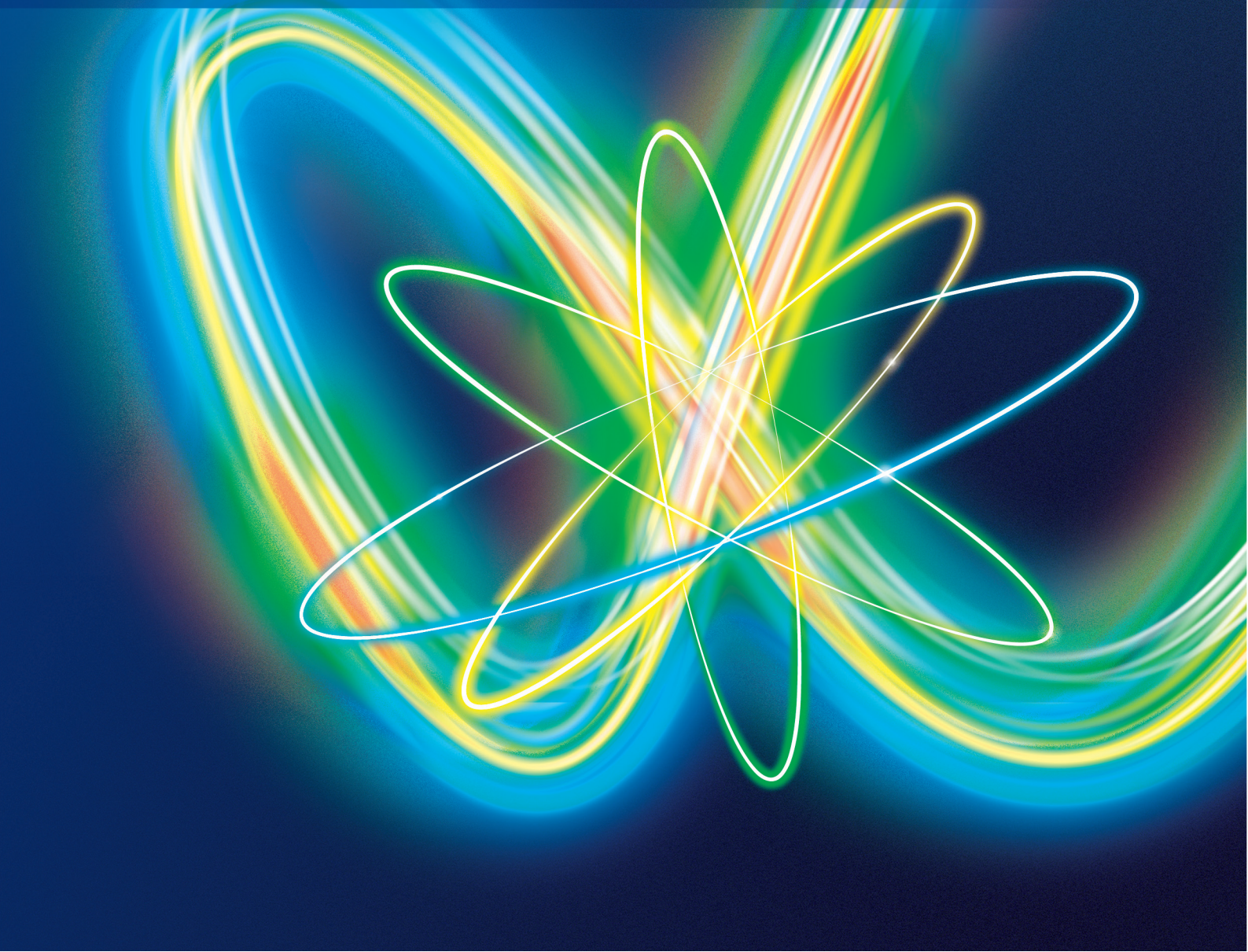
NUTHOS-13

2022 | September 5-10 Hsinchu, TAIWAN

Advancing Sustainable Development of Nuclear Power

13th International Topical Meeting on Nuclear Reactor Thermal - Hydraulics, Operation and Safety

Proceeding Book



Development of turbulent hydrogen combustion CFD solver for OpenFOAM

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ABSTRACT

Significant international efforts are devoted to improving understanding and prediction accuracy of hydrogen combustion phenomena in the containments of nuclear power plants during severe accidents. One of the most challenging issues is simulation of flame acceleration in the presence of turbulence. It is also critical for safety since flame acceleration is directly linked to the posed risk – stronger acceleration leads to powerful shock waves or even DDT. Due to the large scales of the containment applications, relevant state-of-the-art employs simplifications, allowing running models with affordable resources, while obtaining sufficiently accurate results. Used simplified approaches are turbulence modeling based on RANS and combustion models based on progress variable and turbulent flame speed correlations.

