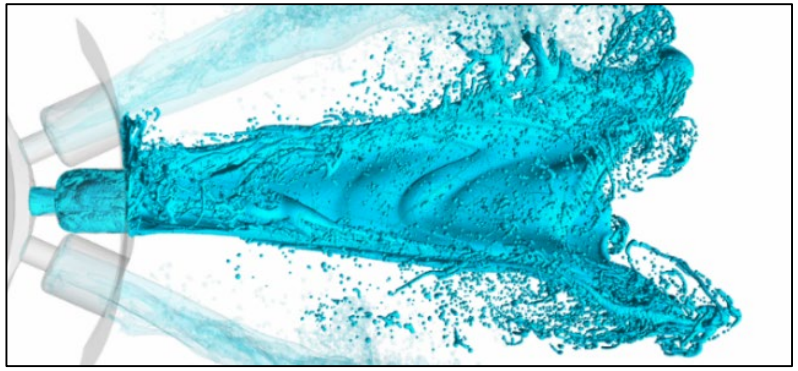
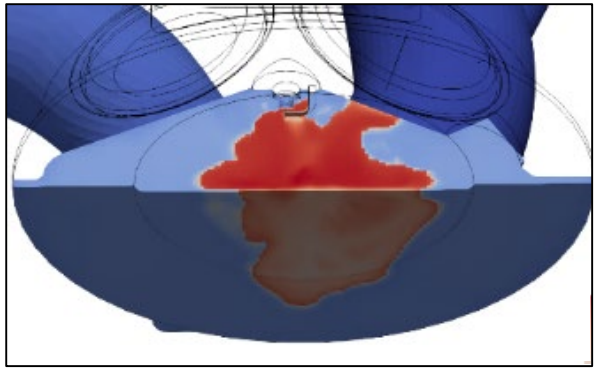
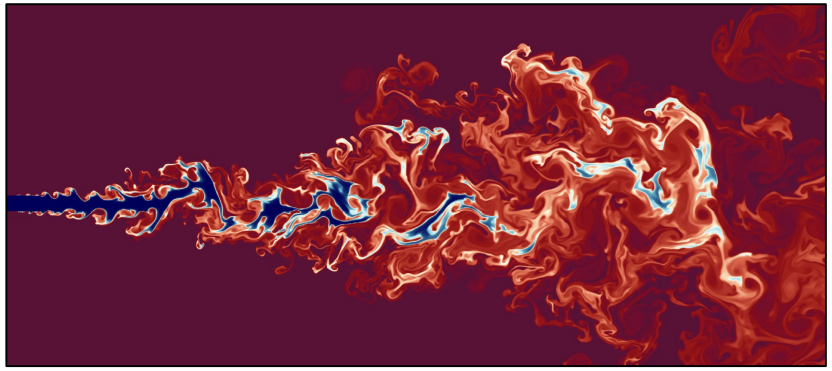

Accelerating multi-phase flow simulations with neural network models in OpenFOAM for fuel-air mixing under transcritical conditions

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Outline

- Introduction
  - Background
  - Motivation for NN
- Computational aspects
  - Governing equations and thermophysical models
  - CFD numerical framework
  - Real-fluid data sets and NN model training
  - Coupling between NN models and openFoam
- Results
  - GH2-LOX test case
  - Comparison between NN-version and original-version
  - Performance
- Conclusion
  - Summary and Future work

Background and motivation

Context:

- Increase in energy costs
- Stringent emission policies toward climate neutrality and decarbonization

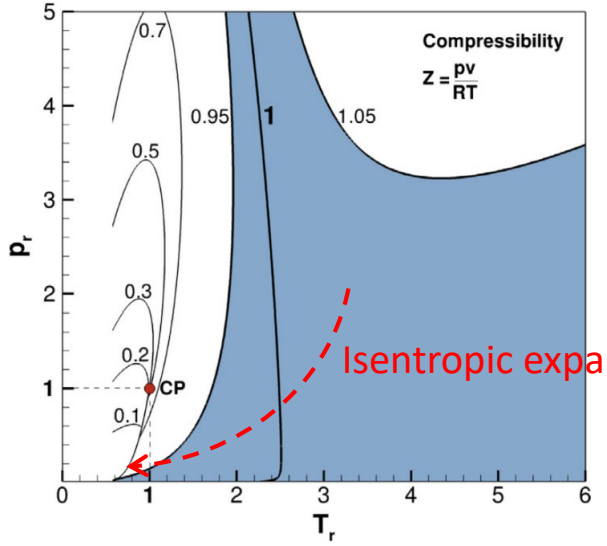
E-fuels including **hydrogen** and hydrogen carriers **(ammonia,..)** are part of the solution

