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SIMMER AS A SAFETY ANALYSIS TOOL

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ABSTRACT

SIMMER has been used for numerous applications in fast reactor safety, encompassing both accident and experiment analysis. Recent analyses of transition-phase behavior in potential core disruptive accidents have integrated SIMMER testing with the accident analysis. Results of both the accident analysis and the verification effort are presented as a comprehensive safety analysis program.

INTRODUCTION

Development of the SIMMER[1,2] (S_n, Implicit, Multifield, Multicomponent, Eulerian, Recriticality) Program began in 1974 in an effort to predict the extended motions of fast-breeder-reactor core materials during a core disruptive accident. Assessment of recriticality potential and possible subsequent energetics, particularly for the transition phase, has been the primary goal of this program. Since its inception, SIMMER has been used for a wide variety of applications, primarily, but not exclusively, for assessing the safety of liquid-metal-cooled fast breeder reactors. In this paper we present the current status of the SIMMER program by drawing together recent SIMMER analyses.

This paper emphasizes the modeling flexibility of the SIMMER code that permits its application in an integral LMFBR safety analysis program. Such an integral program includes the interplay between whole-core accident analyses that help identify dominant phenomena in the accident sequences and separate-effects studies that help verify that the code is predicting the proper physics. The separate-effects studies may be a direct comparison of calculated results against experimental data, or they may be an assessment of the calculated results against basic physical principles that dominate the accident sequence. Because of nonlinear, transient, and incoherency effects, the basic physical principles cannot directly evaluate the accident consequences. This paper concentrates on the application of SIMMER to transition-phase analysis but also briefly updates the verification effort for postdisassembly expansion analysis. We begin with a short summary of the philosophical approach surrounding the development of SIMMER.

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DEVELOPMENT APPROACH

From a simplistic viewpoint, SIMMER is basically a bookkeeper combined with an integrator. For the fluid-dynamic models the bookkeeping aspect of the code tracks the mass, momentum, and energy of the various materials in a fast reactor core as they change because of thermal and mechanical interactions. The conservation equations provide the bookkeeping function, and although they are important and necessary, they are not the main emphasis of the development program. The larger part of the program is determining the models describing the rates of interaction between the materials. The pressures that develop to exert force on the materials evolve from these rate processes. The mathematical model describing a particular rate process can range from simple to complex. Simple models permit fast computer execution time but may have limited accuracy for a broad range of applications. More complex models reduce the uncertainties for broader applications but involve greater calculational effort. A similar circumstance exists for predicting the reactor neutronic state in that the cross-section treatment in the Boltzmann equation for neutron conservation must balance complexity, applicability, and computational economy.

The integrator function of the code solves the complex nonlinear set of conservation equations and rate models. Not only does this function eliminate the necessity for over simplifying the equation set for analytic solution, but it also allows more complex rate models and greater diversity in spatial and temporal resolution.

Although the SIMMER code has been developed for analysis of core disruptive accidents (CDAs) in LMFBRs, the fluid-dynamic models are generally applicable to many fluid flow problems that have similar mass, momentum, and energy transfer processes. Thus, application is not necessarily limited to the whole-core phenomena that might occur in CDAs. Because the code is not tied to specific accident phenomena and reactor materials, it has considerable flexibility in other applications, particularly analyses of separate effects studies and simulant experiments. This ability to benchmark the code then permits the extrapolation from the small-scale, simulant experiments to the whole-core, real-material system.

POSTDISASSEMBLY EXPANSION VERIFICATION

The proper balance between simple and complex rate models evolves from a verification program that tests the models in experimental thermophysical regimes simulating the expected reactor accident regimes. Model uncertainties are assessed and reduced by testing against available and appropriate experimental data. Testing the SIMMER fluid-dynamic treatment (i.e., the basic conservation equations) has continued for several years.[3] In essence, this testing has shown that, for postdisassembly expansion analysis not involving significant thermal interactions, the SIMMER fluid-dynamic treatment is adequate. Recent Upper Structure Dynamics experiments[4] have added to this data base, indicating that SIMMER properly accounts for the flow resistance of the upper-core structure during postdisassembly expansion. However, inability to accurately predict certain rate processes, such as vapor generation in nucleating bubbly flow encountered outside the test section in these experiments, has indicated that some rate models may need further development. To analyze experiments adequately, further improvements are being considered for these rate process

models even though it is not clear that the processes encountered outside the test section are appropriate to the reactor accident regime being investigated.

