THERMAL STRATIFICATION MODELING FOR SODIUM-COOLED FAST REACTORS: A STATUS UPDATE

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ABSTRACT

Thermal hydraulic behavior in the upper plenum of pooltype sodium-cooled fast reactors (SFRs) is a major concern, as many design challenges are concentrated in this region. As SFR designs aim for licensing and commercialization, it is important to accurately analyze and predict the thermal-hydraulic behavior in this region during accident scenarios, specifically thermal stratification.

Thermal stratification models are currently a major source of uncertainty in most system codes for all types of power plants. Most system codes, including SAS4A/SASSYS-1, a system level code developed by Argonne National Laboratory (Argonne), use very coarse meshes that cannot capture the complexities of the stratification phenomena. While the commonly employed lumped-volume based models for thermal stratification are able to run in a matter of seconds, they result in approximate results and can only handle simple cases. Other 2-D and 3-D methods, such as computational fluid dynamics (CFD) models, can analyze simple configurations with higher fidelity, but come with a relatively large computational expense. Finding a modeling solution that is both accurate and computationally efficient has proven difficult. This paper provides details of a review and gap analysis of the various modeling approaches proposed to date and explores a path forward for future thermal stratification modeling efforts, with a focus on developing new models for the SAS4A/SASSYS-1 system code.

INTRODUCTION

Thermal mixing and thermal stratification in large volumes, such as the upper plena of pool-type liquid metal reactors (LMRs) have been of recent concern with the prospect of licensing and commercializing new system codes and reactor designs in the near future. Thermal stratification is a three dimensional thermal hydraulic phenomenon that could possibly affect the start of natural circulation and decay heat removal in LMRs. Most current system level codes implement highly simplified and conservative 0-D models that result in only approximate results. Using various 3-D CFD methods offer reasonably accurate information on the phenomenon but come with a large computational expense. It is very desirable to have an advanced and efficient thermal mixing and thermal stratification modeling capability in a production-level system analysis code.

THERMAL STRATIFICATION OVERVIEW

Mass, energy and species transport in large interconnected enclosures is of interest in a variety of applications, including nuclear reactor containments, building fires, HVAC systems, chemical processing and pollutant dispersal. The thermal stratification phenomenon we are examining takes place in a large pool when the fluid entering is colder than the fluid contained in the pool and the momentum of the flow is not large enough to overcome the negative buoyant force. A difference in fluid density results in denser cold fluid flowing in the lower region of the outlet plenum while the large upper volume of the fluid remains hot. Thermal stratification can also take place in the reversed situation of a hot fluid flowing into a large cold pool, also creating density differences. Thermal stratification in hot water tanks has been studied extensively for many different purposes. In the solar industry, much research has gone into finding ways of minimizing the mixing of hot and cold water in hot water storage tanks [1]. Stratification is also an important factor in environmental and biological science as well, for example in complex systems such as lakes and oceans [2]. Jaluria and coworkers [3] have used a one-dimensional temperature distribution to develop zone mixing models for enclosure fires. Interest in ecological systems has been motivated by the study of jet and plume dispersal of pollutant discharges.

In the nuclear industry the importance of thermal stratification is a concern beyond large pools in sodium cooled reactors. Several different types of reactor designs are concerned with the phenomenon. In advanced BWR designs such as GE's ESBWR, the suppression pool is an important element in the passive safety system as it serves as a major heat sink and provides emergency cooling water. Thermal stratification of the suppression pool can lead to a surface temperature higher than the bulk temperature which in turn increases the vapor pressure and the total containment pressure [2,4,5]. Newer LWR designs that rely on passive safety systems such as the AP-1000 are concerned with thermal stratification as well, specifically in the core makeup tanks (CMTs). Thermal mixing and stratification in large enclosures is important in the reactor cavity cooling system in High Temperature Gas Cooled Reactors (HTGR), along with gas distributions in the reactor and power-conversion-unit enclosure [6,7]. The Advanced High Temperature Reactor (AHTR) is another liquid-salt cooled pool type reactor that is concerned with this phenomenon.

