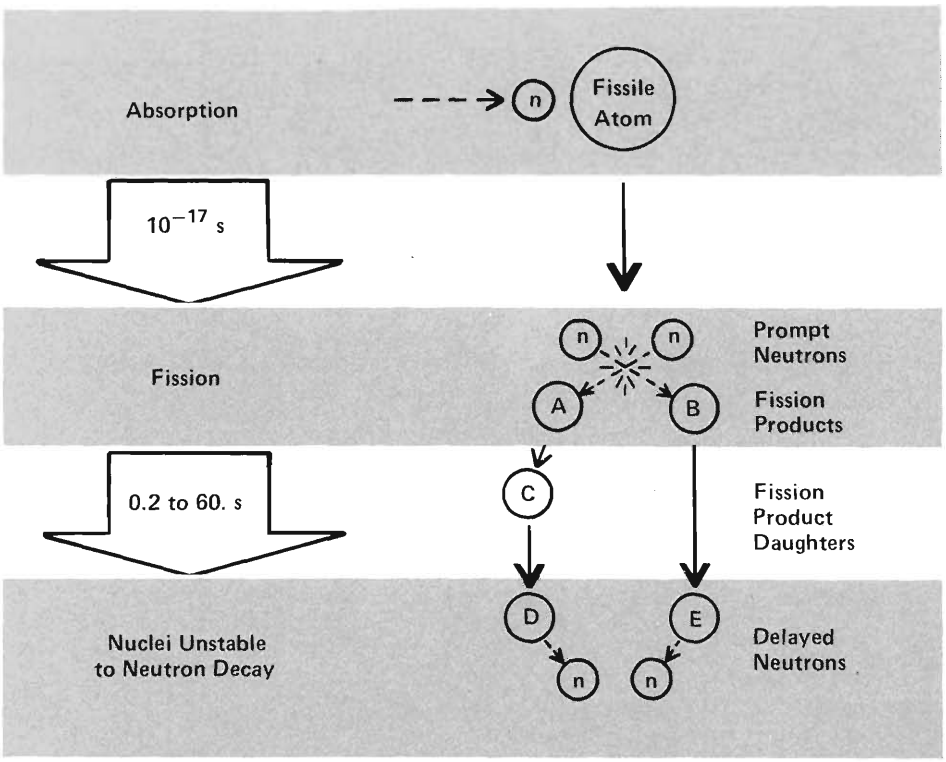


Fig. 3. Prompt neutrons are released during fission almost immediately after absorption of the neutron triggering the event. Delayed neutrons are released considerably later whan a fission product or a fission-product daughter is produced that is unstable to neutron decay. Other radiations have been eliminated for clarity.

very small reactor had a cylindrical core 0.15 meter in diameter and 0.14 meter in length, 35 plutonium metal fuel rods, and used mercury as a coolant. It produced 25 kilowatts at full power.

CORE. The special need of the breeder to generate and harbor neutrons efficiently dictates a core design that differs in several key respects from the thermal-neutron reactor core. First, breeder cores are made compact to minimize the masses of nonfuel materials such as stainless steel and coolant. These materials decrease the average yield by moderating neutron energies and the neutron availability by absorption.

Second, the fuel is highly enriched. While it is true that fast neutrons absorbed by fissile atoms result in high neutron yields (large η), the absorption cross section, that is, the probability for those absorptions to occur in the first place, is several orders of magnitude lower than for thermal neutrons. The solution to this problem is to increase the number of targets by increasing the density of fissile atoms. Thus, a typical breeder fuel is enriched to between 20 and 30 per cent in the fissile isotope compared to 3 per cent in light-water reactor fuel. A further advantage to high fissile-fuel density is that neutron mean free paths are kept small compared to the size of the core, thus

**The same is true of commerical reactors using thermal neutrons (see Fig. 2), except average lifetime is about 10^{-4} second and the approximate tripling time is 0.1 second.*

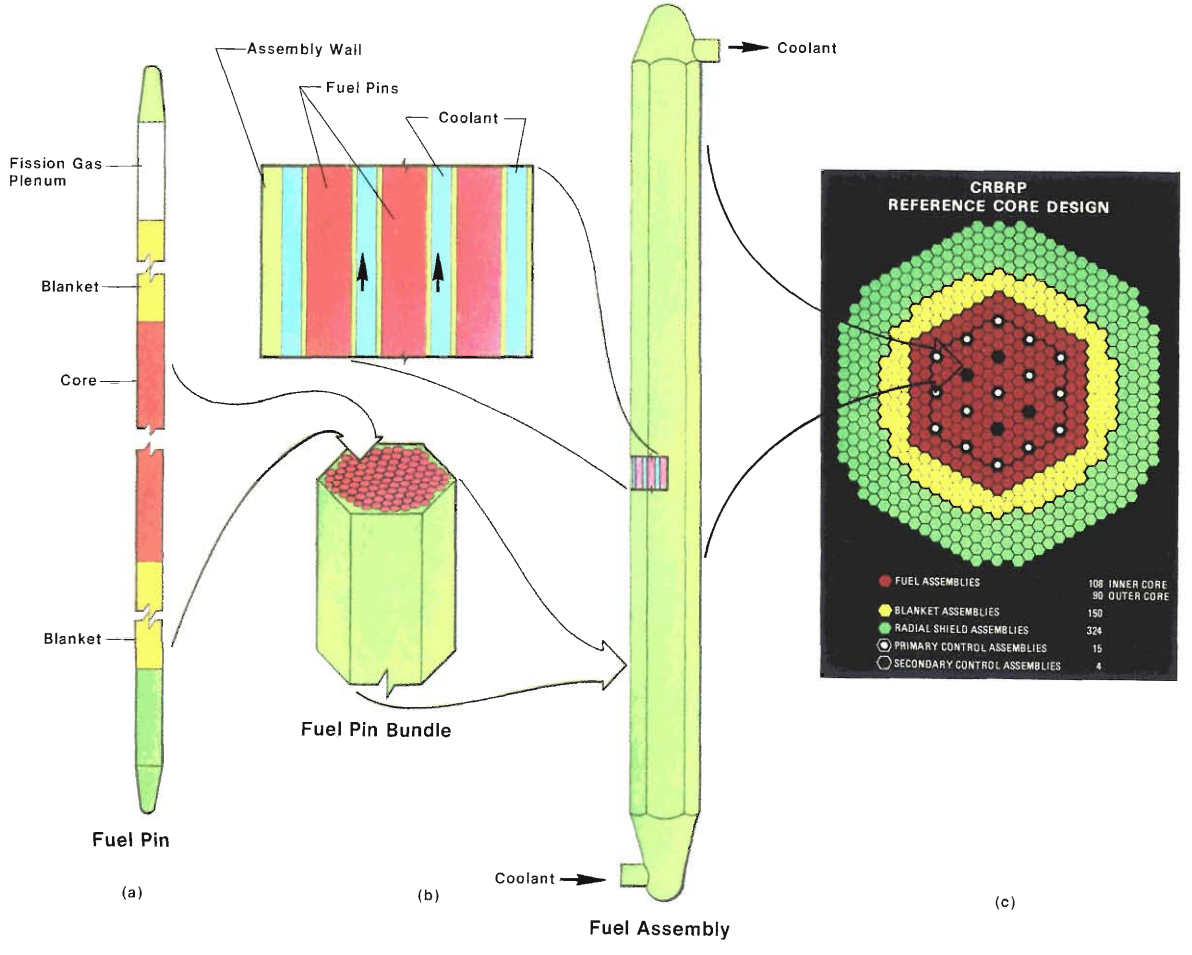


Fig. 4. (a) Fuel pins are long (2.8 meters), narrow (6 millimeters in diameter), and covered with a stainless-steel cladding (0.4 millimeter thick). There are three distinct regions of fuel in each pin with blanket fuel (yellow) placed above and below active-core fuel (red). A hollow region at the top serves as a fission gas plenum. (b) Two hundred seventeen fuel pins are bundled inside each stainless-steel fuel assembly. Liquid sodium coolant (arrows) flows up through the fuel assembly next to the fuel pins. (c) Fuel assemblies (red) are arranged into a core array along with blanket fuel assemblies (yellow) and control assemblies (white for primary, black for secondary). Radiation-shield assemblies (green) surround the array.

reducing neutron leakage.