TRANSITION-PHASE STUDIES

For the past few years, SIMMER applications have emphasized exploratory transition-phase analyses. Again, verification and testing of the code against available and appropriate experimental data have been integral parts of these analyses. Initial exploratory whole-core analyses for loss-of-flow accidents in heterogeneous core LMFBRs helped identify dominant accident characteristics and phenomena. The dominant phenomena then became the focus of the testing program to assess the credibility of the initial results and to provide a basis for improved calculations. In the following we present SIMMER analyses of several dominant transition-phase phenomena identified in these initial whole-core studies.

Freezing and Plugging Analyses

Because retention of the reactor fuel near the original core location enhances the potential for recriticalities, the testing of SIMMER's capability to predict cladding and fuel blockages accurately has been important. Analyses of simulant and real-material blockage experiments have contributed to identifying model deficiencies and sources of uncertainty, but in general SIMMER calculations for a wide range of freezing, melting, and plugging tests have agreed well with experimental data[5]. These experiments have included saturated and superheated (relative to the freezing temperature) water freezing in supercooled tubes and rod bundles, Freon melting of an ice pipe, and thermite injections into rod bundles. Calculations of water freezing in pipes required code modifications to account for the cylindrical pipe (rather than flat subassembly duct wall), the contact resistance between the ice crust and tube wall, and interfacial (rather than bulk) freezing and melting. Agreement with the experimental data was good after the modifications were made. Except for inadequate modeling of entrance effects, SIMMER predictions of the melting rate of an ice pipe by hot refrigerant-11 also have been good.

Analyses[6] of Argonne National Laboratory's (ANL's) thermite freezing and plugging experiments[7] have shown that, for the experimental conditions of low fuel superheat and thin steel cladding, SIMMER predictions agree well with the experimental data shown in Table I. However, the modifications to allow interfacial freezing and melting have not been tested against real-material data; thus, SIMMER predictions of fuel penetration distances must still be verified for conditions in which significant temperature gradients occur in the structure.

Intersubassembly Gap Studies

An important potential fuel removal path in the transition phase is the gap between subassemblies. In heterogeneous cores, gaps between internal blanket assemblies may be available for fuel removal if the corners of duct walls of nearby driver assemblies fall into those intervening gaps. Several SIMMER analyses have investigated the thermal-hydraulic phenomena occurring during fuel ejection into and through the gaps. For example, SIMMER has been used to analyze the ANL GAP1 experiment[7] in which thermite was injected downward through a dry gap test section; experimentally no blockages were

