U.S. Sodium Fast Reactor Codes and Methods: Current Capabilities and Path Forward

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Abstract. The United States has extensive experience with the design, construction, and operation of sodium cooled fast reactors (SFRs) over the last six decades. Despite the closure of various facilities, the U.S. continues to dedicate research and development (R&D) efforts to the design of innovative experimental, prototype, and commercial facilities. Accordingly, in support of the rich operating history and ongoing design efforts, the U.S. has been developing and maintaining a series of tools with capabilities that envelope all facets of SFR design and safety analyses. This paper provides an overview of the current U.S. SFR analysis toolset, including codes such as SAS4A/SASSYS-1, MC^2-3, SE2-ANL, PERSENT, NUBOW-3D, and LIFE-METAL, as well as the higher-fidelity tools (e.g. PROTEUS) being integrated into the toolset. Current capabilities of the codes are described and key ongoing development efforts are highlighted for some codes.

Key Words: safety analysis codes, steady state analysis, severe accident modeling

1. Introduction

The United States has extensive experience with the design, construction, and operation of sodium cooled fast reactors (SFRs) over the last six decades. Design and operation experience spans a range of SFR configurations, including loop and pool type primary systems, oxide and metallic fuel, and a variety of core geometries. Despite the closure of facilities such as EBR-I, FERMI-I, EBR-II, and FFTF, the U.S. continues to dedicate research and development (R&D) efforts to the design of innovative experimental, prototype, and commercial SFR facilities. Accordingly, in support of ongoing design efforts, the U.S. has been developing and maintaining a series of tools and methods with capabilities enveloping all facets of SFR design and safety analyses in the R&D realm.

This paper provides an overview of the current U.S. SFR design and analysis toolset, including more recently developed high-fidelity codes. As the U.S. has primarily utilized metal fuel, this paper focuses on tools appropriate for metal fuel SFR analyses. **Section 2** of this paper provides a high-level overview of the key phenomena addressed by the toolset. Current capabilities of the codes are described in **Section 3**; key ongoing development efforts are highlighted for some codes in this section as well. All codes discussed in this paper are maintained by institutions within the U.S. DOE National Laboratory framework, with the majority being maintained by Argonne National Laboratory.

2. SFR Functional Areas

The key functional areas highlighted in this section provide a complete characterization of the behaviour of an SFR during normal operation and transient conditions. Steady state characterization is required to ensure the reactor and its associated systems behave as expected during normal operation. This analysis step is also important to the definition of plant conditions prior to the onset of transients. Assessments of the neutronic performance of the core, progression of the fuel cycle and fuel performance, and status of the heat transport

systems must be performed. Additionally, performance of the plant and supporting systems during transients must be characterized to predict the degree of satisfaction of predetermined safety metrics (e.g. peak clad temperature, margin to sodium boiling, etc.). Accordingly, the fuel performance, including fission gas behaviour and fuel/clad motion, status of heat transport systems, structural response, and source term must be analysed. Phenomena unique to SFRs, including sodium-water interactions, sodium fire, and inherent reactivity feedback, must also be assessed.

TABLE I: Steady State Phenomena and Analysis Tools

Phenomenon	**Code**	**Role**
Cross-section Preparation	MC^2-3	*Primary*
Neutron and Gamma Diffusion/Transport	DIF3D/VARIANT	*Primary*
Fuel Cycle Performance	REBUS	*Primary*
	ORIGEN	*Secondary*
Fuel Performance	LIFE-METAL	*Primary*
Core-Wide Thermal Hydraulics	SAS4A/SASSYS-1	*Primary*
	SE2-ANL	*Primary*
Single-Assembly Thermal Hydraulics	Nek5000	*Primary*

TABLE II: Transient Phenomena and Analysis Tools

Phenomenon	**Code**	**Role**
Fission Gas Behaviour	LIFE-METAL	*Primary*
	SAS4A/SASSYS-1	*Primary*
Fuel and Clad Motion	SAS4A/SASSYS-1	*Primary*
	LIFE-METAL	*Secondary*
Primary/Intermediate System Heat Transport	SAS4A/SASSYS-1	*Primary*
Structural Response	NUBOW-3D	*Primary*
	SAS4A/SASSYS-1	*Primary*
Inherent Reactivity Feedback	PERSENT	*Primary*
	SAS4A/SASSYS-1	*Primary*
Passive Heat Removal	SAS4A/SASSYS-1	*Primary*
Sodium-Water Interactions	SWAAM-II	*Primary*
Sodium Fires	MELCOR	*Primary*
	CONTAIN-LMR	*Secondary*
Source Term	ORIGEN	*Primary*
	MELCOR	*Primary*
	CONTAIN-LMR	*Secondary*

Table I and Table II provide listings of the phenomena that must be assessed to provide a complete characterization of steady state and transient plant performance, respectively. These tables also identify the analysis tools that correspond to each of these areas, and indicates the role of the tool. Note that codes with a primary role are utilized as the main computational tool, while codes with a secondary role perform supporting calculations. Of the codes

identified in Tables I and II, six (MC^2-3, DIF3D, REBUS (utilizing both DIF3D and TWODANT), PERSENT, and SE2-ANL) have been incorporated into a code suite that provides initial power and temperature profiles to the systems analysis code SAS4A/SASSYS-1.

