Validation of Hydrogen Gas Stratification and Mixing Models

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Abstract

Two validation benchmarks confirm that the BMIX++ code is capable of simulating unintended hydrogen release scenarios efficiently. The BMIX++ (UC Berkeley mechanistic MIXing code in C++) code has been developed to accurately and efficiently predict the fluid mixture distribution and heat transfer in large stratified enclosures for accident analyses and design optimizations. The BMIX++ code uses a scaling based one-dimensional method to achieve large reduction in computational effort compared to a 3-D computational fluid dynamics (CFD) simulation. Two BMIX++ benchmark models have been developed. One is for a single buoyant jet in an open space and another is for a large sealed enclosure with both a jet source and a vent near the floor. Both of them have been validated by comparisons with experimental data. Excellent agreements are observed. The entrainment coefficients of 0.09 and 0.08 are found to fit the experimental data for hydrogen leaks with the Froude number of 99 and 268 best, respectively. In addition, The BIX++ simulation results of the average helium concentration for a enclosure with a vent and a single jet agree with the experimental data within a margin of about 10% for jet flow rates ranging from 1.21×10^{-4} to 3.29×10^{-4} m³/s. Computing time for each BMIX++ model with a normal desktop computer is less than five minutes.

Keywords

- Hydrogen leaks
- Buoyant jets
- Enclosure mixing
- Hydrogen Stratification

1. Introduction

The distribution and mixing of hydrogen with air is a crucial safety issue for two fields. One is the commercial use of hydrogen such as hydrogen-based vehicles and another is nuclear power plants. During a severe accident in a water-cooled nuclear reactor, large quantities of hydrogen can be released into the containment systems. The hydrogen generated by reactions between the steam and the superheated fuel cladding material can form a flammable and detonable mixture which may initiate a combustion. This combustion can damage and jeopardize the integrity of the containment systems. In the worst case, the safety function can be lost. The hydrogen explosions during the Fukushima Daiichi accident in March 2011 have showed that the hydrogen risk is a critical safety issue for nuclear power plants. One major factor of hydrogen deflagration or detonation is the local composition of the hydrogen-air mixture. Therefore an efficient prediction of the distribution of hydrogen in a large enclosure is critical to nuclear safety analyses.

Two thermal-hydraulic approaches have been used for the prediction of the hydrogen concentration in the containment systems: the lumped parameter (LP) models and the computational fluid dynamics (CFD) method. The LP models can provide a quick estimate on the averaged hydrogen distribution in the containment systems, so they are adapted by current major nuclear safety analysis codes such as RELAP5 (The RELAP5-3D® Code Development Team, 2005), TRAC (Spore et al., 2000), and MELCOR (US Nuclear Regulatory Commission, 2005). However, the accuracy of the LP models is severely limited due to the lack of consideration of general gas mixing and stratification. These models thus have limited or no ability to simulate the local composition of the hydrogen concentration for complex gas stratification and mixing situations.

High resolution 2-D or 3-D CFD codes can provide detailed information on hydrogen concentration and local phenomena. Therefore many researchers have been using CFD methods for studies on hydrogen distribution in nuclear reactor containments (Manninen et al., 2002; Prabhudharwadkar et al., 2011; Visser et al., 2012). However, these CFD codes require very fine grid resolution to resolve thin substructures, such as jets and wall boundaries. These codes are thus limited to analyze simple scenarios due to computational expenses. In addition, studies in the European Union show that current CFD analyses can not accurately predict the gases

distribution for complex mixing cases (Paladino et al., 2010). Therefore, it is desired to find other high fidelity and efficient gas mixing and stratification methods to improve the accuracy of nuclear safety analyses at reasonable computational cost. Houf and Schefer (2008) have reported a fast-running and slow-leak model for computing the trajectory of a buoyant jet and the decay of hydrogen concentration along the jet trajectory. El-Amin and Kanayama (2009) also have developed a similar model to predict the behavior of a hydrogen-air buoyant jet resulting from a small-scale hydrogen leakage in the air. El-Amin (2009) has further investigated the behavior of a vertical axisymmetric non-Boussinesq buoyant low-density jet.