TABLE I

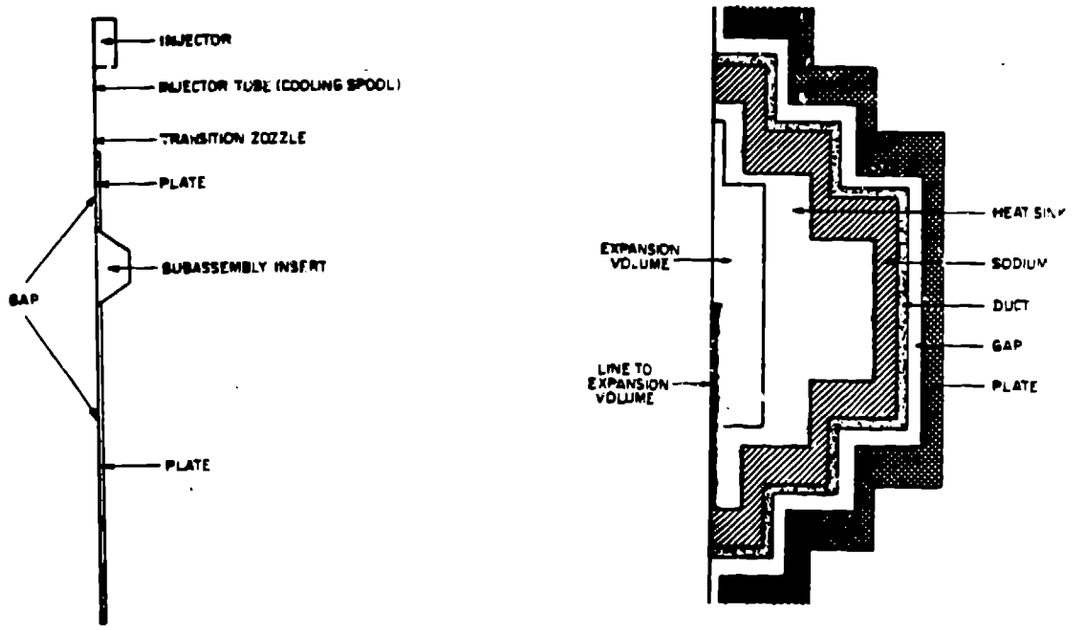
Comparison of Calculated and Experimental Penetration Distances for Thermite Injection Tests

Test Conditions			Penetration Distance (m)	
Injection Pressure (MPa)	Cladding Temperature (K)	Thermite Mass (kg)	SIMMER	Experimental
6.6	1173.0	0.5	0.45	0.43
5.5	873.0	0.5	0.30	0.43
2.5	573.0	2.0	0.35	0.34
3.7	573.0	2.0	0.37	0.41
5.0[a]	1173.0	2.0	1.00	1.40

[a]Estimated due to instrument failure.

formed and the thermite shot through to the test-section bottom. Analyses of this experiment used three SIMMER models: a front view perpendicular to the duct wall, an edge view of the gap between the simulated ducts walls, and cylindrical model with appropriate material volume fractions and surface areas. All three models predicted similar results and reproduced the extensive thermite penetration to the test-section bottom. However, other detailed GAP1 experimental results, such as crust thickness and distribution, were not matched, in part because experimental conditions could not be controlled resulting in duct warping and gas venting. Further, pretest investigations for the effect of sodium initially in the gap indicated that the reduced expansion volume would retard the fuel injection into the test section. Two-dimensional calculations showed fuel being entrapped by recirculating sodium; the resulting fuel-coolant interaction pressures were strongly dependent on heat-transfer assumptions. Simulation of the GAP2 experiment, which included a hexagonal can containing sodium inserted in the path of the flat-plate duct, required modeling the hexagonal shape with a series of right angle turns shown in Fig. 1 to obtain results similar to those obtained experimentally. Further refinements of the calculations would be necessary to match the maximum pressures that occurred after the hex can failure and the final fuel distributions in the test section. Although these initial studies of the GAP experiments indicated the need for more refined data and for further modeling improvements to understand better the phenomena occurring during fuel flow through gaps, the studies did demonstrate that the flexibility of the SIMMER code permits its use in such analyses.

Further studies of the flow of materials in gaps between blanket assemblies have extended the analyses beyond the conditions found in the GAP experiments. Exploratory calculations for flow downward through the gap have varied both the environment and the modeling. Examples of environmental parameters varied include the driving pressure, the stream composition (molten fuel, molten steel, fuel particulate), stream temperature, duct wall temperature, and the presence of sodium. Modeling variations have included the value of the particle viscosity and the ablation characteristics of the duct wall. Without ablation, crust growth on the wall, as shown in Fig. 2, has matched conduction-controlled freezing models. Furthermore, for all cases in which a driving pressure of a few atmospheres exists, no blockages were predicted within the one-meter test length regardless of any reasonable modeling or environmental variation. With ablation, the addition of molten steel into the flow stream caused fuel to freeze and form a slurry of molten fuel, molten steel and fuel particulate. The enhanced viscosity from the particulate slowed the flow stream and, for driving pressures less than one atmosphere, led to blockages near the end of the one-meter calculational mesh



(a) Full-length Model

(b) Subassembly Insert Details

Fig. 1. SIMMER edge-view model for the GAP2 experiment.