The combined result of a compact core and high fuel density is high power density, typically about 300 megawatts per cubic meter. This necessitates a coolant system with good heat-transfer properties: for example, liquid-metal coolant flowing over large surface areas of the fuel.

Finally, a breeder core contains both an active core that supports the chain reaction and a blanket of fertile fuel that completely surrounds this core and captures escaping neutrons.

The manner in which these features are brought together for the proposed Clinch River Breeder Reactor, chosen for construction near Oak Ridge, Tennessee, is shown in Fig. 4. To create the necessary heat-transfer area, the fuel is encapsulated in thousands of small-diameter (6-millimeter) pins clad with stainless steel. Each of these pins is long (2.8 meters) and consists of several sections. The center section contains the active-core fuel, typically an oxide of the fissile isotope plutonium-239 mixed with the oxide of the fertile isotope uranium-238. Above and below the core section are blanket sections of fertile fuel, usually "depleted" uranium (99.8 per cent uranium-238 and 0.2 per cent uranium-235). A hollow section at the top of the fuel pin serves as a fission-gas plenum that collects the gaseous fission products diffusing out of the fuel below.

Between 200 and 300 of these fuel pins are bundled into a hexagonal array within a fuel assembly. Liquid sodium coolant enters the assembly at the bottom, flows upward among the fuel pins, then out the top.

Fuel assemblies are themselves positioned in arrays to form the active core. Blanket assemblies of fertile fuel are arranged about the active core to complete the blanket horizontally. Control rods are included among the fuel assemblies, and shield assemblies encircle the entire array to block escaping radiation. In some core designs, blanket assemblies are placed within the active core to enhance breeding.

The main features of the reactor vessel for the Clinch River Breeder are shown in Fig. 5. The vessel is approximately 6 meters in diameter and 17 meters in length. The active core, 1.8 meters in diameter and 1 meter in length, requires a fissile inventory of approximately 2 metric tons.* Two types of control rods with completely independent actuation systems assure reactor shutdown when demanded either by the automatic response of the control system or by the operators. Since the coolant is liquid sodium, which readily burns in air, the vessel must be carefully sealed and given an inert atmosphere. The closure head is, therefore, a complex structure of thermal shields and rotating, eccentric plugs that allow remote-control refueling operations. The sodium enters at the bottom (arrows), moves up through the fuel assemblies, mixes in the upper sodium pool, and finally flows out of the vessel to heat exchangers.

Despite high chemical reactivity with air and water, liquid sodium has several properties that make it an excellent coolant for fast breeders. First, it is a relatively poor moderator.** Second, its thermal conductivity allows for rapid transfer of heat within the high-power-density core and so eliminates concerns about local boiling, surface dryout, and fuel overheating. Third, the metal is a liquid over a large temperature range. Thus, the operating temperature can be high enough to achieve high thermal efficiencies of about 40 per cent, yet is still 300 kelvin below the boiling point. Finally, the system operates at atmospheric pressure.

The characteristics of low operating pressure and the capability of large heat removal prior to coolant boiling have led many engineers to argue that the liquid-metal fast breeder is generically safer than the light-water reactor. If control and safety systems function as intended, the possibility of a core meltdown should be no higher, and perhaps even less likely, than for the light-water reactor.

The Severe Accident

REACTIVITY CHANGES. Despite those generic safety features, certain aspects of the fast breeder raise a special safety threat in many people's minds. These aspects center, once again, on the neutron.

Unlike the light-water reactor, the core of a liquid-metal fast breeder is not in its most reactive configuration. Typically, there are several critical masses of fuel present in the breeder core. This fact, in conjunction with the core's high power density, led people to conjecture accidents in which the fuel melted and slumped into a supercritical configuration. Any similar slumping and compaction of fuel in a light-water reactor would eliminate coolant, which is important as a moderator. With the elimination of coolant, the population of thermal neutrons driving the chain reaction in the light-water reactor would decrease. In contrast, elimination of coolant in a breeder would actually increase the neutron population.

This concern about meltdown led to an emphasis on hypothetical core-disruptive accidents for liquid-metal fast breeders. Why hypothetical? Accidents become severe when there is a sustained inability to remove heat from the fuel at a rate commensurate with its generation. For this to happen, two major systems must fail. For example, if the reactor control system fails to control the power level, the safety system will scram or shut down the reactor. But if both systems fail, then a major thermal or heatup excursion can occur. Likewise, a severe acci-

A commercial light-water reactor of the same power capacity (1000 megawatts thermal) requires only 1 metric ton of fissile material.

***The hydrogen atoms of water have a mass equal to that of the neutron and so can absorb a large portion of the neutron's energy in a single collision; the heavier sodium atoms (atomic mass = 23) cannot.*

