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An Overview of Modeling Methods for Thermal Mixing and Stratification in Large Enclosures for Reactor Safety Analysis

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ABSTRACT

Thermal mixing and stratification phenomena play major roles in the safety of reactor systems with large enclosures. Depending on the fidelity requirement and computational resources, 0-D steady state models, 0-D lumped parameter based transient models, 1-D physical-based coarse grain models, and 3-D CFD models are available. Current major system analysis codes either have no models or only 0-D models for thermal stratification and mixing, which can only give highly approximate results for simple cases. While 3-D CFD methods can be used to analyze simple configurations, these methods require very fine grid resolution to resolve thin substructures such as jets and wall boundaries. Due to prohibitive computational expenses for long transients in very large volumes, 3-D CFD simulations remain impractical for system analyses. For mixing in stably stratified large enclosures, UC Berkeley developed 1-D models where the ambient fluid volume is represented by 1-D transient partial differential equations and substructures such as free or wall jets are modeled with 1-D integral models. This allows very large reductions in computational effort compared to 3-D CFD modeling. This paper presents an overview on important thermal mixing and stratification phenomena in large enclosures for different reactors, major modeling methods and their advantages and limits, potential paths to improve simulation capability and reduce analysis uncertainty in this area for advanced reactor system analysis tools.

KEYWORDS

Thermal mixing, stratification, large enclosure

1. INTRODUCTION

Thermal mixing and stratification phenomena play major roles for safety of reactor systems with large enclosures, such as post-LOCA gas transport between containment compartments and hydrogen distribution in operating LWRs, long-term passive containment cooling in AP-1000, and steam condensation and mixing in the suppression pool and isolation condenser pool of ESBWR. It is important to accurately predict the temperature, density, and/or concentration distributions for both design optimization and safety analysis. However, the individual transport mechanisms governing mixing in containments are characterized by time and length scales that can differ by orders of magnitude. Large volumes and complexity of the interactions of different flow and thermal structures make analysis a daunting task. The accompanying large analysis uncertainty often casts doubt about the claimed large safety improvement by Gen-III+ passively safe LWRs over the operating Gen-II actively safe LWRs. Due to these reasons, large-scale projects like programs performed at PANDA (PSI, Switzerland) have been continuously investigating these phenomena over the past two decades [1].

Current major system analysis or severe accident analysis codes (such as RELAP5 [2], TRAC [3], MELCOR [4], etc.,) either have no models or only 0-D models for thermal mixing and stratification in large enclosures. The lack of general thermal mixing and stratification models in those codes severely limits their application and accuracy for safety analysis, especially for passively safe ALWRs, where the primary system and containments are more strongly coupled together. While 2-D or 3-D CFD methods can be used to analyze simple configurations, these methods require very fine grid resolution to resolve thin substructures, such as jets and wall boundaries, yet such fine grid resolution is difficult or impossible to be provided for studying the reactor response to transients due to prohibitive computational expenses. Therefore, new high fidelity and efficient thermal mixing and stratification methods are needed to improve the accuracy of safety analysis and reduce modeling uncertainty.

Previous scaling analysis [5] has shown that stratified mixing processes in large stably stratified enclosures can be described using 1-D partial differential equations, with the vertical transport by free and wall jets modeled using standard integral techniques, which can have different varying flow directions besides the vertical direction. This allows very large reductions in computational effort compared to 3-D numerical modeling of turbulent mixing in large enclosures. The BMIX++ (Berkeley mechanistic MIXing code in C++) code was originally developed at UC Berkeley to implement such ideas [6, 7, and, 8]. The BMIX++ code has been successfully validated against multiple benchmark problems. Various problems with different combinations can be solved by the BMIX++ code, such as: multi-species fluid, variable enclosure cross section area in vertical direction, multi-enclosures connected with openings, and multiple jets, plumes, and sinks within one enclosure. When steam-water jet and condensation models are available, the code can be applied for containment analysis.

Section 2 will discuss several important thermal mixing and stratification phenomena in large enclosures for different reactors; section 3 will review major modeling methods and their advantages and limits, and discuss potential paths to improve simulation capability and reduce analysis uncertainty for advanced reactor system analysis tools.

