Advances in the Development of the SAS4A Code Metallic Fuel Models for the Analysis of Prototype Gen-IV Sodium-cooled Fast Reactor Postulated Severe Accidents

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Abstract. The SAS4A safety analysis code, originally developed for the analysis of postulated Severe Accidents in Oxide Fuel Sodium Fast Reactors (SFR), has been significantly extended to allow the mechanistic analysis of severe accidents in Metallic Fuel SFRs. The new SAS4A models track the evolution and relocation of multiple fuel and cladding components during the pre-transient irradiation and during the postulated accident, allowing a significantly more accurate description of the local fuel and cladding composition. The local fuel composition determines the fuel thermo-physical properties, such as freezing and melting temperatures, which in turn affect the fuel relocation behavior and ultimately the core reactivity and power history during the postulated accident. The models describing the fission gas behavior, fuel-cladding interaction, clad wastage formation and cladding failure models have been also significantly enhanced. The paper provides on overview of the SAS4A key metal fuel models emphasizing their new capabilities, and presents results of SAS4A whole core analyses for selected Prototype Gen-IV Sodium Fast Reactor (PGSFR) postulated severe accidents.

Key Words: Sodium Fast Reactors, Metal Fuel, Severe Accidents, SAS4A Safety Analysis Code.

1. Introduction

Development of the SAS family of codes began in the early 1960s with the SAS1A code. Subsequent versions were named SAS2A, SAS3A, and SAS3D. Development of SAS4A [1] began in the mid-1970s, and continued until the cancellation of the US advanced reactor program in 1994. Early versions of SAS4A focused on oxide fuel clad with stainless steel. Around 1985, modeling of metallic fuel began. It was recognized that differences between the metal and oxide fuels which influence the reactor core response during the accidents will require the extension of the previous oxide fuel models. A SAS4A metal-fuel model development effort was initiated and initial metal-fuel whole core analyses illustrated the favorable response of metal fuel cores during postulated severe accidents [2]. These analyses also identified the needs for significant further development of the SAS4A metal-fuel models. However, as attention at Argonne shifted away from severe accidents and focused on inherent, passive safety phenomena, the development and validation of the metal fuel severe accident models was discontinued.

The renewed interest in the analysis of metal fuel severe accidents in the context of the PGSFR development requires renewed emphasis on the development and validation of the SAS4A metal fuel models that play an important role in describing the accident sequence. A significant metal fuel model development and validation effort has been undertaken at Argonne National Laboratory as part of a collaboration with Korea Atomic Energy Research Institute (KAERI). This paper provides on overview of the SAS4A key metal fuel models

emphasizing their new capabilities, and presents results of SAS4A whole core analyses for selected PGSFR postulated severe accidents.

2. Metal Fuel Model Development Needs

The metal-fuel development needs are driven by several important phenomena that occur in metal fuel pins but are not present in the oxide fuel pins: a) the migration of the U-Zr and U-Pu-Zr fuel components during irradiation, which leads to the formation of radial fuel regions with different composition, b) the formation of the fuel-cladding eutectic at the interface between the fuel and cladding, which leads to changes in the local composition of both fuel and cladding failure and fuel ejection in the coolant channel, which affects fuel freezing and cladding ablation, and d) the presence of the in-pin sodium in the molten fuel cavity which can affect the cavity pressure and molten fuel ejection after cladding failure. The changes in the local composition of the fuel and cladding the melting and freezing properties. These changes in turn can affect the timing and magnitude of cladding failure and material relocation events, and therefore the reactivity feedbacks that determine the core response.