3. Codes and Methods

3.1. MC^2-3: Multigroup Cross Section Generation

The MC^2-3 code [1] is a multigroup neutron and gamma cross section generation code for fast reactor analysis developed and maintained by Argonne National Laboratory. The code was developed by improving the resonance self-shielding and spectrum calculation methods of MC^2-2 and integrating the one-dimensional cell calculation capabilities of the SDX transport solver. A homogeneous medium or a heterogeneous slab or cylindrical unit cell problem can be solved in ultrafine (~2000) or hyperfine (~400,000) group levels. Pointwise cross sections are reconstructed with Doppler broadening at specified isotopic temperatures in the resolved resonance range. The pointwise cross section are used directly in the hyperfine group calculation, whereas for the ultrafine group calculation self-shielded cross sections are prepared by numerical integration of the pointwise cross sections based on the narrow resonance approximation. Neutron and gamma libraries contain all isotopes of the ENDF/B-VII data relevant to SFR applications. Multigroup cross sections are written in the ISOTXS format for a user-specified group structure.

Significant verification and validation efforts have been completed using numerous fast reactor benchmarks and experiments. The cross section data generated by MC^2-3 has seen considerable code-to-code comparisons (especially with Monte Carlo solutions) as well as comparisons to experimental measurements [2,3]. Modern validation efforts have shown that the MC^2-3 software can provide solutions that compare very well to experimentally measured quantities.

3.2. DIF3D: Neutronics Solver

The DIF3D code [4] obtains solutions to the steady state, multi-group diffusion and transport equations using the finite difference approximation (one-dimensional slab, sphere, and cylinder, two-dimensional Cartesian, hexagonal, and r-z, and three-dimensional Cartesian, hexagonal prism, and r-θ-φ), the transverse integrated nodal method (two-dimensional Cartesian and hexagonal and three-dimensional Cartesian and hexagonal prism), and a hybrid finite element method (two-dimensional Cartesian and hexagonal and three-dimensional Cartesian and hexagonal prism). It also has a spherical harmonics transport capability built on the hybrid finite element method which provides solutions to the even-parity transport equation.

The GAMSOR processing code enables a sequence of DIF3D calculations that allows users to run a coupled neutron-gamma calculation needed for neutronics calculations. We combine them here because DIF3D is used to solve the neutron and gamma flux problems in two separate calculations via GAMSOR.

The DIF3D code has seen considerable code-to-code comparisons along with comparisons to analytic solutions of the diffusion equation. The validation comparisons have been completed throughout the last 30 years, and have included excess reactivity, reaction rate foils, and flux spectrum measurements. Modern validation efforts have shown that the DIF3D software can provide solutions that compare well to experimentally measured quantities. There are ~100

papers on verification and validation of the DIF3D software over a 30-year period; recent examples include [3] and [5].

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3.3. PROTEUS: High-Fidelity Transport Solver

PROTEUS [6], developed at Argonne National Laboratory, is a high fidelity code that encompasses a set of transport solves and a cross section application programming interface (API) for thermal feedback. The S_N solver completes a second-order discrete ordinate formulation of the even-parity transport equation. This massively parallel solver is based on a fully unstructured finite element mesh, can handle more than 10^{12} degrees of freedom, and includes an adiabatic quasi-static kinetics formulation. PROTEUS also contains a Method of Characteristics (MOC) solver for unstructured finite element meshes. The three-dimensional MOC solver is practical only for small problems due to high memory requirements. An MOCEX solver is also available, which is based on the combination of the two-dimensional MOC method with the discontinuous Galerkin finite element method in the axial direction for axially-extruded geometries. The cross section API of PROTEUS allows transport solvers to generate self-shielded multi-group cross sections on-the-fly. The API accounts for the effects of heterogeneous geometry, temperature, and composition. It was originally developed as a functional module and can be easily adapted to other transport codes with fixed source solvers.

