COMPUTATIONAL ADVANCES IN TRANSITION PHASE ANALYSIS

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ABSTRACT

In this paper, historical perspective and recent advances are reviewed on computational technologies to evaluate a transition phase of core disruptive accidents in liquid-metal fast reactors. An analysis of the transition phase requires treatment of multi-phase multi-component thermohydraulics coupled with space- and energy-dependent neutron kinetics. Such a comprehensive modeling effort was initiated when the program of SIMMER-series computer code development was initiated in late 1970s in the U. S. A. Successful application of the latest SIMMER-II in U. S. A., western Europe and Japan have proved its effectiveness, but, at the same time, several areas that require further research have been identified. Based on the experience and lessons learned during the SIMMER-II application through 1980s, a new project of SIMMER-III development is underway at the Power Reactor and Nuclear Fuel Development Corporation (PNC), Japan. The models and methods of SIMMER-III are briefly described with emphasis on recent advances in multi-phase multi-component fluid dynamics technologies and their expected implication on a future reliable transition phase analysis.

1. INTRODUCTION

The evaluation of the so-called transition phase of core disruptive accidents (CDAs) has been one of major concerns in the safety of liquid-metal fast reactors (LMFRs). Even though CDAs are lately categorized as events postulated as beyond the design basis of a LMFR plant, because of extremely remote probability of their occurrence, the consequences of CDAs have been extensively analyzed to evaluate a safety margin of the plant or potential risk to the public. Mechanical energy release resulted from a recriticality event during the transition phase may directly challenge the integrity of a double containment system consisting of the primary reactor vessel boundary and the containment vessel. The energetics potential of a recriticality event is dependent on the core design parameters such as the core size, fuel inventory and its reactivity worth, and determined from the mode, scale and rate of fuel motion. Therefore the evaluation of the transition phase requires simulation of an entire core and modeling of key thermohydraulic and neutronic phenomena occurring during accident progression. Realistic (or less conservative) evaluation must be made to appropriately bound the energetics potential and hence to rationalize the consequence assessment. This is only made possible by developing a comprehensive evaluation method, taking advantage of advanced computational techniques in multi-phase, multi-component fluid dynamics and space-dependent neutron kinetics.

The objective of this paper is to review the history and recent advances in computational technology in the transition-phase analysis. Especially the features are highlighted of a most up-to-date computer program, SIMMER-III, being developed at the Power Reactor and Nuclear Fuel Development Corporation (PNC). At this moment, the problems involved in the transition phase are not conclusive due mainly to limited experimental knowledge. Further the core behavior during the phase depends strongly on the core size, fuel types, neutronic parameters

and other design specifications. Regardless of these uncertainties in phenomenological understanding, core design parameters and so on, significant improvement is expected with advanced computational technologies in accuracy and reliability in the future transition phase analysis.

2. HISTORICAL PERSPECTIVE

The evaluation of a potential energy release from a recriticality event was first attempted by Bethe and Tait in 1956 [1]. In their analysis, a hypothetical scenario of collapsing an upper half of a molten core toward a lower half was postulated, and the maximum potential energy release was estimated. A similar approach was taken in the safety analysis in early LMFRs [2]. This is a historical reason why a CDA has been sometimes called as a Bethe-Tait accident. The approach taken at that time is overly simplistic and conservative, assuming core-wide coherency of fuel collapse that results in hydrodynamic core disassembly with a reactivity insertion rate of hundreds of dollars per second. As the understanding on CDA behaviors improved especially for the initiating phase of the accident, an inherent nature of core meltdown turned out to be incoherent event progression and gradual core meltout. The most probably scenario of initiating phase accident progression is no longer a direct entry to the disassembly phase. This is especially true in a small- or intermediate-sized core.

The importance of the transition phase of CDAs was first identified when an unprotected loss-of-flow accident in Fast Flux Test Facility was analyzed in early 1970s by the SAS3A code [3, 4]. Early studies on the transient phase already identified the importance of boiling pool behavior of a molten core pool consisting of liquid fuel and steel [5]. Fauske studied phenomenological aspects of the transition phase and discussed that the boiling pool in nature tends to be dispersive and this prevents coherent collapse of the pool inserting large reactivity [6]. Several comprehensive review reports are available that describe these early studies on phenomenology and treatment of the transition phase [7-10].