Up to now the majority of the simulations are performed using commercial CFD codes with in-house modifications. Other proprietary specialized solutions are also prevalent, e.g., FLACS or EUROPLEXUS. This situation motivated us to develop an open-source solver for turbulent premixed combustion. The current version of our solver, flameFoam, is built with the OpenFOAM toolkit version 9. flameFoam basis are standard solvers rhoPimpleFoam, buoyantPimpleFoam, and chtMultiRegionFoam, included with the OpenFOAM. flameFoam is not a straight copy of these standard solvers but a combination of them. The presented initial solver version has been developed and tested for the combustion of homogeneous hydrogen-air mixtures.

The current development status of the solver is presented in the paper, with its ongoing validation, recent applications, and performed research. Recent, yet unpublished implementation of laminar burning velocity estimation based on artificial intelligence model is highlighted and discussed.

KEYWORDS

premixed combustion, turbulence, CFD, OpenFOAM, flame propagation

1. INTRODUCTION

The containment of nuclear power plant is the last barrier protecting the environment from radioactive contamination in the case of a severe accident. Containment integrity is threatened by several possible threats during the severe accident, with significant risk posed by possible hydrogen combustion or explosion. To manage this risk adequate understanding of the combustion process and efficient numerical solutions are needed.

One of the most important phenomenological hydrogen combustion issues for safety is the flame acceleration due to obstacle-induced turbulence. At the same time, this issue still poses significant challenges for both analytical investigations and numerical studies.

Therefore, to possess the capacity required for the adequate managing of the severe accidents and risks present due to possible hydrogen combustion, international efforts are devoted to improving understanding and prediction accuracy of hydrogen combustion phenomena in the containments of nuclear power plants during severe accidents.

Due to the large scales of the containment applications, relevant state-of-the-art employs simplifications, allowing running models with affordable resources, while obtaining sufficiently accurate results. Used simplified approaches are RANS turbulence models and combustion models based on progress variable, turbulent flame speed closure (TFC) approach [1] and turbulent flame speed correlations.

Up to now the majority of the simulations available in literature or demonstrated in the international benchmarks [2–4] have been performed using commercial CFD codes with in-house modifications [5–13]. Other proprietary specialized solutions have also been prevalent, e.g., GASFLOW-MPI [14–16], FLACS [17] or COM3D [18, 19].

So far open-source contributions compose only a smaller, albeit significantly increased in recent times, fraction. Such dominance of in-house modified commercial and other proprietary solutions for the state-of-the-art applications impedes collaborative, open and free innovation in the field.

This situation motivated us to develop an open-source solver for turbulent premixed combustion. To be practically applicable in the nuclear safety context and based on the relevant state-of-the-art we based our solver initially on RANS and TFC approaches, with LES and more detailed combustion models foreseen for more detailed and fundamental studies.

We decided to base our solver on OpenFOAM CFD [20] as the most popular open-source CFD solution. It implements a finite volume method and allows the development of custom solvers. 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 are some solvers dedicated to the simulation of reacting flows already distributed with OpenFOAM (version 9):

- 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
- reactingFoam – models combustion using chemical kinetics simulations

Older versions of OpenFOAM also have other custom open-source solvers, e.g. reactingFoam-SCI [21] or blastFoam [22].

None of the combustion solvers distributed with OpenFOAM are based on a progress variable approach with TFC and practically applicable for the simulation of turbulent premixed combustion in severe accident-relevant conditions. The closest in terms of the formulation is XiFoam solver, which is based on the regress variable, approach basically equivalent to progress variable, but its combustion source is modeled using a flame surface wrinkling approach. Therefore, in order to flexibly apply TFC model we developed a new solver, called flameFoam [23–25].

The paper presents the status of the development version of flameFoam solver, including implemented models and initial validation examples. Extended TFC model was implemented into the development version of flameFoam, validation efforts in progress. LES combustion model with Charlette correlation was implemented and initially validated using the University of Sydney laboratory-scale chamber experiment. The last presented improvement is an AI-based model of laminar burning velocity.

2. FLAMEFOAM SOLVER

The development version of flameFoam is built on the OpenFOAM toolkit version 9. 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 complimented with custom combustion modeling. The

presented initial solver version has been developed and tested for the combustion of homogeneous hydrogen-air mixtures.

Base elements of flameFoam solver are standard buoyant compressible Navier-Stokes equations complemented with progress variable equation and combustion source terms.

