Development and verification of a multi-species gas transport solver

Vijaya Kumar G, IIT Madras, India & Forschungszentrum Juelich, Germany

Manohar Kampili, Forschungszentrum Juelich, Germany

Stephan Kelm, Forschungszentrum Juelich, Germany

Hans-Josef Allelein, Forschungszentrum Juelich, Germany

During a severe nuclear reactor accident, large amounts of hydrogen, steam and other non-condensable gases are released into the reactor containment. Hydrogen gas can accumulate in significant proportions in some parts of the containment, and subsequent hydrogen combustion (like in Fukushima Daiichi NPP) may result in structural failures, which may allow the release of harmful radioactive material into the environment. Hence, it becomes essential to predict hydrogen and steam distribution in containment for the design and assessment of effective hydrogen mitigation methods. Ongoing work at Forschungszentrum Juelich aims at developing a dedicated solver 'containmentFOAM' which has the capabilities to handle multi-species turbulent gas transport, conjugate heat transfer, aerosol/particle transport, and radiative heat transfer. The 'reactingParcelFoam' solver available in OpenFOAM-6 is chosen as the base solver for 'containmentFOAM'. Multi-species gas transport is the focus of this paper. In the application mentioned above, gas mixing phenomenon occurs among gases with significant difference in specific enthalpies $(C_p \text{ of } H_2 = 14.32 \text{ kJ/kg.K}, C_p \text{ of } Air = 1.01 \text{ kJ/kg.K}, C_P \text{ of } H2O = 1.864 \text{ kJ/kg.K})$. The base solver has deficiencies in modeling such multi-species gas transport phenomenon and produces incorrect temperature field even on isothermal cases. Incorrect enthalpy transport equation results in a wrong temperature field and hence an incorrect density field, eventually leading to solver instability and poor results. The energy equation was modified to account for (i) enthalpy transport due to inter-species diffusion (ii) varying specific enthalpy values of different species. The overall solver stability is improved by introducing an additional density corrector step in PIMPLE algorithm. The paper discusses the successive modifications and highlights their effects systematically based on simple 1D cases. Finally, the general applicability of the solver is demonstrated on a 2D mixing layer case.

1 Background and Motivation

During a severe accident in water-cooled nuclear power plants, large amounts of hydrogen and steam are released into the reactor containment building. Hydrogen so released can accumulate in flammable proportions in certain parts of the containment and eventually result in combustion (like in Fukushima Daiichi NPP). This may challenge the structural integrity of the containment and may result in release of harmful radioactive materials to the outside environment affecting civilian life in the vicinity of the power plant. To have effective hydrogen mitigation methods, simulation tools to predict the hydrogen gas distribution in severe accident scenarios are nec-

essary.

Since several years CFD models, mostly based on commercial CFD codes [6, 7] are used to predict hydrogen gas distribution and mixing in a containment in severe accident scenarios. In recent times, the open source CFD code OpenFOAM is gaining attention among users in industry and academia alike. OpenFOAM has seriously improved in the recent years with respect to increased choice of models and robust numerical schemes. The most attractive feature of OpenFOAM is the complete source code accessibility because this permits for continuous improvement of the existing models.

Though OpenFOAM is getting popular in Nuclear safety research field, all the works seems to be tar-

Arul Prakash K, IIT Madras, India

geted towards specific phenomena only. A dedicated solver which can perform an integral analysis of a severe accident sequence is not available at the moment. For instance, in the fire safety research field there is a dedicated solver called as 'fire-FOAM', developed by FM Global aims at modeling fire spreading and suppression. It comprises robust models for the analysis of turbulent combustible gas and smoke transport, pyrolysis, combustion, thermal radiation, sprinklers and fire suppression systems [8]. It is successfully used to disseminate knowledge and thus ensure improved mitigation concept design and safety concepts. Taking a cue from 'fireFOAM', ongoing work at Forschungzentrum Juelich aims to develop and validate a tailored solver 'containmentFOAM' along with relevant model libraries to analyse the different scenarios that may arise during a severe accident in a nuclear reactor containment.