2. SAFETY IMPORTANT THERMAL MIXING AND STRATIFICATION PHENOMENA IN REACTOR SAFETY ANALYSIS

Thermal mixing and stratification phenomena play major roles in safety of reactor systems with large containments and enclosures. For both current operating LWRs with active safety features and advanced LWRs with passive safety features, post-LOCA gas transport between containment compartments and hydrogen distribution have been identified by several international expert groups as high-ranking phenomena since they mostly affect the risk of containment failure [1]. Buoyancy driven flows, potentially augmented by break-jet momentum, will play a key role in the transport as shown in Fig.1 [5]. More generally, enclosure flows driven by free buoyant jets and wall boundary layers are important in nuclear systems experiencing fires, using passive autocatalytic recombiners, and removing aerosols following severe accidents.

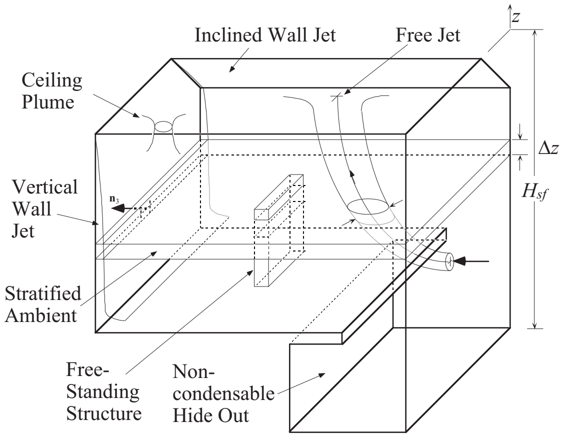


Fig 1 Large Containment Mixing at Later Stage of A LOCA.

Gen-III+ LWRs like ESBWR and AP-1000 rely on passive safety grade containment systems to reduce cost and improve safety. As a result, some phenomena that were previously of little interest for design-basis accidents in earlier version of LWRs, such as thermal mixing and stratification in large enclosures, have become important. Moreover, a stronger coupling between the primary system and containment in accident conditions requires integrated simulation of both systems [9]. In the passive safe BWRs, the long-term post-accident containment pressure is determined by a combination of the noncondensible gas pressure and steam partial pressure in the wet well gas space. The suppression pool surface temperature, which determines the vapor partial pressure, is very important to the overall containment pressure response [10]. Separate-effects tests with a 1/10th scaled-down ESBWR suppression pool indicated that significant thermal stratification is likely to exist after the steam blowdown and direct contact condensation in the pool [11]. Without taking into account the thermal stratification, any analysis predicting the containment pressure response will be non-conservative. Therefore, the thermal stratification of the suppression pool due to blowdown is of primary importance.

AP-1000 design uses passive containment cooling system (PCCS) to remove decay heat. Mass transfer is the dominant means of containment heat removal on both inner and outer steel shell surfaces [12]. On the inside, condensation on the containment shell dominates heat removal and is strongly influenced by the distribution of steam and noncondensible gases. During the post-blowdown phase of a LOCA transient, mixing due to break flow momentum may be neglected by assuming momentum to be dissipated within the break compartment, conservatively minimizing source momentum-induced mixing. One or more buoyant plumes will rise from openings in the operating deck, and a wall boundary layer induced by heat and mass transfer to the containment shell will flow downward. Both the plume and wall layer entrain bulk mixture, acting to circulate the bulk mixture. The fluid dynamics leads to a time-averaged vertical gradient of steam concentration. The containment design used several highly conservative assumptions regarding mixing and condensation. Improved thermal mixing modeling capability would increase the confidence on the passive containment performance and allow further power uprate to improve economics.

In summary, it is important to accurately predict the temperature, density, and/or concentration distributions for both design optimization and safety analysis. However, the individual transport mechanisms governing mixing in containments are characterized by time and length scales that can differ by orders of magnitude. The large volumes and complexity of the interactions of different flow and thermal structures make analysis a daunting task. The accompanying large analysis uncertainty often casts doubts about the claimed large safety improvement by Gen-III+ passively safe LWRs over the operating Gen-II actively safe LWRs. Due to these reasons, large-scale experimental projects, such as programs performed at PANDA (PSI, Switzerland) have been continuously investigating these phenomena over the past two decades [1, 13]. The SETH project investigates mixing and distribution of steam/air/helium at large scale in multi-dimensional, multi-compartment geometry in order to resolve some safety-related issues in containment thermal-hydraulics.