3.4. REBUS: Fuel Cycle Analysis and Depletion

REBUS [7] is a general purpose fuel cycle analysis code built around DIF3D with features specific to a commercial fast reactor industry. Unlike thermal spectrum systems, fast spectrum systems typically require (and benefit from) using recycled used fuel as the initial enrichment. The addition of breeding blankets within fast spectrum reactors allows them to progressively eliminate the need for external enrichment feeds as fast spectrum reactors can generate a larger amount of fissile material than they destroy to create power. To model these aspects of the fuel cycle analysis, REBUS contains a fuel fabrication system that can handle multiple feed materials and multiple sources (i.e. different spent fuel feeds from the same reactor including blankets). The fuel fabrication process allows for spent fuel cooling and allows the user to select how effective the reprocessing plant is at separating out the minor actinides and fission products.

The REBUS code has seen considerable code-to-code comparisons. The validation comparisons have been done over the course of 20 years looking at chemical assays of spent nuclear fuel on the EBR-II reactor [8-10]. Modern validation efforts have shown that the REBUS software can provide solutions that compare well to experimentally measured quantities [11].

3.5. VARI3D/PERSENT: Perturbation and Sensitivity

The perturbation and sensitivity analysis code PERSENT is based upon the hybrid finite element method available in DIF3D called DIF3D-VARIANT [12]. PERSENT is considered to be a replacement of VARI3D. Its core function is to compute the space-energy breakdown of proposed perturbations and linear cross section sensitivity coefficients for uncertainty quantification calculations. Perturbations of material densities, material constituents, and microscopic cross section data are allowed, although most reactivity coefficients are computed using the material constituent option. Sensitivity calculations are allowed on eigenvalue, reactivity coefficients, reaction rate ratios (foils), power fraction, and reaction rates.

PERSENT is primarily used for generating reactivity coefficients for point kinetics analysis codes. The primary focus for safety analysis systems is PERSENT's ability to give the spatial distribution of the reactivity coefficient which then can easily be converted into input for safety analysis codes. For general reactor physics uses, it provides not only the spatial breakdown of the proposed perturbation but also the area (core, reflector, etc.) and balance edits (reaction types by area). It also produces a visualization of the perturbation as output, which can be used to understand the space-energy details of the perturbation.

The other aspect of PERSENT that is unique is its capability to generate cross section sensitivity coefficients for three-dimensional transport calculations; PERSENT is the only known code to possess this ability for metal fuel. Sensitivity coefficients are primarily used as part of an uncertainty evaluation for experimental measurements or new reactor designs. The cross section data that all Argonne neutronics calculations are based on is experimentally measured and thus has errors. The cross section sensitivity coefficients, combined with a covariance matrix, allows computation of the uncertainty associated with any quantity of interest, such as a reactivity coefficient due to the cross section errors.

The PERSENT code was verified against VARI3D [13], its predecessor, noting that VARI3D can only produce diffusion theory perturbation results. For all transport related quantities, results had to be verified using direct perturbation computations. For the sensitivity calculations, there are no analytic approaches, so finite difference perturbations of the base cross section data were used to obtain sensitivity coefficients which were compared directly to the PERSENT-generated quantities. PERSENT relies upon DIF3D for its validation to physical problems and only exercises the mathematical perturbation and sensitivity operations on the base DIF3D solver. More recent efforts on verification of PERSENT are available in [14,15].

3.6. SUPERENERGY: Subchannel Thermal Hydraulics

The SUPERENERGY code [16] is a multi-assembly, steady state subchannel thermal hydraulics code designed to perform core-wide coolant temperature profiles in liquid metal cooled reactors. The user provides coolant mass flow rates, radial and axial assembly power profiles (derived from DIF3D coupled neutron-gamma calculations), and linear heat generation rates (derived from power distribution and assembly pin geometry). It uses a subchannel model within each assembly with a simplified energy mixing model (porous body model).

The Argonne staff has modified the SUPERENERGY code to include hot spot analysis methods as well as fuel and cladding temperature calculation models that give both average and two-sigma temperatures. SUPERENERGY was involved in validation calculations for the EBR-II reactor system.

3.7. Nek5000: Single Channel Thermal Hydraulics

Nek5000 [17] is an open source spectral element method computation fluid dynamics (CFD) solver developed at Argonne National Laboratory. The code utilizes Reynolds-averaged Navier-Stokes and large eddy simulation for turbulence formulation. Nek5000 contains finite volume method (FVM), finite difference method (FDM), and spectral element method (SEM) discretization techniques on an unstructured grid. Incompressible and weakly-compressible flows can be modeled; two-phase boiling model development is currently underway.

Nek5000 is designed to simulate unsteady Stokes, unsteady incompressible Navier-Stokes, low Mach-number flows, heat transfer and species transport, and incompressible

magnetohydrodynamics (MHD) phenomena. High-order accuracy at a low cost in enabled via extremely rapid (exponential) convergence and third-order accuracy in time. The code is also highly scalable through the use of fast scalable multigrid solvers and the ability to scale to more than 290,000 processors.