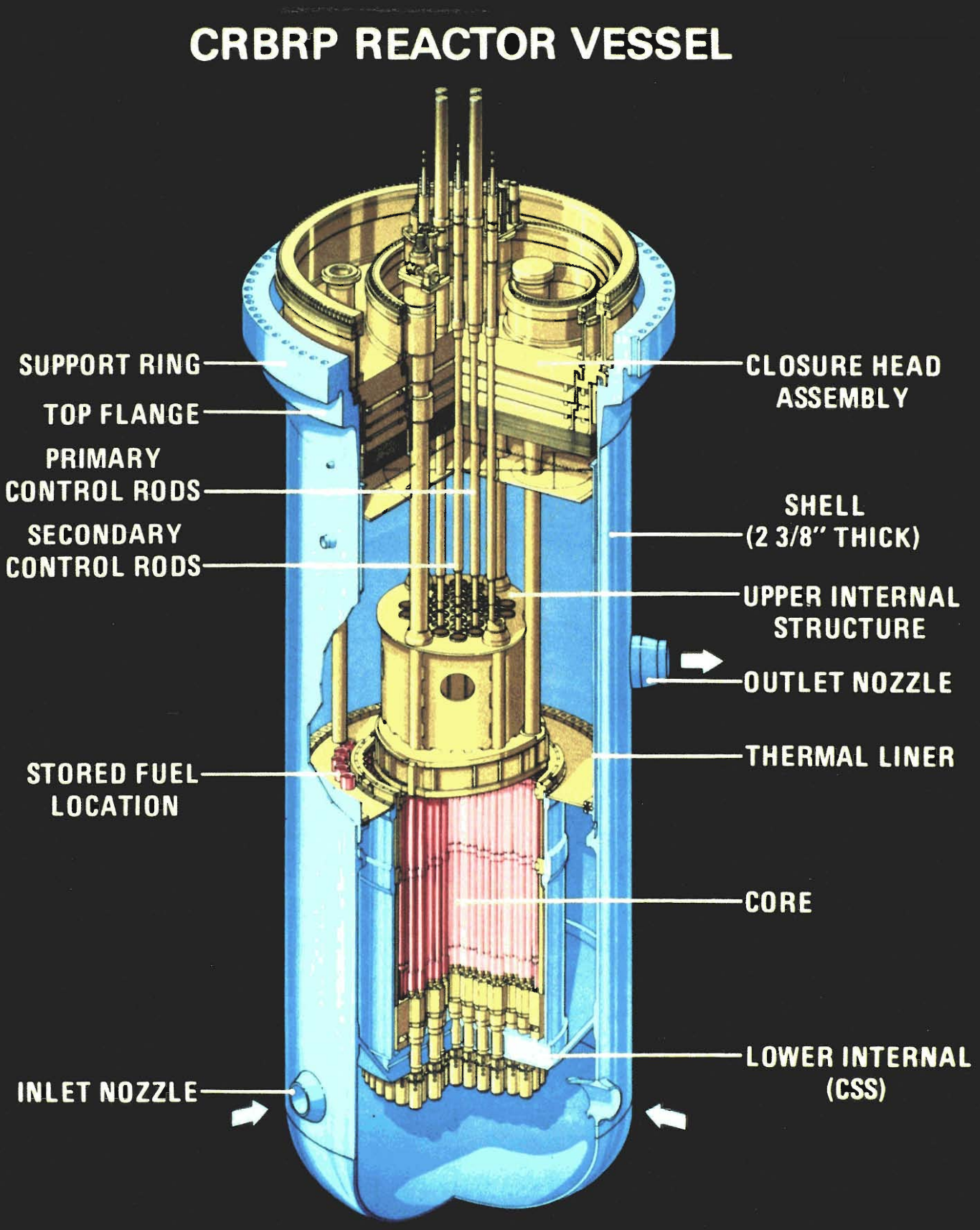


Fig. 5. The reactor vessel for the proposed Clinch River Breeder Reactor plant (CRBRP). Illustrated are the array of fuel assemblies, the associated control mechanisms, the core-support structure (CSS), and the primary containment vessel. Liquid sodium coolant enters at the bottom, flows up through the core and fuel assemblies, and out the vessel to the heat exchangers. (Courtesy CRBRP Project Office, Oak Ridge, TN 37830.)

dent will happen when heat transport from the core deteriorates due to pump failures or extreme pipe breakage, but again, only when coupled with failure of the safety system to scram. Other possibilities are associated with malfunctions of the redundant heat removal systems.

The system failures described can, in some cases, result in disruptive feedback: the failure causes heatup, which can melt fuel; if the fuel collapses, it creates excess neutrons and a power increase which accelerates the heatup. Central to this feedback are changes in the neutron balance called "reactivity." Positive reactivity involves the creation of excess neutrons, which, of course, increases the disruptive feedback; negative reactivity would moderate or decrease the feedback.

If the generation of excess neutrons is large enough, the controlled balance maintained by the delayed neutrons will be destroyed and there will be a sudden and very rapid rise in power. The reactor has gone "super-prompt-critical," a potentially dangerous condition that, in severe cases, will terminate only after the high pressures of hot, vaporizing core materials have dispersed the fuel.

Unfortunately, the liquid-metal fast breeder core designs that are most desirable in terms of performance and economics also have an undesirable domination of positive reactivity during severe heatup transients. For instance, core structural materials and coolant both absorb neutrons and moderate neutron energies. Loss of these materials contributes to positive reactivity both by increasing available neutrons and by causing a shift to higher neutron energies and, thus, higher neutron yields (Fig. 2). This happens if the liquid sodium boils or otherwise voids around the fuel pins, or if the stainless-steel cladding melts and flows from the core.

Fortunately, the positive reactivity is moderated by several inherent negative reactivities. The release of fission-product gases and the thermal expansion of core materials tend to disperse the fuel. Specific core design features can be incorporated that aid dispersal during a core-disruptive accident. Also, more neutrons are absorbed in the fertile fuel as temperature increases (the Doppler effect*).

AN ACCIDENT SCENARIO. The analysis of a postulated accident is designed to determine, with reasonable confidence, the degree of any positive reactivity, its transient behavior, and its potential for damage. Details of one accident scenario—failure of all primary sodium coolant pumps and complete failure of the reactor shutdown system—will provide perspective on the complexity involved in this chore.

First, there is gradual loss of heat transport from the core as coolant circulation slows to a stop. Different fuel assemblies have different power levels and flow rates, so they heat up at different rates. The Doppler effect and thermal expansions of sodium, fuel, and steel help keep reactivity feedbacks and power changes small. Soon, though, sodium boiling and voiding in fuel assemblies with the highest ratio of power to coolant flow lead to a net positive reactivity effect and accelerated heatup; then voiding begins in other fuel assemblies.

During this phase (the first 10 to 30 seconds) the dominant phenomena are the transfer of heat between materials, boiling and voiding of the coolant, and condensation of sodium vapor on cold structures at the ends of the various assemblies. Neutronics remains relatively smooth throughout the core. The analysis of this phase is simplified by the constant geometry of the core and the quasistatic character of the phenomena.

In the second phase, heat removal is highly degraded because the coolant has voided. Melting of fuel and cladding occurs on the order of a second after sodium voids are formed in a particular fuel assembly. The resulting complex situation is shown schematically in the opening figure of the article. The melted fuel pins in the central portion of the active core form a two-phase column of liquid fuel, liquid steel, fuel fragments, fission gas, fuel vapor, and steel vapor. The liquid components are immiscible, with greatly different melting points, viscosities, and thermal conductivities. The gaseous phase has been generated primarily near the midplane where the fission power was initially highest. The pressure from the gas and vapors expels liquids and fragments to the ends of the active core and into the colder axial blankets.

Analysis of this phase of the accident thus requires multiphase, multicomponent fluid dynamics and variable core geometry. Moreover, characteristics of the fluids vary greatly depending on initial conditions, time into the accident, and status of individual fuel assemblies.

The fission process causes the fuel to have a higher temperature than the other materials within the fluid mixture. Thus, a bewildering variety of heat-transfer processes and associated phase changes are possible. Some of the possible phase changes are illustrated in Fig. 6. All these processes are transient and have feedback effects on fluid displacement that, in turn, produce feedback effects on neutronics, reactor power, and fuel temperatures. The feedbacks are not only strong, but also highly nonlinear due to exponential relationships between liquid temperatures and vapor pressures and between material displacements and power. In fact, neutronic response changes from a relatively smooth core-wide distribution to one with local distortions and sudden peaks.

Although this complex, chaotic behavior occurs within individual fuel assemblies, the

Intermediate-energy neutrons are strongly absorbed at specific energies in the resonance region between thermal and fast neutrons (Fig. 2). As the temperature increases, these absorptions broaden, allowing absorption of a larger range of energies and, therefore, a larger fraction of the limited numbers of these neutrons.