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \Delta \cdot \left(\rho \vec{U}\right) = 0 \tag{1}$$

Momentum equation:

$$\frac{\partial \rho \vec{U}}{\partial t} + \Delta \cdot \left(\rho \vec{U} \times \vec{U}\right) = \nabla \cdot \hat{\mathbf{t}}_{eff} - \nabla p + \rho \vec{g} \tag{2}$$

Energy equation:

$$\frac{\partial \rho h}{\partial t} + \Delta \cdot \left(\rho \vec{U} h\right) + \frac{\partial \rho K}{\partial t} + \Delta \cdot \left(\rho \vec{U} K\right) = \frac{\partial p}{\partial t} + \nabla \cdot \left(\alpha_{eff} \nabla h\right) + \rho\left(\vec{g} \cdot \vec{U}\right) + S_h \tag{3}$$

The mixture composition and flame propagation simulation are based on the progress variable approach. The progress variable c is defined as

$$c = \frac{Y_0^{H_2} - Y^{H_2}}{Y_0^{H_2} - Y_\infty^{H_2}} \tag{4}$$

The progress variable c can have values from the interval [0, 1]. Value 0 corresponds to the fresh mixture, while value 1 to burnt. The thermophysical properties of the mixture depending on its composition (molar mass, specific enthalpy and others) are linearly interpolated from the properties of burnt and unburnt mixtures and the value of c.

The combustion process is simulated using a transport equation of progress variable:

$$\frac{\partial \rho c}{\partial t} + \Delta \cdot \left(\rho \vec{U} c\right) = \nabla \cdot \left(\frac{\mu_{Eff}}{Sc_T} \nabla c\right) + S_c \tag{5}$$

The progress variable transport equation can be closed using several approaches. The stable version of flameFoam has only TFC closure implemented:

$$S_c = \rho_u S_T |\nabla c| \tag{6}$$

Closing progress variable equation requires estimation of turbulent flame velocity S_T. This can be done in several ways. In the stable version of flameFoam S_T can be estimated using one of three universally established correlations – Zimont [26], Bradley [27] and Bray [28].

All three S_T correlations require values of laminar flame velocity S_L. In the stable version, S_L can be defined by the user (constant value) or be estimated from the Malet correlation [29].

The stable version of flameFoam has been validated against several turbulent combustion experiments from the French ENACCEF and ENACCEF2 facilities, including blind simulations in the frame of the ETSON-SAMHYCO-NET benchmark [4], and Australian laboratory-scale chamber [25]. Results of these simulations have been reported elsewhere [23–25] and will not be repeated here. Instead, the further section of the paper presents recent improvements of flameFoam implemented in the development version.

3. CURRENT DEVELOPMENT STATUS OF FLAMEFOAM

2.1. Extended TFC Model

TFC model, implemented in the stable flameFoam version, is a simplified turbulent combustion model, which is widely used and has been shown to provide adequate results in various turbulent cases. However, it is universally accepted that this model has shortcomings when combustion is close to the laminar regime since it does not model laminar combustion and transition between regimes [30]. To address these deficiencies, Lipatnikov and Chomiak proposed the extended TFC model (ETFC), which should account for flame development phenomena and allow modeling of quasi-laminar combustion in addition to turbulent regime.

ETFC has been recently implemented in flameFoam by modifying the diffusion and source terms in the progress variable equation:

$$\frac{\partial \rho c}{\partial t} + \Delta \cdot \left(\rho \vec{U} c\right) = \nabla \cdot \left(\rho(\alpha/Le + D_{T,t})\nabla c\right) + S_c \tag{7}$$

$$S_c = \frac{S_L^2}{4(\alpha/Le + D_{T,t})} \rho_u c(1-c) + \rho_u S_{T,t} |\nabla c| \tag{8}$$

Where

$$S_{T,t} = S_T \sqrt{1 + t_L/t_{fd}\ (e^{-t_{fd}/t_L} - 1)} \tag{9}$$

$$D_{T,t} = D_{T,\infty}(1 - e^{-t_{fd}/t_L}) \tag{10}$$

$$D_{T,\infty} = \frac{1}{Sc_T}\frac{k}{\omega} \tag{11}$$

$$t_L = \frac{D_{T,\infty}}{u'^2} \tag{12}$$

with the flame development time t_{fd} assumed to be equal to the time passed since the ignition.

The ETFC progress variable source term, eq. (8), is composed of two parts, quasi-laminar and turbulent, the latter being similar to TFC progress variable source term. At low turbulence intensities, the quasi-laminar part is inversely proportional to the chemical timescale $\alpha/(LeS_L^2)$.