In addition to the LWRs, thermal mixing and stratification phenomena in large pools or enclosures are also very important for safety analysis in several Gen-IV reactor systems, such as the cold and hot pool mixing in pool type sodium cooled fast reactor systems (SFR) [14] and reactor cavity cooling system behavior in High Temperature Gas Cooled Reactors [15]. For SFRs as shown in Fig 2, the hot pool and cold pool mixings directly affect the reactor inlet temperatures and natural circulation flow rate through the reactor core, which affects the peak clad temperature, one of the most important parameters to evaluate the SFR safety. For HTGRs, buoyancy-driven flows play a key role in heat and mass transfer in the reactor cavity cooling systems. Air and steam ingress following loss-of-coolant accidents is also strongly affected by gas distributions in the reactor and power-conversion-unit enclosures.

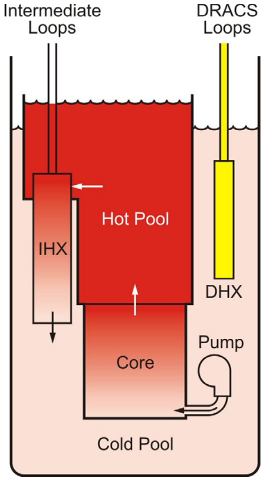


Fig 2 Schematic View of the Existing Pool Type Design of SFRs.

3. MODELING METHODS FOR THERMAL MIXING AND STRATIFICATION IN SAFETY ANALYSIS

In term of modeling and simulation efforts in large enclosure mixing, two opposite trends can be observed. One is along the traditional system analysis approach by using decoupled, highly simplified and conservatively 0-D models to study mixing in large enclosures. Another path is to try expensive and inefficient 3-D CFD simulations. Considering the limitations of inadequate 0-D models and inefficient 3-D CFD methods, new high fidelity and efficient thermal mixing and stratification methods are needed to improve analysis accuracy and reduce modeling uncertainty, especially for system analysis. There existed a middle path that tries to obtain the physical insights with combinations of different 1-D methods, like the

BMIX++ code uses. This section will review all these methods and show some examples.

3.1. 0-D Methods

Current major system analysis codes have no general models for thermal stratification in large enclosures. The lack of general thermal mixing and stratification models in those codes severely limit their application and accuracy for safety analysis for reactor systems with large enclosures. For example, Fig. 3 shows the peak clad temperature sensitivity for different cold pool mixing models according to preliminary RELAP5-3D simulations for a pool type of SFR design as shown in Fig 2. We can note that the peak clad temperature is very sensitive to different pool mixing models. RELAP5-3D has no thermal stratification models for large enclosures. If analysts are not familiar with the physical phenomena and use one large control volume (implying well mixed case) to represent either the hot or cold pool, the code will give non-conservative results.

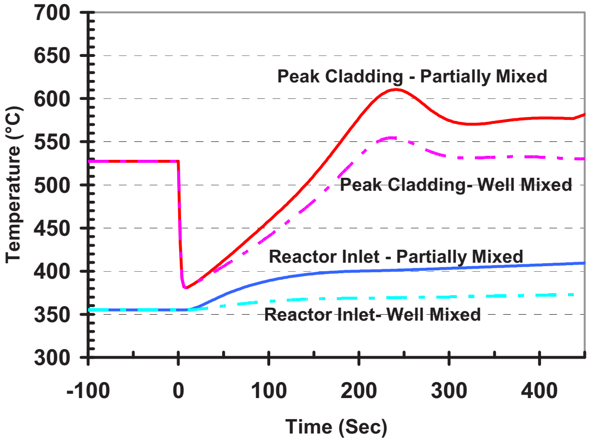
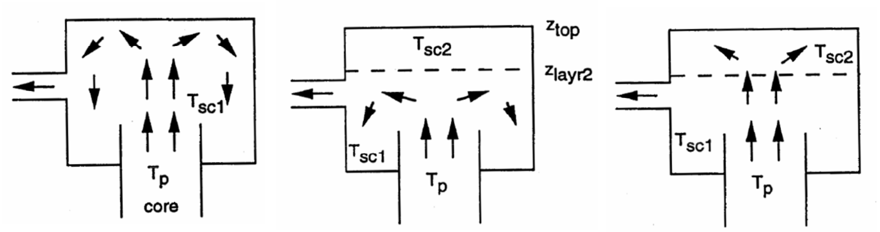


Fig 3 Peak Clad Temperatures Predicted by RELAP5-3D Simulation for A SFR Design, for Two Different Cold Pool Mixing Models: Well Mixed and Partially Mixed (credit of Hongbin Zhang, INL).

