### flameFoam: An OpenFOAM Based Solver For Practical Turbulent Premixed Combustion Simulation

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### Initial motivation



• The highest risk to containment integrity is related to hydrogen combustion

Adequate simulation of flame acceleration due to turbulence is still challenging
Model complexity and applicability balance

### Timeline

2018 V Thoughts about solver creation

- Proprietary CFD solutions were extensively used
- Additional challenge for the independent newcomers in the field
- When we started our transition from system codes and faced this situation, it and other personal experiences motivated us to develop an open-source solver
- Difficult (no-)start due to experience, personnel and time issues



- Additional motivation start of a new benchmark project
- Only practically-relevant simulations at a larger laboratory scale
   Need to run models with affordable computer resources, and at the same time obtain sufficiently accurate results
  - RANS for turbulence
  - TFC with for combustion
- OpenFOAM

 rhoPimpleFoam, buoyantPimpleFoam, chtMultiRegionFoam (later)



POVILAITIS, M., JASELIŪNAITĖ, J., Simulation of ENACCEF2 Premixed Hydrogen-Air Mixture Deflagration Experiment Using OpenFOAM. Proceedings of the 2020 28th International Conference on Nuclear Engineering, ICONE28 August 4–5, 2020, Virtual.



POVILAITIS, M., JASELIŪNAITĖ, J., flameFoam: An open source CFD solver for turbulent premixed combustion, Nucl. Eng. Des. 383 (2021) 111361 POVILAITIS, M., JASELIŪNAITĖ, J., Simulation of Hydrogen-Air-Diluents Mixture Combustion in an Acceleration Tube with flameFoam Solver, Energies 14 17 (2021) 5504 JASELIŪNAITĖ, J., POVILAITIS, M., STUČINSKAITĖ, I., RANS- and TFC-Based Simulation of Turbulent Combustion in a Small-Scale Venting Chamber, Energies, 14 18 (2021) 5710



- Extending to quasi-laminar and transitional regimes of turbulence
- Implementing LES combustion model
- Developing of AI method for estimation of laminar burning velocity

Developing flame

#### TFC

### flameFoam

https://github.com/flameFoam/flameFoam

ETFC

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot \left( \rho \vec{U} c \right) = \Delta \left( \frac{\mu_{Eff}}{S c_T} c \right) + S_c$$
$$c = \frac{Y_0^{H_2} - Y^{H_2}}{Y_0^{H_2} - Y_\infty^{H_2}}$$
$$S_c = \rho_u S_T |\nabla c|$$



$$\begin{aligned} \frac{\partial \rho c}{\partial t} + \nabla \cdot \left(\rho \vec{U} c\right) &= \Delta \left(\rho \left(\frac{\alpha}{Le} + D_{T,t}\right) c\right) + S_c \\ c &= \frac{Y_0^{H_2} - Y^{H_2}}{Y_0^{H_2} - Y_\infty^{H_2}} \\ S_c &= \rho_u S_{T,t} |\nabla c| + \rho_u \frac{S_L^2}{4(\alpha/Le + D_{T,t})} c \left(1 - c\right) \\ t_{t,t} &= D_{t,\infty} \left[1 - exp\left(-\frac{t_{fd}}{\tau_L}\right)\right], S_{t,t} = S_t \left[1 + \frac{\tau_L}{t_{fd}} \left[exp\left(-\frac{t_{fd}}{\tau_L}\right) - 1\right]\right]^{\frac{1}{2}} \end{aligned}$$



LES combustion

### flameFoam

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RANS

Turbulent flame-speed closure (TFC) combustion model:  $S_c = \rho_u \mathbf{S_T} |\nabla c|$ 

Turbulent flame-speed Bradley correlation:  $S_T = u' 0.88 (Ka \ Le)^{-0.3}$ 

$$u' = \left(\frac{2}{3}k\right)^{\frac{1}{2}} Ka = 0.157 \left(\frac{u'}{S_L}\right)^2 Re_T^{-\frac{1}{2}}$$
$$Re_T = \frac{u'l_t^B}{\nu} \qquad l_t^B = \left(\frac{3}{2}\right)^{\frac{3}{2}} \frac{u'^3}{\varepsilon}$$

LES

Flame surface density (FSD) combustion model:

 $S_c = \rho_u \boldsymbol{S_L} \boldsymbol{\Xi_\Delta} |\nabla c|$ 

Charlette sgs flame wrinkling factor correlation:  $\mathcal{E}_{\Delta} = \left(1 + \min\left[\frac{\Delta}{\delta_F}, \Gamma \frac{u_{\Delta}'}{S_L}\right]\right)^{1.4}$ 







Velocity, [m/

# Deep Neural Network of

14/21

## Laminar Burning Velocity





#### flameFoam

https://github.com/flameFoam/flameFoam

DNN: 3000 datapoints (33% experimental), tanh and ReLU activation functions











Laminar burning velocity, m/s

Challenges

Balancing between application and research

Resources – time, manpower, financing

#### Rushed work

Conclusions

20/21

- We made stuff
- It was fun... at the beginning...

• It is difficult to sustain development based solely on the scientific output



## Thank you !

21/21

Any questions? You can find me at mantas.povilaitis@lei.lt