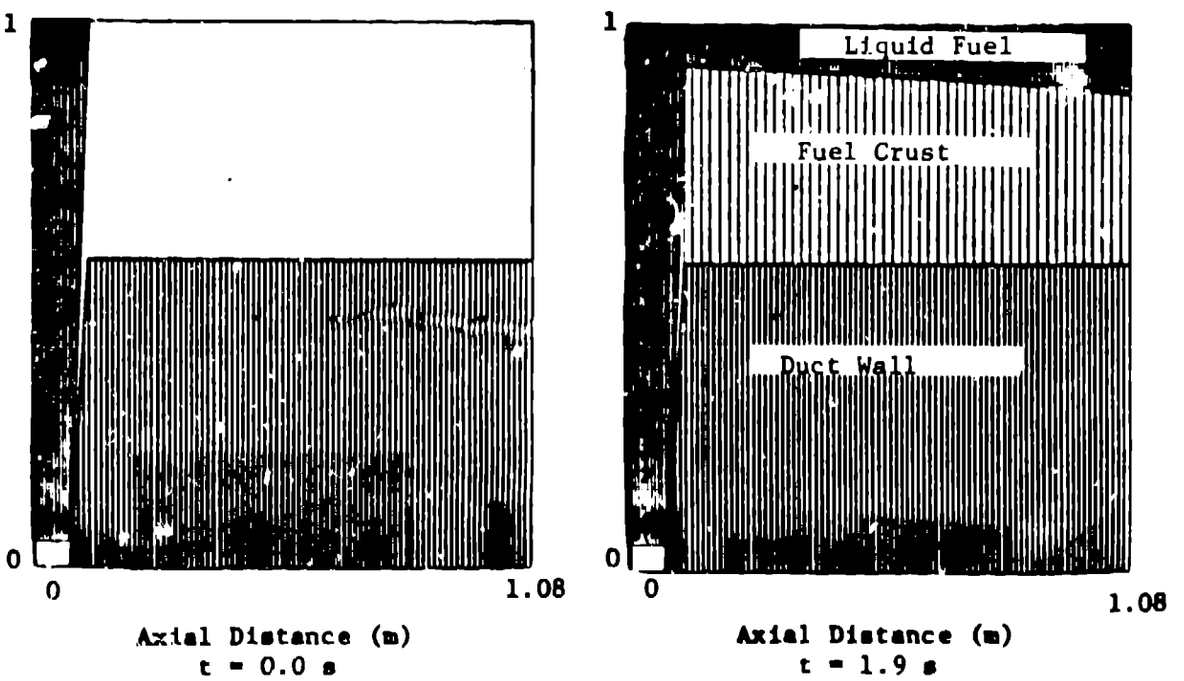


Fig. 2. SIMMER predictions of crust growth in subassembly gaps in the absence of ablation.

as indicated in Fig. 3. For initial duct-wall failure near the axial midplane, downward flow of fuel thus would reach the cold lower blanket and shield and move radially through these regions. In addition, the internal blanket duct wall is probably sufficiently hot that it would fail prior to development of a blockage. Also, as ablation occurs, the flow path for fuel removal widens and the resistance to flow decreases.