The SASSYS code developed by Argonne National Laboratory (ANL), one of the major SFR system analysis codes, only provides lumped-volume-based 0-D models that can only give very approximate results and can only handle simple cases with one mixing source [14]. The models were derived according to simulant experiments for specific SFR upper plenum design configurations [16 and 17]. Fig 4 shows several mixing configurations in the hot pool. Depending on the momentum and buoyancy of the outlet flow from the reactor core, well mixed case, two-zone with a negative buoyant jet case, two-zone with a positive buoyant jet case, even more complex three-zone cases may form. The total jet entrainment, zone interface location, average temperatures in each zone can be estimated by empirical correlations. Since the methods are based on scaled experimental data, using those models for SFR designs with different hot/cold pool configurations tend to have larger uncertainty.

The modeling method is very similar as the zone models widely used for room fire analysis [18, 19]. Zone models may be grouped into two types based on the number of the control volumes (zones) in each compartment: one-zone models and two-zone models. One-zone models were widely used in the analysis of post-flashover fires, as well as the smoke movement in the compartments remote from the fire room (network models). Two zone models divide the gas in a compartment into two distinct zones: an upper, higher-temperature zone and a lower, lower-temperature zone. These zones are a result of buoyancy induced thermal stratification. For each zone, the mass, energy conservations are used to drive four ordinary differential equations describing mass, energy variables. In this type of models, the physical details of the gas within a zone are not considered, while mass and energy exchange between zones is calculated by modeling the sub-structure processes, such as buoyant jet and wall boundary flow. The 2-zone models give more detailed information about the average temperatures in two layers and the interface location. However, it cannot provide the distribution of temperature, density, and pressure in the enclosure.



Fully mixed case

Two layer, cold (negative) buoyant jet case

Two layer, hot buoyant jet case

Fig 4 Several Hot Pool Mixing Cases in SFR Safety Analysis [14].

3.2. 2-D or 3-D CFD Methods

2-D or 3-D CFD codes have been widely used for laminar problems and some turbulent problems with simple geometry configurations. For example, natural convection problems in enclosures have been extensively studied in both the laminar and the turbulent flow regimes [20, 21, 22, 23]. COMMIX code developed by ANL used CFD methods to analyze simple configuration small-scale thermal stratification problems and achieved limited success [24, 25]. However, the restrictiveness and shortcomings of such applications have been recognized and further research needed to extend the applications to large complex pool mixing systems have been highlighted in the review report by ANL [25].

For large enclosure mixing problems, as illustrated in Fig. 1, very fine grid resolution is required to resolve thin jet structures when one attempts to numerically solve the multi-dimensional mass, momentum, and energy equations with CFD codes, yet such fine grid resolution is difficult or impossible to provide due to the computational expense, particularly in geometrically complex volumes. With multiple interconnected enclosures, 3-D CFD analysis becomes more difficult. Moreover, for strongly stratified flows, the rate of convergence can be extremely slow because of the vastly differing time-scales present in this type of flow [26]. In the framework of the 5th EU-FWP project ECORA, the CFD capabilities for simulating flows in the containment of nuclear reactors were evaluated [27]. The assessment included a first attempt to use Best Practice Guidelines (BPGs) for the analysis of long, large-scale, transient problems. Due to the large computational overhead of the analysis, it was concluded that the application of the BPGs to full containment analysis is out of reach with the currently available computer power. Without fully following BPGs, the CFD simulation uncertainty cannot be quantified.

3.3. 1-D Methods

Depending on mixing sources strength and the aspect ratio, scaling analysis [5] has shown that the ambient fluid between jets and boundary layer flows tends to organize into either a homogeneously mixed condition or a vertically stratified condition that can be described by a 1-D temperature and concentration distribution. Thus, we can describe stratified mixing processes in large, complex enclosures using 1-D differential equations, with transport in free and wall jets modeled using 1-D integral models. The detailed geometry of the enclosure becomes unimportant, and only the horizontal cross-sectional area and perimeter must be specified as a function of elevation. This allows very large reductions in computational effort compared to the 3-D numerical modeling of turbulent mixing in large enclosures.