The code has seen extensive validation and verification over 25 years via a significant number of users and platforms worldwide. A large test suite containing over 400 tests is completed after each build to ensure verified source code, and more tests are continuously being added. Comparisons to experiments include the OECD/NEA Blind Benchmarks, in which Nek5000 ranked first in temperature in the 2010 T-Junction test and first in the rms velocity in the 2012 Matis test. Good agreement has also been found with Argonne National Laboratory's MAX jet-mixing experiment, and JAEA's sodium jet-mixing experiment.

3.8. LIFE-METAL: Fuel Performance

The LIFE-METAL code [18] represents the metallic fuel version of the LIFE series of fuel performance codes that have been developed in the U.S. to evaluate the thermo-mechanical behavior of fuel elements in fast reactors. Development of LIFE-METAL continued up to the termination of the Integral Fast Reactor (IFR) program in the early 1990s. The recent interest of academia and industry in the development of advanced sodium cooled fast reactors has renewed interest in these fuel performance codes, as they can be utilized for design and licensing activities as well as for verification and validation of other newly developed fuel performance codes. Over the past decade, the LIFE-METAL code has been used extensively to support design evaluation and licensing efforts by Toshiba and KAERI in relation to licensing of the 4S and PGSFR reactors, respectively.

LIFE-METAL includes physical, mechanical, thermal, and irradiation property correlations for test and design cladding materials such as SS316, D9, and HT9 alloys. The code also includes correlations for wastage due to sodium/cladding interaction as well as time and strain failure correlations. Models were developed for Ni depletion from D9 cladding and carbon depletion from HT9 cladding due to fuel-cladding chemical interaction (FCCI). Code predictions that are of interest to nuclear design are changes in fuel length and fissile content with burnup. Thermal predictions of fuel temperature and design margins to fuel melting are also of interest, in addition to predictions of FCCI. Mechanical predictions useful to designers are fuel-cladding mechanical interaction (FCMI), cladding deformation and design margin to significant coolant flow area reduction, and cladding damage and design margin to cladding failure due to fuel and fission-gas-pressure loading.

LIFE-METAL was calibrated and validated using the large Post Irradiation Examination (PIE) database from metallic fuel irradiated at both EBR-II and FFTF. Examples of PIE data used for code validation and calibrations include fission gas release, fuel volumetric change, cladding diameter change, cladding wastage and fuel axial growth. Re-validation and verification of LIFE-METAL-R16 is in progress using PIE data in the EBR-II Fuels Irradiation and Physics Database (FIPD) which is being developed at Argonne.

LIFE-METAL was validated and verified using PIE data from EBR-II and FFTF irradiation experiments. Details on LIFE-METAL validation and validation can be found in [19].

3.9. SAS4A/SASSYS-1: Liquid Metal Systems Analysis

Development of the SAS series of codes began in the mid-1960s to model the initiating phases of hypothetical core disruptive accidents. SAS1A originated from a sodium-boiling model and included single- and two-phase coolant flow dynamics, fuel and cladding thermal

expansion and deformation, molten fuel dynamics, and a point kinetics model with reactivity feedback. By 1974, SAS evolved to the SAS2A computer code which included a detailed multiple slug and bubble coolant boiling model which greatly enhanced the ability to simulate the initiating phases of loss of flow (LOF) and transient overpower (TOP) accidents up to the point of cladding failure and fuel and cladding melting.

The SAS3A code added mechanistic models of fuel and cladding melting and relocation. This version of the code was used extensively for analysis of accidents in the licensing of the Fast Flux Test Facility. In anticipation of loss of flow and transient overpower analysis requirements for licensing of the Clinch River Breeder Reactor Plant, new fuel element deformation, disruption, and material relocation models were written for the SAS4A version of the code which saw extensive validation against TREAT M-Series test data [20]. In addition, a variant of SAS4A, named SASSYS-1 was developed with the capability to model ex-reactor coolant systems to permit the analysis of accident sequences involving or initiated by loss of heat removal or other coolant system events. This allows the simulation of whole-plant dynamics feedback for both shutdown and off-normal conditions. Although SAS4A and SASSYS-1 are sometimes portrayed as two computer codes, they have always shared common code architectures, the same data management strategy, and the same core channel representation. Subsequently, the two code branches were merged into a single code referred to as SAS4A/SASSYS-1.