The BMIX++ (UC Berkeley mechanistic MIXing code in C++) code is developed for solving transient mixing and heat transfer problems in stably stratified enclosures accurately and efficiently. Density, pressure, enthalpy, concentration, and temperature of the ambient fluid for each control volume are calculated in the BMIX++ code. In addition jet local information such as velocity, width, temperature, or concentration are also calculated by different jet models. This code is built upon the fact that the ambient gas mixture between hydrogen jets tends to organize into either a homogeneously mixed condition or a vertically stratified condition which can be described using 1-D partial differential equations (Peterson, 1994). The computational cost of a BMIX++ simulation is thus reduced dramatically compared to multi-dimensional CFD numerical modeling (Zhao, et al., 2014). The BMIX++ code has been successfully validated against multiple benchmark problems such as stratification in a water tank due to a heat source, stratification by multiple plumes and thermal stratification in a suppression pool (Christensen and Peterson, 2001; Zhao, 2003; Zhao and Peterson, 2009; Zhao, et al., 2014).

This paper reports two newly developed validation benchmarks of the BMIX++ code against a set of air-hydrogen and a set of air-helium experimental data, respectively. The mathematical and physical models included in this code and used in this benchmark validation work are the focus of the next section. Section 3 details the validation of the BMIX++ code by comparisons with experimental data, and Section 4 concludes the paper.

2. Mathematical and Physical Models in the BMIX++ code

This section summarizes the mathematical and physical models in BMIX++ used in this validation work including three models used in three distinct constituents—ambient fluid, a jet and a vent—in this enclosure. The general 1-D governing equations for mixing in a stably stratified enclosure are presented first. The Lagrangian method for the ambient fluid is briefly described next; following is Schatzmann's model for circular free curved buoyant jets; finally is the vent model. Note that the BMIX++ code is designed for generic mixing and heat transfer simulation including variable cross section areas, multiple jets and vents at different locations, wall heating or cooling, and multiple numbers of constituents. These along with the comprehensive mathematics and physics behind can be found in (Christensen and Peterson, 2001; Zhao, 2003; Zhao and Peterson, 2009).

2.1 One-Dimensional Governing Equations for Mixing in Stably Stratified Enclosure

Large enclosures mixed by buoyant plumes and jets can normally be assumed stratified. In addition, the transition between the well-mixed and stratification condition can be predicted [Peterson, 1994]. For example, the ambient fluid in an injected buoyant jet case is considered stably stratified when

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

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

$$Ri_{bjo} = \frac{(\rho_a - \rho_o)gd_{bjo}}{\rho_a U_o^2}, \quad (2)$$

where ρ_a is the ambient fluid density (kg/m³), ρ_o the source fluid density (kg/m³), g the gravity constant (m/s²), and U_o the jet source speed (m/s).

Therefore stratified mixing processes in large, complex enclosures can be predicted by 1-D differential

equations, with transport in free and wall jets modeled using integral models (Peterson, 1994). For a stratified enclosure, the governing equations for the ambient fluid can be written as the following form (Zhao and Peterson, 2009):

$$A(z) \frac{\partial \mathbf{G}}{\partial t} + \frac{\partial \mathbf{F}}{\partial z} = \mathbf{S}, \quad (3)$$

where $A(z)$ represents the horizontal cross sectional area of the ambient fluid at elevation z (m^2); $\mathbf{G}$ is the vector of conserved quantities,

$$\mathbf{G} = \begin{pmatrix} \rho \\ 0 \\ \rho h \\ \rho \chi_1 \\ \vdots \\ \rho \chi_{ns-1} \end{pmatrix},$$

where ρ is the mixture density of the ambient fluid ($\text{kg}\cdot\text{m}^{-3}$), h is the enthalpy of the ambient fluid ($\text{J}\cdot\text{kg}^{-1}$), χ is the mass fraction of each constituent of the ambient fluid, and the subscript ns denotes the total number of species; $\mathbf{F}$ is the vector of conserved fluxes,

$$\mathbf{F} = \begin{pmatrix} \rho Q_{sf} \\ P \\ \rho h Q_{sf} - Ak \frac{\partial T_{sf}}{\partial z} \\ \rho \chi_1 Q_{sf} - \rho AD \frac{\partial \chi_1}{\partial z} \\ \vdots \\ \rho \chi_{ns-1} Q_{sf} - \rho AD \frac{\partial \chi_{ns-1}}{\partial z} \end{pmatrix},$$

