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MODELING AND SIMULATION NEEDS FOR FUTURE GENERATION REACTORS

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ABSTRACT

Advances in modeling and simulation (M&S) are needed for the development and design of future generation reactor plants, particularly for providing the desired *a priori* assurance that performance, safety and economic goals are met. This paper summarizes the M&S needs for two types of reactor systems, the Sodium Cooled Fast Reactor (SFR), which enables multi-recycle of actinides to avoid nuclear waste accumulation and improve uranium utilization, and the Very High Temperature Reactor (VHTR), which enables high temperature applications of nuclear energy including the efficient generation of electricity and hydrogen. Near term development of the SFR and VHTR systems requires specific improvements of existing M&S tools and validation of these tools for their intended applications. In addition to these near term needs, which are for the most part system specific, a number of farther reaching advances in M&S are attainable through use of leadership class computers and advances in computing resources, tools, and methods. These advances promise to reduce reliance in the future on large-scale, dedicated experiments or mockup facilities for reactor development than is the case today, and may ultimately allow rapid “numerical prototyping” of reactor components and systems.

1. INTRODUCTION

Design of a new reactor system and confirmation of its safety require a validated set of M&S tools for representing system behavior and determining performance and safety characteristics. For each plant component or subsystem, e.g., the reactor core, these tools are comprised of modeling approaches/abstractions (which generally involve simplifications of geometry and the relevant physics), mathematical formulation of governing and constitutive equations of the model, solution methods and their implementation in computer codes, databases of model parameters and their main dependencies, and procedures for accessing the data and making the results available for display or for use in subsequent, dependent calculations. Figure 1 illustrates the use of these tools as part of the iterative reactor design process, which is aimed at meeting performance, safety and economic objectives through specification of system design parameters and operating conditions. Analysis tools are used to establish major system performance and safety characteristics, including:

- Excess reactivity and control element insertion as a function of time.
- Evolution of fuel composition with burnup and, in the case of the SFR, with recycle.
- Fission heat generation and its deposition within the reactor.
- Distribution of coolant flows within the core and in other regions or components of the primary and secondary coolant circuits.
- Distributions of temperatures, in relation to thermal limits of materials.
- Fuel behavior, including swelling, restructuring, fission gas release, and possible chemical interaction with cladding or coating layers.

- Stresses on cladding or coating and damage from irradiation (strain, wastage, loss of ductility or strength).
- Static and transient mechanical loads on components and structures, e.g., due to temperature gradients and changes and seismic events.

This paper addresses the M&S needs for development and design of future generation reactor systems. Some of these needs are system specific, and in the U.S. they arise from near-term requirements for design and safety evaluation of two comparatively mature advanced reactor systems [1]:

- The Sodium Cooled Fast Reactor (SFR), which has been identified in the U.S. as the primary technical option for a fast-spectrum actinide transmutation system designated as the Advanced Burner Reactor (ABR); its main missions are consumption of actinides recovered from discharged light water reactor (LWR) fuel and generation of electricity.
- The Very High Temperature Reactor (VHTR), identified in the U.S. as the primary option for the Next Generation Nuclear Plant (NGNP); its main application is delivery of heat at high temperature for efficient generation of electricity and hydrogen, and possibly for use in industrial applications.

In addition to specific needs associated with the design of these two systems in the near term, this paper also summarizes methods advances that are more crosscutting in nature. Some of these crosscutting advances are farther reaching and would in the somewhat longer term greatly facilitate the development of high-performance future generation reactor systems.