Beyond the release of SAS4A/SASSYS-1 v 2.1, revisions to SAS4A/SASSYS-1 continued throughout the Integral Fast Reactor program between 1984 and 1994 [21] culminating with the completion of SAS4A/SASSYS-1 v 3.0 in 1994 [22]. During this time, the modelling emphasis shifted towards metallic fuel and accident prevention by means of inherent safety mechanisms. This resulted in 1) addition of new models and modification of existing models to treat metallic fuel, its properties, behaviour, and accident phenomena, and 2) addition and validation of new capabilities for calculating whole-plant design basis transients, with emphasis on the EBR-II reactor and plant [23], the IFR prototype. The whole-plant dynamics capability of the SASSYS-1 component plays a vital role in predicting passive safety feedback. Without it, meaningful boundary conditions for the core channel models are not available, and accident progression is not reliably predicted. By the mid 1990s, SAS4A/SASSYS-1 v 3.1 had been completed as a significant maintenance update, but it was not released until 2012 [24].

Several benchmark models have been developed for validation of whole-plant passive safety response based on EBR-II tests conducted in the 1980s. Two of these tests, Shutdown Heat Removal Tests 17 and 45R [25], are the basis of an International Atomic Energy Agency Coordinated Research Project lead by Argonne. DOE and Argonne are currently preparing additional validation models based on FFTF testing conducted in 1986. Beyond these benchmark activities, a validation and verification test suite examining the majority of the fundamental models and capabilities has recently been developed.

In an effort to address U.S. advanced reactor licensing barriers, a SAS4A/SASSYS-1 Software Quality Assurance (SQA) Program has recently been developed which seeks to satisfy the regulatory requirements for safety analysis software used in a license application. The Program establishes SQA best practices and provides valuable support to vendors for commercial-grade dedication of the tool. Additionally, SAS4A/SASSYS-1 has been coupled with RAVEN [26] and Dakota [27], prominent U.S. uncertainty analysis tools, to explore the capabilities of the coupled code systems and provide insight on uncertainty quantification for SFRs [28].

3.10. SWAAM-II: Sodium-Water Interactions

The SWAAM computer code analyzes the pressure transients in an SFR secondary system produced by a sudden tube break in a steam generator. The tube break injects tube-side water/steam at high pressure into shell-side sodium at low pressure, resulting in an energetic sodium/water chemical reaction. The coupled physical phenomena include: propagation of rarefaction waves through the steam piping system caused by the sudden depressurization at the break, including possible phase changes of the fluid; thermochemical dynamics of the chemical reaction and formation of a reaction products bubble resulting from the sodium/water mixing at the break; pressure-pulse propagation in the sodium system resulting from the interface interaction, including the effects of fluid cavitation and possible inelastic deformation of the piping; dynamic buckling rupture of curved rupture disk sets; and subsequent filling of relief systems. Extensive system modelling capability is provided by a variety of junction types in both the sodium and water systems. Code input is designed to be user friendly. SWAAM was originally developed to perform pre-test predictions and post-test analyses of Large Leak Test Rig (LLTR) experiments completed in support of the CRBR Project. SWAAM was validated using results of the LLTR and SWAT-3 experiments [29]. The sodium system module of SWAAM was also developed as a separate pressure transient analysis code PTA-2. PTA-2 was validated using Stanford Research Institute experiments on severe pressure transients in piping [30, 31].

3.11. NUBOW-3D: Core Restraint Structural Analysis

NUBOW-3D, a special purpose structural analysis code developed to support design of core restraint systems, analyzes core deformations using detailed mechanical analyses. The code models the core in 3-D space using 1-D beam elements and determines the transverse displacements of the beam (axial displacement is not included). The code includes the effect of core restraint systems as part of the boundary conditions. Inelastic effects of irradiation creep and swelling are included as is duct-to-duct contact. The code requires thermal and flux information as input. NUBOW-3D calculates the displacement response over time and at varying power to flow ratios. If reactivity displacement worths are available, NUBOW-3D will calculate the reactivity change as a post-processing step.

The main assumptions of the NUBOW-3D code are that the hexcans act like beams that control the deflection. Any coupling or stiffening provided by the fuel pin bundle or shielding is ignored. Friction is not included. Contact is assumed to occur through the centerline and as such duct rotation is ignored. As with all models, there are dependencies on the material property correlations (stiffness, thermal expansion, creep, swelling) and on the inputs (temperature and neutron flux). Further, the reactivity change calculation assumes that the reactivity can be expressed purely as a linear combination of duct displacement.

A set of verification/validation problems from International Atomic Energy Agency (IAEA) working group problems has been applied to NUBOW-3D. This includes 10 verification problems that verify the correct calculation of the thermal bowing, contact forces, and inelastic bowing. There was good agreement in these cases. This same group of problems included three validation problems that only cover thermal bowing and contact. These were single and ten row problems. There was fair agreement in these models, with the discrepancy attributed to uncertainty in assembly tolerances. NUBOW-3D's calculated results in the validation problems were in agreement with nine other similar codes used in the benchmark study.