The 'containmentFoam' solver is developed to handle multicomponent gas mixing, conjugate heat transfer along with thermal radiation heat transfer and steam condensation. Supplementary libraries are developed to handle radioactive nuclear aerosol transport. This paper discusses the details of the 'containmentFOAM' solver development only within the purview of multicomponent gas mixing. The 'reactingParcelFoam' (RPF) solver available in OpenFOAM-6 is chosen as the base solver for 'containmentFOAM' because it has the capability to handle multicomponent gas transport and heat transfer. It is also well integrated with libraries to compute aerosol transport and thermal radiation phenomenon. In section 2, the governing equations used to model multicomponent gas flows are summarized. The deficiencies present in the governing equations of the base solver are identified and suitable corrections are made to 'containment-Foam' solver. In section 3, the algorithm present in the 'containmentFoam' solver is discussed in detail. In section 4, the base solver instability is identified and is mainly caused due to incorrect equations and deficiency present in the PIMPLE iterative algorithm. In section 5, a series of systematic test cases are discussed by isolating the individual phenomena present in multicomponent gas flows such as (i) binary diffusion (ii) heat conduction and (iii) convective transport. Finally, the correctness of the 'containmentFoam' solver is finally verified by simulating a two dimensional mixing channel test case where all the three major phenomena coexist along with turbulence.

2 Governing Equations

2.1 Mass conservation equations

2.1.1 Species mass conservation

If there are n species of gases in the multicomponent system, the species mass conservation for specie i can be written as

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{U}) = -\nabla \cdot F_i, \quad i \in S \qquad (1)$$

where ρ_i is the mass density of specie *i*, **U** is the mass averaged flow velocity, F_i is the diffusion flux of the *i*th specie and *S* is the set of the gas species indices given by $S = \{1, 2, ..., n\}$.

The species mass fractions $Y_i, i \in S$ are defined by,

$$Y_i = \frac{\rho_i}{\rho}, \quad i \in S \tag{2}$$

where ρ is the total density given by

$$\rho = \sum_{i \in S} \rho_i \tag{3}$$

Due to Eqn. 3, the species mass fractions Y_i satisfy the condition,

$$\sum_{i \in S} Y_i = 1 \tag{4}$$

The species mass conservation equation (Eqn.1) can be rewritten in terms of the species mass fractions as

$$\frac{\partial \left(\rho Y_{i}\right)}{\partial t} + \nabla \cdot \left(\rho \mathbf{U} Y_{i}\right) = -\nabla \cdot F_{i}, \quad i \in S \qquad (5)$$

where F_i is the diffusive flux of specie *i* given by

$$F_i = -\rho D_i \nabla Y_i \tag{6}$$

where D_i is the effective molecular diffusivity of the specie i in the multi-component gas medium. Since the present discussion is restricted to two species,

$$D_i = D_{12} \tag{7}$$

where D_{12} is the binary diffusivity of two gas species calculated in accordance with the Fuller model [2].

However, in the RPF solver, the kinematic viscosity ν is used instead of the effective molecular diffusivity D_i .

2.1.2 Total mass conservation

The n species mass conservation equations can be summed to derive the total mass conservation equation in terms of total density.

$$\sum_{i \in S} \frac{\partial \left(\rho Y_{i}\right)}{\partial t} + \sum_{i \in S} \nabla \cdot \left(\rho \mathbf{U} Y_{i}\right) = -\sum_{i \in S} \nabla \cdot F_{i}, \quad i \in S$$
(8)

The diffusive flux F_i is only due to motion of the gas molecules and there should not be any net bulk flow caused to diffusion i.e. the sum of diffusive mass fluxes should go to zero.

$$\sum_{i \in S} F_i = 0 \tag{9}$$

From the relations in Eqn.4 and Eqn.9, the total mass conservation equation (Eqn.8) becomes

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \tag{10}$$

2.1.3 Methods to solve the mass conservation equations

It must be noted that the *n* species mass conservation equations (Eqn.5) and the total mass conservation equation (Eqn.10) are linearly dependent. Hence, it is only possible to either solve for *n* species mass conservation equations with the unknowns $(Y_1, Y_2, ..., Y_n)$ or solve the total mass conservation equation along with the species mass conservation equations for n - 1 species with the unknowns $(\rho, Y_1, Y_2, ..., Y_{n-1})$ and evaluate the species mass fraction of n^{th} specie Y_n by imposing the constraint in Eqn.8 as

$$Y_n = 1 - \sum_{i \neq n} Y_i \tag{11}$$

The latter method is used in the RPF solver as well [3].