A recriticality potential during the transition phase has been a central question, because it determines the severity of mechanical energy release during a CDA and thus it is closely connected to the accident containability and potential risk to the public. A classical approach to evaluate this concern during 1970s consists of: identification of probable recriticality modes, estimation of a reactivity insertion rate for each mode, an analysis of the disassembly phase to estimate neutronic energy yield and evaluation of mechanical work potential based on a thermodynamic method such as assuming isentropic expansion of fuel. These are so-called a "bounding" approach where the recriticality energetics are evaluated in a sufficiently conservative fashion under idealized initial and boundary conditions. A representative computer code used is VENUS-II developed at the Argonne National Laboratory [11]. German KADIS [12] and Japanese VENUS-PM have a similar capability. These codes model two-dimensional hydrodynamic disassembly of a completely molten core coupled with a point reactor kinetics. One-dimensional transport codes were also developed such as PAD [13]. The development of an advanced disassembly code coupled with space-dependent kinetics, FX-2/VENUS-III, was also attempted [14]. In such an approach, short transients of 10 ms at most during prompt-critical power excursion are analyzed for "snapshots" of postulated recriticality modes [7, 8, 15]. Advances in evaluation of mechanical energies are discussed in Refs. [16, 17].

The above "snapshot" analyses of recriticality events are non-mechanistic in nature and do not exactly trace the core behavior following the initiating phase of CDAs. More mechanistic modeling of the early transition phase was tried in the TRANSIT-HYDRO code [18], but this has not completed to the level to be applied to reactor calculations. A mechanistic analysis of the transition phase was first made possible by the development of the SIMMER computer code at the Los Alamos National Laboratory as discussed in the next chapter.

3. SIMMER-SERIES CODE DEVELOPMENT

The objective of the SIMMER-series codes, SIMMER-I [19] and later SIMMER-II [20, 21], was to provide a generalized framework of multi-field, multi-component fluid dynamics coupled with space-dependent neutron kinetics. All the LMFR core materials are modeled in structure (fuel pins and subassembly duct walls), liquid (liquid materials and solid particles) and vapor (mixture of vapor species) fields, together with mass, momentum and energy exchanges among them. The code has limitations that only two moving fields (liquid mixture and vapor mixture) are modeled and only a single flow regime (dispersed droplet flow) is treated. The SIMMER-II code was applied for the first time to the integral analysis of the transition phase, successfully simulating a whole core accident progression sequence based on the initial condition supplied form CDA's initiating phase calculation [22]. This analysis demonstrated the importance of consistently treating various competing thermohydraulic phenomena occurring simultaneously, in tight coupling with core neutronic behavior. SIMMER-II then were used widely in Japan and some European countries for the transition phase calculations [23, 24]. Later the code was applied to a transition phase analysis in a large heterogeneous-core LMFR [25], an independent assessment of CRBRP CDA energetics [26] and an integrated analysis within a framework of probabilistic safety assessment [27].

The successful applications of this code to the transition phase were epoch making, but at the same time they revealed the needs for further improvement of the computational technology. The improvement in accuracy and efficiency of the cross-section handling in the code was already included in the latest version of SIMMER-II [21, 28]. The improvement of the fluid dynamics portion was considered to require more basic research. Therefore, to further develop advanced fluid-dynamics techniques, an AFDM code development program was conducted at Los Alamos by an international team participated by PNC, the Kernforschungszentrum Karlsruhe (KfK), the Commissariat à l'Energie Atomique (CEA), and the Commission of the European Communities (CEC), Ispra [29]. This program studied the fundamental fluid-dynamics methods for a three-velocity-field convection algorithm coupled with multiple flow-regime modeling; it is noted again SIMMER-II is a two-field and single flow-regime code. The application of AFDM was only limited, but sufficiently demonstrated that there existed a basis to develop a next-generation code.