The validation of the ETFC model and implementation is still ongoing. Preliminary results show that for hydrogen-air flames where S_L is of the order of m/s or tens of cm/s, obtained source term S_c is unphysically large for the quasi-laminar regime at low turbulence intensities due to relatively small value of thermal diffusivity and large ratio S_L^2/α. This issue has been encountered previously in the literature [11], where Holler et al. had to introduce a multiplication factor (lower than 1) for S_L to obtain realistic slow flame propagation results with ETFC implementation. However, ETFC has also been shown to provide good results with hydrogen concentrations below 10%, when laminar flame speed is sufficiently low [8, 9].

2.2. LES Combustion Model

While initially flameFoam solver was developed targeting practical nuclear safety (containment) applications with computationally efficient RANS and TFC modeling, it can also be used as a basis for more fundamental studies employing more detailed simulations. Initial work has been performed in the development version of flameFoam in this direction. To enable a more detailed simulation of turbulence and combustion, LES-suitable combustion models had to be implemented. LES itself is supported by the underlying OpenFOAM framework, which provides numerous options to simulate sub-grid scale viscosity.

In the implemented LES combustion model the turbulent flame velocity S_T in the progress variable source term S_c (eq. 6) is reformulated following the flame surface density approach through the laminar velocity S_L and the sub-grid scale flame wrinkling factor Ξ_Δ:

$$S_T = S_L \Xi_\Delta \tag{13}$$

For the estimation of Ξ_Δ, Pitsch – Duchamp de Lageneste [31] and Charlette [32] correlations were implemented. Initial validation attempts showed poor accuracy when using Duchamp de Lageneste correlation and promising results with Charlette.

Figure 1 presents LES simulation results of the University of Sydney laboratory-scale chamber experiment [33] using a 3D mesh of 0B0S configuration (Figure 2). Vented combustion of 22.5 % hydrogen-air mixture was simulated. While simulation slightly over-estimates the pressure, the qualitative agreement is good. Failure to obtain better agreement with the experiment might be related to missing support for quenching in flameFoam. Quenching would not only reduce the average speed of flame propagation, diminishing the level of over-estimation, it could also allow to better reproduce the shape of pressure curve since local flattenings of the curve might be related to intense quenching behind the obstacles due to increased turbulence and mixing. Another reason for missing local flattenings is the use of constant S_L value in these simulations, since RANS simulations with ANN S_L estimation, presented further manage to reproduce such flattening.

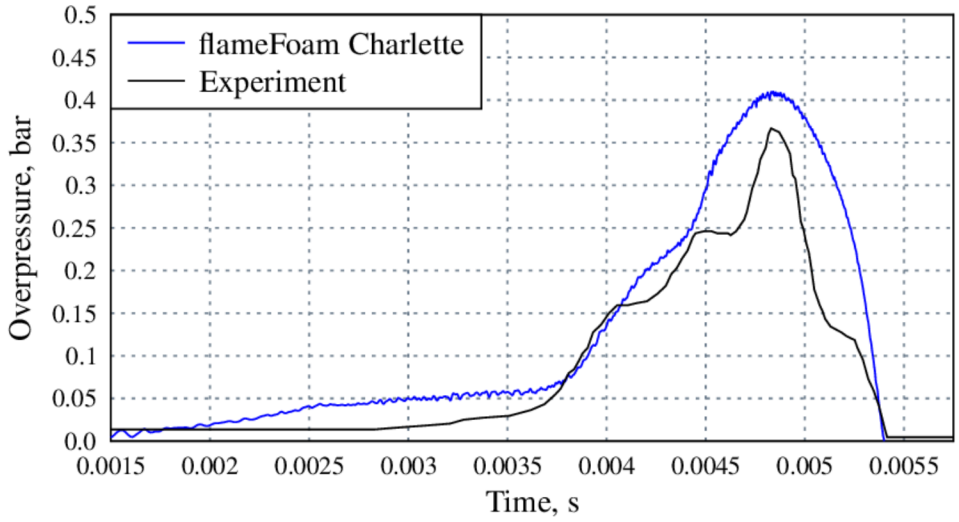

Figure 1 LES results (pressure evolution) of University of Sydney laboratory-scale chamber experiment 0B0S configuration [33]

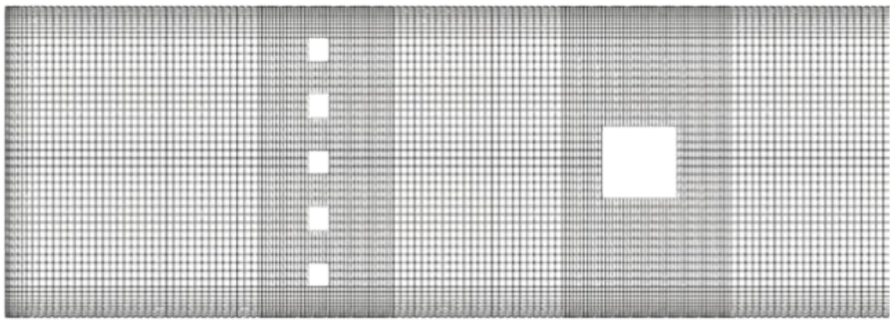

Figure 2 Mesh geometry (2D view) of the 0B0S chamber configuration used for 3D LES (rotated view, up is right)

Figure 3 shows an example of the flame surface and fluid velocity streamlines obtained with flameFoam-LES. Flame surface wrinkling by turbulent flow and disturbances by obstacles, including vortices behind the upper obstacle, are visible.