3. SAS4A Metal Fuel Models

In order to address these metal fuel model extension needs, a significant model development and validation has been undertaken for the following SAS4A models:

- SSCOMP-A: pre-transient metal fuel characterization
- DEFORM-5A: transient metal fuel pin mechanics
- PINACLE-M: pre-failure in-pin metal fuel relocation
- LEVITATE-M: post-failure metal fuel relocation

To allow an accurate description of the local fuel composition, the new metal fuel models track twelve fuel components, including: U235, U238, Pu239, Pu240, Pu241, Pu242, Actinides, Fission Products, Lanthanides, Zirconium, Iron, and a Residual component that includes all the mass not included in the previous eleven components. The in-pin sodium and fission gas are also tracked. The changes in the local composition of the fuel have led to significant changes in the reactivity feedback calculation. The reactivity feedback is now calculated by taking into account the axial distribution of each fuel component and its corresponding reactivity worth, while in the previous SAS4A version the fuel composition was assumed to remain unchanged and only one fuel component distribution was used to calculate the reactivity feedback. The impact of the variable fuel composition on reactivity tends to become more pronounced after the cladding failure, because the relocating molten fuel tends to have a composition different from the stationary still-solid fuel. The validation of the new metal fuel models is performed through analyses of the TREAT metal fuel TOP experiments and recent results are presented in a companion paper at this conference [3]. The severe accidents analyzed with the new models include Loss of Flow (LOF), Transient Over-Power (TOP), and Assembly Flow Blockage (AFB) accidents in the PGSFR metal fuel reactor.

3.1. SSCOMP-A: The Pre-transient Metal Fuel Characterization Model

SSCOMP-A describes the metal fuel behavior during the pre-transient irradiation. The model captures essential physical phenomena taking place during normal operation. The main processes simulated are redistribution of fuel constituents, fuel swelling, porosity evolution, fission gas release, plenum pressurization, solid fission product swelling, radial and axial stresses, strains, and displacements for the fuel and cladding, formation of the fuel phases,

lanthanide migration to the cladding and formation of brittle layer at the clad inner surface, iron migration to the fuel surface and formation of complex iron bearing layers, sodium infiltration to the fuel, burnup dependent formation of various nuclide groups and corresponding reactivity feedback coefficients, and clad failure margin assessment. Some of these processes are depicted in FIG. 1.

SSCOMP-A was validated against EBR-II normal operation database using the real irradiation histories [4] up to 19 % peak burnup. The module predicted satisfactorily essential parameters such as fuel swelling, fission gas release behavior, fuel axial elongation, fuel constituent redistribution, clad wastage formation due to lanthanide attack, clad strain, and clad failure margin.



3.2. DEFORM-5A: The Transient Metal Fuel Pin Mechanics Model

DEFORM-5A describes the metal fuel transient performance [3]. The model is the extension of SSCOMP-A model, addressing transient-related issues such as rapid changing conditions during the transient, eutectic formation between fuel and cladding, gas bubble behavior, creep of the soft fuel and clad failure. FIG. 1 depicts the processes being modeled. Several important models related to transient fuel modeling include:

- Fuel Mechanics: During the transients, occurrence of fuel liquefaction at the fuel cladding interface and formation of single gamma phase leads to frictionless and soft metallic fuel, which is prone to expansion or contraction. The mechanical analysis model captures these phenomena by allowing creep of the fuel driven mainly by the fission gas swelling and thermal expansion. This is an important axial relocation mode for the metallic fuels.

- Fuel Swelling and Fission Gas Behavior: The evolution of the fission gas bubbles are captured by modeling three different groups of bubbles. The small, medium, and large bubbles based on their atom number and phases present. The large bubble formation takes place during the transient at elevated temperatures or upon the fuel liquefaction.

- Fuel-Clad Chemical Interaction: Upon eutectic formation between fuel and cladding the eutectic penetration of the clad is driven by iron dissolution and actinide diffusion. The models are validated using the results of furnace tests [5].

- Clad Failure Models: The failure margin for HT9 cladding is modeled using: 1) Combined Cumulative Damage Fraction (CDF) and 2) Mechanistic Creep Fracture (MCF) models. The combined CDF is an empirical model, covering a wide range of data. MCF is a constrained diffusion cavity growth model, tracking the nucleation, growth, coalescence of the cladding grain boundary cavities. It is validated using the HT9 failure database.