The development of a totally new code, SIMMER-III, began in late 1980s at PNC, initially in collaboration with Los Alamos under the agreement with the United States Nuclear Regulatory Commission (NRC). This program has been based on the technologies developed and lessons learned in the former SIMMER-II and AFDM. As described in the next chapter, the first fluid-dynamic system code has been completed [30], and the assessment program is underway in collaboration with KfK and CEA.

4. SIMMER-III CODE DEVELOPMENT

4. 1 Overall framework of SIMMER-III for transition-phase analysis

SIMMER-III is a two-dimensional, three-velocity-field, multi-phase, multi-component, Eulerian, fluid-dynamics code coupled with a fuel-pin model and a space- and energy-dependent neutron dynamics model. A conceptual overall framework of SIMMER-III is shown in Fig. 1. The entire code consists of the three elements: the fluid-dynamics model, the structure (fuel pin) model, and the neutronics model. The fluid-dynamics portion, which constitutes about two thirds of the code, is interfaced with the structure model through heat and mass transfer at structure surfaces. The neutronics portion provides nuclear heat sources based on the mass and energy distributions calculated by the other code elements. The basic geometric structure of SIMMER-III is a two-dimensional R-Z system as shown in Fig. 2, although optionally an X-Z or one-dimensional system can also be used for various fluid-dynamics calculations.

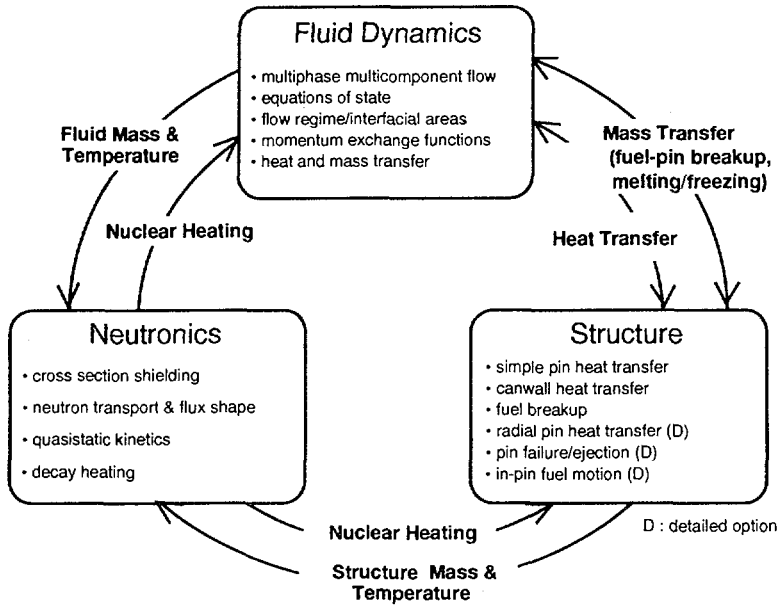

Fig. 1. SIMMER-III overall structure.

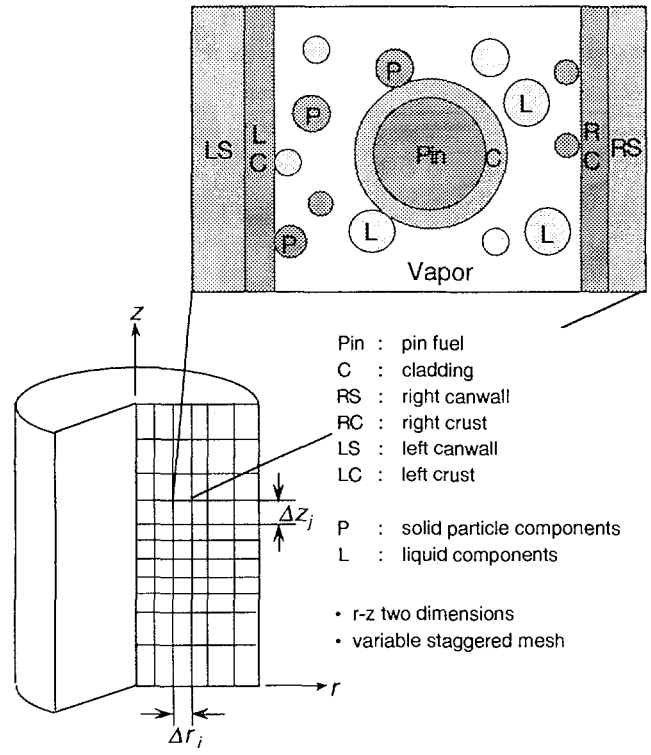

Fig. 2. SIMMER-III mesh-cell geometry.