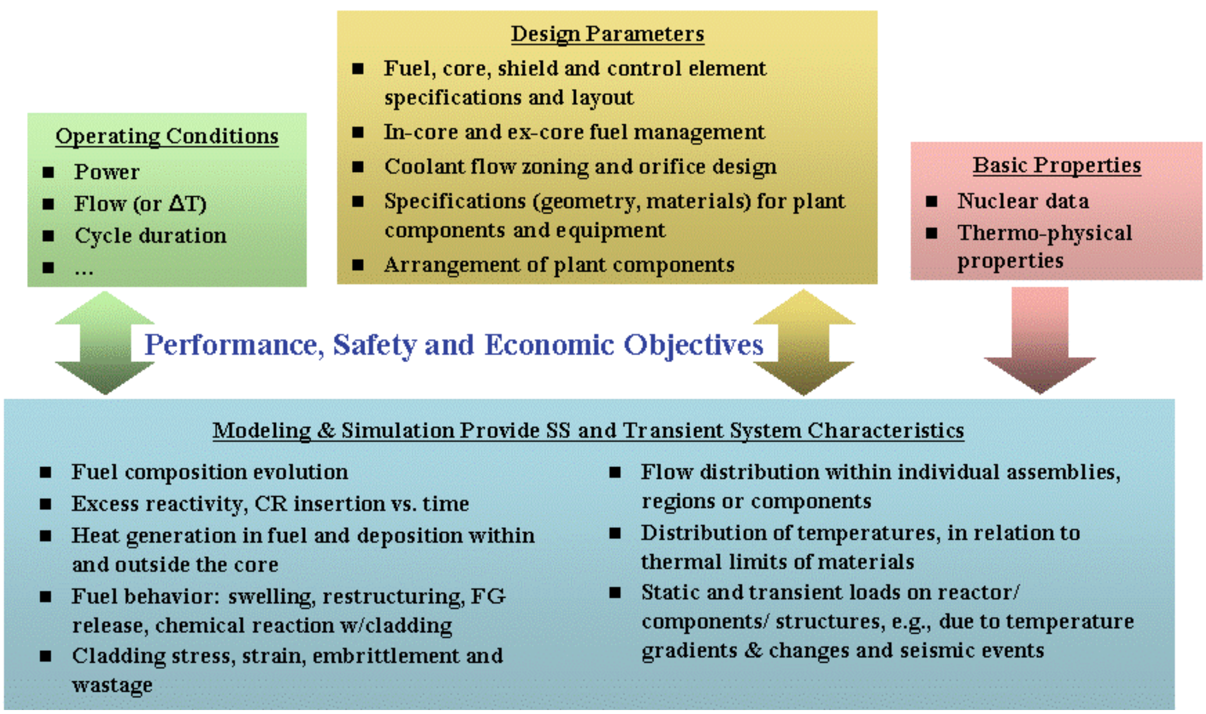

Figure 1. Abstraction of Reactor Design Process.

2. SYSTEM CHARACTERISTICS AND ANALYSIS REQUIREMENTS

As shown in Table I, the SFR and VHTR differ greatly in their design features and operational characteristics from existing or advanced LWR plants. Moreover, they may differ significantly from sodium or gas-cooled reactors that were designed and operated in the past, reflecting their contemporary missions and design goals [1]. For the SFR, significant new features include potentially much higher fuel enrichment (with a mix of transuranics, including minor actinides, as the fissile material), elimination of breeding blankets for TRU burner designs, and potential use of supercritical CO_2 as the secondary coolant with a Brayton power conversion cycle. For the VHTR, new features include elevated temperature and coupling of the reactor to systems for hydrogen production or process heat delivery. It should be noted that these systems may employ a range of configurations and technical options. For example, the VHTR may employ prismatic block type core or a pebble core, and the SFR may employ oxide or metallic fuel. Modeling and simulation tools must therefore accommodate a relatively wide range of possible system features and performance characteristics.

Table I. Comparison of reactor characteristics.

	ALWR	*VHTR*	*SFR*
Applications	electricity generation	electricity generation, heat supply	electricity generation, actinide management
Power, MW_{th}	3000-4500	600-800 (block) ~300 (pebble)	800-3500
Power Density, W/cm^3	50-100	≤ 6.5	200-400
Primary Coolant (T_{Outlet}, °C)	H_2O (300-350)	He (850-1000)	Na (510-550)
Primary System Pressure (MPa)	15.5	7.1	0.1
Fuel Material	UO_2	UO_2, $UC_{0.5}O_{1.5}$	(U,TRU) oxide, metal alloy
Fuel Form	pellet	Triso coated particle	pellet or slug
Fuel Element / Assembly	square pitch pin bundle	hex block, pebble	triangular pitch pin bundle w/duct
Moderator	light water	graphite	None
Number of coolant circuits	2	1 or 2	3
Core Structural Material	zirconium alloy	graphite	ferritic steel
Power Conversion Cycle	steam Rankine	direct or indirect He Brayton	superheated steam Rankine, or S-CO_2 Brayton

Near-term design and development of the VHTR and SFR (as required for the NGNP and ABR projects, respectively) will be carried out using evolutionary improvements of analysis tools that are currently available at research and commercial organizations worldwide. For the most part, these tools were developed more than twenty years ago, although some relevant advances of methods and codes have been made more recently. Desired improvements include (a) increased integration of tools to facilitate system optimization and enhance user efficiency, (b) enhancement of the fidelity of specific models, (c) enhancement of solution efficiency through improvement of numerical methods and effective utilization of modern computer and software capabilities, (e) modernization of databases of input parameters, (f) improvement of capabilities for sensitivity calculations and uncertainty propagation, and (f) verification and validation of the models and their implementation to modern standards.