2.1.4 Gas mixture properties

The gas mixture properties such as dynamic viscosity (μ), specific heat capacity (C_p) and thermal diffusivity (α) are calculated by assuming an ideal mixture relation. Any arbitrary mixture property ϕ can be computed from the specie properties ϕ_i and specie mass fractions Y_i , $i \in S$.

$$\phi = \sum_{i \in S} Y_i \phi_i \tag{12}$$

2.2 Momentum conservation equation

The momentum conservation equation to evaluate the average flow velocity \mathbf{U} is given by

$$\frac{\partial \left(\rho \mathbf{U}\right)}{\partial t} + \nabla \cdot \left(\rho \mathbf{U} \otimes \mathbf{U}\right) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g}$$
(13)

where τ is the viscous stress tensor, p is the pressure and **g** is the acceleration due to gravity. The viscous stress tensor is given by

$$\tau = \rho \nu \left[\nabla \mathbf{U} + (\nabla \mathbf{U})^T - \frac{2}{3} \delta \nabla \cdot \mathbf{U} \right]$$
(14)

where ν is the kinematic viscosity of the gas mixture and δ is the Kronecker delta.

2.3 Energy conservation equation

The energy equation implemented in the RPF solver is in the total enthalpy form (Eqn.15). From here on, the enthalpy and kinetic energy mentioned correspond to the specific properties (per unit mass) only. The source terms due to radiation and particles are irrelevant for the present work and hence a discussion on them is ignored here.

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{U}h) + \frac{\partial(\rho K)}{\partial t} + \nabla \cdot (\rho \mathbf{U}K) = \frac{\partial p}{\partial t} + \rho \mathbf{U} \cdot \mathbf{g} - \nabla \cdot \mathbf{Q} - \nabla \cdot \sum_{i=1}^{n} F_i h_i$$
(15)

All the terms in the LHS together constitute the material derivative of total enthalpy h_{tot} defined by

$$h_{tot} = h + K \tag{16}$$

where h is the static enthalpy, K is the total kinetic energy and \mathbf{Q} is the conductive heat flux. K is defined by

$$K = \frac{|\mathbf{U}|^2}{2} \tag{17}$$

The first and second terms in the LHS of the energy equation (Eqn.15) correspond to the material derivatives of static enthalpy. Since, static enthalpy h is the unknown, these terms are implicit i.e. **fvm** terms in OpenFOAM parlance. The third and fourth terms in the LHS is to account for the material derivative of total kinetic energy K and are treated as explicit terms i.e **fvc**. The first and second terms in the RHS of the energy equation accounts for the rate of change of potential energy respectively. The third term in the RHS represents the heat conduction term due to temperature gradients.

2.3.1 Heat conduction

The third term in the RHS of the energy equation (Eqn.15) represents the contribution of heat conduction. Two formulations $\mathbf{Q_T}$ and $\mathbf{Q_h}$ of the conductive heat flux \mathbf{Q} are considered. According to Fourier's law of heat conduction, the heat flux $\mathbf{Q_T}$ is defined in terms of gradient of temperature as

$$\mathbf{Q_T} = -\lambda \nabla T \tag{18}$$

where λ is the thermal conductivity of the gas mixture. But in the RPF solver, **Q** is implemented in terms of gradient of static enthalpy as

$$\mathbf{Q_h} = -\alpha \nabla h \tag{19}$$

where α is the thermal diffusivity of the gas mixture. α and λ are related by

$$\alpha = \frac{\lambda}{C_p} \tag{20}$$

where C_p is the specific heat capacity of the gas mixture at constant pressure.

The two formulation $\mathbf{Q_T}$ and $\mathbf{Q_h}$ are not identical. The enthalpy of the gas mixture h in terms of specie enthalpies $h_i, i \in S$ is

$$h = \sum_{i=1}^{n} h_i Y_i \tag{21}$$

The static enthalpy of an ideal gas specie i is defined by

$$h_i = h_{ref,i} + \int_{T_{ref}}^T C_{p,i} dT \tag{22}$$

where $h_{ref,i}$ is the enthalpy of formation of the specie *i* at reference temperature T_{ref} and $C_{p,i}$ is the specific heat capacity of the gas specie *i* at constant pressure. In the present work only sensible enthalpy formulation is used ($h_{ref,i}=0$) and the reference temperature is absolute zero ($T_{ref}=0$). If the ideal gas assumption is made, $C_{p,i}$ is only a function of temperature.