The thermal hydraulics in the upper plenum of a sodiumcooled fast reactor (SFR) has been labeled as a major concern, as many design challenges are concentrated in this region. Tenchine et al. [8] provided an excellent overview of important thermal-hydraulic challenges in the development of SFRs thermal stratification being near the top of this list. Refined modeling of the concerned regions is needed in order to perform numerical analysis on this phenomenon along with other related phenomena identified in the region. Roelofs et al. [9] built off of Tenchine's efforts but focused solely on fuel assembly and pool thermal hydraulics. This work provided an overview of state-of the-art evaluations for liquid metal fast reactors (LMFRs) and focused on two benchmark activities initiated by the International Atomic Energy Agency (IAEA) concerning the prediction of flow patterns in LMFR pools [9]. Innovative passive shutdown and decay heat removal systems commonly used in SFR designs still require much more research on 3-D flow and temperature distribution of primary sodium under various power levels. Multiple issues, including thermal stratification, thermal mixing, and thermal striping, are being studied all over the world in an effort to develop codes equipped to better analyze the phenomena [10]. Another in-depth overview of current modeling methods of thermal mixing and thermal stratification was provided by Zhao and Peterson [6].

Two trends are observed in the modeling and simulation of large enclosure mixing: the traditional system analysis approach using decoupled, highly simplified and conservative 0-D models to study mixing, or 3-D CFD methods. Existing major system analysis codes only provide lumped-volume based models for thermal stratification, which result in approximate results and can only handle simple cases. In the lumped models, the fundamental assumption is that the volume is homogeneously mixed. Several attempts have been made to introduce artificial control volumes within the large lumped model, but this introduces non-physical flows between control volumes [23]. Other 2-D and 3-D methods can analyze simple configurations but at a relatively large computational expense. New methods are needed to support design optimization and safety analysis of Generation IV pool type liquid metal reactor systems.

SAS4A/SASSYS-1 CURRENT MODEL

The SAS4A/SASSYS-1 computer code is a system level code developed by Argonne for thermal, hydraulic, and neutronic analysis for power and flow transients in liquid-metal-cooled fast reactors. Its origins date back to the 1960s, since when it has continuously undergone further development. In more recent years, several modeling additions and enhancements have been made to meet U.S. DOE programmatic needs, including efforts to couple the code with external CFD simulations to resolve flow distribution and thermal stratification.

The stratified volume model currently used in the thermal hydraulic solver PRIMAR-4 of SAS4A/SASSYS-1 stems from the older PLENUM-2A model developed by Howard and Lorenz [11]. The newer model is now able to handle up transients as well as down transients, and horizontal discharges, as in the case of the IHX discharging into the cold pool.





Stage 1, fully mixed, 1 layer







Stage 3, case 3.2, 2 layers, interface moving, Tp > (Tsc1 + Tsc2)/2, hot outlet coolant goes to upper layer, entrains from the lower layer as it passes through

т_р



Stage 5, case 5.1, 3 layers, interfaces moving, cool plume liquid goes to layer 1

entrainment from layer 2 at zlayr2 $T_p < (T_{sc1} + T_{sc2})/2$

Stage 4, 3 layers, interface at the core outlet, filling the bottom with cool liquid, plume height < zlavr3



^zlayr2 I sc1 zlayr1 тр Stage 5, case 5.3, 3 layers, interfaces moving, plume passes through layers 1 and 2, goes to layer 3, entraining from

 $(T_{sc2} + T_{sc3})/2$

z_{top}

^zlayr3

moving, plume passes through layer 1 to layer 2, entraining from layer 1 as it passes through, also entraining from layer 3 at zlayr3 layers 1 and 2 as it passes through $T_{sc2} + T_{sc3} > 2T_p > T_{sc1} + T_{sc2}$

Figure 1: Stratified volume stages from SAS4A/SASSYS-1 User's Manual [11].