Prospectives:

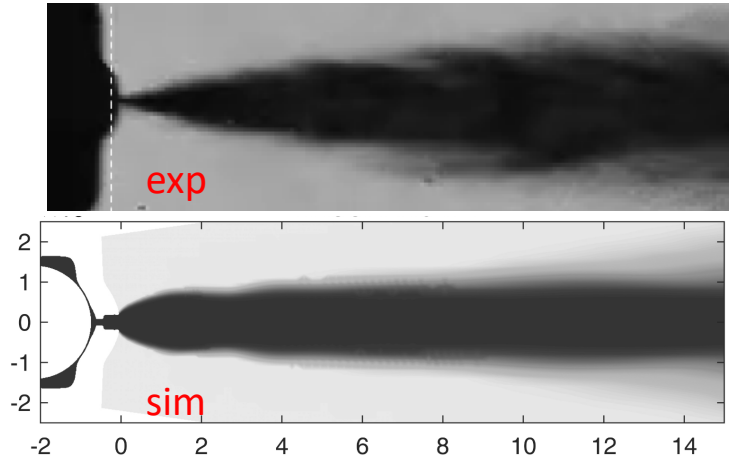
- At high-loads, heavy-duty H2-ICEs performance with DI can be comparable to FCEVs for HD transportation
- Green H2 can become a sustainable/affordable option.

Two-phase flow properties and challenges

- Accurate understanding and prediction capabilities of supercritical, and transcritical jet formation and mixing are important for clean and efficient combustion process.
- Many parameters can have large impacts (inj. pressure, back pressure, temperature, nozzle geometry)
- At high pressure, accounting for real fluids effects may be necessary
- Goal: explorations of the effect of real gas under operating conditions relevant to H2, NH3, other e-fuels, with high pressure, or crossing the two-phase region.



Example of ammonia flash boiling spray



Computational methods: Governing equations

- Mass $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$
- Momentum $\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$
- Energy $\frac{\partial \rho h_T}{\partial t} + \nabla \cdot (\rho h_T \mathbf{U}) = \frac{\partial p}{\partial t} + \nabla \cdot (\mathbf{U} \cdot \boldsymbol{\tau}) - \nabla \cdot \mathbf{q}$
- Species $\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \mathbf{U}) = \nabla \cdot \mathbf{J}_k$

$\boldsymbol{\tau}$ = viscous stresses

$\mathbf{q}$ = heat flux due to conduction and species enthalpy flux

$\mathbf{J}_k$ = species diffusion velocities

- coupled with a turbulence model: RANS, LES
- diffuse interface method

Thermodynamics and transport properties

Thermodynamics

- Real-fluid mixture density (PR EOS with non-linear Van der Waals mixing rules)
- Real-fluid caloric properties (departure functions based on PR EOS for the mixture)

Transport

- Real-fluid transport properties (Chung correlation)

$$p(v,T,x_i) = \frac{RT}{v-b_m} - \frac{a_m}{v^2+2b_m v-b_m^2}$$

$$h_m(p,T) - h_{0,m}(p,T) =$$

$$= pv_m - RT + \frac{1}{2b_m\sqrt{2}}\left[a_m - T\frac{\partial a_m}{\partial T}\right]\left[\frac{v_m + b_m(1-\sqrt{2})}{v_m + b_m(1+\sqrt{2})}\right]$$