4. 2 Fluid-dynamics models and methods

(1) Fluid-dynamics algorithm

The two-velocity-field code, SIMMER-II [21], cannot treat the relative motion of fuel and steel and hence it is not appropriate for analyzing the long-term transition phase in which the fuel/steel separation due to gravity force becomes an important behavior in a molten core pool. In addition, SIMMER-II underestimates the inter-penetration of fuel into a sodium pool. In

SIMMER-III, three velocity fields (two liquids and one vapor) are modeled to simulate these relative motions of different fluid components. The three-velocity-field formulation of fluid convection in SIMMER-III is based on AFDM [29]. Mass and energy conservation equations are solved for 27 density components and 16 energy components, respectively, in order to model complex flow situations during postulated LMFR core disruption. The overall fluid-dynamics solution algorithm is based on a time-factorization approach developed for AFDM [29], in which intra-cell interfacial area source terms, heat and mass transfer, and momentum exchange functions are determined separately from inter-cell fluid convection. A semi-implicit procedure is used for the intercell solution. This type of modularized approach is advantageous and flexible enough to allow future exchange of different intra-cell multi-phase models. A more integrated approach is obviously impractical in a complex multi-phase, multi-component framework of SIMMER-III. A higher-order differencing scheme is also implemented to improve the resolution of fluid interfaces by minimizing numerical diffusion.

(2) Equation-of-state (EOS) model

An EOS model is required to close and complete the basic fluid-dynamic equations set. Moreover it is crucial from the viewpoints of numerical accuracy and stability, and computing efficiency. Thermodynamically consistent formulation and appropriate treatment of the critical point are required. Stability of vaporization/condensation calculations is also sensitive to EOS consistency and accuracy. Neither SIMMER-II nor AFDM were satisfactory from these aspects. In SIMMER–II, inconsistencies in the simple analytic EOS introduced difficulty in determining vapor temperature at high pressure, resulting in numerical problems. In addition, numerical instability upon single/two phase transition due to EOS inconsistency leads to the nonphysical motion of fluid. To resolve these problems, a use of a tabular EOS model was tried in AFDM, but was not successful due to the combined effects of time–consuming table search/interpolation and the iteration to obtain mechanical equilibrium. Based on the past experiences, therefore, an improved analytic EOS model using the flexible thermodynamic functions is newly developed for SIMMER-III [31], which treats the basic reactor-core materials: mixed-oxide fuel, steel, sodium, control (B_4C) and fission gas. These materials are assumed to be immiscible, such that a unique EOS for each material can be defined. Proposed function forms use the polynomial equations for the liquid and solid phases and a modified Redlich-Kwong (MRK) equation for the vapor phase [32]. The latter equation is as simple as the van der Waals equation, but it is much more accurate at high temperature. Temperature and pressure dependent liquid specific volumes are modeled so as to represent single-phase cells appropriately. The EOS functions are fitted using the most up-to-date and reliable data sources available [32, 33, 34]. The present SIMMER-III EOS model has adequate accuracy at high temperature and high pressure and consistently satisfies basic thermodynamic relationships over the wide temperature range from the solid to supercritical state.