Figure 1 shows the various stages and cases considered in the current model. Improvements from the old model include having three regions and five stages, improved from the previous two region model. Stage one represents the beginning of a transient when the fluid is fully mixed and the plume reaches the top of the plenum. As time proceeds through the transient the temperature and velocity drop, causing the plume to no longer be able to reach the top of the plenum; thereby initiating stage two.

In this stage, a boundary layer is formed at the outlet of the core. As liquid enters this layer and fills a quarter of its volume stage three begins, where the interface rises while the plume entrains liquid from the interface into the first layer. If the liquid entering the region is cooler than the bulk temperature, case 3.1 takes place, whereas if the liquid entering the plenum is hotter, case 3.2 is entered. In stages 4 and 5 three layers are developed. These stages occur later in the transient and only if the core outlet temperature starts out rising and later falls, or vice versa if the temperature starts out decreasing and later rises. If the coolant inlet into the volume is horizontal, as in the case with the discharge from the intermediate heat exchanger (IHX) to the cold pool, only stages 1, 3, and 5 are used [11].

The majority of the experiments on the multiple aspects relevant to the phenomenology described above were performed before the current model was developed in the late 1970s [12-15]. Baines (1975) [16] studied entrainment by a plume or jet at a density interface and their results stressed the importance of the Froude number, a dimensionless number that can combine the three parameters on which the phenomenon depends. These studies showed that the Reynolds number was an unimportant parameter and that entrainment was limited to a region about the size of the jet cross section at impingement. Lorenz and Howard used Baines' simplified expression for correlating entrainment data for jets and plumes and slightly modified it to result into equation (1).

$$\frac{Q}{V_j d_j^2} = \frac{\pi}{4} a(Ri)^{-b} \tag{1}$$

Modifications made by Lorenz and Howard include the use of the average jet velocity rather than the centerline jet velocity and the use of the Richardson number, or as they refer to it, the modified Froude number. Their experiments related the volumetric entrainment flux, Q, to the interfacial rise rate, ε , and provided equation (2) as the basis for correlating the data [17].

$$\frac{\varepsilon}{V_j} \left(\frac{D}{d_j}\right)^2 = a(Ri)^{-b} \tag{2}$$

The values of the effective jet diameter at impingement, d_i, and the average jet velocity at impingement, V_i can be determined from the theory of free submerged jets [18]. The expressions used in their experiments for velocity profiles of free submerged jets are the same expressions used in the current stratification model in SAS4A/SASSYS-1. The elevation change from the core outlet to the top of the zone of flow establishment is directly derived from the recommended value $C_1 = 0.111$ within the zone of flow establishment, which is where most of the impingement occurred [11,16]. The constants *a* and *b* were found to be 0.8 and 1.1 empirically. These constants are also used in the current SAS4A/SASSYS-1 model, leading to equations (3)

and (4) listed below for calculating the entrainment at an interface (W_{ent}) and the elevation change from the core outlet to the top of the zone of flow establishment (z_0), where d_j is the plume effective diameter at the interface, V_j is the plume average velocity at the interface, and F_f is the modified Froude number, or simply the Ri number.

$$W_{ent} = .2\pi\rho_{plume}V_i d_j F_f^{-1.1} \tag{3}$$

$$z_0 = \frac{r_0}{.111}$$
(4)

Yang investigated the penetration of a turbulent jet with negative buoyancy in a uniform environment. The motivation for his research is directly related to the current issues being explored, the response in the upper outlet plenum of a liquid metal cooled fast reactor. The mismatch of power-to-flow was identified as the cause of the phenomena consisting of the colder fluid exiting the core, therefore creating a negative buoyancy jet and preventing a full penetration of the jet, leading to stratification- which could have an important effect on the average temperature of the fluid entering the primary loops. Yang replotted measurements taken by Turner (1966) [19] and Lorenz et al. (1975) [20] in terms of the Froude numbers and obtained a single correlation of the penetration distance as a function of only the Froude number. The simple correlation he derived (5) is currently employed in the SAS4A/SASSYS-1 PRIMAR-4 model [21,11].

$$z_m = 1.0484 F r_0^{.785} \tag{5}$$

Yang concluded that the simplified one-dimensional approach presented in his analysis would provide satisfactory prediction of the maximum penetration distance [21].