where Q is the volume flow rate ($\text{m}^3\cdot\text{s}^{-1}$), the subscript sf denotes the stratified ambient fluid, P is the pressure of the ambient fluid (Pa), A is the cross sectional area of the ambient fluid (m^2), k is the thermal conductivity of the ambient fluid ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$), T is the temperature of the ambient fluid (K), and D is the mass diffusion coefficient of the ambient fluid ($\text{m}^2\cdot\text{s}^{-1}$); $\mathbf{S}$ is the vectors of conserved source terms,

$$\mathbf{S} = \begin{pmatrix} -\sum_{k=1}^n (\rho Q')_k + \rho S' - \rho \hat{S}' \\ -\rho g \\ -\sum_{k=1}^n (\rho h Q')_k + \rho S'_h - \rho \hat{S}'_h \\ -\sum_{k=1}^n (\rho \chi_1 Q')_k + \rho \chi_1 S' - \rho \chi_1 \hat{S}' \\ \vdots \\ -\sum_{k=1}^n (\rho \chi_{ns-1} Q')_k + \rho \chi_{ns-1} S' - \rho \chi_{ns-1} \hat{S}' \end{pmatrix},$$

where Q' is the volumetric jet entrainment rate per unit length ($\text{m}^3 \cdot \text{s}^{-1}$), n is the total number of jets, S' is the volumetric jet source per unit length ($\text{m}^3 \cdot \text{s}^{-1}$), $\hat{S}'$ is the volumetric sink per unit length ($\text{m}^3 \cdot \text{s}^{-1}$), S'_h is volumetric energy source per unit length ($\text{W} \cdot \text{s}^{-1}$), and $\hat{S}'_h$ is the volumetric energy sink per unit length ($\text{W} \cdot \text{s}^{-1}$).

Equation (3) is a compact form of the governing equations of the ambient fluid in a stratified enclosure, which can be divided into a user-specified number of horizontal control volumes (CVs). A Lagrangian method is then used to track the physical properties of these CVs for each time step. Fig. 1 shows an illustration of the grids for the ambient fluid (black) and a jet (red), where F_0 indicates the injection. Both grids are functions of location and time (t). The ambient mesh is dynamically determined by the evolution of the Lagrangian CVs and precision control methods such as the gradients of the ambient concentration or temperature, or by the minimal CV size. The size of the jet mesh is controlled by the local transitional error, which can be selected by the user. The jet mesh is along the jet streamline s , which can be a function of vertical (z) and horizontal (y) coordinates as shown later in this paper. The blue arrows indicate the entrainment flow and the jet discharge process. Piecewise linear functions are used for the exchange of information between the ambient and the jet(s).

Fig. 1- Illustration of the distinct grids for the jet (F_0) and the ambient fluid.

2.2 Lagrangian Method for the Ambient Fluid

The following three discrete Lagrangian conservation equations are used to calculate the new position, compositions and enthalpies of the CVs for each time step. The composition and energy are then corrected based on the diffusion terms in the conservation equations (Christensen and Peterson, 2001):

- Conservation of mass:

$$\frac{V_k^{j+1} - V_k^j}{\Delta t} = - \sum_{l=1}^L Q_{k,l}^j + f(k+1) - f(k) + S_k^j - \hat{S}_k^j, \quad (4)$$

where $f(k) = A_k^j \sum_{i=1}^I \dot{V}_{i,k}^j$, where A is the horizontal cross-sectional area of the ambient fluid (m^2), $\dot{V}''$ is the volumetric flow rate per unit area due to molecular diffusion ($\text{m} \cdot \text{s}^{-1}$), the subscript i corresponds to the i th component of the ambient fluid, I is the total number of fluid components presenting in the enclosure, the subscript k indicates the k th CV; the subscript l indicates the l th buoyant jet, L is the total number of buoyant jets presenting in the enclosure, the superscripts j and $j+1$ indicate the time step, Δt is the time step length

(second), V is the volume of the CV (m^3), $Q_{k,l}^j$ is the volumetric flow rate entrained by buoyant jet l within the k th CV ($\text{m}^3 \cdot \text{s}^{-1}$), S is the volume source of the ambient fluid ($\text{m}^3 \cdot \text{s}^{-1}$), and $\hat{S}$ is the volume sink of the ambient fluid ($\text{m}^3 \cdot \text{s}^{-1}$).