3.3. PINACLE-M: The Pre-Failure Metal Fuel In-Pin Fuel Relocation Model

PINACLE-M is an Eulerian, two-phase, transient hydrodynamic model describing the prefailure in-pin relocation of the molten fuel. PINACLE-M retains all the physical models of the earlier PINACLE model [6], but extends them to allow the mechanistic modeling of metallic fuel specific phenomena. It describes the melting and relocation of the multiple fuel components tracked by SSCOMP-A, and uses the composition-dependent thermo-physical properties at each axial location. It also models the relocation and effects of the in-pin sodium present in the molten fuel cavity. During postulated accidents the mismatch between the energy generated in the fuel pin and the energy removed by the coolant may lead to the overheating of the fuel pin. This leads initially to limited fuel relocation due to the axial expansion of the solid fuel pin. As the accident proceeds, the fuel pin begins to melt, leading to the formation of an internal cavity. Due to the radial migration of the U-Zr or U-Pu-Zr metal fuel components, the local composition of the metal fuel pin changes during the pretransient irradiation leading to different local fuel melting temperatures. The formation of an off-center region with lower Zr content and lower melting temperatures favors the formation of an annular molten fuel cavity as illustrated in FIG. 2. The geometry of the molten cavity depends on the irradiation conditions which determine the local fuel composition and the local fuel melting temperature. PINACLE-M uses the fuel composition provided by the SSCOMP-A model to dynamically determine the geometry and growth of the molten fuel cavity. This cavity is filled with a mixture of molten fuel, fission gas and sodium and expands both radially and axially, due to continued fuel melting. The fuel-gas-sodium mixture in the cavity is pressurized due to the presence of fission gas and can move under the influence of the local pressure gradients. As long as the cavity maintains a bottled-up configuration the hydrodynamic fuel relocation is limited. As the cavity continues to expand there is a competition between two effects illustrated in FIG. 2:

1) The radial extension of the cavity and cladding melting which can cause fuel pin cladding failure. The fuel ejection into the coolant channel and subsequent axial relocation that occurs after cladding failure is modeled by the post-failure fuel relocation model LEVITATE-M.

2) The axial extension of the cavity, which can cause the cavity to reach the top of the fuel pin. When the fuel pin top is breached the pressurized molten fuel in the cavity is connected to the lower pressure upper plenum and can relocate suddenly, leading to a potentially significant insertion of negative reactivity. The rapid in-pin molten fuel relocation prior to cladding failure is modeled by the PINACLE-M module.

A schematic representation of the PINACLE-M model domain and interactions with other SAS4A models is illustrated in FIG. 3. Molten fuel, fission gas and sodium present in the molten fuel cavity can be ejected above the fuel pin top when the molten cavity reaches the top of the fuel pin. Freezing of the fuel ejected above the fuel pin top is also allowed.

3.4. LEVITATE-M: The Post-Failure Metal Fuel Relocation Model

The LEVITATE-M model describes the phenomena that occur in a metal fuel assembly after the cladding failure and fuel ejection into the coolant channel. LEVITATE-M retains all the physical models of the oxide fuel LEVITATE model [7], but extends them to allow the modeling of metallic fuel specific phenomena. It describes the post-failure relocation of the multiple fuel components tracked by SSCOMP-A and PINACLE-M both in the coolant channel and in the pin cavities, and uses the composition-dependent thermo-physical properties at each axial location to determine the fuel phase transitions (melting and freezing) and the corresponding mass exchanges between various LEVITATE-M fields. LEVITATE-M has also been extended to model the metal fuel ejection into unvoided coolant channels replacing the PLUTO-2 model still used in the oxide fuel version of SAS4A to simulate TOP accident conditions. A schematic LEVITATE-M configuration illustrating the early postfailure coolant channel conditions is shown in FIG. 4. LEVITATE-M continues the PINACLE-M calculations after the cladding failure, but extends them to model the phenomena that occur in the coolant channel. As the accident proceeds, molten fuel ejected in the coolant channel can relocate axially and freeze in the colder regions of the channel, leading to the formation of blockages or/and solid fuel particles, depending on the local conditions. LEVITATE-M describes a large spectrum of physical phenomena which depend on the metal fuel composition and properties, including fuel pin melting and disruption, cladding ablation due to melting or eutectic formation, multiple fuel and steel flow regimes, fuel fragmentation and freezing, and channel blockage formation due to freezing fuel or/and cladding. The local composition of the moving and stationary fuel fields (molten fuel, fuel chunks/particles, frozen crust on cladding and structure) is carefully tracked, allowing an accurate calculation of the time-dependent reactivity changes.