(3) Flow regime and interfacial area model

In SIMMER-II, only a dispersed droplet flow is modeled. This model overestimates the liquid/vapor inter-phase coupling in a pool with low void fractions. Lack of treatment of channel flows also underestimates the pressure drop along the structures in a core. In addition, SIMMER-II determines the interfacial areas from the instantaneous and local flow conditions in a cell. This tends exaggerate the evolution process of pool boiling. In order to eliminate these problems in SIMMER-II, the interfacial area modeling, successfully attempted in AFDM [35], was extended to the SIMMER-III multi-component system, with more comprehensive representation of flow topologies. To obtain the mass, momentum, and energy transfer terms, binary contact areas must be determined for 42 possible contact interfaces among seven fluid energy components and three structure surfaces (a fuel pin, left can wall and right can wall). Such binary contact areas are determined based on the convectible interfacial areas and a flow regime which describes the geometry of the multi-phase flow. Multiple flow regime treatment is modeled for both the pool flow in which the effect of the structure is negligible and the channel flow which is confined by structure. For the pool flow, bubbly, dispersed and in-between transition regimes are modeled [36]. The channel flow-regime map is defined for the nine flow regimes modeled as the functions of the vapor volume fraction and the liquid

entrainment fraction [30]. The latter is related to the inter-phasic velocity difference, taking the flooding condition into account. The multiple flow-regime treatment in SIMMER-III significantly improves the code applicability to reactor and experiment analyses over the previous SIMMER-II. It is also intended to provide a consistent framework of the flow regime map, over the entire range of void fraction, with smooth and stable transition of the flow regime. This is done by dividing a mesh cell volume locally into the bubbly and dispersed regions as described in Ref. [36]. Momentum constitutive relationships suitable for each flow topology are based on available engineering correlations.

The interfacial area convection model improves the flexibility of SIMMER-III by tracing transport and history of interfaces, and thereby better represents physical phenomena. Ishii [37] proposed a convection equation for the interfacial areas per unit volume in a general form. The problem in implementing Ishii's formulation into an Eulerian code such as SIMMER-III is the difficulty of determining the real velocity of an interface. Therefore, we made a compromise that a convectible interfacial area is defined as a surface area of an energy component and is convected with the same velocity. The total of nine interfacial areas associated to moving energy components are presently convected. A special treatment is modeled to avoid abrupt changes in such situations that the area convection occurs into a cell having a different void fraction. This is done by modeling additional diffusion terms between the bubbly and dispersed regions [36]. The changes of interfacial areas due to hydrodynamic breakup, flashing, turbulence-driven breakup, coalescence, and production of droplets or bubbles are treated as "source terms" in the interfacial area convection equation.

(4) Heat-transfer coefficients model

In SIMMER-III, heat-transfer coefficients must be determined for all the 42 binary contact interfaces. In general the definition of the coefficients corresponds to the heat transfer driven by the difference between the bulk and interface temperatures. The coefficients for solid particles and droplets are simply based on heat conduction. The convective heat transfer in continuous fluids is formulated by Nusselt number empirical correlations. Under severe accident conditions, radiative heat transfer may become important when the high-temperature fuel has difficulty in transferring its heat by other processes, i.e., in a film boiling situation or in the dispersed flow regime. Hence the formulation of film-boiling heat transfer was developed based on sodium and water data [38]. The radiative heat-transfer model is being attempted with some acceptable simplifications based on the phenomenological considerations.

(5) Heat- and mass-transfer model

After the interfacial areas and heat-transfer coefficients are obtained, the conservation equations without convection are solved for intra-cell heat and mass transfer in two steps. The first step is the phase transition processes occurring at interfaces, described by a non-equilibrium heat-transfer-limited model. This is a non-equilibrium process because the bulk temperature does not necessarily satisfy the phase-transition condition when the mass transfer occurs at the interface. The second step of mass and energy transfer is through an equilibrium process occurring when the bulk temperature satisfies the phase-transition condition. At 42 possible interfaces, all the important non-equilibrium mass-transfer processes are modeled, including 30 vaporization/condensation (V/C) paths and 20 melting/freezing (M/F) paths. It is noted that in the V/C transfers condensation processes of fuel or steel vapor on other colder liquids are included to avoid the SIMMER-II/AFDM problem of nonphysical presence of subcooled vapor. The M/F transfers include the crust formation on a can wall that can furnish thermal resistance and steel ablation and particle formation that model fluid quenching and bulk freezing. In addition, 8 equilibrium M/F transfers are performed to eliminate subcooled liquids or metastable solids in consequence of heat transfer and nuclear heating. The mass-transfer processes actually modeled are selected in consideration of their importance in and effects on the transition-phase behaviors.