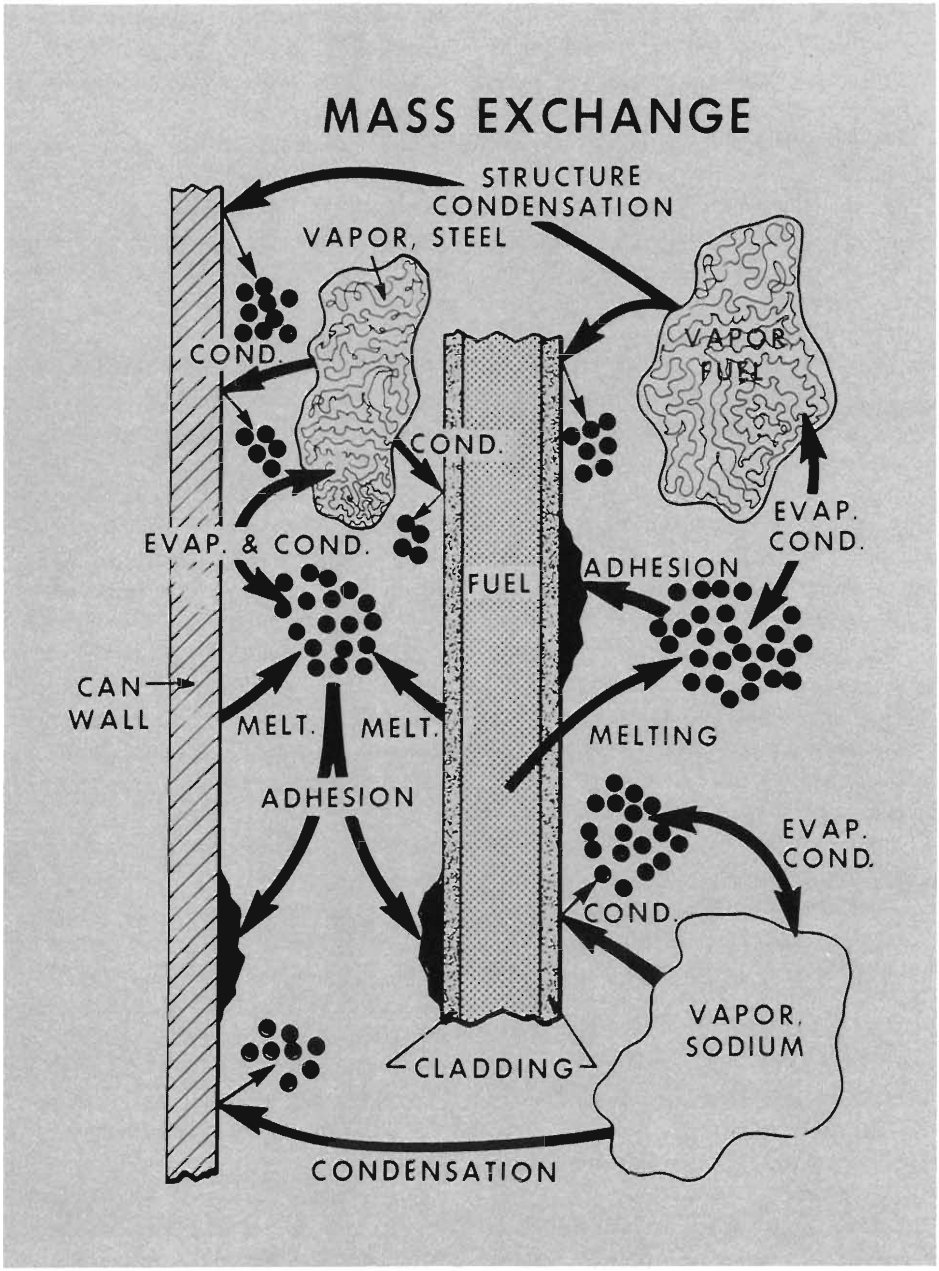


Fig. 6. Typical phase changes possible during a severe accident.

overall disruption process must be viewed on a core-wide basis. Reactor neutronics and power are dependent on the behavior in all the assemblies, and the common boundary conditions prevailing at the inlet and outlet sodium plena produce a core-wide fluid-dynamic coupling.

The third phase, designated the "transition phase," occurs when the fuel-assembly duct walls begin to melt. Now the flow field becomes multidimensional on a core-wide scale. Local fluid dynamics are no more complex than in the previous phase, but the extent of material relocation within the core may be much greater. This results in a difficult neutronics problem because of large voided and compacted regions where neutron mean free paths are no longer small compared to the dimensions of the medium. The large voids introduce strong directional effects, known as neutron streaming, which are important to this phase of the accident.

Neutronic coupling in the transition phase is potentially stronger because disrupted fuel is no longer in discrete assemblies; thus larger masses of fuel are capable of concurrent motion. Changes in reactivity can be both large and rapid. At this point two different outcomes are possible depending on such things as the reactor design or the reactor state at the beginning of the accident. First, if a large fraction of the original fuel has managed to remain within the active core region, a super-prompt-critical excursion can occur that heats the fuel in milliseconds to high temperatures and pressures. The fuel in the core, in essence, blows apart. While the dispersal of the fuel terminates the neutronic excursion, the pressure surge poses a direct mechanical threat and the possibility of breached containment.

On the other hand, if the fuel inventory has been reduced to about half the original amount by gradual leakage, or if large quantities of blanket materials have diluted the fuel, a severe power excursion will probably not occur. Thus, fluid-neutronic coupling becomes weak and of little further importance. The threat along this path is a potential meltthrough at the bottom of the reactor vessel from decay heat sometime within a few days.

SAFETY DESIGN. From this brief description of a severe accident, it is possible to understand why many knowledgeable scientists and engineers have considered detailed mechanistic analyses of these accidents to be an impossible problem. An appropriate description of the thermodynamic,

fluid-dynamic, thermal, and neutronic behavior has been judged beyond the state of the art. As a result, the hypothetical core-disruptive accident has, until recently, been dealt with in two ways.

First, engineers have attempted to design reliable systems with very low probabilities of even entering the severe accident regime. Second, the complexity of the problem has been side-stepped by basing designs on highly conservative bounding estimates of the "damage potential." This is the potential for neutronically heated core materials to produce high pressures damaging to containment structures and is typically based on the assumption of isentropic (reversible and adiabatic) expansion of the fuel. This approach worked well for small breeders such as the second experimental breeder developed by Argonne, EBR-II, which had a thermal power rating of 62 megawatts.

However, for the large breeders being considered today, the bounding approach places difficult if not impossible demands on design. For a hypothetical core-disruptive accident of a given energy-density level, damage potential increases approximately in proportion to reactor size, whereas the ability of reasonable designs to absorb damage scales weakly, or even inversely, with reactor size. As a result, if proof of containment for these accidents is necessary and it is tied to the demands of simple bounding analyses, an impasse may be reached in the licensing process.

SIMMER. Seven years ago, a team of engineers and scientists at Los Alamos decided to tackle this demanding problem. With the support of the Nuclear Regulatory Commission and the Department of Energy and with the use of the computer resources at Los Alamos, work was begun on the SIMMER code in 1974.

The approach adopted was to develop a generalized numerical framework based on the conservation laws of mass, energy, and momentum constrained by the initial and boundary conditions. Models representing the "physics" and consistent with physical laws or state-of-the-art understanding were to be inserted into this framework. This approach permits maximum flexibility for description of the physical interactions among materials, many of which were not well known at the time the work was begun. It also allows modeling sensitivities and uncertainties to be assessed in the interactive context of overall accident simulation. Thus, the impact of imperfections in knowledge can be established in a realistic manner.

EULERIAN FRAMEWORK. The "bookkeeping" needed to follow specific particles of material moving about and mixing together during a core-disruptive accident would be unbelievably complex. As a result, an Eulerian numerical approach was chosen for the fluid dynamics. This approach follows the evolution of material parameters at fixed points in space. The reactor core is divided by a mesh into a collection of cells, and the densities and energies of the material components are calculated at each cell as a function of time. This technique introduces some undesirable smearing of the transported entities within and between cells, but the approximation is considered acceptable.

While the fluid dynamics of core disruption are three-dimensional, considerable symmetry usually exists in the circumferential direction. Accordingly, a two-dimensional, cylindrical approximation is normally used in SIMMER, and each cell is specified by a radial and an axial coordinate.

MULTIPLE FIELDS. Because of the variety of material phases and components, certain simplifications must be incorporated into the fluid dynamics. The first simplification is to treat all materials having the same approximate velocity as a "field." Thus, one momentum equation at most needs to be assigned to each field. SIMMER uses three fields: structure, liquid, and vapor (Table I). The structure field includes all materials that are stationary in space. Besides the expected structural materials, fission gas trapped inside fuel pins and resolidified materials are components of this field. The liquid field includes all materials that flow: normal coolant, melted solids, and solid particles moving with these liquids. The vapor field, the gases, generates the pressure distribution that drives the motion of the liquid field as well as itself.

MULTIPLE COMPONENTS. Each field has a large number of material components, the densities and energies of which must be specified in each Eulerian cell. However, some of these densities and energies can be combined. For example, all gases in the vapor field have short thermal equilibrium times and so all gases in a given cell are given the temperature and energy of the mixture. On the other hand, since the location of fertile and fissile fuel must be considered individually for neutronic purposes, the density is specified separately for both in all three fields.

CONSERVATION LAWS. The Eulerian numerical framework with its three fields and multiple components must be formulated with conservation laws for momentum, mass, and energy as the foundation. There are only two momentum equations, one each for the liquid and vapor fields, but none for the structure field since it is assumed stationary. There are 23 mass equations and 12 energy equations, one for each density or energy component in each field.