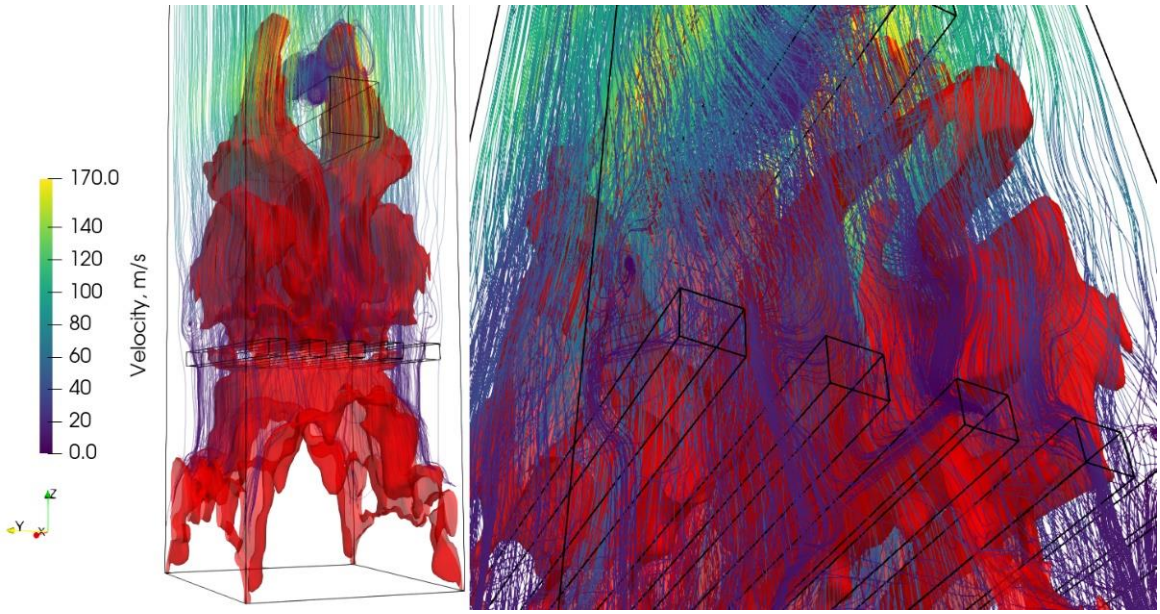

Figure 3 Flame shape and flow distribution at selected time moment obtained with flameFoam-LES

2.3. Artificial Intelligence Based Estimation of Laminar Burning Velocity

The stable version of flameFoam supports two methods for prescribing the value of laminar flame velocity: constant value, given by the user, and estimation from the Malet correlation [29], valid only for lean hydrogen-air mixtures.

To expand the domain of flameFoam application, additional methods of obtaining laminar flame velocity S_L are needed. Obvious candidates would be the inclusion of additional correlations. However, due to the complexity involved with laminar hydrogen flame velocity measurements, there is no universally accepted correlation for S_L. Furthermore, the accuracy of most correlations is uncertain in regions of lower datapoint quantity since empirical correlations relate results obtained from the entire available multi-parameter experimental range using a single, relatively simple expression.

To overcome these limitations and enable more direct use of experimental data for the estimation of S_L, it was decided to develop an artificial neural network (ANN) model of laminar burning velocity. This model would be trained on experimental data from literature and predict S_L based on (currently) three input parameters – hydrogen concentration (equivalence ratio of dry mixture), temperature and pressure.

The development of ANN model for S_L estimation can provide several benefits. First, ANN might provide higher accuracy than empirical correlation based on the same data, but expressed through simplified expression. Second, a single ANN model can be suitable for the whole domain of interest of temperatures, pressures and hydrogen concentrations, while different correlations might be more suitable at different conditions (e.g., Malet correlation for lean conditions). Third, ANN model can be easily retrained each time new experimental data becomes available, at the same time easily retiring old, less accurate data, thus enabling dynamic adaption of prediction values to the newest results in the field.

