COMPUTATIONAL FLUID DYNAMICS MODELLING OF INDUSTRIAL SCALE RELEASES OF HYDROGEN AND NATURAL GAS BLENDS

Lars Hov Odsæter[1], Bjørn Lilleberg[2]
[1]DNV, Trondheim, Norway
[2]DNV, Bergen, Norway

Corresponding author's e-mail address: Lars.Hov.Odsater@dnv.com

Keywords: Hydrogen safety, Computational Fluid Dynamics, Consequence Modelling, Natural Gas Mixture, Accidental Release

ABSTRACT

Blending hydrogen into existing natural gas infrastructure can be a cost-effective approach to introduce more hydrogen into the global energy mix. Blends of natural gas and hydrogen produced from renewable energy sources can be used to generate heat and power with lower CO_2 emissions in hard-to-abate industries which today are fueled by natural gas. However, the safety implications of such solutions are not well enough understood. The physical properties of hydrogen differ from those of natural gas, and the safety implications may not be linearly dependent on the composition of the fuel.

Reliable and predictive engineering tools to estimate the consequences of an accidental release are paramount for safety analysis, e.g., to establish flammability or toxicity contours or thermal radiation hazard distances. In this work we demonstrate the ability of computational fluids dynamics (CFD) modelling to simulate both unignited and ignited releases of hydrogen and natural gas mixtures into surroundings with geometrical obstacles. The simulation results can then readily be used for consequence predictions in safety analysis for industrial scale problems. The advanced industrial CFD tool KFX[1] is used to model the scenarios. KFX has previously been demonstrated to give good results for pure hydrogen jet releases[2].

KFX is a finite-volume CFD code which solves the fundamental conservation equations for three-dimensional, time-dependent turbulent flow and combustion using a non-uniform Cartesian grid. Turbulence is modelled with the standard k-ε model, while turbulent combustion is modelled with the Eddy Dissipation Concept (EDC)[3]. In turbulent combustion, chemical reactions take place in fine structures of the turbulent fluid. This is a complex interplay, and EDC connects the fine scale physics to the larger scale turbulence model parameters. Furthermore, thermal radiation is modelled by the discrete transfer model of Lockwood and Shah[4], while soot formation from combustion of hydrocarbons is modelled by the Eddy Dissipation Soot model. A mean absorption coefficient based on Leckner's model of CO_2 and H_2O absorption are applied, while Felske and Tien's model is used for soot absorption.

A multicomponent approach is applied so that individual species, such as hydrogen, methane, ethane, propane, and air components, are tracked separately. Detailed CAD geometry can readily

be imported into the simulation model, and geometries can be represented either as solid construction cells or by a sub-grid porosity concept to capture the effect of geometries that are smaller than the computational grid. This is a prerequisite for incorporating complex geometries of industrial facilities into the simulation model.

Releases from pressurized storage typically results in under-expanded jets. In such scenarios a pseudo-source concept that models the expansion process at sub-grid level to obtain equivalent expanded flow parameters at atmospheric conditions is used. This model is based on conservation of mass, momentum and energy. The expansion from a stagnation state to the orifice state is modelled as an isentropic expansion, while the expansion from orifice to the atmosphere is modelled as a constant total enthalpy process. Accurate and robust equations of state (EOS) are accessed through the open-source toolbox Thermopack[5]. For this work we employ the GERG-2008 EOS[6], which is the ISO standard for natural gas and similar mixtures.

By comparing simulation results to large-scale experiments, we show that the CFD model captures the fundamental physics of a mixed hydrogen/natural gas release, including dispersion and combustion in the surroundings and heat load to surrounding obstacles. This demonstrates that the model can be used as a reliable and predictive tool for consequence modelling of industrial relevant release scenarios of hydrogen and hydrogen/natural gas blends.

Acknowledgements
The research is partly funded by the JIP “Hydrogen CFD simulation software” with DNV and Equinor as partners.

References
1. KFX v 4.0 User Manual. DNV, October 2023.
2. Rian, K.E., Modelling and Numerical Simulation of Hydrogen Jet Fires for Industrial Safety Analyses – Comparison with Large-Scale Experiments, In: 8th International Conference on Hydrogen Safety, 24-26 September 2019, Adelaide, Australia.
3. Magnussen, B.F., The Eddy Dissipation Concept – a Bridge between Science and Technology, Invited paper at ECCOMAS Thematic Conference on Computational Combustion, 21-24 June 2005, Lisbon, Portugal.
4. Shah, N.G., The Computation of Radiant Heat Transfer, Ph.D. Thesis, University of London, Faculty of Engineering, UK, 1979.
5. Wilhelmsen, Ø., Aasen, A., Skaugen, G., Aursand, P., Austegard, A., Aursand, E., Gjennestad, M.A., Lund, H., Linga, G., and Hammer, M., Thermodynamic Modeling with Equations of State: Present Challenges with Established Methods, Ind. Eng. Chem. Res. 2017, 56, 13, 3503-3515.
6. Kunz, O., and Wagner, W., The GERG-2008 Wide-Range Equation of State for Natural Gases and Other Mixtures: An Expansion of GERG-2004, J. Chem. Eng. Data 2012, 57, 11, 3032-3091.