The equations are in terms of densities, velocities, pressures, and internal energies, but they also include many source and sink terms to account for transfer of heat, mass, and momentum between fields. The mass equations account for vaporization, condensation, freezing, and melting; the momentum equations account for gravity and drag forces; the energy equations account for heat exchange and the various heats generated by phase changes, neutronics, viscous dissipa-

TABLE I.
FIELDS AND COMPONENTS OF SIMMER FLUID DYNAMICS

Field	Energy Components	Density Components	Geometry and Models
Structure (stationary)	Fuel pins Cladding steel Assembly wall steel Fuel crust Control pins	Fertile fuel Fissile fuel Cladding steel Assembly wall steel Fertile fuel crust Fissile fuel crust Contol pins Intergranular fission gas Intragranular fission gas	Fuel assembly geometry Order and thickness of layers on fuel pins Exterior surfaces exposed to liquid field Flow-channel diameters
Liquid (mobile)	Liquid sodium Melted fuel Melted steel Melted control pins Fuel particles Steel particles	Liquid sodium Melted fertile fuel Melted fissile fuel Melted steel Melted control pins Fertile fuel particles Fissile fuel particles Steel particles	Dispersed droplets in continuous vapor field Solid particle size Liquid droplet size from: surface tension internal pressure fluid dynamic forces (drag) coalescence model (collisional)
Vapor (mobile)	Vapor mixture	Fertile fuel vapor Fissile fuel vapor Steel vapor Sodium vapor Control pin vapor Released fission gas	Homogeneous mix Local vapor volume fraction

tion, and pressure-volume work.

EXCHANGE FUNCTIONS. The essential physics is introduced through the source and sink terms in the form of exchange functions. These functions give SIMMER its flexibility because each represents the modeling of a specific, independent physical process. Improvements in the understanding of specific phenomena are reflected as improvements in modeling and, hence, in the exchange functions that are inserted into the conservation equations. Currently, the modeling area receives considerable emphasis through both analysis and experiments.

One modeling area of particular concern is the manner in which materials break up. For instance, what distribution of particle sizes will result when a fuel pin begins to melt and crumble? What fraction will be liquid droplets and what fraction solid particles? Another area of concern is the physical properties of materials at high temperatures.

A typical modeling study starts with an attempt to describe the phenomenon by using standard engineering functions. In these equations appear various coefficients or exponents that correlate forces or material properties; for example, a Reynold's number may be used that relates dynamic pressure and viscous stress for vapor flow over a spherical particle. Many of these coefficients have parameters that depend on the specific geometry of the phenomenon being modeled: particle sizes, flow-channel diameters, heat-transfer contact areas. Thus, an important step in the analysis is a realistic description of the physical configuration.

Next, attempts are made to "benchmark" the model by comparing its predictions with experiments dealing directly with the phenomenon. Some of these experiments are done at Los Alamos, but most are carried out at other laboratories. SIMMER is run using only the exchange functions, the geometry, and those parts of the code necessary to the particular experiment being simulated. At this point, the model can be "fine tuned" by adjusting coefficients until the desired agreement between calculated and experimental results is achieved.

As implied by this discussion, the Eulerian mesh imposes a certain geometrical scale on the problem, but the exchange functions allow for effects due to a finer scale. Each function depends on local cell conditions, including the predicted characteristics of the microscale geometry.

The properties of the microscale geometry in the structure field are based on a typical

TABLE II

TRANSFER PROCESSES INCLUDED IN SIMMER

Source[a]	Process	Sink or Final State[a]
MOMENTUM TRANSFER		
Cladding Assembly wall Fuel or control material	Breakup	Liquid or vapor field
Vapor field	Pressure change	Liquid field
Cladding Assembly wall Fuel or control material	Melting (or freezing)	Liquid field
Liquid field	Vaporization	Vapor field
Steel vapor Fuel or control material vapor	Condensation	Liquid field
——	Viscous coupling transverse to flow	——
——	Liquid-vapor, drag-driven slip flow	——
MASS TRANSFER		
Liquids (fuel, steel, sodium, control material)	Vaporization	Vapor field
Fission gas trapped in fuel	Release	Vapor field
Vapors (fuel, steel, sodium, control material)	Condensing out onto structures	Liquid field
Fuel vapor	Condensation	Liquid fuel
Steel vapor	Condensation	Liquid steel
Sodium vapor	Condensation	Liquid sodium
Control material vapor	Condensation	Liquid control material
Solids (fuel, cladding assembly walls, control material, fuel particles, steel particles, fuel crust)	Melting	Liquid fuel Steel Control material
Liquids (fuel, steel)	Freezing out	Assembly walls
Liquid steel	Freezing out	Cladding
Liquid control material	Freezing out	Control material
Liquid fuel	Freezing	Fuel particles
Liquid steel	Freezing	Steel particles
Solids (fuel, fuel crust)	Breakup	Fuel particles
Solids (cladding, assembly walls)	Breakup	Steel particles

ENERGY TRANSFER

Fuel pins	Heat transfer	Cladding Liquids (fuel, sodium, steel, control material) Vapor field
Fuel crust	Heat transfer	Assembly walls
Fuel particles	Heat transfer	Liquids (steel, sodium, control material)
Cladding	Heat transfer	Control material Liquids (sodium, control material) Vapor field
Assembly walls	Heat transfer	Liquids (sodium, control material) Vapor field
Steel particles	Heat transfer	Liquids (sodium, control material)
Liquid steel	Heat transfer	Solids (cladding, assembly walls, steel particles, control material) Liquids (sodium, control material) Vapor field
Liquid fuel	Heat transfer	Solids (cladding, assembly walls, fuel particles, steel particles) Liquids (sodium, control material, steel) Vapor field
Liquid sodium	Heat transfer	Control material Liquid control material Vapor field
Liquids (fuel, steel, sodium, control material	Vaporization (or condensation)	Vapor field
Fuel	Melting	Liquid fuel
Steel particles	Melting (or freezing)	Liquid steel
Liquid fuel	Freezing	Fuel particles
Liquids (fuel, steel)	Freezing out	Assembly walls
Liquid steel	Freezing out	Cladding
Cladding Assembly wall Fuel or control material	Viscous dissipation during momentum transfer	Liquid field Vapor field
Liquid field	Viscous dissipation during momentum transfer	Vapor field
——	Viscous dissipation during momentum transfer by transverse viscous coupling	——

[a]Source and sink may reverse roles depending on local temperatures.

fuel assembly. Included are flow-channel diameters, the properties of surfaces interacting with the flow of the liquid and vapor fields, and the thicknesses and order of layered materials of the fuel pins, assembly walls, and solidified material.

The liquid field is generally viewed as dispersed immiscible droplets in a continuous vapor field. This concept is extrapolated to simulate situations where the liquid is continuous. Solid particle sizes are specified directly, but liquid-droplet diameters are computed by balancing local fluid-dynamic and surface-tension forces and by tabulating all local coalescenses.

All transfer processes expected to have any significant strength are included in SIMMER as exchange functions. These are listed in Table II. The sheer number of these processes illustrates the high degree of interactivity among physical processes attempted in SIMMER and required of any reliable mechanistic approach.

Also important is the ability of the code to deal with a wide range of transient phenomena in many environments. During an accident, stationary materials become mobile, flow obstructions such as duct walls are removed, and normal flow channels become blocked. This alteration of normal core geometry is included through exchange functions related to structure melting, structure disintegration by local thermal and pressure loads, and freezing of liquids on structures. Also, functions representing microscale geometry provide areas and distributions of particles and droplets for heat transfer, phase change, and coalescence phenomena calculations.

A DROPLET HEAT-TRANSFER MODEL. As an example of the level of detail incorporated in the models used in SIMMER, the liquid-liquid heat-transfer model will be outlined here. This model assumes that each droplet sweeps out a volume determined by its radius and velocity and then collides with other droplets in that volume. The average fluctuating velocity used may differ from the liquid-field velocity or from component to component because of acceleration differences due to droplet sizes and densities. A collision rate between various liquid components is calculated for each mesh cell.