Eqn.22 becomes

$$h_i = \int_0^T C_{p,i} dT \tag{23}$$

On evaluation of gradient of enthalpy ∇h ,

$$\nabla h = \sum_{i=1}^{n} \nabla (h_i Y_i)$$

$$= \sum_{i=1}^{n} h_i \nabla Y_i + \sum_{i=1}^{n} Y_i \nabla h_i$$
(24)

Consider only ∇h_i term in index notation.

$$\nabla h_i = \frac{\partial h_i}{\partial x_j} \hat{\mathbf{e}_j}$$

With specie enthalpy h_i formulation from Eqn.23,

$$\frac{\partial h_i}{\partial x_j} = \frac{\partial}{\partial x_j} \int_0^T C_{p,i} dT$$

Temperature field T varies in space and hence, $C_{p,i}$ which is a function of T also varies in space. By the Liebniz's differential under the integral rule,

$$\frac{\partial h_i}{\partial x_j} = C_{p,i} \frac{\partial T}{\partial x_j} + \int_0^T \frac{\partial C_{p,i}}{\partial x_j} dT$$

$$\nabla h_i = C_{p,i} \nabla T + \int_0^T \nabla C_{p,i} dT$$
(25)

On substitution of Eqn.25 in the second term of Eqn.24,

$$\sum_{i=1}^{n} Y_i \nabla h_i = \sum_{i=1}^{n} Y_i C_{p,i} \nabla T + \sum_{i=1}^{n} Y_i \int_0^T \nabla C_{p,i} dT$$

From Eqn.12,

$$\sum_{i=1}^{n} Y_i \nabla h_i = C_p \nabla T + \sum_{i=1}^{n} Y_i \int_0^T \nabla C_{p,i} dT \quad (26)$$

From Eqn.19, 24, 26 & 20 and after rearrangement,

$$\mathbf{Q_h} = -\alpha \nabla h$$

= $-\lambda \nabla T - \alpha \left(\sum_{i=1}^n h_i \nabla Y_i \right)$
 $-\alpha \left(\sum_{i=1}^n Y_i \int_0^T \nabla C_{p,i} dT \right)$ (27)

The gradient of specie specific heat $C_{p,i}$ arises due its dependence on temperature.

$$\nabla C_{p,i} = \frac{dC_{p,i}}{dT} \,\nabla T \tag{28}$$

It is clear that conductive heat flux \mathbf{Q} evaluated from $\mathbf{Q}_{\mathbf{h}}$ and $\mathbf{Q}_{\mathbf{T}}$ formulations are not identical. In Eqn.27, the enthalpy gradient occurs not only because of temperature gradients (Term 1) but also from the gradients of specie mass fractions (Term 2) and the variation of specie specific heat capacities due to temperature gradients (Term 3).

Two methods are proposed to overcome this issue on the heat conduction term in the energy equation.

- 1. To implement the conduction term in terms of temperature gradient i.e $\mathbf{Q}_{\mathbf{T}}$ (Eqn.18).
- 2. To add a correction term to the $\mathbf{Q_h}$ formulation.

The first method is straightforward but enthalpy h is the unknown in the energy equation (Eqn.15) and hence the heat conduction term with \mathbf{Q} in terms of temperature gradient, can only be added as an explicit source term i.e **fvc**. This will lead to solver instability when the heat conduction term dominates the energy equation.

In the second method (Eqn.29), corrections are added to the $\mathbf{Q}_{\mathbf{h}}$ formulation to arrive at a formulation equivalent to $\mathbf{Q}_{\mathbf{T}}$.

$$\mathbf{Q_{new}} = -\alpha \nabla h + \alpha \left(\sum_{i=1}^{n} h_i \nabla Y_i \right) + \alpha \left(\sum_{i=1}^{n} Y_i \int_0^T \nabla C_{p,i} dT \right)$$
(29)

This renders the heat conduction term partially implicit in enthalpy $(-\alpha \nabla h \text{ term})$ with the corrections as explicit source terms resulting in better solver robustness than the first method. The simulations discussed in the present work are carried out with constant values of species specific heat capacities $C_{p,i}, i \in S$. Hence, the third term in the RHS of Eqn.29 vanishes.

$$\mathbf{Q_{new}} = -\alpha \nabla h + \alpha \left(\sum_{i=1}^{n} h_i \nabla Y_i \right)$$
(30)

2.4 Enthalpy transport due to inter-species diffusion

The different gas species in a multi-component system will have different enthalpy values h_i . As the gases diffuse into one another, the corresponding enthalpy transport should also be considered. Ignoring the enthalpy transport due to inter-species diffusion will result in incorrect temperature field [1]. The fourth term $(-\nabla \cdot \sum_{i=1}^{n} F_i h_i)$ in the RHS of the energy equation (Eqn.15) accounts for the enthalpy transport due to diffusive flux F_i . This term is completely ignored in the RPF solver and therefore added as an explicit source term in the energy equation of 'containementFoam' solver.