4. SAS4A Analyses of Postulated Severe Accidents

To illustrate the capabilities and evaluate the results of the new SAS4A metal fuel models two postulated severe accident scenarios - an assembly inlet flow blockage (AFB) unprotected accident and an unprotected Loss of Flow and Transient Over-Power (LOF-TOP) - are analyzed for both Beginning of Cycle (BOC) and End of Cycle (EOC) conditions. The preliminary SAS4A analyses presented below are conducted for the Prototype Gen-IV Sodium Fast Reactor (PGSFR).

4.1. Pre-transient Irradiation Results

The pre-transient PGSFR analysis, which defines the initial fuel conditions for the transient calculations, is performed using the SSCOMP-A model. The PGSFR fuel pin has U-10Zr fuel slug and HT9 cladding. A three-batch equilibrium core is modeled with the power highest for the fresh fuel and lowest for the thrice-burned fuel. The cycle length is 602 days. End of Life burnup is 10 at %. The fuel pin in the hot channel for the BOC and EOC conditions has 0.9 at% and 4.7 at% burnup, respectively, and the corresponding core average burnup values are 4.9 at% and 7.6 at%, respectively. The fuel swelling calculated during the pre-transient for the BOC low burnup fuel is small (less than 10 %), whereas the EOC medium burnup fuel is predicted to be fully swollen and in contact with the cladding.





FIG. 5. Pre-transient results of SSCOMP-A fuel irradiation simulation

FIGs. 5a.1 and 5b.1 show the distribution of the Zr weight fractions at the end of BOC and EOC, respectively, illustrating the formation of a Zr-rich central region and a Zr-depleted offcenter region. The fuel component migration in the EOC case is more pronounced than that in the BOC case due to the higher burnup. The Zr-depleted off-center region extends to the top of the fuel in the EOC case as shown in FIG. 5b.1, which is not observed in the BOC calculation. The distribution of the U weight fraction at BOC and EOC is illustrated in FIGs. 5a.2 and 5b.2 respectively. The Pu weight fraction is also calculated, but it is not shown due to space limitations. Pu does not migrate radially during irradiation and differences in the Pu weight fraction tend to be small and have a secondary effect on the radial fuel composition variations. The changes in the local fuel composition driven by Zr and U migration lead to changes in the fuel thermo-physical properties, including the fuel melting temperatures, which are shown at BOC and EOC in FIGs. 5a.3 and 5b.3. These composition changes are seen to increase with burnup as expected. The margin to melting in the Zr-depleted annular region (FIGs. 5a.4 and 5b.4) becomes lower than that in the Zr-rich central region, although the fuel temperature is highest in the central fuel region.

These local fuel composition changes determine the initial conditions for the transient accident analysis and influence significantly the subsequent sequence of events calculated by the SAS4A metal fuel transient models. The formation of a Zr-depleted off-center zone in the axial region where fuel component relocation occurs favors the formation of an annular molten fuel cavity during the transient, when the power level and fuel temperatures increase. This effect is more pronounced for the higher burnup fuel pin.