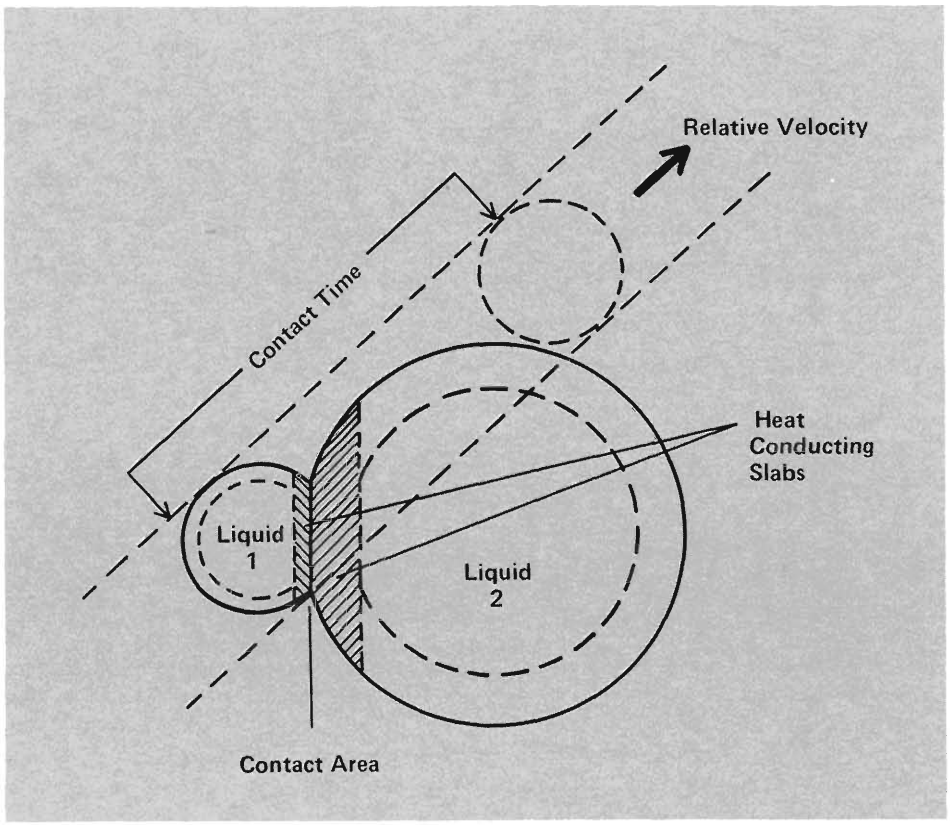


Fig. 7. Droplet-droplet collision and associated heat-transfer parameters.

Figure 7 illustrates three other parameters used in the heat-transfer calculation. The collisional contact area is based on the cross-sectional area of the smaller droplet, but a correction factor is included to approximately account for relative velocity and angle of impact. The heat-transfer rate per unit area is assumed to be quasistatic and is based on conduction between the two slabs of material next to the contact surface. Each slab thickness is taken as 20 per cent of the droplet's radius; this short conduction length is due to the fact that most of the heat capacity in a sphere is effectively near the outer surface. Contact time is estimated from the time the respective droplet volumes intersect.

The heat-transfer rate per unit volume is the product of contact area, time of contact, heat-transfer rate per unit area, collisional rate, and the temperature difference between droplets. The final equation is in terms of cell parameters: the radius and temperature of each droplet, the liquid volume fraction, and the heat conductivities of both components.

EQUATION OF STATE. The multicomponent equation of state that completes the coupling between the fields can take one of two forms in SIMMER. An analytic equation-of-state approach requires direct input of material properties such as specific heats, heats of fusion and vaporization, and vapor pressures. The equations then relate the

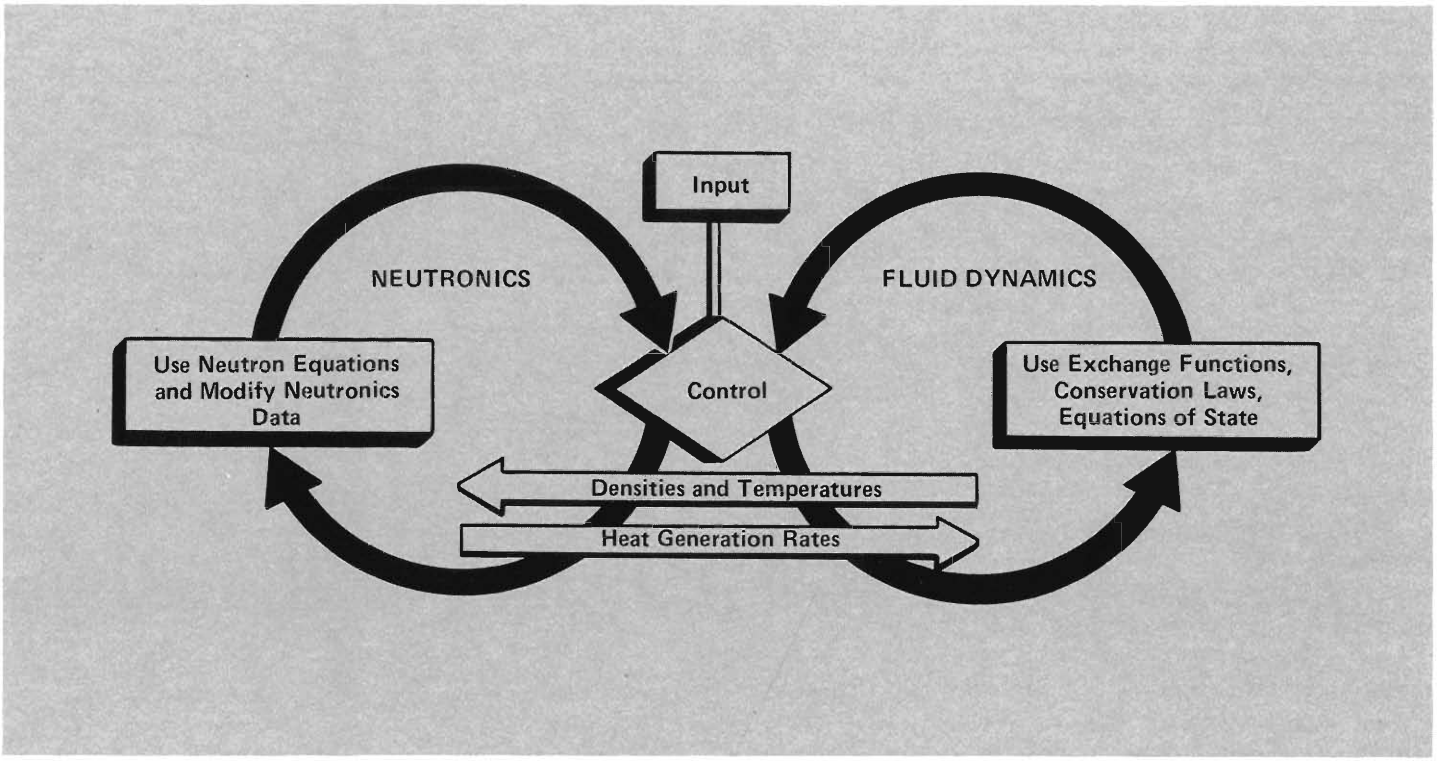


Fig. 8. Schematic of the coupling between the neutronics and the fluid-dynamics calculational loops in SIMMER.

microscopic density and internal energy of the components in each field to the pressure and temperatures. The reference energy states of all materials are synchronized to a temperature of 0 kelvin. Also, the vapor materials are assumed to obey the simple concepts of ideal gas mixtures.

The other approach is a tabular equation of state that enables data from the Los Alamos equation-of-state library, Sesame, to be used. This library provides a wider and more realistic data base than can be obtained with an analytic approach, but the interfacing of the conservation equations and exchange functions with the tables has not yet been fully completed.