2.5 Turbulence contribution

The equations discussed above are valid only for laminar flows where the diffusion terms of momentum, species mass fractions and enthalpy are modelled with kinematic viscosity ν (momentum diffusivity), effective specie diffusivity D_i and thermal diffusivity α respectively. If turbulence modelling is considered, then the turbulence contribution of diffusivity should be added. Turbulence modeling in the present work(wherever specified) is done with the standard $k - \omega - SST$ model by Menter[REF3]. Turbulent eddy diffusivity ν_t is obtained from the turbulence model.

Turbulence contribution to the momentum diffusivity is reflected in the viscous stress tensor (Eqn.14) formulation as

$$\tau = \rho \left(\nu + \nu_t\right) \left[\nabla U + (\nabla U)^T - \frac{2}{3}\delta \nabla \cdot U\right] \quad (31)$$

Turbulence correction to the specie diffusive flux F_i yields

$$F_i = -\rho \left(D_i + \frac{\nu_t}{Sc_t} \right) \nabla Y_i \tag{32}$$

The final form of the conductive heat flux \mathbf{Q} after the addition of turbulence contribution is

$$\mathbf{Q_{new}} = -\left(\alpha + \frac{\rho\nu_t}{Pr_t}\right)\nabla h + \left(\alpha + \frac{\rho\nu_t}{Pr_t}\right)\left(\sum_{i=1}^n h_i \nabla Y_i\right)$$
(33)

3 Algorithm

The multicomponent gas flow modeling involves a tightly coupled set of equations. The PIM-PLE algorithm implemented in the 'containment-Foam' solver is the same as in the base RPF solver with slight modification (Fig.1). The density field change may come about due to change in the species mass fractions or due to the pressuretemperature changes through the ideal gas equation of state. Hence, the density field is kept in two different variables i.e. solver density ρ_{solver} and thermodynamic density ρ_{thermo} for different situations arising in different parts of a PIMPLE iteration. In addition, variable ϕ_f which denotes the mass flux at control volume faces in the discretized equations, is also related to density. This can be explained by the discretization of the continuity equation (Eqn.10) through the finite volume method.

On integration of the continuity equation over the control volume ${\cal V}$

$$\frac{\partial}{\partial t} \int_{V} \rho \, dV + \int_{V} \nabla \cdot (\rho \mathbf{U}) \, dV = 0$$

$$\frac{\partial}{\partial t} \int_{V} \rho \, dV + \int_{S} (\rho \mathbf{U}) \cdot d\mathbf{S} = 0$$
(34)

where S is the surface of the control volume. For simplicity, time discretization here is done with the Euler implicit method.

$$\frac{\rho^n - \rho^0}{\Delta t} V + \sum_f (\rho \mathbf{U}) \cdot \mathbf{S_f} = 0$$
(35)

where ρ^n and ρ^0 are density values at new time step and old time step respectively, Δt is the time step, f denotes the faces of the control volume and S_f is the surface normal vectors of those faces. The mass flux through a control volume face f is given by

$$\phi_f = (\rho \mathbf{U}) \cdot \mathbf{S}_\mathbf{f} \tag{36}$$

It is important that the density value becomes consistent in all the three variables ρ_{solver} , ρ_{thermo} and ϕ_f over the course of a PIMPLE iteration.

At the first step continuity equation/mass conservation equation(10) is solved and the density ρ_{solver}^* becomes consistent with the mass fluxes ϕ_f at that instant. In the momentum predictor step, the velocity field U^* is calculated with the existing pressure field p according to the Eqn.13. The velocity field thus obtained is not the actual solution but only a prediction. Then the species mass fractions are computed using the expression in Eqn.5. As discussed in section 2.2.1, only n - 1 specie mass fraction equations are solved and for the n^{th} specie Y_n is calculated using the Eqn.11. With the new mass fractions Y_i^* , the mixture specific heat capacity C_p^* (using Eqn.12) and effective mixture molecular weight W^* (using Eqn.37) are calculated. Then, the energy equation (Eqn.15) is solved and the new static enthalpy h^* is evaluated.

$$W^* = \frac{1}{\sum_{i \in S} \left(\frac{Y_i^*}{W_i}\right)} \tag{37}$$

3.1 Thermodynamic corrector step

Thermodynamic properties are updated in this step. At first, new temperature T^* is computed from enthalpy h^* based on the enthalpy-temperature relation through the Newton-Raphson method. Then, the thermodynamic density $\rho thermo^*$ and compressibility ψ^* are calculated with ideal gas relations as in Eqn.38.

$$\rho_{thermo}^{*} = \frac{p}{\frac{R_{u}}{W^{*}}T^{*}}$$

$$\psi^{*} = \frac{1}{\frac{R_{u}}{W^{*}}T^{*}}$$
(38)

where, R_u is the universal gas constant with the value 8314.462 $J.K^{-1}.kmol^{-1}$. μ^* and α^* are computed based on the new specie mass fractions Y_i^* using Eqn.12.