While this model has resulted in fairly accurate solutions, it fails to compete with CFD in accuracy and does not provide a complete picture of the phenomena occurring in the upper plena. Having a solution that can obtain the accuracy 3-D techniques achieve along with preserving the speed in which it is able to analyze complex systems is the focus behind this project.

OTHER SYSTEMS CODES WITH STRATIFIED VOLUME MODELS

There is a large number of system level codes previously or currently being developed in many countries to predict safety analysis for all types of nuclear reactor designs. While not all of these codes have stratified layer models, the ones that do contain them are for the most part inadequate for similar reasons as SAS4A/SASSYS-1. More recently, established system codes for light water reactors have been pushed to add stratification-capable models. CONTAIN is a thermal hydraulics code based on control volume formulation used for light water reactors. In order to improve its ability to predict highly stratified conditions, a "hybrid flow solver" was incorporated; however, several limitations in its abilities have been pointed out and can be found in Reference [23]. The GOTHIC code uses a CFD like approach to try to predict thermal stratification in the pressure suppression pools of BWRs. [24, 25].

France's CATHARE system code used for PWR safety analysis has had extensive work done to extend its capabilities to handle more working fluids than just water. Newer versions of the code are able to handle designs including PWR, BWR, SFR, and fast gas cooled reactors. The stratified volume model is performed using several 0D volumes connected to predict stratification during transient conditions. CATAHRE2 is a modified version of CATHARE to treat heavy liquid metals that is currently going through the Verification and Validation (V&V) process. ATHLET is another code originally developed for LWR applications currently being extended to handle SFR designs. Developers of the ATHLET code are relying on connecting the system level code with CFD in order to predict thermal stratification. There have been several system codes developed specifically for pool type reactors, including India's DYANA-P and France's DYN2B. DYANA-P takes the CFD coupling route for thermal stratification while DYN2B employs a 0D zone model based on the Richardson number [26, 27].

The Japanese code Super-COPD is based on the flow network model and has been validated using natural circulation experimental data from the Monju reactor. Its one-dimensional model cannot predict thermal stratification as correctly as threedimensional models, but comparisons of the two methods show good agreement [28,29]. Korea's code MARS-LMR uses a multi-dimensional approach to model large volumes such as the cold pool and the hot pool [30]. Korea is also developing the SSC-K code for the safety analysis in the conceptual design of Korea Advanced Liquid Metal Reactor (KALIMER) and the analysis of the anticipated system transients during operation. In this code, a two-dimensional hot pool model is coupled into SSC-K for a more realistic analysis of thermal stratification phenomenon in the hot pool. The solution domain is divided into a finite number of control volumes and the governing equations are discretized according to the finite volume approach. The convection terms are approximated by a higher-order bounded scheme HLPA developed by Zhu (1991) and the unsteady terms are treated by the backward differencing scheme. Users of SSC-K can select the 2D model or the two-mixing model for hot pool simulations [31].

3-D MODELING OPTIONS

It is common in system codes to experience problems properly predicting the evolution of temperatures during a transient, especially in regions with complex 3-D phenomena or buoyancy effects. The course mesh-control volumes and flow paths in many cases have a difficult time modeling complex 3-D flows. In liquid metal reactor designs these 3-D effects can have a large influence on the behavior of a reactor during a transient. CFD does a good job in defining these complex phenomena, but at a computational expense. This is not always sufficient for design optimization, as the need to quickly analyze designs arises. In order to address this common issue, coupling existing codes to CFD has been proposed. CFD would model regions of 3-D interest and leave the rest of the reactor loop to be modeled by the system code, therefore optimizing computational costs. Several coupled methodologies have already been explored. The assessment of the thermal hydraulic codes, CFD codes, and coupled-codes is one of the main objectives of the THINS Project of the 7th Framework EU Program [27,32]. A multidimensional plenum modeling capability can be developed by coupling a CFD code to a whole-plant system analysis code. By applying the CFD model to only portions of the domain, excessive computational burden is avoided.