NEUTRONICS. Coupled with the fluid dynamics analysis is a calculation of the neutronic and power response of the disrupting core. Thus, as shown in Fig. 8, SIMMER consists of two interacting calculational loops: one for fluid dynamics and one for neutronics.

The mesh structure used for the fluid dynamics calculations is also the basis for the neutronics calculations. However, regions where neutronic effects are known to be negligible can be eliminated. Also, specified regions can be further subdivided when needed to obtain realistic representations of neutronic spatial effects.

The neutronics and fluid dynamics equations are not solved for the same time step, but are required to agree at certain times. This approach is what permits the separation of the two loops. The interaction between loops occurs with the transfer of such key quantities as material temperatures, densities, and heat generation rates.

Three levels of sophistication are provided in SIMMER for the neutronics loop. The simplest approach assumes a uniform neutron distribution in space and an invariant energy spectrum during the transient. Reactivity feedbacks are derived from overall reactivity coefficients and, for each material, a reactivity effect per unit mass. This approach is known as "point kinetics" since it treats the reactor as a single point in space. Because of its simplicity, it appears in SIMMER merely as a step in the fluid dynamics loop.

As the core becomes more disorganized, neutronic characteristics change markedly, requiring an approach that incorporates space, time, and spectral effects. In some cases, a diffusion treatment of neutron transport in space can be used that represents an intermediate level of sophistication and has the advantage of numerical economy. In general, however, an approach using the full neutron transport or neutron conservation equation is necessary. This approach includes the dependence of the neutron distribution on space, time, neutron energy, and

neutron direction. The solution of this equation is formidable and has received much attention from reactor physicists for a number of years. The techniques used in SIMMER are state of the art.

Severe Accident Analysis

The combination of the features discussed above resulted in a flexible code capable of simulating experiments, performing controlled examinations of isolated phenomena, and analyzing severe accident behavior in a variety of reactor configurations. As a result, an interactive approach involving applications and testing was implemented early in the development of the code with very fruitful results.

The first major application came in 1977 when SIMMER I, the first version, was still in a developmental stage. This application involved an investigation of the hypothetical accident already described in which the core suffers a super-prompt-critical excursion producing a state of high thermal energy (fuel temperatures on the order of 4000 to 6000 kelvin and a maximum vapor pressure of approximately 25 megapascals). As previously noted, the isentropic expansion analysis of this event indicates that the pool of liquid sodium should surge up against the reactor head, generating large pressures and structural deformations, and could thus pose a threat to primary containment.

In 1977 the SIMMER I capabilities were adequate for a more realistic analysis of this expansion process. These capabilities included the modeling of a multitude of heat-transfer processes, structural constraints on fluid flows, and mass-transfer effects, all in a transient context. To everyone's surprise, the calculated mechanical energy was only about 5 per cent of that from the isentropic expansion for identical initial conditions.

The impacts of this finding, if substantiated, are fourfold. First, the damage potential of severe accidents was previously being estimated in an overly conservative fashion. Second, the ability of reactor containment systems to withstand severe accidents and thereby protect the public may be substantially greater than thought. Third, the extent to which the highly complex parts of the severe accidents are resolved could be relaxed by allowing some difficult phenomena to retain large uncertainties. Finally, a phenomenological signature of the expansion was established against which concepts and estimates could be tested.

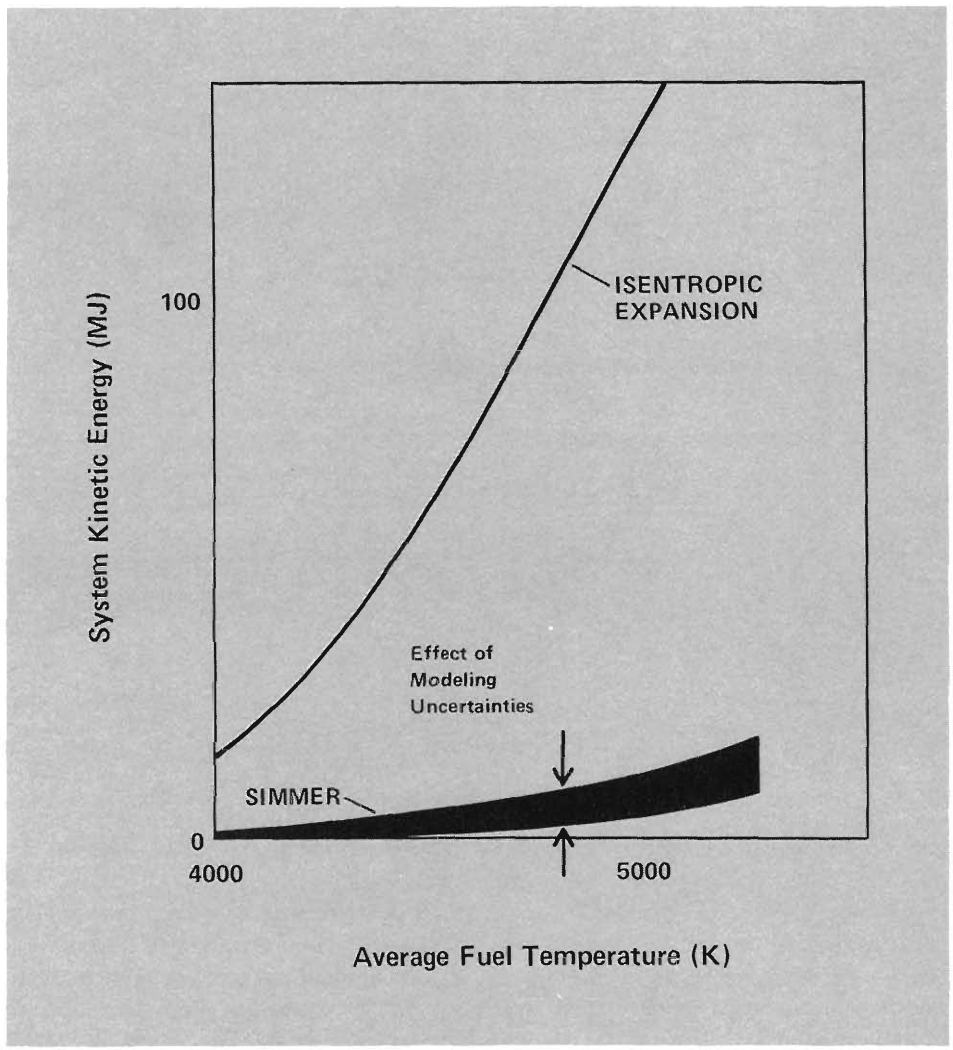


Fig. 9. Reactor damage potential (fluid kinetic energy) versus accident severity (initial fuel temperature) calculated by SIMMER and by assuming an isentropic expansion of the fuel. The band represents the effect of SIMMER modeling uncertainties.

Follow-up investigations with an improved and expanded version of the code, SIMMER II, revealed the reduction in mechanical energy to be due to interactions among the various aspects of the expansion process. For example, the pin structure in the upper core produces a strong throttling effect that prevents rapid discharge of core material into the sodium pool as well as redirecting heat flow so that not all the available energy