Mixture coefficients $a_m = \sum_i \sum_j x_i x_j a_{ij}$ $b_m = \sum_i x_i b_i$

Non-linear blends, interactions coeff., *ij* $a_{ij} = (1-k_{ij})\sqrt{a_i a_j}$

Thermo package:

thermoType	
type	hePsiThermo;
mixture	reactingMixture;
transport	chungMix;
thermo	janaf;
energy	sensibleEnthalpy;
equationOfState	mixturePengRobinsonGas;
specie	specie;

- Rahantamialisoa FNZ, et al., 2021, International Conference on Liquid Atomization and Spray Systems ILASS
- Rahantamialisoa FNZ, et al., 2022, *Journal of Physics: Conference Series* Vol. 2385, No. 1, p. 012051. IOP Publishing.

Computational methods: Numerical frameworks

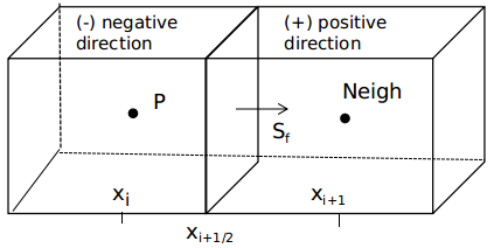
realFluidReactingFoam

- based on **reactingFoam**, with added species transport equations, and real-fluid library
- modified pressure equation to include density changes within the inner loop
- changes in the frequency of updates of other variables (enthalpy, specie)

$$\frac{\partial(\rho_0 - \psi_0 p_0)}{\partial t} + \frac{\partial \psi_0 p}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho \frac{H_P}{A_P}\right) - \frac{\partial}{\partial x_i}\left(\frac{\rho}{A_P}\frac{\partial p^*}{\partial x_i}\right)$$

realFluidHybridFoam

- based on **rhoPimpleCentralFoam**[1], with added species transport equations, and real-fluid library
- with KT/KNP (Kurganov Tadmor / Kurganov Noelle Petrova) schemes for convective terms (flux splitting)

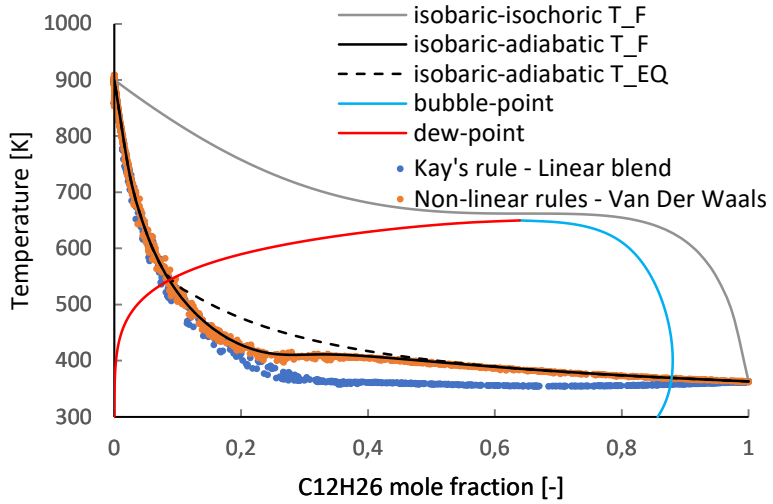


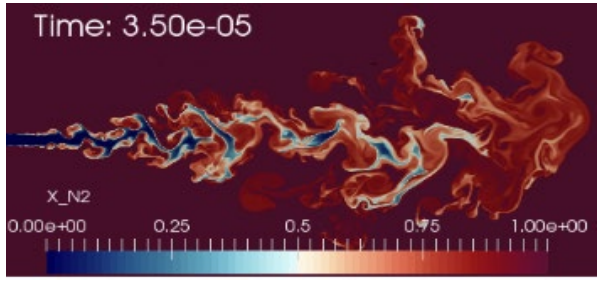
$$\sum_f \phi_f \Psi_f = \sum_f \left[\alpha \phi_{f+} \Psi_{f+} + (1-\alpha)\phi_{f-}\Psi_{f-} + \omega_f(\Psi_{f-} - \Psi_{f+})\right]$$

[1] Kraposhin MV, Banholzer M, Pfitzner M, Marchevsky IK. A hybrid pressure-based solver for nonideal single-phase fluid flows at all speeds. International Journal for Numerical Methods in Fluids. 2018 20;88(2):79-99.

