# flameFoam: an OpenFOAM based solver for praCtical turbulent premixed combustion simulation

M. POVILAITIS

Lithuanian Energy Institute

Kaunas, Lithuania

Email: mantas.povilaitis@lei.lt

J. JASELIŪNAITĖ

Lithuanian Energy Institute

Kaunas, Lithuania

Nuclear power plant containment would be the last barrier preventing environment from the radioactive contamination during a severe accident. The containment integrity would be challenged by a number of threats during the accident progression. The highest level risk during the early and delayed accident phases is related to hydrogen combustion. Consequentially, significant international effort is being devoted to understanding and reliably predicting hydrogen combustion phenomena in the containments of nuclear power plants during the severe accidents.

One of the most challenging issues when modeling hydrogen combustion is adequate simulation of flame acceleration due to turbulence. At the same time it is one of the most important issues to safety, since flame acceleration is directly related to the risk posed by combustion – stronger acceleration can lead to more powerful shock waves or even to deflagration to detonation transition.

In the international benchmarks dedicated to the simulation of turbulent hydrogen combustion in the severe accident relevant conditions, and in the scientific literature, presenting relevant cases, most of the CFD simulations are performed using commercial CFD codes (mainly ANSYS FLUENT and CFX) with more or less privately in-house customized combustion models. Other proprietary solutions also also prevalent, using more specialized licensed codes, e.g., FLACS or EUROPLEXUS.

Compared to the discussed proprietary solutions, open source contributions compose only a smaller (however, continuously increasing in recent time-frame) fraction. Such dominance of commercial, but modified privately in-house, and other proprietary solutions for the state-of-the-art applications (in our opinion) stifles innovation, promotes fragmentation in the community, duplication of efforts and creates additional challenges for the independent newcomers in the field. When we started our own transition from system codes to more detailed simulation of hydrogen combustion and faced this situation, it motivated us to develop a freely accessible open-source solver for turbulent premixed combustion reproducing present (practical) state-of-the-art. In our opinion, such public more or less ready-made open-source CFD solution would promote knowledge dispersion and lower the barriers to gain experience in modeling turbulent premixed combustion.

The state-of-the-art demonstrated in the international benchmarks and scientific publications here concerns only practically relevant simulations of turbulent premixed combustion at slightly larger laboratory scale. Absolute majority of such simulations employ simplified approaches, which allow to run models with affordable computer resources, and at the same time provide sufficiently accurate results. The employed approaches are RANS modeling of

turbulence and combustion models based on progress variable, turbulent flame closure (TFC) and turbulent flame speed correlations.

We chose OpenFOAM CFD toolkit for our open-source turbulent premixed combustion solver. OpenFOAM is the most popular open source CFD solution. It is a broadly used toolkit which allows custom implementations of finite volume method based solvers of partial differential equation systems. OpenFOAM solvers have been developed and applied for the simulations of a wide range of problems -– compressible and incompressible fluid mechanics, heat and mass transfer and reacting flows. There is a collection of solvers already distributed with OpenFOAM, including several among them dedicated to the simulations of reacting flows:

* XiFoam – implements b-Ξ flame surface wrinkling combustion model
* PDRFoam – implements b-Ξ flame surface wrinkling combustion model with porosity/distributed resistance
* chemFoam – single cell solver for comparison against other chemistry solvers
* coldEngineFoam – solver for cold-flow in internal combustion engines
* fireFoam – simulates fires and turbulent diffusion flames with reacting particle clouds, surface film and pyrolysis
* reactingFoam – models combustion using chemical kinetics simulations

reactingFoam also has a numerically improved (outside of OpenFOAM distribution) version, called reactingFoam-SCI. However, none of the reacting flow solvers pre-included with OpenFOAM are based on a progress variable approach with TFC and practically applicable for the simulation of turbulent premixed combustion in the severe accident relevant conditions. The closest in terms of formulation is XiFoam solver, which is based on regress variable, comparable to progress variable, but its combustion source is modeled using different approach than TFC.

Present version of our solver, called flameFoam, is built based on the OpenFOAM toolkit version 7. The basis for the solver are standard solvers rhoPimpleFoam, buoyantPimpleFoam and chtMultiRegionFoam, included with the OpenFOAM distribution. flameFoam is not a straight copy of any of these standard solvers, but is a combination of all three mentioned solvers. Presented initial solver version has been developed and tested for the combustion of homogeneous hydrogen-air mixtures.