Additional verification and validation of NUBOW-3D has previously been performed, however much of that information has been lost and is now unavailable. The NUBOW code was used at FFTF to manage refuelling [32]. The code correctly predicted standby residual bowing shape resulting from inelastic strains and was used to calculate resulting forces due to contact. Results for contact forces were acceptable, with differences in the modelled gap indicated as the biggest cause for error. NUBOW-3D was used to successfully manage over 1000 duct withdrawal/insertions and predict over 20 bow dilation measurements throughout 1730 days of reactor operation. It was found that NUBOW-3D matched core dilation creep fairly well. There was also a duct bow-reactivity feedback test during the acceptance period where it was concluded that NUBOW-3D predicted "Reasonable agreement at higher P/F ratios when gaps are closed" [32].

3.12. ORIGEN: Depletion Assessment

SCALE 6.1.3 [33] can perform depletion calculations for an arbitrary reactor system (e.g. SFR) using the ORIGEN code. Multi-group scalar fluxes are used to collapse ENDF/B-VII based 200- and 238-group cross section libraries to 1-group cross sections required by ORIGEN. The 200-group library has energy boundaries intended for analysis of fast systems and threshold reactions and thus contains more high-energy groups than the 238-group library that is used primarily for thermal systems. Cross section data for materials and reaction processes not available in ENDF/B-VII are obtained from the JEFF-3.0/A special purpose European activation library containing 774 materials, 23 reaction channels with 12617 neutron-induce reactions below 20 MeV. Resonance cross section corrections in the resolved and unresolved range are performed using a continuous energy treatment by data modules in SCALE. All nuclear decay data, fission product yields, and gamma ray emission data are developed from ENDF/B-VII.1 evaluations. Decay data includes all ground and metastable states nuclides with half-lives greater than 1 ms. Advanced neutron source capability is provided by ORIGEN using routines integrated from the SOURCES4C code for (α,n) and spontaneous fission neutrons.

ORIGEN currently tracks 174 actinides, 1149 fission products, and 974 activation product nuclides. The nuclide inventories, source terms, and cross sections can be accessed from the code output or through binary interfaces. Cross section data can be generated using the modules in SCALE or supplied externally as available from other independent neutronics code systems. The final release versions (6.1.1, 6.1.2, 6.1.3) have undergone extensive V&V with comparison to burst fission decay heat measurements, fuel assembly calorimetry experiments, neutron and gamma emission spectra, and destructive analysis of LWR and other international commercial fuel types. The LWR benchmarks are performed using TRITON, which has one-, two-, and three-dimensional transport capability to calculate the neutron energy spectrum, and uses ORIGEN internally as the depletion solver. Additionally, ORIGEN has been used at INL to predict inventories and activities for EBR-II fuel safety studies. The ENDF/B-VII cross section data in 238- and 200-group structures are routinely tested in a comprehensive criticality safety benchmark suite (VALID), which includes fast systems. These same data libraries are used in fuel depletion calculations. The 200-group generally outperforms the 238-group for fast systems, but biases in eigenvalue are acceptable with both group structures. Examples of recent validation studies include [34, 35].

3.13. MELCOR: Systems Analysis

MELCOR is primarily used to model the progression of severe accidents in light water reactor nuclear power plants. In the current version of MELCOR (version 2.1), new models are being

added for SFR applications. This requires implementation of sodium databases and sodium specific models that are modelled in CONTAIN-LMR. Sandia National Laboratories develops and supports MELCOR for the NRC. MELCOR is a second-generation plant risk assessment tool and the successor to the Source Term Code package. Verification and validation of the MELCOR code is an ongoing process. Analytical solutions, separate effects tests, integral tests, and actual plant accidents are used for code assessment. International standard problems are often used for validation because they are well documented, well instrumented, and have been analyzed by other codes and modelling approaches. Actual accidents such as the Three-Mile Island Unit 2 and Fukushima Unit 1, 2, and 3 are used as part of the validation testing. Verification and validation models can be found in Volume III of the code manual [36].

3.14. CONTAIN-LMR: Containment Phenomena

The original CONTAIN code (CONTAIN version 1.0) is used for LWR applications. To meet future SFR design basis analysis needs, new LMR models were added to the CONTAIN code as part of the CONTAIN-LMR code release [37]. The CONTAIN code was developed by Sandia National Laboratories for the NRC. The last version number of the CONTAIN code was version 2 which was released in 1997. CONTAIN-LMR standing as its own version was based on CONTAIN 1.11. Both CONTAIN 2 and CONTAIN-LMR are unsupported codes. CONTAIN-LMR is used to model liquid metal reactors (LMR) only and CONTAIN 2-LMR will be used to model LWRs or LMRs. The LMR models in CONTAIN-LMR that will eventually be incorporated into CONTAIN 2 and MELCOR 2.1 are: aerosol condensation and two-condensable option; upper cell chemistry; sodium spray fires; sodium pool fires; debris bed models; sodium concrete interactions; sodium pool modelling; condensate removal from the atmosphere; and radionuclide production associated with molten core-concrete interactions. For CONTAIN-LMR, there are not many sodium experiments that can be used to verify and validate the models. For sodium spray fires, the Aerosol Behavior Code Validation and Evaluation (ABCOVE) AB5 experiment is used to verify and validate the model. For sodium pool fires, an experiment used to verify the SOFIRE II code is used. The verification and validation of CONTAIN-LMR with these experiments, as well as other information about CONTAIN-LMR, can be found in [38].