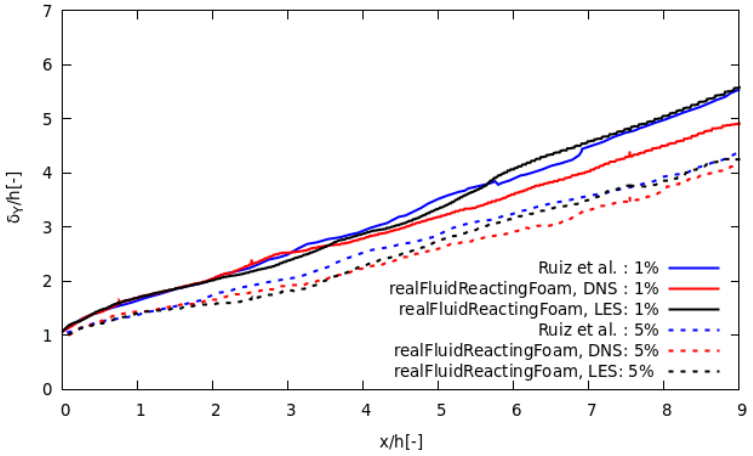
Previous validations

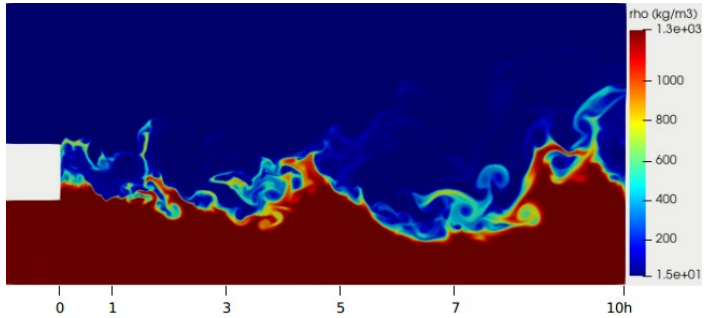
Spray A [1]



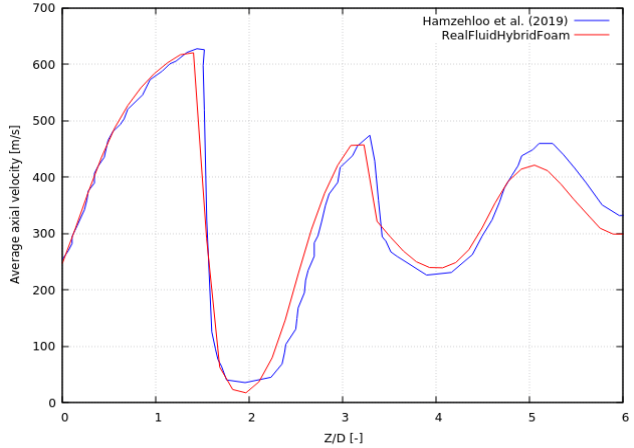


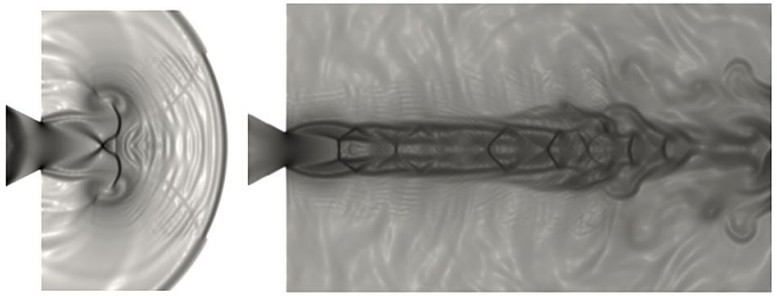
LOX-H2 [2]





H2 jets [3]