2.1. System Specific Modeling and Simulation Needs

Systematic assessments of the existing tools, for VHTR and SFR designs of contemporary interest, is essential to the specification and prioritization among the potential improvements of the methods and their implementation in computer codes. Significant progress has been made on the required assessments of the available tools and their predictive capabilities, in relation to anticipated requirements [2,3]. It should be emphasized, however, that the assessment is iterative and can only be completed as part of a specific design activity in which the establishment of target accuracies for important performance and safety parameters is guided by project needs and consideration of costs and benefits associated with attainment of a given level of accuracy.

Very High Temperature Reactor (VHTR)

Prior to the initiation of the NGNP program in 2003, efforts to advance analysis tools applicable to the VHTR were most recently made in the U.S. as part of the New Production Reactors (NPR) program in the early 1990's and more recently as part of the cooperative program with Russia on use of the Gas-Turbine Modular Helium Reactor (GT-MHR) for plutonium disposition. For the most part, these programs sought to adapt and validate existing tools. A notable exception was the effort to develop an advanced, two-dimensional transport theory code capable of representing the intra-block heterogeneous detail (graphite moderator, coolant holes and fuel and target compacts) using a large number of energy groups [4]. Outside the U.S., South Africa has made concerted efforts in recent years to advance capabilities for analyzing the Pebble Bed Modular Reactor (PBMR), including the dynamic modeling of the direct helium Brayton power conversion cycle [5].

The VHTR will be designed to operate at high coolant outlet temperature (850ºC or higher) to enable efficient generation of hydrogen and electricity. Because of the need to characterize proximity of temperatures to material limits, computational tools must be capable of accurately resolving "hot spots" and calculating other localized effects. Limitations in our ability to model all relevant physical effects from first principles creates a need to discern the most important scenarios and phenomena that computational tools must represent. As part of the NGNP program, significant efforts have been made to structure the identification of modeling needs through development of Phenomena Identification and Ranking Tables (PIRT) [2]. For each operational or transient scenario, important phenomena have been tentatively identified by plant component or system and ranked in their importance and priority.

Guided by the preliminary PIRT and related assessments made by the Generation IV International Forum (GIF) Project Management Board charged with planning cooperative efforts on VHTR Computational Methods Validation and Benchmarks, the following M&S needs have been identified for the VHTR:

Reactor Core Physics

Accurate prediction of VHTR physics parameters (e.g., critical fuel enrichment, power distribution, control rod worths) requires a code system that accurately represents neutron moderation by graphite and resonance absorption by heavy nuclides including plutonium isotopes generated through neutron capture. Generation of condensed (multigroup) cross sections used for deterministic calculations requires proper treatment of the heterogeneous nature of the VHTR coated particle fuel (specifically the "doubly heterogeneity" of fuel elements) randomly distributed in a compact or pebble [5]. Additional challenges are posed by the non-deterministic packing and movement of pebbles in the case of the pebble bed variant of the VHTR and the strong transition of the neutron energy spectrum at the core-reflector interface. The temperature dependence of the effective cross sections is also important to represent, as the VHTR operates with a core temperature rise of several hundred degrees Celsius.

Heterogeneity factors analogous to those previously developed for LWR analysis may be needed to improve the accuracy of global (full-core) calculations performed for homogenized core models [6] with deterministic methods. Moreover, calculation of power deposition in different regions of the core and reflector should account for transport of gamma rays away from their creation sites [7].

Thermal Fluid Dynamics

Design and assessment of the VHTR requires modeling of single-phase coolant flow and heat transfer in complex geometries within and outside the core. Basic needs include the modeling of core heat transfer, fluid behavior in the lower and upper plenum, helium loss from coolant channels (flow bypass), hot channel characteristics in normal operation and accident conditions including natural circulation heat removal following a loss of forced circulation accident.

Existing Computational Fluid Dynamics (CFD) codes can be used to model thermal-fluid behavior in multidimensional geometry, and it is expected that such codes will be needed for predicting the maximum temperature levels reached in the reactor for operational and off-normal scenarios. Several commercial and developmental CFD code systems are available to simulate coolant flow and heat transfer in the VHTR. Major needs related to their use include the systematic testing and qualification of modeling approaches including geometry representation, mesh selection and choice of turbulence models. Phenomena of specific interest include:

- Flow distribution in the core: Thermal expansion and shrinkage of the graphite blocks and the leakage flow from outside of the permanent reflector blocks to inside, bypass flow and cross flow between the fuel blocks affect the fuel temperature and must be well estimated for normal operating and accident conditions.
- Coolant mixing in the upper and lower plenum, hot duct, and turbine inlet: Circulation in the upper plenum is important during the pressurized loss of forced circulation accident scenario, since hot plumes rising from the core may impinge on the upper head structures and overheat portions of the upper vessel. The extent of lower plenum and hot-duct mixing determines both the temperature variations in these regions and the maximum temperatures experienced by the turbine blades and the structural components of the power generation vessel.
- Heat transfer in the reactor cavity cooling system (RCCS): The heat removal capability of the RCCS with air or water used as the heat sink is an important passive safety attribute. Performance of the RCCS affects peak temperatures during an accident and is thus key to the choice of reactor materials (e.g., for the outer vessel wall).