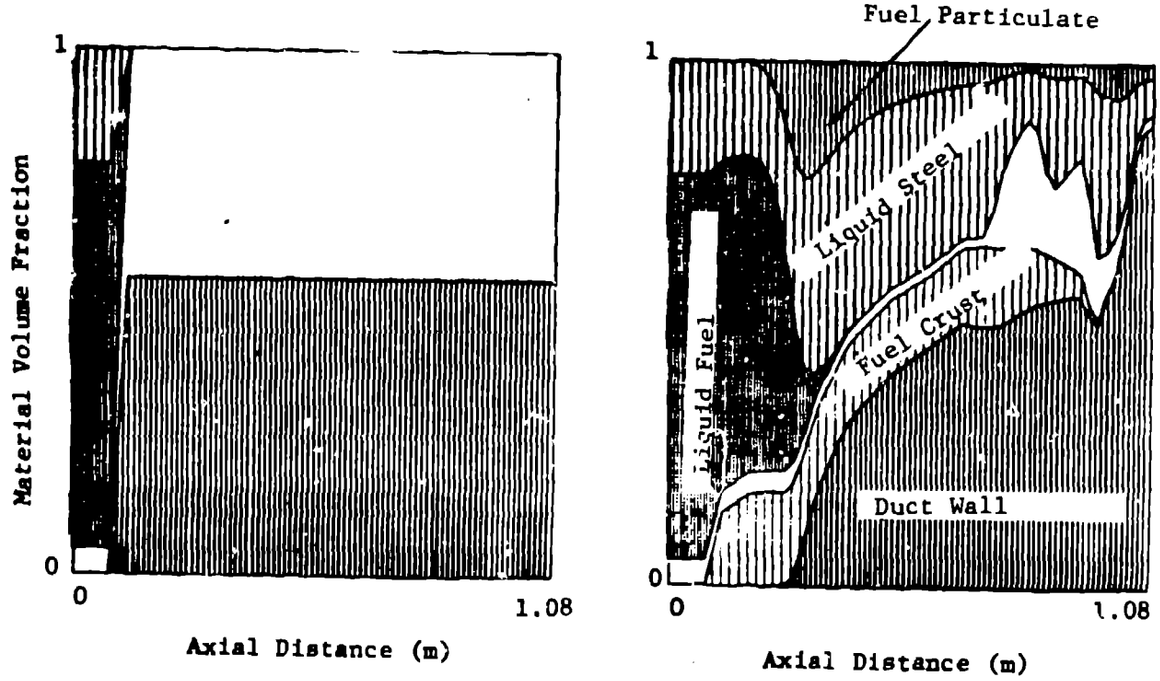


Fig. 3. SIMMER predictions of intersubassembly-gap blockages when driving pressures are low and duct wall ablation occurs.

The importance of fuel removal through the intersubassembly gaps has led to a modification to SIMMER-II that allows calculation of flow axially and radially though a porous medium modeling the gaps. An initial exploratory whole-core calculation with this model indicated that the gaps are potential fuel removal paths that could remove sufficient fuel to decrease the potential for recriticality. However, these exploratory calculations were done without neutronic feedback. Although the fuel removal paths appear to be present, timing of the duct failure, gap width, presence of sodium in the gaps, and core pressure can influence the rate of fuel removal such that there is a competition between the removal process and potential recriticalities. Current analyses at Los Alamos are addressing these concerns using a model of a portion of the Clinch River Breeder Reactor (CRBR) heterogeneous core that includes only the central blanket and first driver region.

Boilup Studies

Another important phenomenon encountered in transition-phase analyses has been fuel-steel boilup caused by steel vaporization near the fuel melting temperature. The transient conditions predicted have not precluded recriticalities and have emphasized the need to assess SIMMER's ability to predict both transient and steady-state boilup.

Two-dimensional SIMMER calculations[9] of steady-state gas-water experiments have indicated that SIMMER's liquid-vapor momentum coupling, which is based primarily on dispersed flow correlations, can reproduce the experimental results shown in Fig. 4 for a wide range of flow conditions. Only in the bubbly flow regime does the model break down, with an overestimate of dispersiveness.