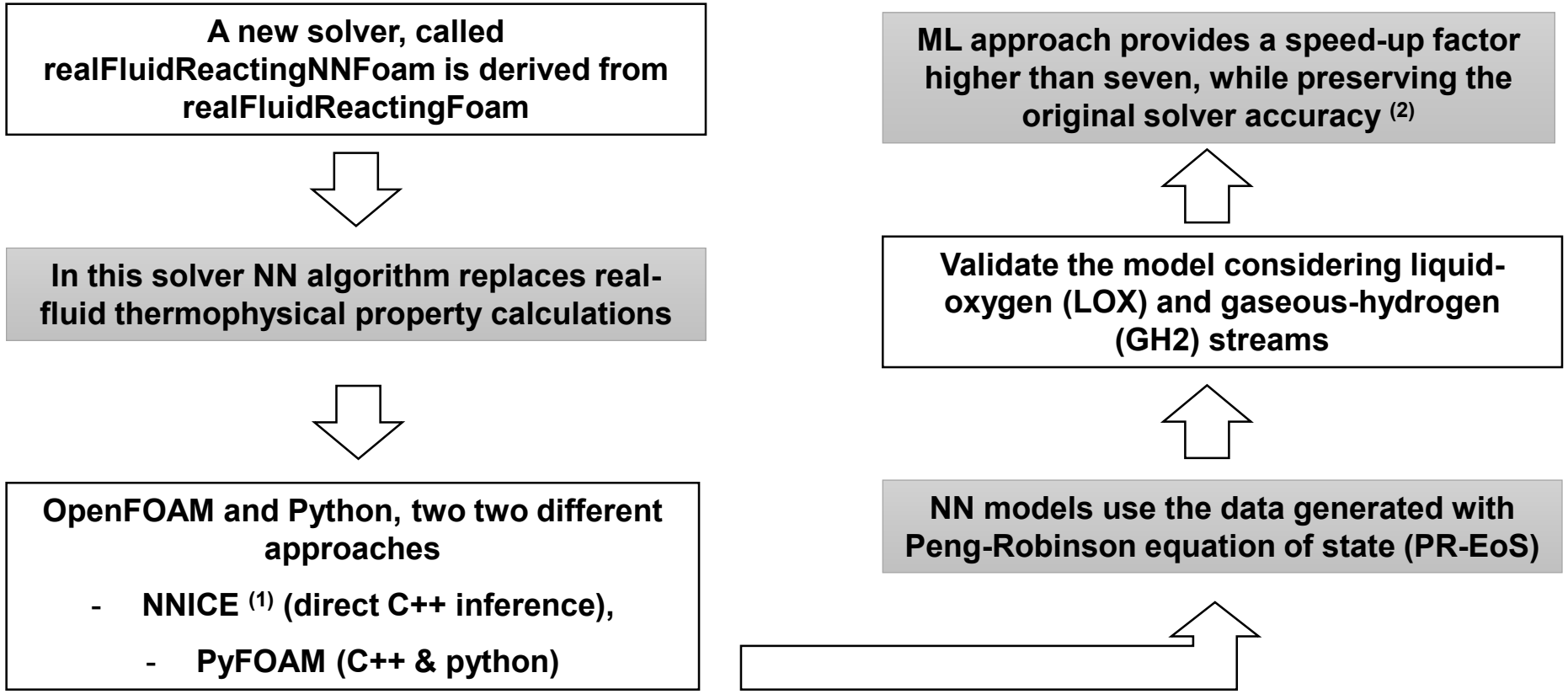




[1] Ningegowda, B.M.; Rahantamialisoa, F.N.Z.; Pandal, A.; Jasak, H.; Im, H.G.; Battistoni, M.; Energies 2020, 13, 5676.
[2] Rahantamialisoa F.N.Z, Pandal A., Ningegowda B.M., Jacopo Z., Nasrin S., H. Jasak, Hong G. Im, Battistoni M., ICLASS 2021.
[3] F Rahantamialisoa, M Battistoni, A Miliozzi, N Sahranavardfard, J Zembi, SAE Technical Paper 2023-01-0312.