3.2 Pressure equation block

Pressure, velocity and density changes with pressure are all computed in the pressure equation block of the code. First, the solver density is set equal to the thermodynamic density updated in the thermodynamic corrector step.

$$\rho_{solver}^{**} = \rho_{thermo}^* \tag{39}$$

With this new solver density, pressure-velocity coupling steps are executed. Here, the momentum conservation equation and continuity equation are combined to give new values of pressure, mass fluxes and velocity i.e. p^* , ϕ_f^* and \mathbf{U}^{**} . The face mass fluxes ϕ_f^* is consistent with the new pressure field p^* , but density values ρ_{thermo}^* and ρ_{solver}^{**} are inconsistent with the pressure field p^* . The thermodynamic density is adjusted for the change in pressure by

$$\rho_{thermo}^{**} = \rho_{thermo}^* + \psi^*(p^* - p) \tag{40}$$

The solver density is made consistent with the face mass flux field ϕ_f^* (or pressure p^*) through the continuity equation.

3.3 Convergence

The turbulence fields are solved for if the turbulence model is activated. The PIMPLE iterations continue till solution convergence or for the maximum number of PIMPLE iterations, whichever comes first.

4 Deficiencies in the 'reactingParcelFoam' solver

The RPF solver available in OpenFOAM-6 was found to have a few deficiencies in its original form.

4.1 Inconsistency in the PIMPLE algorithm

In the RPF solver, the continuity equation is solved only in the final PIMPLE outer corrector step or if the number of outer correctors is set as 1(PISO mode). This clearly violates the conditions discussed in section 2.1.3. And, the solver density is inconsistent with the mass fluxes ϕ_f , if continuity equation is not solved. This results in the usage of incorrect density field in the species mass fraction, momentum conservation and energy equations.

4.2 Incorrect enthalpy transport

The multicomponent flow modeling is tightly coupled in terms of density, specie mass fraction, enthalpy and temperature. Due to the incorrect heat conduction term, the absence of the source term to account for enthalpy transport due to inter-species diffusion and the error present in the PIMPLE algorithm results in the calculation of incorrect enthalpy field. An incorrect enthalpy field means an incorrect temperature field. The temperature field affects the density field through the ideal gas equation of state. Wrong density field again influences the results of species mass transport equations, momentum conservation and energy equation. As the PIMPLE iterations progress, this vicious circle amplifies the errors and results in incorrect solutions. In the next section the impact of the existing errors are shown in a systematic manner and the necessity of the corrections are demonstrated.

5 Model Verification

The necessary corrections to be made to the 'reactingParcelFoam' solver are summarised in Table.1. The 'reactingParcelFoam' solver and the 'containmentFoam' solver use different diffusivity values to model the specie diffusion flux F_i and hence cannot be directly compared. Moreover, temperature divergence or incorrect enthalpy transport is the major issue addressed in the present work. To have consistent modeling of diffusion flux F_i term in the two solvers, the 'reactingParcelFoam' solver is tweaked only to have the F_i term same as 'containmentFoam' solver (Eqn.32) with all the other terms and PIMPLE algorithm as in original Open-FOAM implementation. This modified version of 'reactingParcelFoam' solver from hereon is referred to as 'Without correction' and the 'containment-Foam' solver with all the necessary corrections is called as 'With correction'.



Figure 1: PIMPLE algorithm

Term/Equation	reactingParcelFoam	${\bf containment}{f Foam}$	
Diffusion flux F_i	$F_{i} = -\rho \left(\nu + \nu_{t}\right) \nabla Y_{i}$	$F_i = -\rho \left(D_i + \frac{\nu_t}{Sc_t} \right) \nabla Y_i$	
Conductive heat flux Q	$Q = -\left(lpha + rac{ ho u_t}{Pr_t} ight) abla h$	$egin{aligned} Q &= -\left(lpha + rac{ ho u_t}{Pr_t} ight) abla h \ &+ \left(lpha + rac{ ho u_t}{Pr_t} ight) (\sum_{i=1}^n h_i abla Y_i) \end{aligned}$	
Enthalpy transport due to inter-species diffusion	Ignored	$-\nabla \cdot \sum_{i=1}^{n} F_i h_i$	
PIMPLE algorithm	Continuity equation is solved at the beginning of a PIMPLE iteration only if the total number of PIMPLE iterations per time step is one or if it happens to be the final PIMPLE iteration.	Continuity equation is solved at the beginning of every PIMPLE iteration.	

