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Large eddy simulations of erosion of a stratified layer by a buoyant jet

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ABSTRACT

During a Loss of Coolant Accident (LOCA) accident, leaked hydrogen from the primary circuit can form a stable stratified layer at the top of the containment building. The formation and erosion of a stratified layer is a challenging numerical problem due to the interaction mechanism of the jet flow with the stratified layer. The OECD-NEA conducted an experiment to investigate the erosion of the stratified layer by a vertical air-helium jet from the bottom of the large vessel (height 8 m., diameter 4 m). During the experiment, CFD grade experimental data was generated that could be used for comparative studies.

In this study, the LES (Large Eddy Simulation) numerical methodology is used to validate the PANDA experiment for the nuclear reactor containment safety analysis. Specific attention is given to the analysis of the interaction between a buoyant jet and stratified layer. An understanding of the interaction mechanisms will help to quantify turbulent mass transport of the gas components. Good agreement between the numerical results and the experimental data is observed for temporal velocity, gas concentration and temperature data. FFT (Fast Fourier Transform) analysis is applied to check the numerical grid resolution and POD (Proper Orthogonal Decomposition) is applied to investigate coherent flow structures and turbulent mass transport mechanisms. Horseshoe vortices, which has previously been observed experimentally and numerically for buoyant jets, are observed near the round jet.

1. Introduction

Validation of CFD tools and models used in nuclear reactor safety analyses is vital. During severe accident conditions in light water cooled nuclear reactors, explosive hydrogen gas can be formed due to an oxidation reaction between high temperature zirconium cladding and steam. If the hydrogen gas is released into the containment building, it is possible that a buildup in concentration of the gas occurs to such an extent that a combustible air-hydrogen mixture forms, potentially leading to a hydrogen explosion. An example of such an event is the Three Mile Island accident in 1979. After this accident, extensive research on the mechanisms that lead to this type of accident has been done at both national and international levels. Several experimental facilities around the world have been built to investigate the hydrogen buildup and distribution such as PANDA, MISTRA, TOSQAN, THAI, PHEBUS, HDR, BMC, and HYJET [1]. Furthermore, the Fukushima Daiichi accident in 2011 showed that hydrogen mitigation is an important safety problem. The accident emphasized that more studies were necessary to ascertain what the optimal positioning of hydrogen recombiners needed to be, such that hydrogen build-up in the reactor containment building could be mitigated.

Most of the hydrogen mixing studies in the literature are experimental in nature. However, CFD is the only tool that can be used to fully realize hydrogen temporal distributions in the containment building. To this end, numerical simulations have been performed using Reynolds-averaged Navier-Stokes (RANS) models [2,3]. Problematically for RANS based simulations, a parametric influence study by [4] showed that RANS turbulence model selection has the highest impact on the hydrogen mixing. Another problem is that most of the CFD validation attempts focused on the prediction of single quantities of interest, instead of simultaneous calculations of multiple quantities like velocity, temperature or gas concentration, which are necessary for CFD grade model validation. Thus, RANS simulations were able to predict selected variables accurately, but failed when attempts were made to predict multiple variables simultaneously [5]. In this respect, Large Eddy Simulation (LES) will help to understand flow physics better than RANS. Specifically, LES is able to predict this kind of complex flow. The reason for the complexity of the current flow problem is related to the interaction between the jet and stratified layer, which has strong anisotropy and fluctuations due to buoyancy effect. LES scale studies allows for the identification of weaknesses of the two equation models in accurately predicting the interaction

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between jets and stratified layers. This is due to the LES methods being able to directly simulate turbulent behavior of the investigated phenomena.

The aim of this study is to validate LES methods by comparing their numerical results with PANDA IBE-3 experimental data in the form of temporal velocity, temperature and gas concentration results. As shown in [5], LES analysis predicted erosion time worse than RANS models. Additionally, the previous studies [6,7] showed that jet velocity profile directly impacts the temporal erosion time of the stratified layer, and it was stated that careful implementation of inlet boundary condition would solve this problem. In one other LES attempt by [8], temperature effects were not considered in the simulation, causing a ~3% velocity increment over the simulation due to the density difference of the injection jet and the constant mass flow rate condition. The same study found that the LES results could also not predict the helium concentration as accurately as the RANS results.