Motivation for NN

The purpose is to **reduce computational costs** of multiphase flow simulations using **neural network models** to replace heavy parts related to the calculation of the **thermophysical properties.**

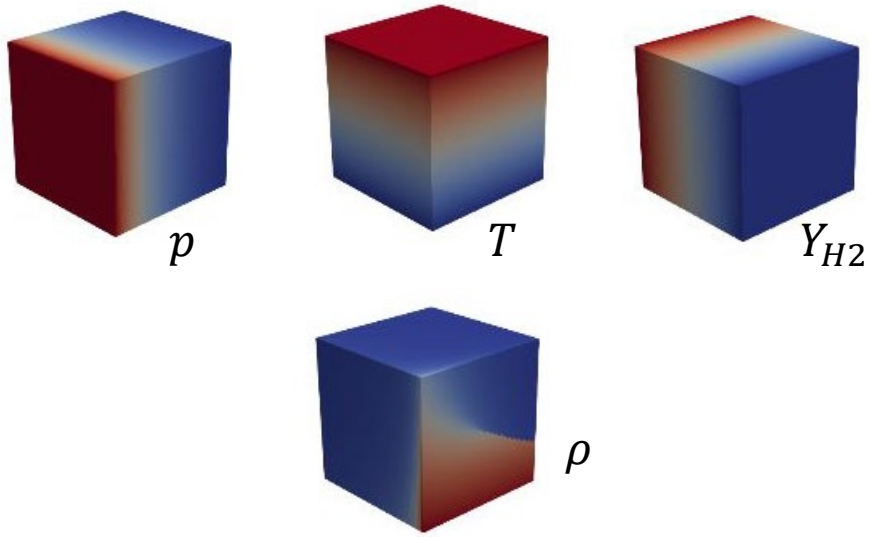


[1] D. Aubagnac (IFP-EN) https://github.com/aubagnacd/NNICE

[2] N. Sahranavardfard, D. Aubagnac-Karkar, C. Habchi, G. Costante, F. N. Z. Rahantamialisoa, and M. Battistoni. “Computation of real-fluid thermophysical properties using a neural network approach implemented in OpenFOAM”, Fluids, MDPI, 2024

Real-fluid Thermophysical Data Generation

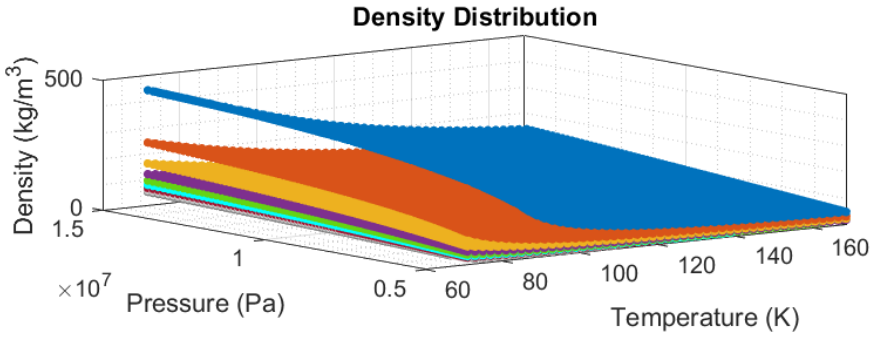
- We have three different inputs, **temperature**, **pressure**, **composition** (hydrogen mass fraction)
- Thermophysical space discretized with **250000** points.
- Data generated through
  - OpenFOAM implemented Peng-Robinson (**realFluidReactingFoam**),
  - or through IFPEN Carnot library