Fluid and solid regions in a simulation domain can be distinguished by the flameFoam solver. Compressible Navier-Stokes equations are solved in the fluid regions. Continuity equations for the mass, momentum, energy and combustion progress variable are solved. Only energy conservation equation is solved in the solid regions. Conjugate heat transfer between the fluid and solid regions is realized using standard OpenFOAM conditions for boundaries between regions. Multiregion support (based on standard chtMultiRegionFoam solver) implemented in flameFoam allows simulation of heat losses from hydrogen flames to solid walls and, if needed, to the environment. Solved mass, momentum and energy continuity equations are the same as in standard OpenFOAM solvers, a sole exception being a combustion heat source term in the (fluid region) energy equation.

The progress variable equation expresses combustion model of the solver. Progress variable shows progression of the combustion from the fresh mixture to the burnt. The equation is closed by the combustion source term calculated using the TFC model expression, based on the turbulent flame speed value. Turbulent flame speed is defined as a function (correlation) of turbulence parameters, e.g. turbulent kinetic energy and dissipation rate. Three different correlations for turbulent flame speed evaluation are implemented in the present flameFoam version – Zimont, Bradley and Bray. Laminar flame speed value, required for the estimation of turbulent flame speed, can be either given by the user (constant) or dynamically calculated according to Malet’s correlation, which is a function of pressure, temperature and concentrations of hydrogen and diluents.

The presented model features implemented in the solver are equivalent to the state-of-the-art demonstrated in the recent international benchmarks and scientific literature. Thus we consider flameFoam to be a part of current state-of-the-art. We have already used it in currently on-going ETSON-SAMHYCO-NET benchmark, including for blind simulations, and obtained results on the same accuracy level as established proprietary solutions. Additionally, solver is being validated with a number of simulations, for both reacting and non-reacting flows. Some selected validation examples are discussed bellow.

Since the solver implementation is new and includes algorithm modifications compared to the standard OpenFOAM solvers, the initial validation and verification of general features was also necessary. One of these is shock tube case, which allows to validate simulated discontinuity evolution against an analytical solution. Obtained pressure, velocity and density profiles in the shock tube case were in good agreement with the analytical results. Both the shock wave and contact discontinuity were resolved. The gradients of thermodynamic parameters along the rarefaction wave were also correctly predicted, as well as its head and tail positions. Other non-reacting case example is backward facing step, which allows experimental validation of turbulence treatment and fluid interaction with no slip boundaries, including boundary layer separation and reattachment due to a sudden cross-section expansion. Obtained numerical results in this case showed accurate agreement with the experiment.

Turbulent premixed combustion modeling was validated on several experiments – hydrogen-air-steam mixtures combustion in ENACCEF facility (CNRS,France), hydrogen-air mixtures combustion in ENACCEF2 facility (CNRS,France) and hydrogen-air mixture combustion in vented small-scale chamber (University of Sydney, Australia). In all cases turbulence was generated by the obstacles present in flame path.

In all these cases the simulations provided good prediction of experimental data. flameFoam was able to capture flame propagation behaviour, including acceleration phases, velocity peaks and following decelerations (if present), including interaction with a reflected pressure wave. In the simulations of ENACCEF facility experiments false flame acceleration in the dome region was obtained due to currently missing quenching model in the solver.

However, currently only initial flameFoam version has been developed with further work still required in order to expand flameFoam application and validation domain, robustness and usability.

The further development is planned to be performed in several directions. First, in order to keep up with the state-of-the-art progress, support for non-homogeneous mixtures is projected to be implemented and validated in the solver in near future. Second, work is required to improve the quality of code, make the solver more user-friendly and keep up-to-date in relation to OpenFOAM releases. Current flameFoam version has simplified mixture composition treatment with some unnecessary restrictions on the definition of mixture properties by the user. This is planned to be fixed together with the porting of solver code to current OpenFOAM version 8 and in preparation for the non-homogeneous mixtures support. Third, with the emphasis on practical application, solver needs to be further developed to be usable with larger simulation domains. In addition to numerical robustness evaluation with coarser grids, next target in this direction is implementation and validation of dynamic mesh refinement. At present unvalidated support for three-dimensional single-region dynamic mesh refinement (standard OpenFOAM functionality) has already been implemented in the internal development version of the solver. Possibility of expanding refinement support to two-dimensional and/or multi-region meshes is currently under consideration. And fourth, in order to support more detailed and physical premixed combustion simulations, development and implementation of combustion model suitable for LES is foreseen in the future.

Current version of the solver is published on github (<https://github.com/flameFoam/flameFoam>)