In addition to their use for conventional thermo-fluids analysis, CFD based capabilities are applicable for modeling the transport of chemical species, including for example, transport and deposition of activation product and fission products in the primary coolant circuit. Execution of such analyses will require effective coupling of the CFD code with tools that represent the other relevant phenomena (e.g., nuclear, chemical, mechanical) at the appropriate level of detail.

Fuel and Materials Behavior

Reliable fuel performance and extremely low failure rates are central to the successful and safe operation of the VHTR plant. As described below in the section on crosscutting needs, there is great incentive to develop mechanistic fuel performance modeling capability based on physical principles, rather than correlations from irradiation and safety tests – both to improve understanding of fuel performance and to provide confidence in the application of the models for conditions other than those for which test results are available.

Because of the diversity and complexity of the phenomena affecting fuel behavior, achievement of a significant capability for predictive modeling of fuel behavior will take many years, so for the shorter term, irradiation and transient/safety tests will continue to provide the empirical information needed to establish and validate existing fuel performance models. Of central importance is the transport of fission products through fuel materials and their release under normal operating conditions and postulated accidents. Data needed for the models include thermo-mechanical properties of kernel and coating materials, gaseous swelling and fission gas release characteristics of the kernel material, thermo-chemical parameters governing kernel migration, interactions between fission products and the fuel coating, and thermal decomposition of the coating. Fission product release from defective particles is also important to characterize, as it can be a major contributor to fission product release from the core.

VHTR design and safety verification would also benefit greatly from improved prediction of the irradiation and temperature dependence of graphite properties (as a function of temperature and stress history) and of possible accumulation of stored energy in the graphite matrix that may contribute to the energy released in accident scenarios.

Mechanics

Mechanical design of VHTR plant components and assurance of the structural integrity of the components and their interconnections requires thermo-mechanical models that characterize stresses and deformations resulting from operational loads and system challenges including seismic events. Available structural code packages can probably be used for most of the analyses, although they will need to be appropriately coupled to descriptions of fluid flow and materials behavior as a function of irradiation history.

Chemistry and Transport

A diverse set of chemical interactions and chemical specie transport phenomena need to be described to assess the operational implications and to confirm the ability of the VHTR to withstand challenging accidents with minimal operational consequence, damage or radioactive releases. The phenomena of interest include:

- Generation and transport of radio-nuclides: Fission products released from fuel and activation products originating from graphite or coolant impurities may be transported as atomic particles or attached to graphite dust. Significant issues include the radioactivity of the reactor coolant gas and the contamination level of the primary circuit surfaces due to settling and lift-off of dust and plate-out of condensable species. In some accident scenario, radio-nuclides transport out of the pressure boundary and through the reactor building and into the environment; the contamination consequences of such accidents need to be assessed.
- Tritium permeation through reactor structures: Tritium is generated through nuclear reactions on light elements and ternary fission. Some may accumulate in the primary helium coolant, and a fraction will permeate through heat exchanger walls and other surfaces of the primary coolant system. Possible consequences include contamination of the hydrogen produced by the plant and exposure of plant workers and the public. Tools are needed to estimate the level of tritium contamination and to assess the effectiveness of design features for controlling tritium release.
- Graphite oxidation in accident scenarios: In large air ingress accidents (beyond the design basis), the graphite may oxidize at high temperature, creating CO_2 and other gaseous species whose chemical reactions can affect the accident progression. Capabilities are needed to estimate or bound the potentially adverse impacts on core structural integrity and the possible damage to fuel particles.

Reactor and Plant Dynamics

Integrated system analysis tools are used to model operational transients (e.g., reactor start up or load change) and to verify safety of the plant's response for a variety of off-normal events, e.g., turbine trip or over-speed, compressor surge, loss of off-site power, and small or large breaks leading to reduced system pressure and possible air ingress. Systems codes generally model the plant regions or components with limited detail/fidelity; for example they solve simplified field equations and employ fairly coarse nodalization. Their simplicity enables modeling coupled physical effects and interactions among plant components and subsystems, including the reactor, intermediate heat transfer circuit (if present), and the balance-of-plant (turbo-machinery and components employed for direct or indirect Brayton cycle power conversion).

A basic need related to plant dynamics modeling is to adapt and validate existing code systems (e.g., the RELAP-5 code [8]) for VHTR characteristics and to couple them effectively with multi-dimensional reactor kinetics models to provide accurate simulation of power transients including anticipated transients without scram (ATWS) and with CFD models that can provide additional detail concerning proximity to safety or materials limits where needed.