A training database of almost 3000 data points (pure experimental and interpolated) was created for the model. Since the developed ANN model has to be adequately usable during the CFD simulation, fast

calculations had to be ensured. This restriction limited model design to 4 hidden layers with 7, 10, 7 and 5 weights. The first hidden layer used *tanh* activation function. Regularization was used to prevent ANN model from overfitting. The model was trained based on a loss function composed from both mean absolute and squared errors.

Since ANN model can be more demanding on computation resources than some other machine learning or interpolation methods, the results of ANN model were compared to several other methods (Figure 4).

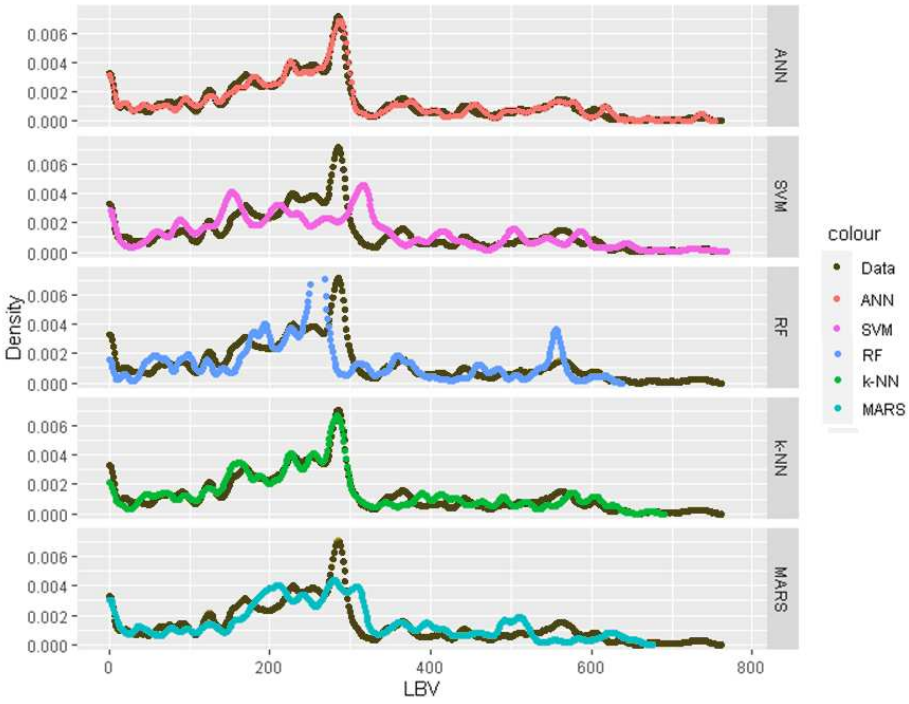

Figure 4 Density plots of ANN and other methods predictions compared to experimental data

Only the k-Nearest Neighbours (k-NN) method had accuracy comparable to the developed ANN model, but it performed worse when predicting higher S_L values.

The developed ANN model of S_L was implemented in the development version of flameFoam in the form of a series of inputs and weights multiplications. Testing simulations have shown so far that the developed model is suitable for the CFD simulations – accuracy seems to be adequate for tested cases and no significant reduction in computation speed was observed.

Figure 5 shows vertical velocity profiles of 13% hydrogen-air mixture flame acceleration experiment performed in ENACCEF2 facility (France, CNRS-ICARE) from ETSON-MITHYGENE benchmark [3]. ENACCEF2 is a closed vertical steel tube of almost 8 m in height. Flame is ignited at the bottom of the facility and propagates upwards. It is accelerated by a series of ring-shaped obstacles (7 in the simulated experiment) installed in the bottom part of the facility. Fragment of the ENACCEF2 geometry and used 2D axisymmetric orthogonal mesh (1 mm cell size) in the obstacles region is shown in Figure 6 (rotated view, up is right). Mesh contained both fluid (gray) and solid (red) regions to simulate heat transfer through the facility wall and loss to the environment. RANS-TFC simulations were performed with S_L estimation by both ANN model and Malet correlation and they display no significant differences. However, local velocity increases at about 1.5 m and 4.5 heights obtained with ANN model are closer to the experimental results, not shown here due to restricted availability.