To explain why a 1-D method can provide enough information to describe mixing and heat transfer in stratified large volumes, we start with the simplest case. Fig 5 shows the classical "filling box" problem, which demonstrates major phenomena in stratified mixings [28]. The heating source gives rise to a thermal plume that rises and spreads over the top of the enclosure, resulting in a stably stratified layer that expands downward with time. The region below the upper stratified layer continues to be at the initial temperature in the enclosure before the onset of the flow. The temperature in the upper heated layer decreases downward from the ceiling to the interface between the upper and lower regions. The flow pattern, the side entrainment into the plume and the downward motion of the heated upper layer are shown in Fig. 5.

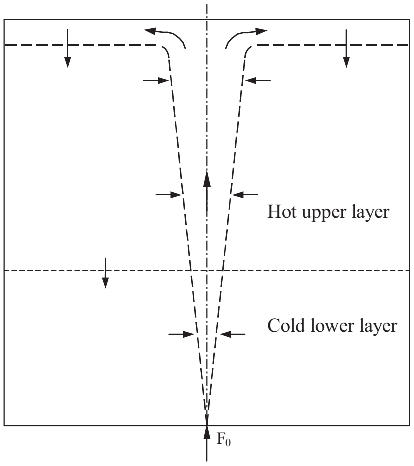


Fig 5 Sketch of Development of a Stratified Environment Due to a Heat Source, Showing the Motions in the Plume and Environment.

In addition to buoyancy induced plumes, momentum jets, buoyancy jets, steam jets that lead to direct contact condensation, and natural convection boundary layer flows (free wall jets) are also common mixing forces to cause stratification. Large enclosures mixed by buoyant plumes and wall jets can normally be expected to stratify. Furthermore, the transition between the well-mixed and stratified conditions can be predicted [5]. For example, for an injected buoyant jet case, the ambient fluid is stably stratified when

$$\left(\frac{H_{sf}}{d_{bjo}}\right) Ri_{bjo}^{1/3} \left(1+\frac{d_{bjo}}{4\sqrt{2}\alpha_T H_{sf}}\right)^{2/3} > 1 \qquad (1)$$

where H_{sf} is the height of an enclosure, d_{bjo} the diameter of the jet source, $\alpha_T = 0.05$ Taylor's jet entrainment constant; and the jet Richardson number (*Ri*) is given by

$$Ri_{bjo} = \frac{(\rho_a - \rho_o) g d_{bjo}}{\rho_a U_o^2} \tag{2}$$

where ρ_a is the ambient fluid density, ρ_o the source fluid density, *g* the gravity constant, and U_o the jet source speed.

A jet is simulated with 0-D or 1-D quasi-steady state integral models. Within this paper, a jet should be understood as a generic concept of any steady continuous flow structure in an ambient volume with a dominant flow direction and a length scale much less than the ambient volume's scale. For example, a plume (due to a heat source), a pure jet (due to an initial momentum source) [29], a buoyant jet (due to both buoyancy and momentum [30, 31], a ceiling jet (a jet below the ceiling due to a jet impingement) [32], a wall jet along a wall surface [33], a wall jet due to a normal jet injection, and a wall boundary flow are all taken as jets. All these different jets have a common character: the jet entrains fluid from the ambient volume and finally discharges into the ambient volume. Fig 6 shows several typical jets.