For the hydrogen production application, the effect of the operational and accident behavior of the hydrogen production system on the reactor system (and vice versa) will need to be determined. This will likely require improved capability for coupling system dynamic codes and software that can treat local phenomena of importance, e.g., local temperatures and stress concentration points. A library of modeling "primitives," from which models of the required fidelity can be assembled may also be extremely valuable. Such primitives would enable or facilitate geometry construction, selection of source and flux terms in conservation equations, and specification of relevant constitutive equations.

<u>Sodium Cooled Fast Reactor</u>

In the U.S., a sustained effort to improve fast-reactor analysis tools was made during the 1985-1994 time period as part of the Advanced Liquid Metal Reactor [9] and Integral Fast Reactor [10] programs. Improvements addressed tools used for neutronic and fuel cycle analysis (including adjoint based methods for depletion-dependent sensitivity analysis [11]), characterization of the isotopic and burnup distributions for irradiated fuel [12], and representation of core structural deformation and associated reactivity feedback in simulation of plant dynamic response in transient sequences including postulated accidents [13]. These efforts resulted in a fairly comprehensive code system for fast reactor core design and safety analysis at Argonne National Laboratory, which is illustrated in Figure 2. A comparable code system has been developed by the French CEA, and many other tools relevant to SFR design and analysis are used in other countries pursuing the development of fast reactors, including Japan, Russia, China and India.

More recently, several advances relevant to SFR have been sponsored in the U.S. by the Advanced Fuel Cycle Initiative and the Generation IV program. They include:

- Implementation of capability to accommodate the ENDF/B-VI and -VII resonance cross section formalisms in preparation of multigroup neutron cross sections used by deterministic reactor physics codes [14].
- Increases of the angular and spatial approximation orders and implementation of new acceleration schemes in the VARIANT nodal transport capability [15,16] employed for whole core flux calculations.
- Incorporation of Monte Carlo (MCNP) and discrete ordinates (TWODANT) flux solvers within the REBUS-3 depletion and fuel cycle analysis codes system [17-19].

- Incorporation of space- and energy-dependent neutron kinetics, based on nodal diffusion or transport theory, and multi-pin representation of fuel assemblies in the SASSYS/SAS4A system dynamics and safety analysis code system [20,21].

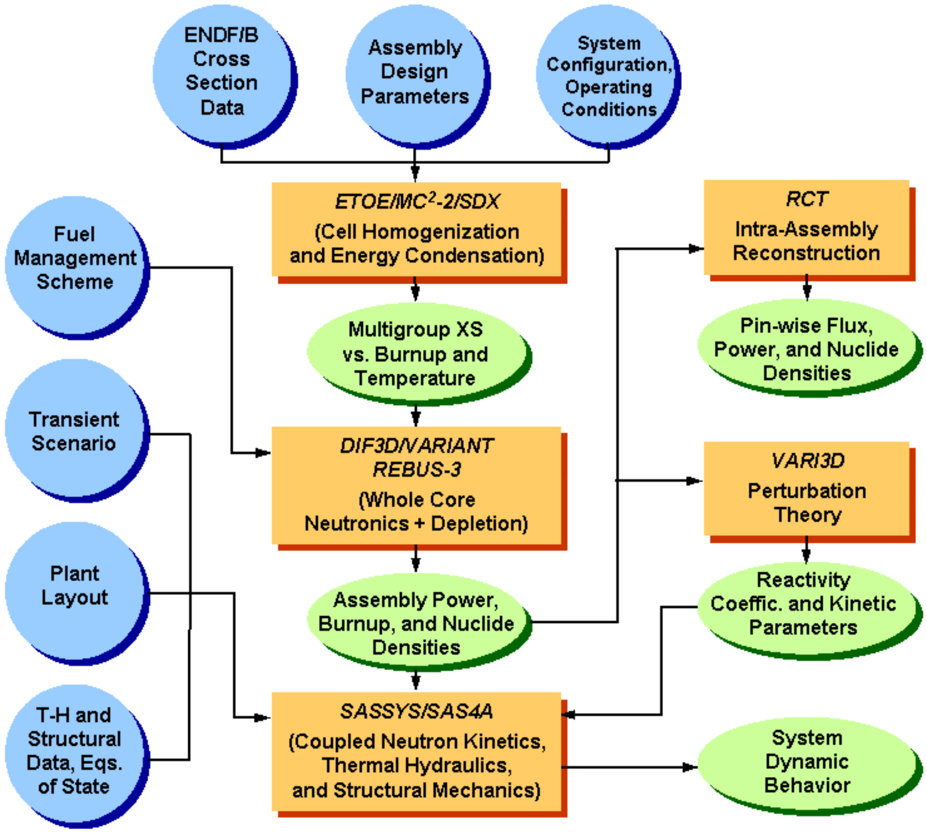

Figure 2. Argonne Code System for Fast Reactor Core Design and Safety Analysis.