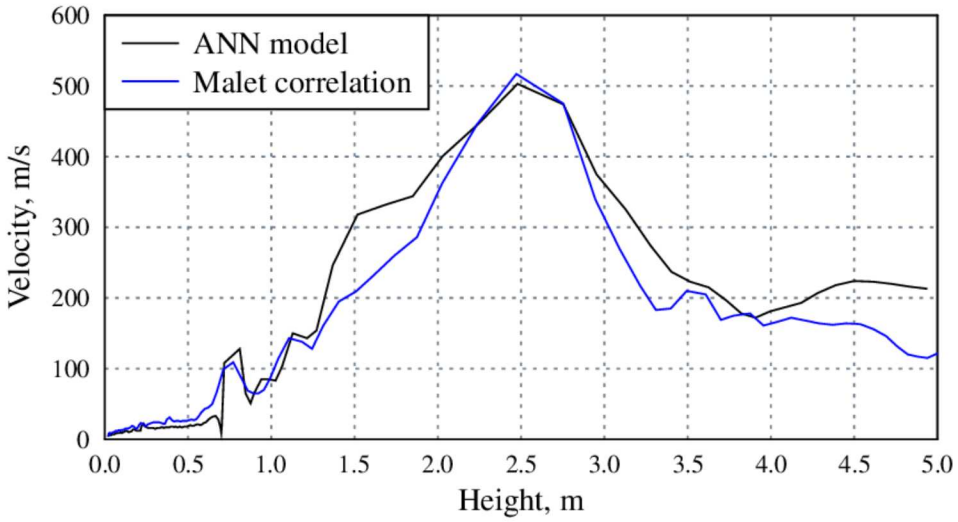

Figure 5 Vertical flame velocity profile of ENACCEF2 facility 13% hydrogen concentration experiment from ETSON-MITHYGENE benchmark obtained with flameFoam RANS-TFC and RANS-TFC-ANN simulations

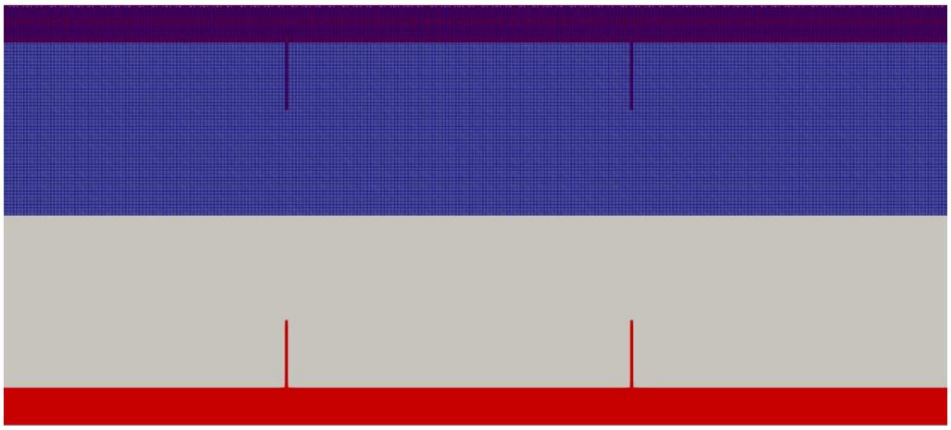

Figure 6 Fragment of ENACCEF2 facility geometry and mesh in the obstacles region, gray – facility volume/fluid mesh, red – facility wall/solid mesh (rotated view, up is right)

Figure 7 presents pressure evolution in the case of the University of Sydney laboratory-scale chamber experiment [33] with BBBS configuration obtained with flameFoam RANS TFC simulation with ANN S_L estimation and 2D axisymmetric orthogonal mesh (Figure 8). Cell sizes in the chamber interior varied from 0.25 mm to 0.03125 mm. Obtained results roughly correspond to the experiment, with a slight overestimation of maximal overpressure value.

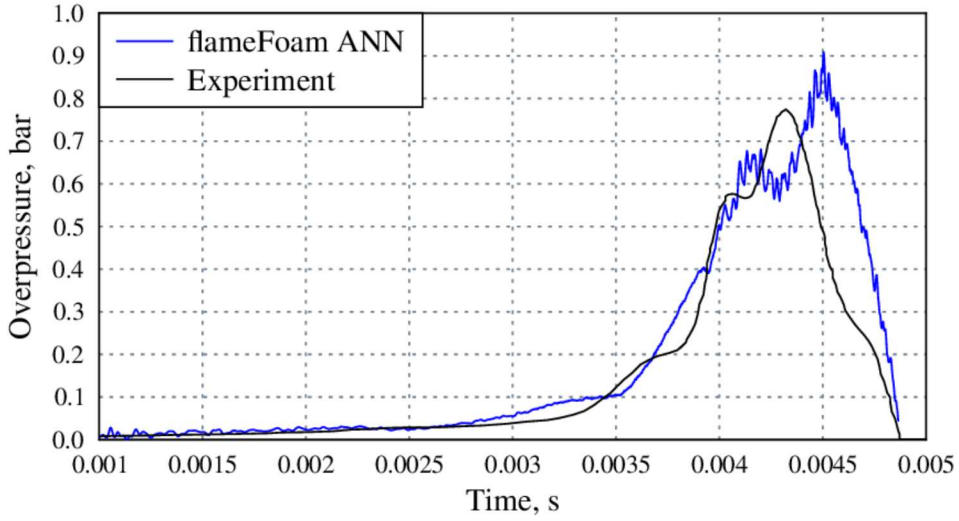

Figure 7 flameFoam RANS-TFC-ANN results (pressure evolution) of University of Sydney laboratory-scale chamber experiment BBBS configuration [33]