4.2. Transient Results

To illustrate the results of the new SAS4A metal fuel models an assembly inlet flow blockage (AFB) and a Loss of Flow combined with Transient Over-Power (LOF-TOP) unprotected accident scenarios are analyzed for Beginning of Cycle (BOC) and End of Cycle (EOC) conditions. Analyses are conducted for the Prototype Gen-IV Sodium Fast Reactor (PGSFR) with the metal fuel version of the SAS4A code. The SAS4A calculations are currently terminated when the in-pin molten fuel freezing is predicted to occur due to low power levels. Future model extensions are planned which will allow the modelling of subsequent low-power events.

4.2.1. Postulated Assembly Inlet Flow Blockage

The AFB unprotected transient resulting from a rapid assembly inlet flow reduction in the peak assembly is modeled by imposing a high pressure-loss condition at the assembly inlet at the beginning of the transient. The assembly inlet flowrate decreases by more than 85% within about 0.1s, which leads to the increase of coolant temperatures and onset of coolant boiling at approximately 3s for both the BOC and EOC cases. The molten cavity size for the BOC case prior to onset of in-pin molten fuel motion is predicted to be significantly larger than that predicted for the EOC case. This is due to higher power levels and fuel temperatures at BOC, caused by different characteristics of the low burnup (BOC) and medium burnup (EOC) fuels. The negative reactivity feedbacks during overheating due to solid fuel axial expansion and Doppler are smaller for the BOC fuel. The BOC solid fuel is not yet in hard contact with the cladding and can expand both radially and axially, whereas the higher burnup EOC fuel is fully swollen prior to the transient and is forced to expand only axially This causes the EOC axial fuel expansion to be larger than at BOC bringing in more negative reactivity and leading to a lower EOC power level.

FIGs. 6a and 6b show the molten fuel cavity evolution in the peak channel at BOC and EOC respectively. A central molten fuel cavity is formed for the BOC case (FIG. 6a), while an annular molten cavity is formed for the EOC case (FIG. 6b). The EOC annular cavity is due to the off-center region where the fuel margin to melting is lower due to Zr migration. At BOC, PINACLE-M initiates at 5.38s. The molten fuel cavity extends to the top of the fuel and in-pin fuel ejection occurs at 5.77s, prior to the cladding failure. Then cladding failure by hoop stress is predicted at the axial segment 9 at 6.75s and LEVITATE-M is initiated. Although the cladding temperature is close to the molten fuel temperature (approximately 1550 K) it remains below the cladding melting temperature (1700 K). The eutectic

penetration, which contributes to cladding failure, is calculated but not shown in the figure. An enhanced visualization capability is under development which will illustrate the cladding penetration. For the EOC case, PINACLE-M initiates at 5.07s and in-pin fuel ejection occurs at 5.40s. Then LEVITATE-M initiates due to cladding failure by hoop stress at the axial segment 14 at 5.54s. It is noted that although the power level is lower in the EOC case, the plenum fission gas pressure is considerably higher at EOC, causing the EOC cladding failure to occur 1.21 s earlier than the BOC cladding failure.



FIG. 6. Molten fuel cavity evolution during transient for AFB accident (Red=molten fuel, Grey=solid fuel, Dark Grey=solid cladding, Yellow=Cladding Failure, Light Blue=liquid sodium)

The post-failure fuel relocation events will be determined by the molten fuel cavity conditions at the time of failure, which differ significantly as shown in FIG. 6. These results illustrate the effects of the variable fuel composition on the accident sequence of events and the need for modelling these effects accurately.

FIG. 7 shows reactivity component history during the transient. The reactivity effects due to the single blocked assembly are relatively small, and the negative reactivity insertion due to fuel motion after in-pin ejection is -0.16\$ at BOC and only -0.005\$ at EOC, respectively.