As a result of these efforts, the tools available for SFR design and analysis appear to be at a somewhat more advanced stage of development and validation than those applicable for the VHTR. It should be noted, however, that a PIRT has not yet been created to guide the further development of M&S tools for SFR applications. A suggested set of SFR-specific M&S needs are summarized as follows; additional, crosscutting needs are suggested in the following section.

Reactor Physics

Recent neutronic studies for a 250 MWt "Advanced Burner Test Reactor" core [22] showed that a fine-group transport model yields accurate solutions for SFR neutronics predictions, but its computational efficiency needs to be improved significantly for routine design calculations. On the other hand, it was found that the accuracy of broad-group diffusion calculations employed in design studies needs to be improved. Suggested directions for future improvements include:

- Incorporation of equivalence theory parameters in broad-group diffusion theory models and development of a computational procedure to calculate the required equivalence parameters.

- Implementation of parallel solution capability and use of modern software tools to improve the efficiency of fine-group transport calculations.
- Development of an integrated, flexible transport equation solver that optionally generates effective cross sections on the fly. For such integrated calculations, a "multi-grid" approach might be employed, consisting of ultra-fine-group MC^2-2 type calculations [23] for different types of pin cells, fine-group transport calculations for individual nodes or assemblies, and broad-group calculations for the whole core with homogenized nodes. Boundary conditions for smaller-domain (more detailed) problems could be obtained from larger-domain solutions, and homogenized/condensed data (e.g., few group node-averaged cross sections) for larger-domain problems could be obtained from smaller-domain solutions. A converged solution would be sought through iteration on the boundary conditions and equivalent parameters. Sub-domain calculations could easily be done in parallel, and a modern parallel computational technique could be adopted for the whole-core calculation as well.

Thermal Fluid Dynamics

The primary needs for SFR appear to be the improvement of the calculation of inlet-plenum flow distribution and of lateral mixing of coolant flows in the assembly to reduce conservatism in the estimation of peak fuel and cladding temperatures. CFD models should be developed, tested and adapted for application to liquid sodium for the relevant flow characteristics and geometric configurations, especially wire-wrapped pin bundles contained within the hexagonal assembly cans.

The accuracy of models used to predict natural circulation flows in loss-of-flow transients and the thermal fluid behavior of passive heat removal systems should be further studied, and improved models based on CFD capabilities should be developed as indicated by results of these studies.

Fuel Behavior

Existing fuel behavior models [24-27] rely extensively on empirical correlations for describing irradiation and chemical phenomena. A major need for the ABR is to improve the ability to predict the behavior of "transmutation fuel" containing a comparatively high concentration of transuranics, including minor actinides. Redistribution of Am in metallic fuel needs to be characterized taking into account its volatility and interaction with other fuel constituents. Another, possibly significant, modeling issue for transmutation fuels is the increased generation of helium gas due to alpha decay of ^{242}Cm (produced following neutron capture by ^{241}Am) and the need to account for the effect of this generation on fuel swelling and on internal stress exerted on the cladding, especially for oxide fuel where gas retention within the fuel might be high.

Additional near term needs for metallic fuels include improvement of existing models for fuel constituent redistribution, fuel cladding chemical interaction (FCCI), and fission gas release. In conjunction with thermo-mechanical modeling capabilities, these improvements would enable better characterization of life-limiting phenomena as well as conditions that affect transient behavior (e.g., fuel-cladding contact).

For oxide fuels, the needs relate primarily to improvement of thermo-mechanical modeling of fuel cladding mechanical interaction (FCMI), particularly localized stress concentration at certain positions along the fuel cladding interface, coupled with improved representation of corrosion effects. Predictive capability will be enhanced by better representation of such phenomena as segregation of volatile fission products, oxygen release, and oxidation of cladding constituents. Recent advances in modeling of oxide fuels behavior in thermal reactors (e.g., gap conductance modeling) should also be adapted for fast reactor applications.

Mechanics

As in the case of the VHTR, the mechanical design of SFR plant components and assurance of the structural integrity of the plant can likely be performed using commercial code systems appropriately coupled to fluid flow and materials behavior models. Capability of plant structures and components to withstand loads during their shipping and initial installation, in operation, and as a result of seismic events and other internal or external challenges will need to be demonstrated.

Improved methods for describing the thermal, irradiation and mechanical behavior of the reactor core are also needed to improve modeling of passive safety phenomena with plant dynamics codes, as well as to verify that contact forces among assemblies do not hinder safe removal of assemblies at the end of their irradiation lifetime.