In the non-equilibrium V/C model, the mass-transfer rates are determined from net energy gain or loss at an interface divided by the effective latent heat, which is defined as the difference

between the interfacial enthalpy and the bulk enthalpy. The net interfacial energy loss/gain is determined by summing the heat flows from/to the interface into/from the respective bulk material. The interfacial energy loss means that condensation must occur to conserve energy, while the interfacial energy gain means that the energy is going into vaporization. The energy- and mass-conservation equations coupled with EOSs are then solved iteratively using the mass-transfer rates obtained. In the solution procedure based on a multivariate Newton-Raphson method, five sensitive variables, three condensable vapor densities, coolant energy and vapor temperature, are updated implicitly, whereas the remaining less sensitive variables are updated explicitly following the convergence of the iteration. The single-phase V/C calculations are performed using the same procedure as two-phase cells except for the energy transfer between liquids. At a liquid/liquid interface, such as fuel/sodium contact in a two-phase cell, the vaporization can occur, and in this case the interface temperature is defined as the saturation temperature of a vaporizing material. In a single-phase cell, however, the interface temperature of the liquid/liquid contact is determined independent of the vapor state. Therefore, no vaporization is allowed in a single-phase cell due to the energy transfer between the liquids. Instead, phase transition occurs only when the liquid temperature increases sufficiently to cause vaporization at a liquid/vapor interface.

The M/F calculation is based on the two modes: a non-equilibrium and an equilibrium processes. The former is similar to the V/C processes; however all the variables are updated explicitly except for the coolant energy, which is identified as sensitive. After calculating the heat and mass transfer resulting from non-equilibrium processes and structure heat transfer, the equilibrium M/F rates are determined by comparing the updated component energy with its liquidus energy for freezing or its solidus energy for melting.

4. 3 Structure and neutronics models

(1) Fuel-pin and can-wall model

In SIMMER-III, the fuel-pin and can wall model represents the stationary structure in the core as well as their time-dependent disintegration behaviors. The standard fuel-pin model is rather simple with a pellet interior modeled by a single temperature node and with its breakup modeled only by a thermal (melt fraction) criterion. However the separated treatment of a pellet surface node provides better thermal coupling with the fluid. Because of relatively large thermal inertia of the pellet interior, the fuel-pin heat-transfer calculation is performed with time steps larger than the fluid-dynamics steps. This simplified model is considered to be sufficient for simulating the fuel-pin behavior in a voided channel typical in the transition phase, but obviously further sophistication is desired for simulating transient overpower situations. For this reason, the development of an optional detailed model is in progress, which may include the calculations of: fuel-pin radial heat transfer, molten cavity growth and pressurization, fuel-pin failure prediction, fuel/fission gas ejection from the cavity, intra-pin fuel motion, plenum fission-gas blowdown.

Unlike SIMMER-II, the can wall model treats separated left and right can walls assumed to be located at the mesh cell boundaries for improved simulation of a core melt-out behavior during the transition phase. The presence of the can wall at a cell boundary eliminates radial fluid convection. Frozen crust fuel can attaches on a can wall when the heat- and mass-transfer model predicts this. Inter-cell heat transfer also is calculated when one of the two can walls at a cell boundary is missing.

(2) Neutronics model

The neutronics model is based on the previous SIMMER-II because the model is judged to be sufficiently advanced to be coupled with SIMMER-III. The space dependence of neutron flux is modeled by an S_n transport theory and the dynamics is treated by an improved quasi-static method. Coupling with the fluid-dynamics portion is carefully designed, because the neutronic state of an LMFR core during CDAs is determined primarily from time-dependent mass and energy distribution of the core materials. It is because of this time dependence that

the calculations of shielded macroscopic cross sections are also performed in the code. An additional feature included in SIMMER-III is a simple decay heating model, which provide a consistent treatment with the SAS-series accident initiating-phase analysis code [39].