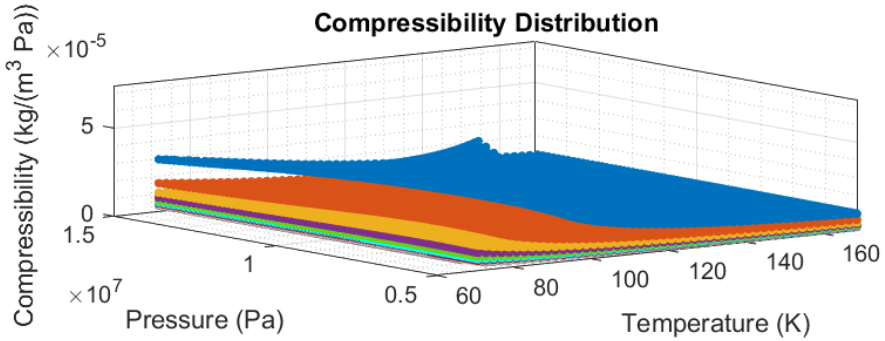


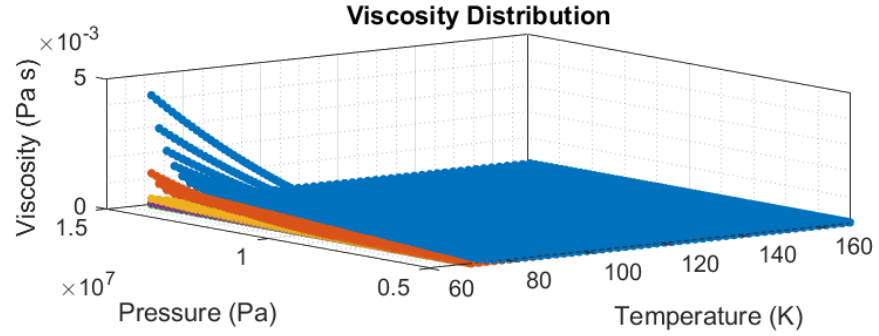
Inputs		Outputs
Variable symbol (code name)	**Definition [units]**	
Y_{H2} (Y)	Fuel mass fraction [-]	all output variables
T (T)	Temperature [K]	all output variables (except T)
p (p)	Pressure [Pa]	all output variables
h (he)	Enthalpy [J/kg]	T

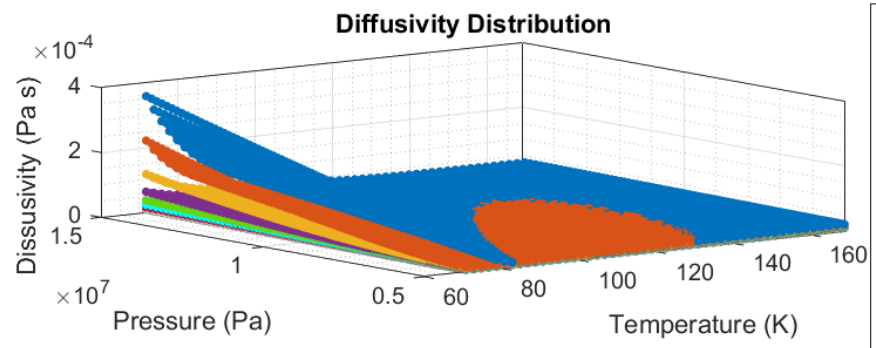
Variable symbol (code name)	**Definition [units]**
ρ (rho)	Density $[kg/m^3]$
μ (mu)	Viscosity $[Pa\ s]$
α $(alpha)$	Thermal diffusivity $[Pa\ s]$
h (he)	Specific enthalpy: $h = sie + p/\rho$ $[J/kg]$
ψ (psi)	Compressibility $\psi = 1/(ZRT)$ $[kg/(m^3 Pa)]$
T (T)	Temperature (K)