Depending on the simulation being attempted, RANS models are known to potentially over- or under-predict turbulent flow quantities. As a result, RANS models have the potential to correctly predict the concentrations of helium during the simulation, while failing to appropriately predict velocity and temperature. However, all of these parameters may have an impact on the risk of a hydrogen explosion, and must therefore be properly predicted. Moreover, one other objective is contributing to validation studies of CFD for nuclear safety applications, specifically to investigate flow structure and the physics of turbulent mass transport. Thus, some computational techniques are applied here to investigate flow physics in more detail. Proper orthogonal decomposition method (POD) is applied to extract coherent structures. Additionally, Fast Fourier Transform (FFT) is applied to check numerical grid resolution, whether it is resolving enough scale or not. In Section 2, the numerical models are briefly described. In Section 3 the experimental test facility, and test details are explained, followed by CFD modeling details. In Section 4, FFT, temporal experimental and numerical results are presented, followed by POD. Finally, conclusions are discussed in Section 5.

2. Numerical models

In the PANDA experiment, there are two complex flow phenomena. The first is a turbulent buoyancy-momentum driven jet and the second is the interaction of the jet and stratified layer. To model this complex flow behavior, the LES technique is used. LES directly solves the large scales of motion in a turbulent flow, while the smaller scales are modelled. Solving larger scales directly and modeling smaller scales allow for significantly less uncertainty than conventional RANS modeling, since the modeling of the smaller scales is based on the hypothesis that smaller eddies are self-similar and thus they can easily modelled due to its universal structure independent from flow geometry. In the current study, the Energy and Species Transport equation are solved as well due to the temperature variation of the gas mixture and mixing of the two different gases. The density is computed by using the ideal gas law with and the temperature computed using the energy equation. Buoyancy is accounted for in the current study due to the variable density at the stratified layer. In Section 2.1, the Multi-Species Transport Equation is detailed, while the turbulence modeling details are explained in Section 2.2.

2.1. Multi-species transport equation

The transport equation for the mass fraction Y_i of the i^{th} species is solved as in Eq. (1)

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (\rho D_{i,m} \nabla Y_i + \alpha_t \nabla Y_i) \tag{1}$$

where D_m is the molecular diffusivity calculated using the Chapman-Enskog model Eq. (2). The diffusion coefficient for molecular diffusivity used is $7 \times 10^{-5}\,\frac{\mathrm{m}^2}{\mathrm{s}}$, α_t is the turbulent diffusivity, and ρ is the density.

$$\mathrm{D}_{1,2} = \frac{1.858 \times 10^{-3} T^{3/2}}{p\sigma_{12}^2 \Omega} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}} \tag{2}$$

where M_1, M_2 are the molecular masses of the gas components, p is the pressure, T is the temperature, σ^2 is the average collision parameter and Ω is the temperature dependent collision integral. The diffusion coefficient for helium and air mixture is $7 \times 10^{-5}\,\frac{\mathrm{m}^2}{\mathrm{s}}$ at $T = 298$ K and $p = 1$ atm.

2.2. Turbulence modeling

CFD applications have commonly been used for turbulent flow in the last three decades. Although there are several turbulent models available, including hybrid variations, a general purpose turbulence model has not been developed yet. Each model has its own specific advantages or disadvantages according to the flow structures. Although the turbulent flow can be resolved directly by solving the Navier-Stokes equations, Direct Numerical Simulation (DNS) it is not feasible for current engineering problems due to its significant computational cost. As a compromise between accuracy and computational cost, turbulence models have been developed. Large Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) are used extensively for most of the current engineering problems.

In the present study, LES is used to investigate its capability for a containment level safety analysis As a sub-grid scale (SGS) model, the Dynamic Smagorinsky model is used in STAR-CCM+ 10.06 [9]

The turbulent viscosity in the Dynamic Smagorinsky SGS model is defined as in Eq. (3)

$$\mu_t = \rho \Delta^2 S \tag{3}$$

where;

$$\Delta^2 = C_s^2 V^{2/3} \tag{4}$$

The difference between the Dynamic Smagorinsky and the Standard Smagorinsky version is that C_s is not constant and it is computed dynamically as a function of test-filtered variables to achieve a more global SGS model. Further details about dynamic SGS modeling can be found in [10]

2.3. Proper Orthogonal Decomposition

The POD algorithm to investigate coherent structures in turbulent flows was first proposed by Lumley [11]. The methodology is based on extracting an orthogonal set of spatial eigenfunctions from the random field.

The main goal of POD is to find the optimal representation of the field by solving a Fredholm integral eigenvalue problem given in Eq. (5).

$$\int R(x, x')\phi(x')dx' = \lambda\phi(x) \tag{5}$$

However, the direct solution of this problem is computationally expensive. Sirovich [12] proposes a solution to this problem, which is known as the Method of Snapshots. The method considers a set of M linearly independent flow realizations. Applying the method of snapshots results in following equation.