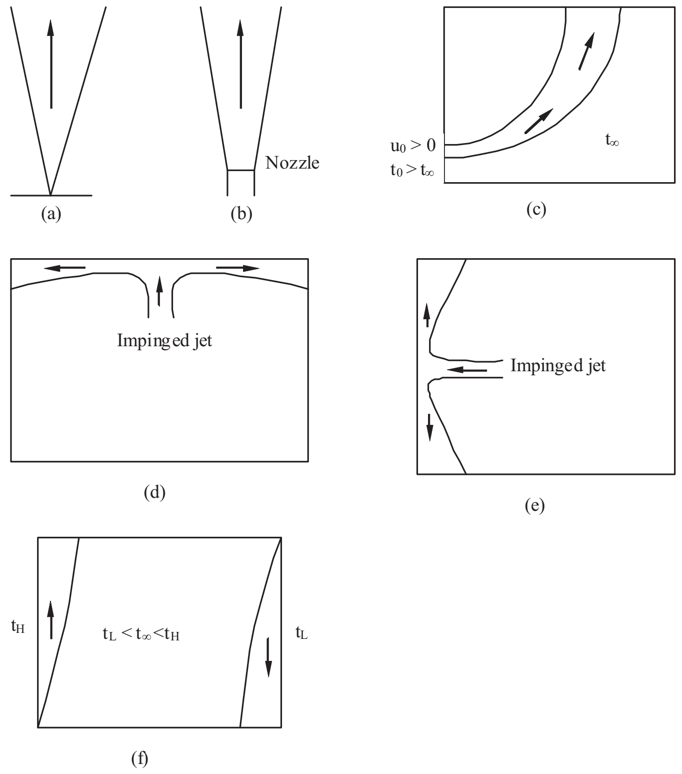
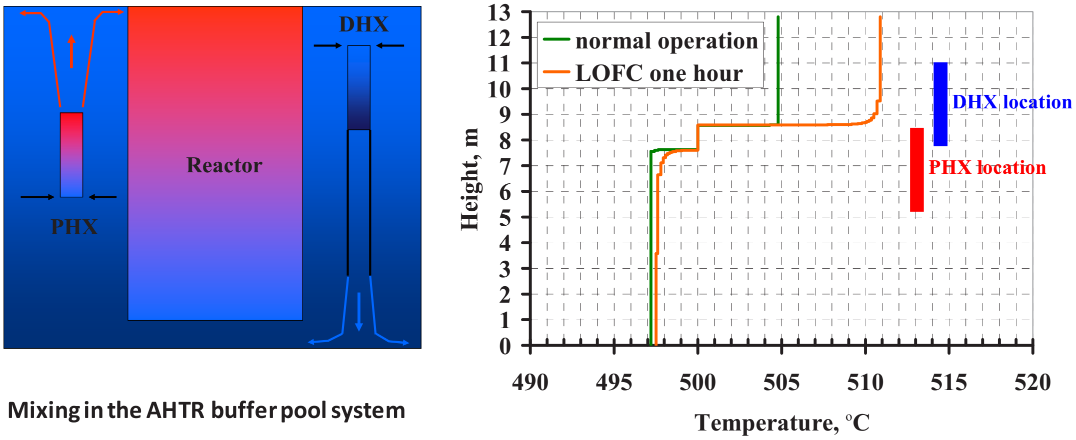


Fig 6 Typical Jet Types. (a) Pure Plume; (b) Pure Jet; (c) Buoyant Jet; (d) Ceiling Jet; (e) Wall Jet Due to Impinged Jet; (f) Free Wall Jet Due to Wall Boundary Flow.

The BMIX++ code was developed at UC Berkeley to implement such ideas [6, 7, 34, and 8]. This code solves mixing and heat transfer problems in stably stratified enclosures. The code uses a Lagrangian approach to solve 1-D transient governing equations for the ambient fluid in order to preserve strong gradients in hyperbolically dominated flows. The traditional first order discretization procedures inherently introduce artificial diffusion terms. Typically, these extra diffusion terms impose severe limitations on the maximum size of the computational control volume for the computed solution to be reasonably accurate. The Lagrangian approach [6] eliminates “false diffusion” even with coarse grid and larger time step. This first-order scheme algorithm could be further improved to reach a 2nd or higher order accuracy with advanced discretization schemes in space [35] and in time [36]. The BMIX++ code includes a jet model library including several free jet models for plumes and buoyant jets, a buoyant wall jet model, a ceiling jet model, and two line jet models. In addition, 1-D transient conduction model for the solid boundaries is included to calculate heat loss through the enclosure walls. Opening models are included to analyze the exchange flow through connections between enclosures.

The BMIX++ code has been successfully validated against multiple benchmark problems, such as stratification in a water tank due to an internal heater, water tank exchange flow experiment simulation [6], stratification produced by multiple plumes [8], and the UCB large containment mixing experiment, which is composed of a rectangular enclosure with an isothermal cooling wall and a hot air jet injecting [34].