- Conservation of species mass:

$$\frac{\bar{\chi}_{i,k}^{j+1} V_k^{j+1} - \bar{\chi}_{i,k}^j V_k^j}{\Delta t} = -\bar{\chi}_{i,k}^j \sum_{l=1}^L Q_{k,l}^j + g(i, j, k+1) - g(i, j, k) + S_{i,k}^j - \hat{S}_{i,k}^j \quad (5)$$

$$\text{for } i = 1, 2, \dots, (I-1),$$

where $g(i, j, k) = A_k^j \dot{V}_{i,k}^j$, and $\bar{\chi}_{i,k}$ is the volume-averaged mass fraction of the i th component of the ambient fluid within the k th CV.

- Conservation of energy:

$$\frac{\bar{h}_{k,mix}^{j+1} V_k^{j+1} - \bar{h}_{k,mix}^j V_k^j}{\Delta t} = -p1(j, k) + p2(j, k+1) - p2(j, k) + p3(j, k), \quad (6)$$

where $\bar{h}_{mix}$ is the volume-averaged mixture enthalpy ($\text{J} \cdot \text{kg}^{-1}$),

$$p1(j, k) = \sum_{i=1}^I \bar{h}_{i,mix}^j \bar{\chi}_{i,k}^j \sum_{l=1}^L Q_{k,l}^j,$$

$$p2(j, k) = A_k^j \sum_{i=1}^I \bar{h}_{i,a_{i,k}}^j \dot{V}_{i,k}^j,$$

$$p3(j, k) = \frac{1}{\bar{\rho}} (A_{k+1}^j q_{k+1}^{''j} - A_k^j q_k^{''j} + S_{h,k}^j - \hat{S}_{h,k}^j),$$

where $\bar{\rho}$ is the volume-averaged total density ($\text{kg} \cdot \text{m}^{-3}$), q'' is the heat flux due to heat diffusion ($\text{W} \cdot \text{m}^{-2}$), S_h is the source of energy per unit time (W), and $\hat{S}_h$ is the sink of energy per unit time (W). The subscript $a_{i,k}$ is defined by

$$a_{i,k} \equiv \begin{cases} k, & \frac{\partial \chi_{i(z_k)}}{\partial z} > 0. \\ k-1, & \text{otherwise} \end{cases}$$

In addition, two volume-based grid managements are available in the BMIX++ code for long simulation time. The first one is based on the relative minimal volume of CVs. The second one is based on the relative minimal concentration of one user-specified constituent or temperature difference between two neighboring CVs. These two volume-based grid management algorithms search all the CVs, find out CVs whose volumes are less than the user-specified minimal value, and merge those CVs with their smaller neighbor CVs. The user should be cautious in choosing the values of these grid management parameters since they affect the coarseness of the ambient fluid mesh. The mesh tends to be merged into few big volumes if large values of the management parameters are used; the mesh will become over-refined with time if very small values are used. The recommended relative minimal volume value and relative minimal concentration value are between 10^{-2} and 10^{-4} . In this paper, simulations use values of around 10^{-3} .

The evolution of the ambient fluid has a close relationship with the injected jets. The BMIX++ code includes several jet models such as a plume (due to a heat source), a pure jet (due to an initial momentum source), a buoyant jet (due to both buoyancy and momentum), a wall jet along a wall surface, and a wall boundary flow. The mathematical expression for circular buoyant jets used in this validation work is briefly introduced in the next section. Information on other jet models of BMIX++ can be found in (Zhao, 2003).

2.3 Schatzmann's Model for Circular Free Curved Buoyant Jets

Schatzmann's model is based on the differential equations for the conservation of mass, momentum, thermal energy, and concentration with a trajectory equation. The simplified Schatzmann's model for the quiescent ambient is implemented in the BMIX++ code with the following governing equations:

- Mass conservation equation with the entrainment assumption by Teixeira and Miranda (Teixeira and Miranda, 1997):

$$\frac{d}{ds} \left[\left(\rho_a + \frac{\lambda^2}{\lambda^2 + 1} \rho^* \right) u^* b^2 \right] = 2\rho_a b u^* \left(3\beta - \frac{(2\lambda^2 - 1)\lambda^2 \sin \theta}{\lambda^2 + 1} \frac{1}{Fr^2} \right), \quad (7)$$

where ρ_a indicates the density of the ambient fluid ($\text{kg}\cdot\text{m}^{-3}$), λ is the ratio of the spreading of the density and

velocity profiles, ρ^* is the centerline excess density over the ambient value ($\text{kg}\cdot\text{m}^{-3}$), u^* is the jet centerline velocity ($\text{m}\cdot\text{s}^{-1}$), b is the characteristic jet width (m, see Fig. 2 for an illustration), β is a coefficient in entrainment models which should fall in the range from 0.08 to 1.0 (Cariteau et al., 2011), θ is the angle with the horizontal direction (radian), and

$$Fr^2 = \frac{(u^*)^2}{(gb)\frac{\rho^*}{\rho_a}}, \quad (8)$$

where g is the gravitational acceleration ($\text{m}\cdot\text{s}^{-2}$).

- s-direction momentum conservation equation (s is the distance along the jet axis. See Fig. 1 for an illustration):

$$\frac{d}{ds} \left[\left(\frac{1}{2}\rho_a + \frac{\lambda^2}{2\lambda^2+1}\rho^* \right) (u^*)^2 b^2 \right] = -\lambda^2 b^2 \rho^* g \sin \theta. \quad (9)$$

- θ -direction momentum conservation equation:

$$\frac{d\theta}{ds} = -\frac{\lambda^2 g \rho^* \cos \theta}{(u^*)^2 \left(\frac{1}{2}\rho_a + \frac{\lambda^2}{2\lambda^2+1}\rho^* \right)}. \quad (10)$$

- Energy conservation equation:

$$\frac{d}{ds} \left[\left(\frac{\lambda^2}{\lambda^2+1}\rho_a + \frac{\lambda^2}{\lambda^2+2}\rho^* \right) b^2 u^* T^* \right] = -\left(\frac{dT_a}{ds} \right) (b^2 u^*) \left(\rho_a + \frac{\lambda^2}{\lambda^2+1}\rho^* \right). \quad (11)$$

where T^* is the centerline excess temperature over the ambient value (K) and T_a is the ambient temperature (K).

- Mass concentration of component i equation:

$$\frac{d}{ds} \left[\left(\frac{\lambda^2}{\lambda^2+1}\rho_a + \frac{\lambda^2}{\lambda^2+2}\rho^* \right) b^2 u^* c_i^* \right] = -\left(\frac{dc_{ia}}{ds} \right) (b^2 u^*) \left(\rho_a + \frac{\lambda^2}{\lambda^2+1}\rho^* \right) \quad (12)$$

$$\text{for } i = 1, 2, \dots, I-1,$$

where c_i^* is the mass concentration of component i of the jet (kg/kg), c_{ia} is the mass concentration of component i of the ambient fluid (kg/kg), and I is the total number of components in the enclosure.

- Trajectory equation:

$$\frac{dx}{ds} = \cos \theta, \quad (13)$$

$$\frac{dz}{ds} = \sin \theta. \quad (14)$$

Fig. 2 - A coordinate system used for buoyant jet analysis (Zhao and Peterson, 2009).

In addition to these conservation equations, two more equations are necessary to predict a gas mixing behavior. As a jet exits a leak, the turbulent mixing fluid layers at the edges of the jet begin to grow and eventually expand to merge at the centerline of the jet. At this point, the jet is considered to be in the zone of the established flow and it is found that the time-averaged jet velocity profiles are nearly Gaussian and of the form:

$$\frac{u_{(s,r)}}{u^*_{(s)}} = e^{-r^2/b_{(s)}^2}, \quad (15)$$

where r is the distance from jet centerline (m, see Fig. 2 for an illustration) and $u_{(s,r)}$ is the velocity at location (s, r) ($\text{m}\cdot\text{s}^{-1}$). The profile of the time-averaged jet scalars is also Gaussian within the zone of the established flow:

$$\frac{\rho_{(s,r)} - \rho_a}{\rho^*_{(s)}} = e^{-r^2/(\lambda b_{(s)})^2}, \quad (16)$$

where $\rho_{(s,r)}$ is the density at location (s, r) ($\text{kg}\cdot\text{m}^{-3}$) (Houf and Schefer, 2008).