Table 1: Summary of corrections

The plots of temperature fields are made in conjunction with the species concentration fields to emphasize the importance of various model corrections necessary for accurate enthalpy transport especially in the regions of sharp species concentration gradients. Three major phenomenon namely i) Binary diffusion ii) Heat conduction and iii) Convection are tested separately with one-dimensional simulations. Finally, the model is applied to a two-dimensional mixing channel case where all three phenomena coexist and the general applicability of the model is shown. Turbulence modeling is considered only for the two dimensional mixing channel simulation.

5.1 Test Case I - Binary diffusion (1D)

Case Description:

To test the model only under the conditions of binary diffusion of gases, the other effects of convection and heat conduction are masked. Convection phenomenon is made impotent by setting the velocity initial field to null value. Heat conduction is prevented by setting the thermal diffusivity of the species $\alpha_i = 0, i \in S$. The one dimensional domain is of length 1m, discretized into 100 uniformly spaced grid points. Two gas species Helium (HE) and Air (AIR) with very different specific heat capacities (C_p of Air = 1004.4 J/kg.K & C_p of Helium = 5240 J/kg.K) are considered. This is to emphasize the importance of enthalpy transport due to inter-species diffusion. Since only two gas species are considered, the species mass fraction equation (Eqn. 5) is solved only for the Helium species with a constant diffusivity D_i and the mass fraction of Air is computed by enforcing the constraint in Eqn.11. The initial conditions are summarized in Table 2. One half of the domain is completely filled with Helium and other half is fully filled with Air and the gases are allowed to diffuse for t = 10s.

Variable	Value		
Species Mass Fraction			
HE	$\begin{cases} 1 & 0 \le x \le 0.5 \\ 0 & 0.5 < x \le 1 \end{cases}$		
AIR	1 - HE		
Temperature [K]	303.15		

Table 2: Binary Diffusion - Initial Conditions

Discussion of results:

The results of the Helium volume fraction field and temperature is shown in Fig.2. For the model without corrections, there is a non-physical temperature divergence in places of species concentration gradients. This can be explained by the absence of the source term to account for enthalpy tranpsort due to inter-species diffusion in the energy equation $(-\nabla \cdot \sum_{i=1}^{n} F_i h_i)$. Physically, this means the Helium and Air species diffuse into each other (through F_i term in the species mass transport equation Eqn.5) but do not carry along their individual enthalpies $(h_i, i \in S)$. In the corrected model, the expected isothermal temperature field is obtained.

5.2 Test Case II - Heat Conduction(1D)

Case Description:

In this test case, the validity of the solver is investigated only under the condition of heat conduction. The flow domain and the initial conditions are same as the previous case(Binary diffusion). Species diffusion is made irrelevant by setting binary diffusivity $D_i = 0$. Appropriate species thermal diffusivity values($\alpha_i, i \in S$) are defined for Helium and Air. Discussion of results:

From the results (Fig. 3), it is clear that the model without corrections exhibit nonphysical temperature values in regions of species concentration gradients. With the 'reactingParcelFoam' solver, the conductive heat flux (Q) is in terms enthalpy gradient (Eqn.19). And, in regions of sharp species concentration gradients, the gradient of enthalpy (h) is non-zero even when the gradient of temperature field (T) is zero, resulting in incorrect heat flux (Q). After the addition of correction term (Eqn.29), the expected temperature field is obtained.

5.3 Test Case III - Convection(1D)

Case Description:

The test case is formulated to check the solver only under the condition of bulk motion. Species diffusion and heat conduction phenomena are made insignificant by defining species diffusivity (D_i) and thermal diffusivity values to zero. The flow domain is one dimensional with only three control volumes of uniform size with an inlet and an outlet as shown in Fig.4a. The initial and boundary conditions are summarised in Table.3. The domain is completely filled with Air initially and Helium is injected into the domain through the inlet. The case is isothermal. The simulation is carried out for a total of 1s with a time-step of 1s with only one PIMPLE iterative loop.

Discussion of results:

At the first time-step as the Helium specie enters the domain, non-physical temperature field is observed in the model without corrections. This behaviour can be only attributed to the incorrectness in the PIMPLE algorithm implemented in the 'reactingParcelFoam' solver(Ref. section 3.1). The continuity equation should be definitely solved in conjunction with the species mass transport equation, if only n-1 species mass fraction equations are solved and constraint(Eqn.11) is used. After rectifying this error, the isothermal temperature field is retained.