The BMIX++ code was recently extended to analyze liquid salt pool systems in an Advanced High Temperature Reactor (AHTR) design [8]. Fig 7 shows the temperature profile in the AHTR buffer salt pool, as calculated by the BMIX++ code, along with the mixing schematic in the buffer pool system. Ambient buffer salt enters the bottom of PHX (Pool reactor auxiliary cooling system Heat eXchanger) modules as mass sinks (relative to ambient fluid) and warmer buffer salt rises from the top of PHX modules as buoyant jets; ambient buffer salt enters the top of DHX (Direct reactor auxiliary cooling system Heat eXchanger) modules as mass sinks and colder salt flows downward from the bottom of DHX modules as buoyant jets. Due to the competing effects by one group of upward hot buoyant jets, one group of downward cold buoyant jets, and two groups of mass sinks, there are two thermal fronts: the upper one for the hot jets and the lower one for the cold jets. Thermal stratification in the buffer salt is divided into three regions: the top region above the PHX, the lower region below the DHX, and the middle one between the PHX and DHX. Under LOFC (Loss of Forced Circulation) transient conditions, the PHX heating power increases and the driving force for thermal stratification becomes stronger. Therefore, the thermal stratification in the buffer salt becomes larger. In Fig. 7, the thermal front profiles are very sharp. Similar analysis can be performed for SFRs and the BMIX++ code can be coupled with a system analysis code to provide better prediction of thermal stratification in pool systems.



Mixing in the AHTR buffer pool system

Fig 7 Temperature Profiles in AHTR Buffer Salt Tank.

3.4. Multi-Fidelity Structures in Advanced Reactor System Analysis Tools

As discussed in previous sections, current major reactor system analysis or severe accident analysis codes lack general modeling capabilities for thermal mixing and stratification in large enclosures. The existing stand-along analysis packages such as commercial CFD software, thermal hydraulic codes with CFD options like GOTHIC [37], or BMIX++ code, need users to provide initial and boundary conditions either by decoupled system analysis code runs or manually constructed. Such practice is not efficient and may result in large uncertainty for strongly coupled transient problems. Therefore, it should be a priority to integrate general large enclosure mixing models in advanced system analysis codes.

Multi-fidelity models consistent with the uncertainty requirement and computation resource should be included in a system analysis code. For example,
- ✓ 0-D models for well mixed cases, for simple configuration with strong experimental data support, or for very fast low fidelity calculation or pre-conceptual design scoping analysis;
- ✓ 1-D models for stably stratified cases, or fast calculation;
- ✓ Coarse grain 2-D, 3-D CFD models for transition cases, potentially for other cases with higher fidelity requirement;
- ✓ Fine grid, converged, validated CFD simulation to provide fundamental understanding and closure models for lower fidelity models.

One of the most difficult tasks is to develop efficient and effective models for transition cases where the fully stratified ambient or well mixed ambient assumptions break down. Transition cases in nature are multi-dimensional and transient. Fine grid converged 3-D transient simulations are too expensive for large volume complex mixing cases while coarse grid 3-D simulations have too large uncertainties due to numerical errors and missing key physical processes. New models need to capture key physical structures with limited computational cost so that important figures of merit such as containment pressure, maximal temperature, maximal species concentration, etc, can be preserved. One potential path is to develop innovative LANS-α (Lagrangian-Averaged Navier-Stokes alpha) based turbulent models [38], which require less resolution to capture major flow structures than the conventional Eulerian-Averaged turbulent models [39]. Another method, recirculation speed method [34], is more experimental based. When a forced jet is injected into an enclosure, it induces a large-scale recirculating flow due to the entrainment of ambient fluid into the jet. These large-scale flows can augment heat and mass transfer. Consideration of the strength of this recirculating flow can allow the heat and mass transfer augmentation to be predicted. The strength of this recirculating flow can be characterized by a velocity scale. Here this characteristic velocity scale is called the recirculation speed. The recirculation speed can be evaluated through an enclosure mechanical energy balance.

4. CONCLUSIONS

Thermal mixing and stratification phenomena play major roles in the safety of reactor systems with large enclosures. However, current tools and methods are not adequate. Scaling based 1-D methods such as BMIX++ code used can give satisfying results for complex thermal mixing problems under stable stratification condition without resorting to expensive CFD simulation, therefore are well suited to couple with system analysis codes for Gen IV reactors and advanced LWRs. The efforts to fill the analysis gaps need to be coordinated with advanced analysis code development and a multi-fidelity modeling strategy need to be developed for different mixing stages and uncertainty requirements.

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