Seven variables are to be solved for the above equation set: the centerline velocity, u^* ; the

characteristic jet width, b ; the centerline temperature excess, T^* ; the angle, θ ; the horizontal coordinate, x ; the vertical coordinate, z ; the mass concentration of component i , c_i . In addition, the jet source conditions are necessary for solving the abovementioned equations. For buoyant jets with an initial flow rate, the initial conditions have been derived from the results of several experiments [Davidson, 1986]. For the benchmark BMIX++ models presented in this paper, the initial point of buoyant jets, S_0 , with an initial flow rate is set as

$$S_0 = n \times d, \quad (17)$$

where d is the diameter of the jet source (m) and n is a constant value of 6.0. The jet trajectory angle of the initial point is given empirically as

$$\theta_0 = \theta_j, \quad (18)$$

where j is the jet source condition. The initial values of the rest of the jet variables are obtained by balancing fluxes through the flow development region with an assumption of no entrainment from the ambient fluid. This assumption is obtained by observed experimental studies on jet behaviors that the jet-ambient boundary is smooth in the developing region and the jet can entrain ambient fluid only after the vortex begins to form at the boundary. This is generally true when a jet comes from a long pipe. The initial values of the rest of the jet variables are

$$u_0^* = u_j^*, \quad (19)$$

$$b_0 = \frac{d}{\sqrt{2}}, \quad (20)$$

$$T_0^* = T_j^* \frac{\lambda^2 + 1}{2\lambda^2}, \quad (21)$$

$$c_{i0}^* = c_{ij}^* \frac{\lambda^2 + 1}{2\lambda^2}, \quad i = 1, 2, \dots, I - 1. \quad (22)$$

This jet model is one significant portion of the vent model, which is introduced next.

2.4 The Vent Model

The definition of “vent” in the BMIX++ code is an opening connecting an enclosure with a steady, large ambient environment. The vent model is formed with a pair of a jet model and a sink model. The states of the

jet model and the sink model are dynamically changed according to the opening flow. The flow inside the vent is assumed unidirectional.

If the fluid inside the enclosure is flowed out of the enclosure, the jet is set to be zero injection and the flow rate of the sink is computed using the following two equations:

$$\dot{m} = CA\sqrt{2\rho\Delta P}, \quad (23)$$

where $\dot{m}$ is the mass flow rate ($\text{kg}\cdot\text{s}^{-1}$), C is the coefficient of the opening flow set as 0.7, A is the cross sectional area of the vent (m^2), ρ is the density of the fluid at the source side ($\text{kg}\cdot\text{m}^{-3}$) and ΔP is the absolute value of the pressure difference between the enclosure and the ambient environment (Pa). The system pressure is solved with the following equation:

$$\frac{dP}{dt} = \frac{(\gamma-1)}{V} \left(\sum_{i=1}^I \dot{m}_i h_i + \sum_{j=1}^J Q_j \right), \quad (24)$$

where t is time (second), γ is the ratio of specific heats, V is the total compressible volume of the enclosure (m^3), h_i is the enthalpy of the i th constitute ($\text{J}\cdot\text{kg}^{-1}$), and Q_j is the j th heat input or output of the enclosure ($\text{W}\cdot\text{m}^{-2}$). Equation (24) is the energy conservation equation for the lumped compressible volume (Fu and Hadjisophocleous, 2000). For the enclosure connected with a stable ambient environment through an opening, Equations (22) can be discretized as

$$\frac{P^{n+1}-P^n}{dt} = \frac{(\gamma-1)}{V} \left(\sum_{i=1}^I \dot{m}_i^n h_i^n + \sum_{j=1}^J Q_j^n \right) + \frac{(\gamma-1)}{V} \dot{m}_V^n h_V^n, \quad (25)$$

where the superscript $n + 1$ indicates the next time step, the superscript n indicates the current time step, and the subscript V indicates the vent flow. Equation (23) is solved using the bipartition method (Teodorescu P. et al., 2013).

If the outside fluid is flowed into the enclosure through the vent, the mass flow rate of the jet is computed using Equations (23) and (25), and the flow rate of the sink is set to be zero. Note that in this in-flow

case, the vent is considered as a jet with the outside condition as the source. If the fluid flows out of the enclosure, the mass flow rate of the sink is computed using Equations (23) and (25) and the flow rate of the jet is set to zero.