5. IMPROVEMENT IN TRANSITION PHASE EVALUATION

In the previous chapter, the models and methods of SIMMER-III are briefly described with emphasis on recent advances in multi-phase multi-component fluid dynamics technologies. Although the first fluid-dynamic system code has been successfully completed and the assessment program is underway, results relating to the transient-phase assessment have not been available yet. However, we can discuss that advanced technologies implemented into SIMMER-III will significantly improve the reliability and accuracy in the transition phase analyses in future LMFRs. The main expected features of the advanced model for the transition-phase analysis are summarized as follows:

1. The three-velocity-field fluid-dynamics model allows us to adequately simulate relative fluid motions, such as fuel/steel separation in a molten core pool and inter-penetration of fuel into sodium. The semi-implicit solution procedure coupled with the time-factorization approach improves the numerical stability of fluid-dynamics algorithm. The implementation of the high-order differencing scheme reasonably improves the resolution of fluid interfaces.

2. The improved analytic EOS model has adequate accuracy at high temperature and high pressure and consistently satisfies basic thermodynamic relationships over the wide temperature range without deterioration of the computing efficiency. This model eliminates numerical difficulties in vaporization/condensation calculations and the numerical instability upon single/two phase transition.

3. The code applicability to reactor and experimental analyses is significantly improved by the multiple flow-regime treatment, such as bubbly flow for a pool flow with low void fractions and a channel flow confined by structure. The interfacial area convection model provides smooth and stable transition between flow regimes over the entire void fraction range. The source term treatment in the interfacial area convection equation better represents the physical phenomena relevant to the change of interfacial areas. For example, the transient boilup and the resultant sloshing of a fuel/steel mixture pool may be reasonably simulated by modeling source terms, such as flashing of steel droplets, with an equilibrium value and a time constant. Thus an energetic recriticality event induced by sloshing of the whole core pool, which was formerly exaggerated, can be suitably mitigated.

4. If fuel-coolant interactions are involved in a transient-phase calculation, the current heat-transfer coefficient model, appropriately including the film-boiling mode, can better represent the phenomena.

5. The mass-transfer processes are modeled in consideration of their importance in and effects on the transition-phase behaviors. In the non-equilibrium phase transitions, condensation processes of fuel or steel vapor on other colder liquids are included. This avoids the problem of nonphysical presence of subcooled vapor.

6. The simplified pin model may sufficiently simulate the fuel-pin behavior in voided subassemblies typical in the transient phase. A detailed pin model is also being attempted to better connect from the initiating of CDAs in a physically consistent way.

7. The can walls with refrozen crust fuel attached on them are distinguished between left and right cell boundaries. This improves the simulation of a core melt-out behavior during the transient phase.

6. CONCLUSIONS

The transient phase of CDAs was formerly treated as a "black box," because of limited experimental data relevant to key phenomena involved and lack of integral computational tools. Snapshots of postulated recriticality modes were analyzed to conservatively bound the transient phase energetics. Significant advances have been made in computational technology incorporated in SIMMER-series codes to directory simulate coupled thermohydraulic and neutronic behaviors during the transition phase. The development of the SIMMER-III code has successfully reached the milestone that integrated code application can be initiated. Major physical models have been completed and they have been integrated into a fluid-dynamics code system. The full version of the code, which couples the neutronics model, will be completed within a few years. An extensive code validation and improvement program is underway in cooperation with KfK and CEA. It is believed that the mechanistic assessment of the transient phase is possible using advanced computational technologies developed thus far. The future research along this line including further up-grading SIMMER features, such as adding a three-dimensional capability, is expected to significantly improve the reliability of LMFR safety analyses.

ACKNOWLEDGMENT

The development of computational technologies in this area was mainly led by researchers at national laboratories in the United States at least until mid-1980s. The authors are grateful especially to W. R. Bohl of the Los Alamos National Laboratory for his inevitable contribution to forming the basis of SIMMER-III. The authors would also like to express our gratitude to Drs. L. L. Smith, C. R. Bell, L. B. Luck, F. R. Parker and other staff of the Los Alamos National Laboratory for their pioneering effort to develop the SIMMER-II code, and to Nuclear Regulatory Commission for their leadership and promotion of international cooperation. The efforts are also acknowledged of many contributors to the AFDM project from Los Alamos, PNC, KfK, CEA and CEC.

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