Reactor and Plant Dynamics

Improved representation of passive safety mechanisms and phenomena, including their dependence on irradiation effects would increase confidence in the ability of a SFR plant to withstand ATWS without core damage. Particular emphasis should be placed on higher fidelity representation of expansion phenomena, including core radial expansion, axial expansion of fuel, and vessel and control rod driveline expansion. Modeling of the transient redistribution of coolant flow may also be needed for simulation of some transients. Finally, improved modeling of fuel behavior and response during ATWS or other postulated severe challenges is important for establishing or bounding the consequences of such transients.

Future fast reactors may be coupled to advanced power conversion cycles, for example a compact Brayton cycle system employing supercritical carbon dioxide (S-CO_2) as the working fluid [28,29]. Coupling to a pool-type SFR would likely require an intermediate sodium circuit, whereas coupling to a loop-type SFR could be accomplished with or without an intermediate circuit. Assessment of the performance and safety of a SFR plant employing S-CO_2 power conversion requires adaptation of relevant models for all components of the power conversion system and integration of these models within a plant dynamics code. This code would model plant behavior, including the effect of potential control mechanisms and systems, for a variety of transients and postulated accidents, including rupture of the CO_2 pressure boundary. It should be capable of describing the shaft dynamics and accounting for compressible flow effects, effects of such impurities as carbon monoxide and tritium on fluid properties, and effects of CO_2 property variations within components.

2.2. Crosscutting Modeling and Simulation Needs

This section summarizes advances of M&S tools for which the need is common to multiple types of reactor systems. It should be recognized however that these crosscutting improvements would generally be implemented for a specific set of tools, which would not generally be applicable to all systems.

<u>Increased Integration of Analysis Tools</u>

Improved integration and automation of the design analysis procedures for both SFR and VHTR would greatly advance the ability to develop high performance designs. Existing code suites simulate parts of a nuclear power plant in a weakly coupled manner. Examples include the more-or-less standalone modeling typically carried out for neutron physics and nuclide transmutations in the reactor core, of coolant flows in the reactor and power conversion system, and of the mechanical behavior of plant structures and components. As a result, the relevant coupling among different phenomena and components may not be represented with sufficient accuracy, and resulting limitations in accuracy and internal consistency make it difficult to establish defensible estimates of prediction uncertainties. Existing limitations in code integration also make the overall design process time-consuming and inefficient, and the piecemeal nature of this process makes it vulnerable to shortcomings in human performance, organizational skills, and project management. Desired improvements include (a) use of common geometry descriptions, possibly derived from CAD models, and databases of physical properties to ensure internal modeling consistency; (b) increased automation of multi-step analysis sequences, including information transfers among the analysis steps and associated code modules; and (c) improved facilities for assessment and visualization of results.

Improved Sensitivity and Uncertainty Assessment

Tools currently available for estimation of uncertainties are insufficient for establishment of tight yet defensible uncertainty estimates for predicted performance and safety characteristics. Improved uncertainty estimates would greatly advance our ability to optimize designs within safety limits. A significant challenge is presented by the need to account for a very large number of uncertain parameters (e.g., in databases of nuclear data and thermo-physical properties) and tolerances in dimensions, geometric configuration and material compositions. Current approaches for estimating and propagating these uncertainties are neither comprehensive nor sufficiently systematic, and they are too dependent on expert judgment for translation from experiment/test conditions to the actual conditions for the system of interest. Principal needs include (a) systematic compilation and improved characterization of data uncertainties; (b) better tools for sensitivity calculation and uncertainty propagation, accounting for nonlinear dependencies and complicating factors such as discrete events; and (c) sound formalisms for using relevant separate-effects and integral measurements to characterize and reduce uncertainties for the system design and operating conditions of interest.

Increased Modeling Fidelity

Modeling of some major aspects of reactor plant behavior, particularly fuels and materials behavior, thermal-fluid dynamics, and thermo-mechanical response of core structures, currently depends substantially on empirical information and correlations from dedicated experimental campaigns requiring large facilities. Fuel behavior modeling, for example, depends extensively on time consuming and expensive irradiation campaigns and transient testing for a range of fuel burnup levels under prototypic conditions. The need for this empirical approach is evident from the enormous complexity of the conditions and phenomena affecting the performance characteristics of interest. Fuel behavior models must be able to predict the thermal and mechanical performance of a fuel element with multiple constituents and non-ideal features such as impurities and defects, while accounting for heat transfer (multi-dimensional conduction, convection and radiation), irradiation effects (local damage, dislocation, transmutation), microstructure evolution (creep, swelling, cracking), chemical species diffusion, aggregation/precipitation of fission products, fuel-cladding mechanical interaction, and chemical reactions of the cladding internally with fission products and externally with corrosive chemical species in the coolant.