Equations (3) to (25) implemented in the BMIX++ code are used in two newly developed BMIX++ benchmark models. The next section details the validation.

3. Validation of the BMIX++ code

The BMIX++ simulations are compared to the results of the experiments performed at Sandia National Laboratories and DEN/DANS/DM2S/SFME/ Laboratoire. These simulations are run in a desktop computer with Intel Core 2 Duo CPU E6550 @ 2.33 GHz x2 and 7.7 GiB memory. The operation system is 64-bit Ubuntu 12.04 LTS. The computational time for each BMIX++ simulation is less than 5 minutes.

3.1 Validation of the BMIX++ Code Against Air-Hydrogen Experimental Data

The first BMIX++ benchmark simulations were compared to the results from Houf and Schefer's slow leak experiment (Houf and Schefer, 2008) with two Froude numbers, $Fr=99$ and $Fr=268$. Note that the BMIX++ jet model is designed for general use and these are just two validation cases. The Froude number is defined in equation (8). The condition of the gas exiting the jet was same as the ambient condition of 21°C and 100 kPa. The jet source was at the ground level and orientated vertically upward in an open space; and a constant cross-sectional area of the ambient fluid was assumed. The injection was assumed to be pure hydrogen.

For the first case with the Froude number of 99, the volume flow rate of the injected hydrogen was $1.424 \times 10^{-4} \text{ m}^3 \cdot \text{s}^{-1}$ with the diameter of the jet tube of 1.91 mm. The entrainment coefficient (β) was 0.09 and the ratio of spreading of the density and velocity profile (λ) was 1.16. The Reynolds number of 900 is 1.8% greater than that provided by the experimental data. Fig. 3 shows the time-average jet velocities from the experiment and simulation along jet centerline as a function of normalized axial distance, which is defined as the ratio of the axial distance (z) to the jet exit diameter (d). Fig. 4 shows the time-average mass fractions of

hydrogen from the experiment and simulation as a function of normalized axial distance. The present BMIX++ data show excellent agreement with experimental data.

Fig. 3 - Comparison of simulation of hydrogen centerline velocity in turbulent non reacting hydrogen jets ($Fr=99$, $Re=900$) with the experimental data ($Fr=99$, $Re=884$) from Schefer et al. (2008).

Fig. 4 - Comparison of simulation of hydrogen mass fraction in turbulent non reacting hydrogen jets ($Fr=99$, $Re=900$) with the experimental data ($Fr=99$, $Re=884$) from Schefer et al. (2008).

Fig. 5 and Fig. 6 show the computed hydrogen mass fractions and the hydrogen centerline velocities with $Fr = 268$ compared to experimental data from Schefer et al. (2008). Excellent agreement is observed. The

BMIX++ model is exactly the same as that described in the previous case except for the entrainment coefficient and the volume flow rate. The entrainment coefficient used here is 0.08 and the volume flow rate of $3.837 \times 10^{-4} \text{ m}^3 \cdot \text{s}^{-1}$ with Reynolds number of 2425 which is 1.7% greater than that provided by the experimental data.

Fig. 5 - Comparison of simulation of hydrogen centerline velocity in turbulent non-reacting hydrogen jets ($Fr=268$, $Re=2425$) with the experimental data ($Fr=268$, $Re=2384$) from Schefer et al. (2008).

Fig. 6 - Comparison of simulation of hydrogen mass fraction in turbulent non-reacting hydrogen jets ($Fr=268$, $Re=2425$) with the experimental data ($Fr=268$, $Re=2384$) from Schefer et al. (2008).

Note that the entrainment coefficient of 0.09 and 0.08 were found to fit the experimental data with

$Fr=99$ and $Fr=268$ best, respectively. These values agree with Cartieau et al.'s observation (2011). Schefer et al. (2008) observed that a transition from the jet limit to the plume limit begins at about $Z/d = 40$. It can be seen in Fig. 3 through Fig. 6 that the BMIX++ simulation with Schatzmann's model fit the plume (buoyancy-dominated) regions better than the jet (momentum-dominated) regions.

