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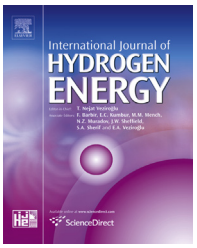

GASFLOW-MPI: A new 3-D parallel all-speed CFD code for turbulent dispersion and combustion simulations
Part I: Models, verification and validation

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ABSTRACT

The objective of the presented work is to develop an efficient and validated approach based on a multi-dimensional computational fluid dynamics (CFD) code for predicting turbulent gaseous dispersion, conjugated heat and mass transfer, multi-phase flow, and combustion of hydrogen mixtures. Applications of interest are accident scenarios relevant to nuclear power plant safety, renewable energy systems involved in hydrogen transport, hydrogen storage, facilities operating with hydrogen, as well as conventional large scale energy systems involving combustible gases. All model development is conducted within the framework of the high-performance scientific computing software GASFLOW-Multi-Physics-Integration (MPI). GASFLOW-MPI is the advanced parallel version of the GASFLOW sequential code with many newly developed and validated models and features. The code provides reliability, robustness and excellent parallel scalability in predicting all-speed flow-fields associated with hydrogen safety, including distribution, turbulent combustion and detonation. In the meanwhile, it has been well verified and validated by many international blind and open benchmarks.

The recently developed combustion models in GASFLOW-MPI code are based on the transport equation of a reaction progress variable. The sources consist of turbulence dominated and chemistry kinetics dominated terms. Models have been implemented to compute the turbulent burning velocity for the turbulence controlled combustion rate. One-step and two-step models are included to obtain the chemical kinetics controlled reaction rate. These models, combined with the efficient and verified all-speed solver of the GASFLOW-MPI code, can be used for simulations of deflagration, detonation and the important transition processes like flame acceleration (FA) and deflagration-to-detonation-transition (DDT), without additional need for expert judgment and intervention. It should be noted that the major goal is to develop a reliable and efficient numerical tool for large-scale engineering analysis, instead of resolving the extremely complex physical phenomena and detailed chemistry kinetics on microscopic scales. During the course of this development, new verification and validation studies were completed for phenomena relevant to hydrogen-fueled combustion, such as shock wave capturing, premixed and

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non-premixed turbulent combustion with convective, conductive and radiation heat losses, detonation of unconfined hydrogen–air mixtures, and confined detonation waves in tubes. Excellent agreements between test data and model predictions support the predictive capabilities of the combustion models in GASFLOW-MPI code. In Part II of the paper, the newly developed CFD methodology has been successfully applied to a first analysis of hydrogen distribution and explosion in the Fukushi Daicchi Unit 1 accident.

The major advantage of GASFLOW-MPI code is the all-speed capability of simulating laminar and turbulent distribution processes, slow deflagration, transition to fast hydrogen combustion modes including detonation, within a single scientific software framework without the need of transforming data between different solvers or codes. Since the code can model the detailed heat transfer mechanisms, including convective heat transfer, thermal radiation, steam condensation and heat conduction, the effects of heat losses on hydrogen deflagrations or detonations can also be taken into account. Consequently, the code provides more accurate and reliable mechanical and thermal loads to the confining structures, compared to the overly conservative results from numerical simulations with the adiabatic assumptions.

Predictions of flame acceleration mechanisms associated with turbulent flames and flow obstacles, as well as DDT modeling and their comparisons to available data will be presented in future papers. A structural analysis module will be further developed. The ultimate goal is to expand the GASFLOW-MPI code into an integral high-performance multi-physics simulation tool to cover the entire spectrum of phenomena involved in the mechanistic hydrogen safety analysis of large scale industrial facilities.

Introduction

If hydrogen is not effectively removed during the early stage of a severe accident in a typical water reactor, wide combustion regimes, from slow laminar deflagration to global detonation, would occur in the containment [1]. For 100% Zircaloy oxidation in a 1500-MW PWR unit, ~1750 kg hydrogen will be generated. If it is released and homogeneously distributed in a containment with the volume of 75,000 m^3, the hydrogen concentration in dry air will reach 22%. When the steam volume fraction drops below 35%, namely H_2 14.3 vol% and air 50.7 vol%, the homogeneous mixture will enter the detonable regime, as shown in Fig. 1. The real situation during the accident could be even worse because most of the hydrogen will accumulate in the dome and local steam condensation could lead to higher hydrogen concentration in the detonable regime. Even for a partial Zircaloy oxidation, it is still difficult to completely remove the risk of hydrogen explosion in local area due to the effects of buoyancy and local steam condensation. In the dedicated studies of severe accidents in nuclear power plants [2–7], large scale hydrogen explosion, which damages the integrity of the containment and leads to radioactivity release into the environment, has been clearly identified. These studies have shown that a design criterion shall be established for the construction of the containment building which withstands the mechanical and thermal loads due to the hydrogen explosions. Therefore, it is of high significance to evaluate the structural response of the containment in case of unmitigated accidents, as we have learned from the devastating hydrogen explosions at Fukushima Daiichi [8].

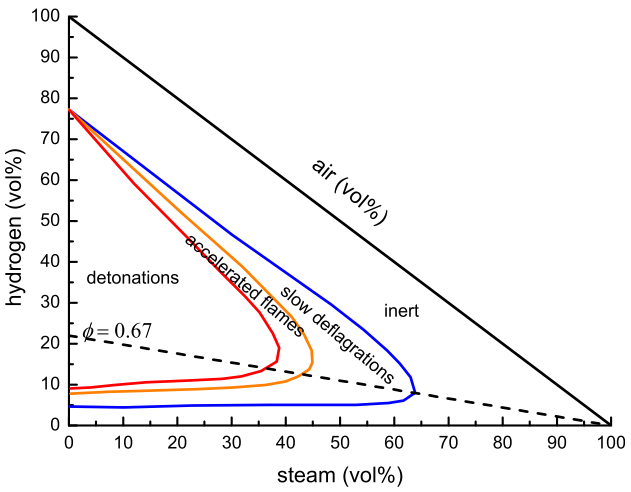

Fig. 1 – Combustion regimes of hydrogen–air-steam mixtures at a typical temperature (373 K) in containment during severe accident.

Three-dimensional numerical simulations of hydrogen safety issues have been requested by nuclear regulatory authorities especially after the Fukushima Daiichi accidents. During the past decades, various numerical codes have been developed and used to simulate hydrogen deflagration, detonation and transition processes, such as DET3D [1,9], COM3D [6,10], TONUS [11,12], FLACS [13–16], REACFLOW [17], CFX [17–19], FLUENT [20] and OPENFOAM [21–25]. Hasslberger [25] used the density-based explicit solver in OPENFOAM to simulate different regimes of combustion within one software framework in a real scale pressurized water reactor. It is a big step forward to the idea of using one single software framework for hydrogen safety analysis. However, the hydrogen distribution phase, which provides initial conditions for

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