4. Summary

As demonstrated by this paper, the U.S. maintains a variety of codes and methods that are suitable to address all facets of metal-fuelled SFR safety analysis. While historical R&D codes focused on best-estimate, lumped-parameter modelling techniques, increases in computational capabilities and resources has allowed for the addition of higher fidelity tools for neutronic and thermal hydraulic modelling to the computational toolset, where the benefit of these tools is a potential increase in safety margins due to reductions in phenomenological uncertainties. As the U.S. realigns its focus on deployment of advanced reactors [39, 40] in the commercial realm, a key activity for many of the legacy codes will be the development and documentation of a software pedigree adequate to satisfy the commercial licensing process in the U.S.

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6. References

[1] LEE, C. H. and YANG, W. S., "An Improved Resonance Self-shielding Method for Heterogeneous Fast Reactor Assembly and Core Calculations," in Proceedings of Mathematics and Computational Methods (M&C), Sun Valley, ID (2013).

[2] LEE, C. H. and YANG, W. S., "Verification and Validation of Multigroup Cross Section Code MC^2-3 for Fast Reactor Systems," in Transactions of the American Nuclear Society **106** (2012) 711-714.

[3] SMITH, M. A., et al., "MC^2-3/DIF3D Analysis for the ZPPR-15 Doppler and Sodium Void Worth Measurements," in Proceedings of ANS MC2015 – Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method, Nashville, TN, American Nuclear Society, LaGrange Park, IL (2015).

[4] SMITH, M. A., et al., "DIF3D-VARIANT 11.0, A Decade of Updates," ANL/NE-14/1, Argonne National Laboratory, Argonne, IL (2014).

[5] SMITH, M. A. and LELL, R. M., "Improved ZPR Analysis with the Argonne Reactor Physics Codes," in ANS Transactions of the U.S. Role in a Global Nuclear Energy Enterprise, Reno, NV, American Nuclear Society, LaGrange Park, IL (2014).

[6] SHEMON, E. R., et al., "PROTEUS-SN User Manual," ANL/NE-14/6, Rev. 2.0, Argonne National Laboratory, Argonne, IL (2015).

[7] TOPPEL, B. J., "A User's Guide to the REBUS-3 Fuel Cycle Analysis Capability," ANL-83-2, Argonne National Laboratory, Argonne, IL (1983).

[8] MCKNIGHT, R. D., Unpublished information, Argonne National Laboratory, Argonne, IL (1975).

[9] MCKNIGHT, R. D., Unpublished information, Argonne National Laboratory, Argonne, IL (1991).

[10] MCKNIGHT, R. D., Unpublished information, Argonne National Laboratory, Argonne, IL (1994).

[11] MCKNIGHT, R. D., Unpublished information, Argonne National Laboratory, Argonne, IL (2000).

[12] SMITH, M. A., et al., "VARI3D & PERSENT: Perturbation and Sensitivity Analysis," ANL/NE-13/8, Argonne National Laboratory, Argonne, IL (2013).

[13] ADAMS, C. H., "Specifications for VARI3D – A Multidimensional Reactor Design Sensitivity Code," FRA-TM-74, Argonne National Laboratory, Argonne, IL (1975).

[14] ALIBERTI, G. and SMITH, M. A., "PERSENT: Need of a Deterministic Code for Sensitivity Analysis in 3D Geometry and Transport Theory," in Proceedings of the American Nuclear Society Reactor Physics Topical Meeting (PHYSOR), Kyoto, American Nuclear Society, LaGrange, IL (2014).

[15] SMITH, M. A., et al., "Perturbation and Sensitivity Tool Based on the VARIANT Option of DIF3D," in Transactions of the American Nuclear Society **107** (2012).

[16] BASEHORE, K. L. and TODREAS, N. E., "SUPERENERGY-2: A Multiassembly Steady-State Computer Code for LMFBR Core Thermal-Hydraulic Analysis," PNL-3379, Pacific Northwest National Laboratory, Richland, WA (1980).

[17] FISCHER, P., et al., "Nek5000 User Documentation," Argonne National Laboratory, Argonne, IL (2016) http://nek5000.github.io/NekDoc/Nek_users.html.