3.2 Validation of the BMIX++ code Against Air-Helium Experimental Data

The computational result from the second BMIX++ benchmark model was compared to the experimental measurements by Cariteau et al. (2011). Inside the tightly-sealed enclosure was a vent of 200 mm diameter located 160 mm above the floor. The height of the enclosure was 2.42 m. The temperature and pressure of the jet were assumed the same as those of the steady air in the enclosure. An isothermal condition of 19°C was adopted even though the temperature of the experiment was between $18.1 \pm 0.2^\circ\text{C}$ and $20.9 \pm 0.3^\circ\text{C}$. There was no information on the pressure, and 101,325 Pa was used in the simulation. The initial condition of this enclosure was full of steady air. Helium was injected through a 70 mm diameter vertical nozzle which exited 210 mm above the floor. Fig. 7 shows the schematic BMIX++ simulation model. The jet and the sink are simulated with the Schwartzman's jet model and the vent model, respectively. The entrainment coefficient used was 0.08. The cross-sectional area of the ambient fluid of the enclosure was assumed as a constant value of 17.0496 m^2 .

Fig. 7 - Schematic BMIX++ simulation model for the air-helium mixing experiment.

Since the BMIX++ code computed the mass fractions of the ambient fluid while the experimental data were the volume fractions of the ambient fluid, a conversion equation was needed for each CV,

$$volume\ fraction\ of\ CV = \frac{1}{1 + \left(\frac{1}{mass\ fraction\ of\ CV} - 1 \right) \frac{\rho_{(He)}}{\rho_{(air)}}}, \quad (26)$$

where $\rho_{(He)}$ was the density of helium with a value of $0.167\ (kg \cdot m^{-3})$, and $\rho_{(air)}$ was the density of air with a value of $1.2125\ (kg \cdot m^{-3})$. The total volume fraction of helium in the enclosure was obtained by the equation,

$$volume\ fraction = \frac{\sum_{i=1}^I (volume\ fraction\ of\ CV_i) \times V_i}{total\ volume}, \quad (27)$$

where the subscript i corresponds to the i th CV, I is the total number of CVs, and V_i is the volume of the i th CV (m^3). Fig. 8 compares the BMIX++ simulation results with jet flow rates ranging from 1.21×10^{-4} to $3.29 \times 10^{-4}\ m^3/s$ to experimental data from Cariteau et al. (2011), and it is found that the error is within a margin of about 10%. Fig. 8 also validates that the vent model of the BMIX++ code can be applied to these complex gas stratification and mixing situations.

Fig.8 - Comparison of simulations of helium average volume fractions in the ambient fluid to the experimental data from Cariteau et al. (2011) for jet flow rates ranging from 1.21×10^{-4} to $3.29 \times 10^{-4}\ m^3/s$.

4. Conclusions

The BMIX++ code is developed to accurately and efficiently simulate fluid mixing and heat transfer in large stratified enclosures. This code includes the scaling based one-dimensional model for the ambient fluid, several one-dimensional buoyant jet models, and a vent model. These models were used to develop two benchmark simulation models for two sets of experimental data. One BMIX++ benchmark model is for a single buoyant jet in an open space and another is for a gas mixing experiment in a large sealed enclosure with both a jet source and a vent near the floor. Both BMIX++ benchmark models are validated by comparing the computational results with experimental data. The entrainment coefficient of 0.09 and 0.08 are found to fit the experimental data for hydrogen leaks with the Froude number of 99 and 268 best, respectively. In addition, the BMIX++ simulation results of the average helium concentration for a enclosure with a vent and a single jet agree with the experimental data within a margin of about 10% for jet flow rates ranging from 1.21×10^{-4} to 3.29×10^{-4} m³/s. Simulation time for each of the abovementioned BMIX++ models with a normal desktop computer is less than five minutes.

Although the BMIX++ code is designed as a general mixing and heat transfer code which can predict the mechanical properties of fluids with multiple jets and multiple vents at different locations in enclosures with variable cross section areas, this paper only validates the single hydrogen jet model and the simple one jet and one vent mixing model. Therefore, future work should include more validation works covering a wider range of mixing configurations and more complex cases. In addition, for larger openings, in-flow and out-flow through the opening may exist at the same time. A large opening model had been developed in the BMIX++ code for fire analysis (Zhao, 2003); however, the application of the large opening model for hydrogen mixing needs to be validated in the future. For severe accident applications, it is necessary to develop condensation jet models for hydrogen mixing in a nuclear power reactor containment where air, hydrogen and steam often co-exist.

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