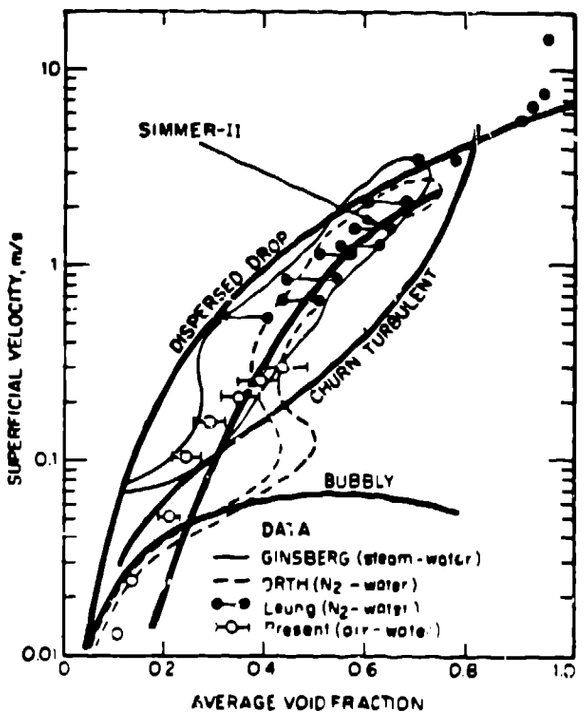


Fig. 4. Comparison of SIMMER-II predictions with experimental data and flow regime boundaries (see Ref. 5).

Separate effects studies[9] with SIMMER have successfully simulated steady-state boilup for fluid-dynamic conditions. Analyses were performed for a two-dimensional pool of molten fuel and steel with a uniform power equal to 10% of nominal full power and with a condenser region at the top of the pool for heat removal. Variations in the condenser strength, in noding size, and in momentum coupling through the vapor fraction dependence and the droplet size found the strongest dependence to be on the liquid droplet size.

The 10% of full nominal power required to sustain boilup in these analyses was greater than expected and was subjected to further investigation. Comparison of the thermodynamic properties of water systems and fuel/steel systems yields a larger gravity head and a weaker dependence of vapor pressure on temperature in the real material system. Because of the difference in properties in the two systems, the axial temperature gradient must be much greater in the real material system than in the water system to overcome the higher pressure and to produce vapor in the lower part of the pool. However, recirculation and mixing of the material in the pool inhibits the establishment of the necessary temperature gradient, thereby reducing the local vaporization in the lower part of the pool and preventing overall boilup. To offset this effect and regain an extensively boiled-up pool,

SIMMER calculations indicate the energy input must be increased to levels greater than decay heat levels for the real material system.

Current experiments at Los Alamos and ANL are expected to provide additional information for verification of SIMMER's ability to predict transient boilup phenomena. Initial comparisons of calculations with experimental data[10] for a two-phase mixture subjected to a pressure pulse have been good. To obtain the correct transmission speed of the pressure pulse, a "virtual mass" term had to be added to the momentum exchange term, but the gross motion of the liquid phase has been reproduced even though the initial flow regime is churn-turbulent and the code simulates it with a dispersed, liquid droplet flow.

Even if a closed boiled-up fuel/steel pool can develop, its maintenance is probably difficult because the pool is likely to be perturbed by changes in condenser behavior, failure of duct walls, or entrapment of sodium. Although the hot, molten pool is likely to drive sodium from its proximity, considerable sodium exists in the system and completely excluding its availability from interaction with the pool seems unreasonable. Vaporization of sodium can affect the pool dynamics in two ways: (1) the resulting local pressure can start large-scale motions of the pool, and (2) the sodium vapor can reduce condensation, pressurize the pool, suppress the steel vaporization, and collapse the pool. A series of calculations with SIMMER was performed to investigate the consequences of introducing approximately 120 g of sodium in a previously established boiled-up fuel/steel pool of size equivalent to whole-core involvement. The sodium was placed in various positions in the pool and the heat transfer to it was varied two orders of magnitude. The final state in all cases was a collapsed pool. In addition, in many cases the sloshing of the pool rapidly led to temporary fuel configurations that potentially could be highly super critical. Further analyses of these dynamic pools coupled with neutronic calculations are being considered.