Reduced reliance on empirical correlations and experience from dedicated experimental facilities is a central goal for future M&S tools. Improved ability to model and simulate the relevant physical effects from first principles, or from systematically established models that are amenable to validation testing, will require (a) enhanced understanding of the relevant physical phenomena, (b) effective methods for spanning and inter-connecting the different spatial and temporal scales between the basic physical phenomena and the engineering quantities of interest, and (c) high quality basic data. A sustained effort will be required, with experimentation tightly integrated as part of the effort – to guide the modeling and to provide data against which predictions can be tested.

Enhanced Solution Accuracy and Efficiency

Significant incentive exists to reduce the computer execution time required to attain a desired level of accuracy for numerical solution of the equations that describe reactor phenomena, particularly for transient calculations of coupled effects with large or highly detailed models. Examples of computations requiring long execution time include full-core, heterogeneous neutron transport calculations and detailed CFD calculations for complex flows. In addition to reducing the (computer) execution time for such detailed models, there is a great incentive to reduce the time and effort needed on the part of the analyst to choose the appropriate solution method and associated solution parameters, e.g., the discretization of independent variables. Identifiable needs include:

- Implementation of alternate solution techniques for model equations that allow trade-off between accuracy and efficiency, depending on the purpose of the analysis, which may be to investigate particular design or safety issues or to perform design analyses ranging from scoping studies to in-depth evaluations.
- Improved numerical methods, including acceleration techniques, to enable greater accuracy to be achieved for a given expenditure of computer resources. A notable example is the need for acceleration of the fission source estimation in Monte Carlo neutronic simulations of large cores.
- Enhanced capability for automated, adaptive selection of the appropriate solution options and parameters, consistent with the objectives of the analysis and associated accuracy needs.

Validation of Tools to Modern Standards

Although the topic of validation is not covered in detail in the present paper, its importance cannot be overstated. A major need is to qualify existing and future analysis tools to modern standards of quality. For this reason, significant efforts have recently been made in the U.S. to assess the relevance, quality and completeness of available information on measurements that can be used to validate model predictions [30,31]. Primary validation needs for the VHTR include detailed distributions of power deposition and temperature, flow distribution of outlet plenum, and passive cooling of reactor vessel in accident situations. Validation needs for the ABR include passive safety behavior and consequences of hypothesized bounding events.

Initial assessments [32] indicate that limitations in the scope or quality of the existing database of validation measurements will likely necessitate additional measurements addressing the phenomena of interest under the relevant conditions. While these measurements are essential for establishing the validity of analysis tools and methods, they are often of an integral nature, for quantities related but not identical to the performance parameters of direct interest, and are frequently made under representative (versus actual) conditions. Hence they are generally insufficient for establishing accuracy at the conditions of interest or for probing specific or detailed aspects of the analysis tools. For this reason, assessments of analysis tools against less approximate methods and higher fidelity models play a crucial role in testing these tools and discerning specific improvement needs. In addition, improved measurements that can be used to test predictions at a more detailed, fundamental level are needed.

3. FUTURE GENERATION TOOLS

To the extent possible, improvement of M&S tools should be pursued in a manner that culminates in a modern and more easily upgradeable set of tools. The existing code systems were initiated more than thirty years ago and were designed to function using the computing resources, tools and methods that were available at the time. Advances in computing capabilities should be exploited for the development of a future generation set of tools that would enable a vastly superior process for development, design and licensing of future reactors. This process would integrate all significant aspects of the design to influence optimized design choices at the conceptual stage of the design. It would also support evolution from the conceptual stage to the detailed design of realizable components. Finally, it would provide for automated transfer of design specifications to instructions for manufacture and assembly, enabling the manufacture of parts and components to close tolerances and assured fit at the time of assembly. Major features of the envisioned capability would include:

- Modular code architecture with flexible connectivity allowing incorporation of advances in individual modules or substitution of faster-running approximations.
- Increased capability to model reactor plant systems from first principles.
- Robust capability for characterization of prediction uncertainties.
- Integrated validation database and associated procedures for establishing validity of the overall code system as well as its individual components.

4. CONCLUSIONS

High levels of performance, assured safety and attractive economics are major goals for future-generation reactors. Improved M&S capabilities are needed to establish that these goals are met and, equally significantly, to reduce reliance on protracted or large-scale experiments for design development or validation of design analysis tools.

Because near term design of sodium fast reactor and the high-temperature gas cooled reactor systems will be done primarily using existing tools, an important short-term need is to address some specific limitations in these existing tools and to qualify their predictions through verification and validation testing. To the greatest extent possible, the improvement of existing tools should exploit advances in computer and software capabilities and should be pursued in a manner that culminates in a modular, flexible code system with validated prediction and uncertainty estimation capabilities.

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