The coupling has been performed for several codes. TRIO_U is a CFD code that has been coupled with CATHARE. In transient calculations, the hot pool, cold pool and upper-core structure are modeled in CFD. The pumps and the core are modeled in CATHARE and the coupling is done through the overlapping method. The system code delivers the mass flow rate and temperature conditions at the CFD boundaries. Miscalculation during the transition between forced and natural regime were noted. The calculation was done on 50 recent processors (4 cores by processor) and took four days [27].

Open Field Operation And Manipulation CFD Toolbox (OpenFOAM) is an open source CFD software package that was coupled with ATHLET. The mass flow rate, temperatures, and pressure must be exchanged from ATHLET to OpenFOAM as boundary conditions. The full transient is iterated between ATHLET and OpenFOAM – as soon as exchanged values show non-significant changes at boundaries the iterations are stopped. A python program was created to handle the iterations. The time for one full iteration is strongly dependent on the CFD calculation performance and takes approximately 8 days for this method [27].

A coupling algorithm implemented in Java controls the time-step, input modification and execution of RELAP5 and STARR-CCM+ with a boundary data transfer between the codes. During a coupling time step, the CFD code runs first with time-extrapolated and cross-section-averaged inlet mass flow and temperature boundary conditions. Next the system level code iteratively computes the energy/sink needed to match the temperature on both solutions. The coupled simulation results differ from the single system level code results. ATHLET was coupled with ANSYS-CFX and compared to results using just ATHLET. The detailed results in the complex 3-D regions differed as expected when adding the 3-D CFD analysis;

however, the overall predictions for the entire transient progression in the facility were very similar [32].

In order to better predict the conditions of thermal stratification during a transient, SAS4A/SASSYS-1 was coupled with STAR-CD. Earlier attempts to couple the two codes resulted in a "one way" data transfer from SAS4A/SASSYS-1 to STAR-CD, with no feedback from STAR-CD to SAS4A/SASSYS-1. In more updated work by Fanning and Thomas, the STAR-CD prediction of the core and IHX inlet temperatures and pressures were provided back to SAS4A/SASSYS-1 and the evaluation of the influence of thermal stratification in the outlet plenum is now possible. The coupled simulations on a quad-core machine required approximately 39 hours [33].

Thomas et al. [34] coupled STAR-CCM+ with SAS4A/SASSYS-1 and compared the results to the data recorded in the SHRT-17 tests, which involved a complete loss of all pumping power to the EBR-II plant while operating at full power and flow, followed by a scram. In this coupling, the STAR-CCM+ cold pool model is linked to the SAS4A/SASSYS-1 model of the EBR-II primary coolant system at the flow boundaries. The STAR-CCM+ model of the cold pool replaces the control volume (CV) in SAS4A/SASSYS-1. The system code provides the flow rate and temperature at the CFD inlet boundary. CFD calculations then update the temperature at all outlet flow boundaries and updates the pressure at all boundaries in order to provide SAS4A/SASSYS-1 with a gravity head that reflect the temperature distribution in the plenum. During the coupled phase of simulation, SAS4A/SASSYS-1 and STAR-CCM+ exchange information about the flow boundaries at the beginning and end of each SAS4A/SASSYS-1 time step. The coupled analysis required 160 hours of time on a workstation with 32 processor cores [34].

MORE RECENT EFFORTS ON THERMAL STRATIFICATION MODELING IMPROVEMENTS

Scaling and modeling of stratified mixing in large enclosures requires detailed and accurate empirical models for wall and free jets. Considerable research has been devoted to the study of transport by jets, plumes, and wall boundary layers in large-scale stratified systems. List [32] reviewed the available literature on jets and plumes and identified major gaps that deserve research attention. After this review, Peterson (1994) [33] showed that the onset and breakdown of stratification can be predicted by governing equations he derived for mixing of stratified fluids in large enclosures. Zuber (1991) [34] presented a hierarchical, two-tiered scaling analysis that works for selecting the height, volume, and power scales for an integral facility. Peterson applied Zuber's hierarchical, two-tiered scaling analysis (HTTSA) method, which divides a complex system into subsystems, modules, constituents, and phases. The fluid volume was subdivided at the phase geometry level into cylindrical control volumes around the buoyant jets and thin, horizontal control volumes slicing the stratified fluid [5,33].