Additional information needed for predicting transient boiled-up states are the heat removal rates from the molten pool to surrounding structures and the condensation rates on the remaining upper core structures that aid in maintaining the boiled-up states. At this time, accurate prediction of these rates has not been tested against experiments.

Neutronics Testing

Predicting the criticality and power of the reactor core during a core disruptive accident is as important as predicting the material interactions and motions. Therefore, the SIMMER neutronics models have been tested against experimental results from steady-state distorted core geometries.[8] Static reactivity changes induced by gross material relocation were predicted well by the SIMMER neutron transport model whereas the neutron diffusion model predictions were not reliable. Further investigations of the cross-section treatment and experimental methods are needed to explain remaining uncertainties resulting from anisotropic streaming, composition heterogeneities and the resonance self-shielding treatment. Testing of the predictive capability for transient neutronics models is also considered necessary because of the significant transient flux shape changes predicted in whole-core transition-phase calculations.

WHOLE-CORE ANALYSIS

Whole-core accident analyses with SIMMER ultimately are intended to predict the consequences of potential accidents in LMFBRs. Specific, detailed accident paths predicted by SIMMER help identify dominant phenomena but are not considered the ultimate answer for the accident sequence or the accident consequences. Instead uncertainties in modeling, data and initial conditions lead to a range of accident paths from which we hope to characterize the accident sequence, identify possible thresholds, and establish the probable consequences of the accident.

The phenomena studies presented earlier in this paper have resulted from the whole-core accident analyses for a 1000 MWe heterogeneous reactor design and preliminary calculations for CRBR. For the 1000 MWe reactor design,[12] the calculations have suggested the following as a possible transition-phase sequence.

At the beginning of the transition-phase calculation, initiating-phase phenomena are predicted to continue, characterized first by within-subassembly fuel slumping and draining with possible prompt-critical bursts and then, as sufficient energy is accumulated, by within-subassembly transient boilup of the fuel-steel mixture. During this latter period, melt-through failure of driver assembly duct walls is predicted, expanding the disrupted region and coupling the individual boiled-up assemblies. In addition, high heat losses to entrained blanket fuel and to duct-wall steel collapse the boiled-up state. For some cases this results in a prompt-critical burst that disperses much of the fuel from the core region. The increased energy in the remaining fuel causes boilup to occur again over a much greater region. Disruption of annular and radial blankets results in additional poisoning of the fuel mixture with the lower-enrichment blanket fuel. Finally a slow collapse results as vapor de-entrains from the pool and escapes through blanket and control assemblies and heat is transferred from the pool to structure and cold blankets. The final state of the core appears to be a molten, dilute subcritical pool leading into conditions for post-accident heat-removal analysis. In general, as the accident continues, the fuel losses from the core compete with the loss of structural integrity. The fuel losses decrease the probability of recriticality, but increased coherence of fluid-dynamic motions increases the severity of potential recriticalities.

The 1000 MWe whole-core analyses, the experiment analyses, and the separate-effects studies have helped to define additional necessary experiments and to improve accident calculations. They form the basis for future analyses of potential core disruptive accidents to be performed for the CRBR. These CRBR analyses will again include whole-core accident calculations, separate-effects studies, and comparison with experimental data when available.

CONCLUSIONS

In this paper we have shown various safety analysis applications of SIMMER to fast reactor safety. The unique flexibility of the code permits its use in whole-core analysis, separate-effects studies and experiment analysis. It allows extrapolation from small-scale, simulant experiments to the whole-core, real-material system. As SIMMER verification efforts have begun to complement the accident analyses, the code is gaining credibility as

a safety analysis tool. SIMMER whole-core analyses still require careful examination and corroboration with additional separate-effects studies and experimental evidence, but further verification efforts and code modifications continue to increase confidence in the results of SIMMER safety analyses. Of course, all safety analysis should be subject to such detailed scrutiny.

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