[18] YACOUT, A. M. and BILLONE, M. C.," Current Status of the LIFE Fast Reactors Performance Codes," in Proceedings of the International Conference on Fast Reactors and Related Fuel Cycles: Safe Technologies and Sustainable Scenarios, Paris (2013).

[19] WALTERS, L., et al., "Sodium Reactor Fuels and Materials: Research Needs," SAND2011-6546, Sandia National Laboratories, Albuquerque, NM (2011).

[20] TENTNER, A. M. and KALIMULLAH, Unpublished information, Argonne National Laboratory, Argonne, IL (1993).

[21] TILL, C. E., "Fast Reactor Directions: The LMR Integral Fast Reactor Program at Argonne," in Proceedings of the International Fast Reactor Safety Meeting, Snowbird, UT (1990).

[22] CAHALAN, J. E., et al., "Advanced LMR Safety Analysis Capabilities in the SASSYS-1 and SAS4A Computer Codes," in Proceedings of the International Topical Meeting on Advanced Reactor Safety, Vol. 2, Pittsburgh, PA (1994) 1038-1045.

[23] SACKETT, J., et al., "EBR-II Test Programs," in Proceedings of the International Fast Reactor Safety Meeting, Snowbird, UT (1990).

[24] FANNING, T. H., ed., "The SAS4A/SASSYS-1 Safety Analysis Code System: User's Guide," ANL/NE-12/4, Argonne National Laboratory, Argonne, IL (2012).

[25] SUMNER, T. and MOISSEYTSEV, A., "Simulations of the EBR-II Tests SHRT-17 and SHRT-45R," in Proceedings of the 16th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-16), Chicago, IL (2015).

[26] RABITI, C. et al., "RAVEN User Manual," INL/EXT-15-34123, Rev. 2 Draft, Idaho National Laboratory (2015).
[27] ADAMS, B. M., et al., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.0 User's Manual," Sandia Technical Report SAND2014-4633, (2015).
[28] ZHANG, G., et al., "Dakota-SAS4A/SASSYS-1 Coupling for Uncertainty Quantification and Optimization Analysis," M&C 2017 – International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20 (2017).
[29] U.S. DEPARTMENT OF ENERGY, "Evaluation of the LLTR and SWAT-3 Large-Leak Sodium-Water Reaction Data with SWAAM-1 Code," in Second US/Japan Steam Generator Seminar, Sunnyvale, CA (1981).
[30] YOUNGDAHL, C. K., et al., "Pressure Transient Analysis in Piping Systems Including the Effects of Plastic Deformation and Cavitation," Journal of Pressure Vessel Technology **102** (1980).
[31] YOUNGDAHL, C. K., et al., "Pressure Transient Analysis of Elbow-Pipe Experiments Using the PTA-2 Computer Code," Journal of Pressure Vessel Technology **103** (1980).
[32] HECHT, S. L. and TRENCHARD, R. G., "Fast Flux Text Facility Core Restraint System Performance," Westinghouse-Hanford Technical Report WHC-SA-0683 (1990).
[33] Oak Ridge National Laboratory, "Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design," ORNL/TM-2005/39, Version 6.1 (2011).
[34] ILIAS, G. and GAULD, I., "SCALE Analysis of CLAB Decay Heat Measurements for LWR Spent Fuel Assemblies," Annals of Nuclear Energy **35** (2008) 37-48.
[35] GAULD, I., et al., "Re-evaluation of Spent Nuclear Fuel Assay Data for the Three Mile Island Unit 1 Reactor and Application to Code Validation," Annals of Nuclear Energy **87** (2016) 267-281.
[36] HUMPHRIES, L. L., et al., "MELCOR Computer Code Manuals Vol. 3: MELCOR Assessment Problems," SAND2015-6693R, Sandia National Laboratories, Albuquerque, NM (2015).
[37] MURATA, K. K., et al., "CONTAIN-LMR/1B-Mod. 1, A Computer Code for Containment Analysis of Accidents in Liquid-Metal-Cooled Nuclear Reactors," SAND91-1490, Sandia National Laboratories, Albuquerque, NM (1993).
[38] LOUIE, D. L. Y. and HUMPHRIES, L. L., "MELCOR/CONTAIN-LMR Implementation Report – FY14 Progress," SAND2014-19183, Sandia National Laboratories, Albuquerque, NM (2014).
[39] U.S. Department of Energy, Office of Nuclear Energy, "Vision and Strategy for the Development and Deployment of Advanced Reactors," DOE/NE-0147 (2017).
[40] U.S. Nuclear Regulatory Commission, "NRC Vision and Strategy: Safely Achieving Effective and Efficient Non-Light Water Reactor Mission Readiness," ML16139A812 Draft Rev. 1 (2016).