Peterson performed scaling for a large volume enclosure with arbitrary geometry and a characteristic height H_{sf} . The equations of mass, momentum, energy, and species conservation inside the enclosure and the Boussinesq approximation for the convective terms of the momentum equations were used. His scaling process resulted in non-dimensional parameters which govern when the onset and breakdown of stratification occurs for enclosure flows driven by wall and free jets. According to Peterson, once the ambient fluid in a large enclosure stratifies, the temperature and species distributions become one-dimensional and can be modeled by simple governing equations, using standard empirical relationships for jet entrainment [5,36]. This work served as the basis for Berkeley's in house BMIX++ code.

The BMIX++ (Berkeley mechanistic MIXing code in C++) solves transient mixing and heat transfer problems in stably stratified enclosures using a Lagrangian approach to solve 1-D transient governing equations or 1-D integral models to compute substructures [38]. The code was validated against a number of experimental tests; however, it is only applicable for relatively stable stratified conditions or well-mixed volumes. Details of transition from stratified to mixed conditions and the time scale for such process were not addressed [2]. In the future, a dynamic solution must be formed to better analyze the phenomena in a timely fashion.

Reduced order modeling (ROM), also known as model reduction, is another possible approach to modeling complex phenomena such as thermal mixing and stratification. ROM commonly uses a small number of solutions generated by a high fidelity model to construct a computationally cheaper model [40]. Argonne is currently developing an advanced system analysis tool SAM to be used as a system-level modeling and simulation tool for advanced reactor safety analysis [41]. SAM is currently slated to implement a reduced-order threedimensional module to predict thermal mixing and stratification modeling in large enclosures during transients. More information for this approach can be found in [42]. While more work is needed for this, including closure model developments and continued V&V preliminary results show promise.

Machine learning methods have also been closely examined in the last few years to assist with turbulent model development for CFD, and could help with the process of developing more cost effective models for thermal mixing and stratification. Shifting attention to the use of machine learning in thermal hydraulic reduced order modeling could alleviate computational expense in modeling and simulating complex 3-D phenomena occurring in new reactor designs.

CONCLUSION

Two trends are observed in terms of modeling and simulation efforts in large enclosure mixing – traditional system

analysis approach using decoupled, highly simplified and conservative 0-D models or computationally expensive and inefficient 3-D CFD methods. Both of these pose serious issues, as one provides a very approximate solution while the other requires high computational costs. The SAS4A/SASSYS-1 code currently only includes lumped-volume-based 0-D models that result in very approximate results and can only handle simple cases with one mixing source. Additionally, the models used in the code are based on experimental data for specific geometries, and they may not be applicable to all problems.

A 1-D approach seems like a sensible approach to attempt to minimize the drawbacks of the two above trends. BMIXX++ has already shown promising results in complex stratified problems without the computational expense of CFD simulations. The development of a similar approach for the new SAS4A/SASSYS-1 stratification models will be informed by the new experimental data being collected by the UW-Madison collaborators, and by the associated CFD models analyzed by MIT collaborators. A 2-D approach should be looked further into as well as ROM options.

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NOMENCLATURE

- Q : volumetric entrainment flux
- V_j jet velocity
- di: effective jet diameter
- *a*,*b* : constants
- Ri: Richardson number
- $\boldsymbol{\epsilon}$: interfacial rise rate
- D : vessel diameter from experiment
- W_{ent} : entrainment rate at an interface
- ρ_{plume} : density of the plume
- F_f: modified Froude number (Richardson number)

 $z_0\colon$ elevation change from core outlet to the top of the zone of flow

- r₀: core effective radius
- z_m: height of the jet
- Fr₀ : Froude number

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