5.4 Test Case IV - Mixing channel(2D)

Case Description:

The test case is designed to investigate the solver correctness in a scenario where all three major phenomena of (i) species diffusion, (ii) heat conduction



Figure 2: Binary diffusion a) Helium volume fraction, b) Temperature



Figure 3: Heat Conduction a) Helium Volume Fraction, b) Temperature

Variable	Initial conditions	Inlet BC	
Species Mass Fraction			
HE	0	1	
AIR	1	0	
Temperature T[K]	303.15	303.15	
Velocity U [m/s]	0	0.1	

Table 3: Convection - Initial & boundary conditions

and (iii) convection coexist. Turbulence modeling is also considered to verify the general applicability of the solver. The flow domain of is a two dimensional mixing channel of a total length of 0.6m and channel height of 0.05m with two inlets and one outlet(Fig. 5). Helium gas enters through the inlet on the top while steam enters from the bottom inlet. The gas species come into contact at 0.1 m downstream of the inlets and form a mixing layer. As in the previous cases, an isothermal temperature field



Figure 4: Convection - Impact of algorithm correction

is used to investigate the temperature divergence problem. The initial and boundary conditions are summarized in Table 4.

Discussion of results:

Helium volume fraction and the temperature values along the plot line(Fig.5) is shown in Fig.6. The model without corrections suffer from the same temperature divergence issue discussed in the previous one dimensional test cases. The solver with corrections gives the correct temperature field across the mixing layer where sharp species concentration gradients exist.





Variable	Initial conditions	inlet 1 BC	inlet 2 BC
Y_{HE}	$\begin{cases} 1 & 0 \le x \le 0.5 \\ 0 & 0.5 < x \le 1 \end{cases}$	1	0
Y _{H2O}	$1 - Y_{HE}$	0	1
Normal Velocity U [m/s]	0	0.75	0.5
Temperature T [K]	300	300	300

Table 4: Mixing Channel - Initial & boundary conditions



Figure 6: Mixing channel a) Helium Molar Fraction, b) Temperature

6 Summary and Conclusions

A thorough review of the existing capabilities of OpenFOAM to model multi species gas transport is given and the deficiencies are identified. A new solver 'containmentFoam' is developed with necessary improvements to the governing equations and PIMPLE algorithm for modeling multi-component gas mixing in nuclear reactor containment flows. The solver is compared with original base solver in OpenFOAM on simple one-dimensional and twodimensional test cases and the impacts of the corrections are shown. At present, the solver is applied to simulate Helium layer erosion in large scale three-dimensional geometries at Forschungzentrum Juelich with reasonable success [4, 5].

7 Acknowledgements

The authors gratefully thank the RWTH Aachen -IIT Madras strategic partnership for funding the research work. We gratefully acknowledge the HITEC Graduate School at Juelich for partial funding of PhD position.

References

- Andrew W. Cook. Enthalpy diffusion in multicomponent flows. *Physics of Fluids*, 21(5):055109, 2009.
- [2] Edward N. Fuller, Paul D. Schettler, and J. Calvin. Giddings. New method for prediction of binary gas-phase diffusion coefficients. *Industrial Engineering Chemistry*, 58(5):18–27, 1966.
- [3] Vincent Giovangigli. Multicomponent Flow Modeling. Birkhauser, 1999.
- [4] M. Kampili, G. Vijaya Kumar, S. Kelm, K. Arul Prakash, and H.-J. Allelein. Validation of multicomponent species transport solver- impact of buoyancy turbulence in erosion of a stratified light gas layer. 14th OpenFOAM Workshop, 2019.
- [5] S. Kelm, M. Kampili, G. Vijaya Kumar, K. Sakamoto, X. Liu, C. Druska, A. Kuhr, K. Arul Prakash, and H.-J. Allelein. Development and first validation of the tailored cfd solver containmentfoam for analysis of containment atmosphere mixing. *NURETH* 18, 2019.
- [6] S. Kelm, J. Lehmkuhl, W. Jahn, and H.-J. Allelein. A comparative assessment of different experiments on buoyancy driven mixing processes by means of cfd. Annals of Nuclear Energy, 93:50 – 57, 2016.

- [7] J. Malet, E. Porcheron, and J. Vendel. Oecd international standard problem isp-47 on containment thermal-hydraulicsâ"conclusions of the tosqan part. *Nuclear Engineering and Design*, 240(10):3209 – 3220, 2010.
- [8] G. Maragkos, P. Rauwoens, and B. Merci. Application of fds and firefoam in large eddy simulations of a turbulent buoyant helium plume. *Combustion Science and Technology*, 184(7-8):1108–1120, 2012.