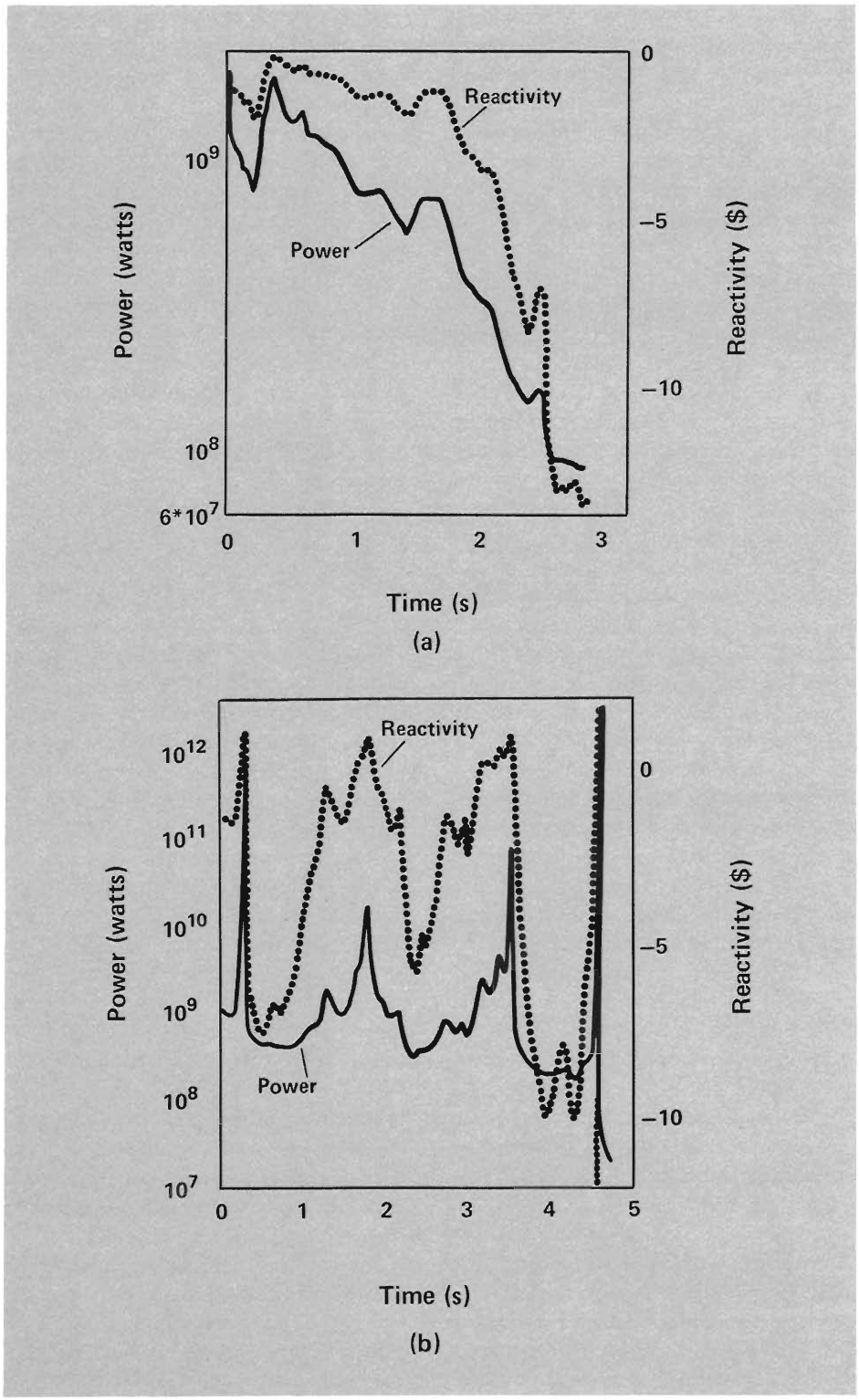


Fig. 10. Two examples of the power and reactivity response calculated by SIMMER for a liquid-metal fast breeder during a hypothetical accident. Initial conditions are identical except in a) large amounts of fuel are able to escape through the axial blanket sections while in b) the channels within the axial blanket sections of the fuel pins are clogged and only slight amounts of fuel escape. (The unit of reactivity is the dollar; one dollar is the reactivity change between delayed-critical and prompt-critical conditions.)

is delivered to the sodium. Nonuniform expansion, resulting from interaction with core structure and from preferential expansion of the hottest fuel, also leads to a considerable drop in the effective expansion pressures.

The investigations also showed that the reduction was highly insensitive to modeling uncertainties. This result is summarized in Fig. 9, where the calculated fluid kinetic energy due to the expansion is plotted against accident severity in terms of the initial fuel temperature at the start of the expansion. The band on the figure represents the combined interactive influence of modeling uncertainties; it was determined by assigning estimated uncertainties to 25 exchange processes important to the accident, randomly selecting values within these uncertainty ranges, and then repeatedly redoing the SIMMER calculations. The result shows that known modeling inadequacies can be tolerated without compromising the gratifying reduction in damage potential.

As a result of this early work, there is presently an international interest in SIMMER and its capabilities. Major laboratories and government agencies in the United Kingdom, West Germany, Italy, and Japan, as well as industrial contractors in the United States, are actively utilizing SIMMER.

The second major application of SIMMER was initiated in 1979. This was the first

attempt to simulate an actual core meltdown transient on a whole-core scale with coupled space-time neutronics and comprehensive thermal-fluid dynamics. The results of two calculations are shown in Fig. 10. The initial conditions and modeling assumptions are identical for both calculations except that the result shown in Fig. 10a assumed easy fuel transport through the axial blankets and thereby considerable fuel escape from the active core regions while the result shown in Fig. 10b assumed rapid freezing of the fuel in the escape paths and thereby slight fuel escape. This approach illustrates the method of dealing with modeling uncertainties by varying one key aspect and so bracketing the phenomenon of interest between two extremes.

Comparison of the transient power for these two extremes indicates the crucial effect of fuel removal. When fuel can escape easily, power dwindles to low levels within 3 seconds and at no time does it get much higher than 10^9 watts. However, when fuel escape is clogged, the result is continued power excursions with peaks of 10^{12} watts as late as 5 seconds into the accident.

This second application of SIMMER provided major insights into the characteristics of core disruption from a transient point of view and called into question qualitative views derived from steady-state perceptions. This latter point of view suggested that a few generic physical processes control the accident behavior, such as a material boilup in the core that permanently disperses the fuel and prevents recriticality. The transient context indicated that these processes may not be continuously operative; for example, even after boilup the fuel could flow back together into another critical mass.

Since full-scale, severe accident experiments are not considered desirable or feasible, there is a need to test the predictive capability of SIMMER through application to a wide spectrum of specialized experiments. One example of the various experiments simulated by SIMMER II has to do with the previously mentioned freezing and plugging phenomenon that may occur during a severe accident. Experiments conducted at Argonne National Laboratory examined this phenomenon, using a hot, molten thermite injected into the channel between steel-clad blanket fuel pins. The molten thermite contains molybdenum, which represents melted stainless steel, and uranium oxides, which represent melted fuel. The full experiment simulates the pressurized flow of melted fuel up into the blanket region of the core. The code successfully simulated the degree of transport of thermite into the channels, the plugging phenomenon, and the amount of destruction of the pins for a variety of initial conditions.

Conclusions.

Because of these SIMMER analyses, the necessary conditions for avoiding severe accidents are becoming discernible. As a result, research directions are being reassessed and the discussion of these accidents is turning from broad opinions to factual support of specific models.

The analytical results obtained so far have encouraged us to feel it is possible to unfold the accident path in a way that adequately represents reality. The fact that development of mechanistic computer codes has been supported by various parties in the breeder community for a number of years indicates a strong desire by the industry to also face that reality.

Moreover, since it is not reality, but rather the uncertainty surrounding a vague possibility, that leads to greater fear in the minds of people, it is necessary to continue refining the analytic tools and extending the experimental base for the study of severe accidents in the fast breeder. Only then can informed decisions be made concerning the safety of this potentially very beneficial modern alchemy. ■

AUTHOR

Charles R. Bell has been a staff member at Los Alamos since 1975. He received his Bachelor of Science degree in mechanical engineering from the University of Cincinnati in 1965 and his Ph.D. in nuclear engineering from the Massachusetts Institute of Technology in 1970. From 1970 to 1975 he worked for Atomics International, assessing severe core-disruptive accidents on breeder reactors. Also, he led the effort to design, develop, test, and apply a system analysis capability to investigate tube breaks in large sodium-water steam generators. At Los Alamos he has been working to develop and apply advanced techniques for detailed assessment of severe breeder reactor accidents. He has played a major role in establishing new perspectives on accident characteristics and in integrating these new perspectives into national and international research and development programs. He is a member of the American Nuclear Society.

Further Reading

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