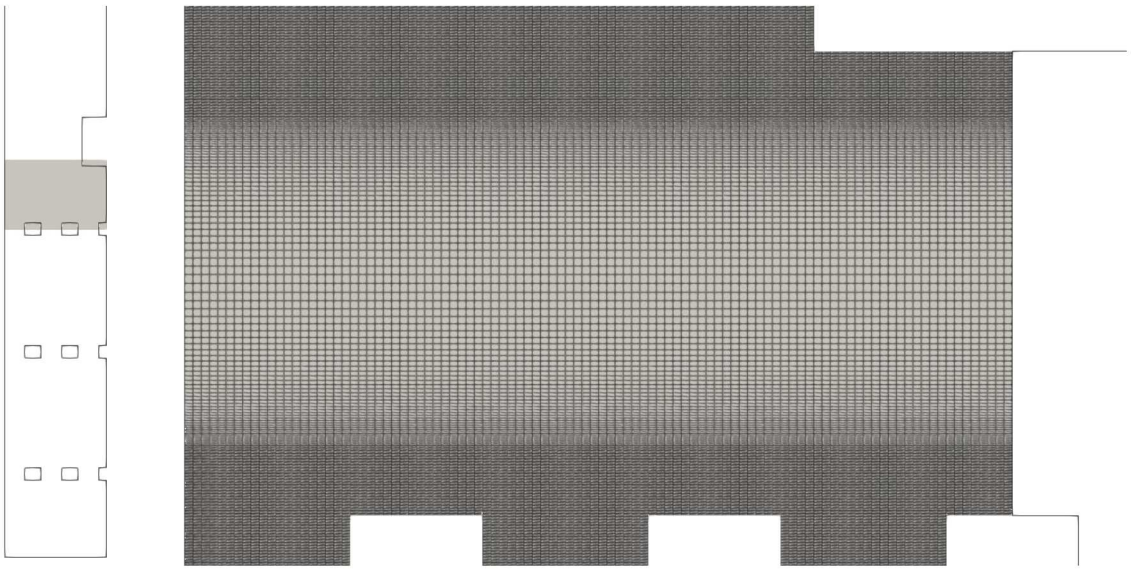

Figure 8 Schematic view of the chamber mesh with BBBS configuration, with a close-up of mesh in the highlighted area

3. CONCLUSIONS

Development status of an open-source turbulent premixed combustion solver flameFoam based on OpenFOAM toolkit was presented. Solver, stable version of which is based on RANS and TFC approach, is being actively developed in several different aspects:

1. Implementation of ETFC model has been completed, however, validation of the model has been unsuccessful so far and needs further work.
2. LES-suitable combustion model based on surface density approach has been implemented together with Pitsch – Duchamp de Lageneste and Charlette correlations for SGS flame wrinkling factor. Initial validation of the model with Charlette correlation showed promising results.
3. A fast ANN model of laminar flame velocity based on experimental data has been developed and implemented into flameFoam. The model showed promising results in both accuracy and calculation efficiency.

NOMENCLATURE

c	combustion progress variable
$D_{T,t}$	time-dependent turbulent diffusivity
g	gravitational acceleration
h	enthalpy
k	turbulent kinetic energy
K	kinetic energy
Le	Lewis number
p	pressure
S_c	combustion progress variable source
S_h	combustion energy source
S_L	laminar flame velocity
S_T	turbulent flame velocity
$S_{T,t}$	time-dependent turbulent flame velocity
Sc_T	turbulent Schmidt number
t	time
t_{fd}	flame development time
t_L	Lagrangian time scale
U	velocity
$Y_0^{H_2}$	initial hydrogen mass fraction
Y^{H_2}	hydrogen mass fraction
$Y_\infty^{H_2}$	final hydrogen mass fraction
α_{eff}	molecular thermal diffusivity
α_{eff}	effective thermal diffusivity
μ_{eff}	effective viscosity
Ξ_Δ	the sub-grid scale flame wrinkling factor
ρ	density
ρ_u	density of a fresh mixture
τ_{eff}	effective shear stress
ω	specific turbulent dissipation rate

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