FIG. 7. Reactivity during transient for AFB accident



FIG. 8. Power and net reactivity during transient for AFB accident

FIG. 8 shows power and net reactivity during the transient. The relative power at the time of clad failure is approximately P=0.84P0 at BOC and 0.96P0 at EOC. The post-failure fuel reactivity contribution depends on the failure location. At BOC the cladding failure is located just below the core centerline. A modest fuel reactivity increase is seen in FIG. 7a immediately after failure, as the in-pin fuel is accelerated towards the failure location and the amount of fuel in the channel is still small. The effect of the in-pin fuel relocation dominates the coolant channel fuel relocation effect during this period. After approximately 0.5 s the coolant channel fuel contribution becomes dominant and the decrease of the fuel reactivity resumes. For the EOC case the failure location is located above the core centerline at approximately 75% of the core height. The early in-pin fuel contribution remains neutral or slightly negative and the post-failure fuel reactivity continues to decrease after failure.

4.2.2. Postulated Unprotected LOF-TOP

A PGSFR postulated LOF-TOP unprotected transient is analyzed. As transient initiators, rapid inlet coolant pressure decrease (DP = 5% DP0 at 1 second) and reactivity insertion at a rate of 0.02\$/s to the maximum 0.6\$ at 30s are specified. The 0.02\$/s reactivity insertion rate is based on the conservative assumption that one control rod is withdrawn at a rate approximately five times higher than the maximum rate. The hot channel contains 10 fuel assemblies out of a total 112 fuel assemblies.

FIGs. 9a and 9b show the molten fuel cavity evolution in the peak channel at BOC and EOC, respectively. Similar to the AFB accident analysis discussed above the molten fuel cavity size at BOC is significantly larger compared to the EOC case. This is due again to smaller negative solid fuel expansion and Doppler reactivity contributions during the BOC transient. The large cavity formed for the BOC case leads to an extensive in-pin fuel ejection, which causes the fuel reactivity to decrease rapidly to -2.2\$ at the time of cladding failure (FIG. 9a and 10a). At EOC a smaller molten cavity forms due to the lower power level (FIG. 9b. Annular molten fuel cavities are formed at the off-center zone where the fuel margin to melting is lower due to Zr migration (FIG. 5b). The negative fuel reactivity due to in-pin fuel ejection and post-failure fuel ejection at EOC is significantly smaller compared to the BOC case due to the small amount of molten fuel present (FIG. 10b). Significant coolant boiling and core voiding occurs in both BOC and EOC cases prior to cladding failure. At the time of cladding failure the lead channel core region is entirely voided for the BOC case and 70% voided for the EOC case. Due to the overall negative void reactivity of the PGSFR core the coolant reactivity shown on Figure 10 is negative in both cases.



FIG. 9. Molten fuel cavity evolution during transient for LOF-TOP accident (Red=molten fuel, Grey=solid fuel, Dark Grey=solid cladding, Yellow=Cladding Failure, Light Blue=liquid sodium)



FIG. 10. Reactivity during transient for LOF-TOP accident



FIG. 11. Power and net reactivity during transient for LOF-TOP accident

At BOC, PINACLE-M initiates at 18.56s. The molten fuel cavity extends to the top of the fuel and in-pin fuel ejection occurs at 18.62s, prior to the cladding failure. Then cladding failure by hoop stress occurs at the axial segment 17 and LEVITATE-M initiates at 20.83s. For the EOC case, PINACLE initiates at 21.90s and in-pin fuel ejection occurs at 21.99s. Then LEVITATE-M initiates due to cladding failure by hoop stress at the axial segment 20 at 22.05s. FIG. 11 shows the power and net reactivity during the transient. The relative power at the time of clad failure is approximately P=0.3P0 at BOC and 0.8P0 at EOC.

5. CONCLUSIONS

The SAS4A code major models have been significantly extended to describe the phenomena associated with the metal fuel pre-transient irradiation and the transient accident events up to and beyond cladding failure. These models allow the tracking of the metal fuel composition changes that occur during the irradiation and the effect of these changes on the events that occur during postulated severe accidents. Future work will focus on the enhancement of the post-cladding-failure metal fuel relocation models and analyses of postulated accidents for the PGSFR safety analysis.

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