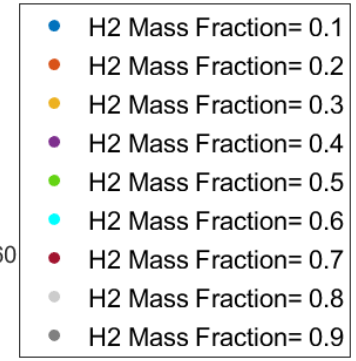
Thermophysical Data Visualization

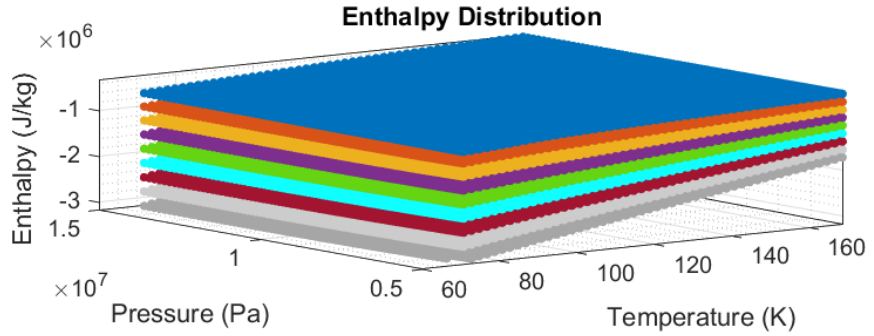


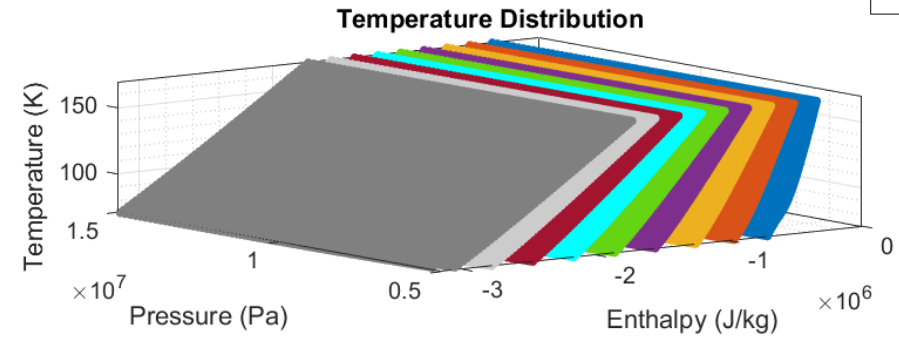




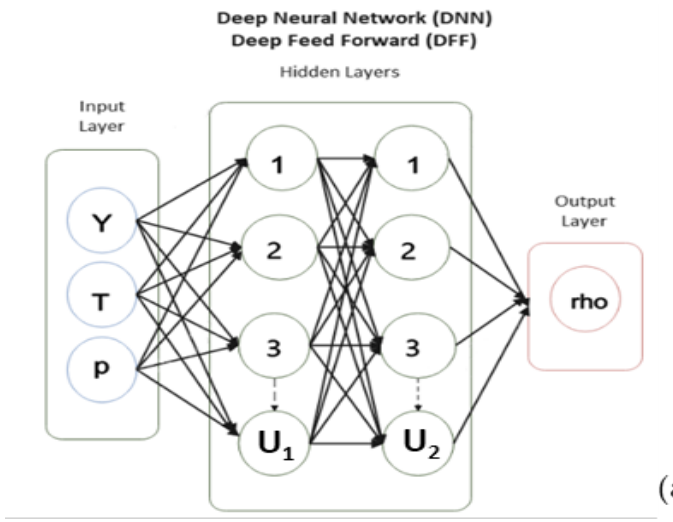




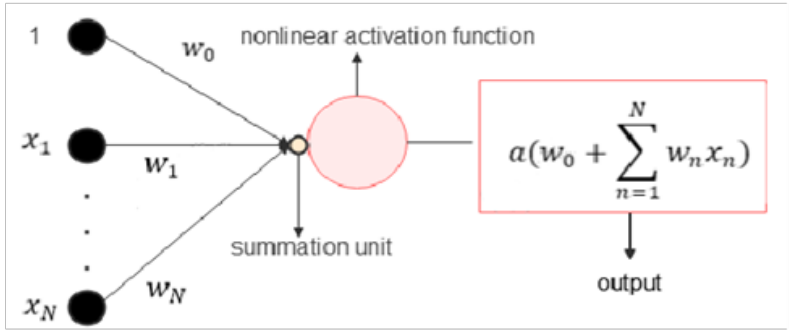




NN model equations



(a)



(b)

$$f_j^{(1)}(\boldsymbol{x}) = \left(v_j(\boldsymbol{x})\right)$$

$$v_j(\boldsymbol{x}) = \boldsymbol{w}_j^{(1)T}\boldsymbol{x} = w_{0,j}^{(1)} + \sum_{n=1}^{N} w_{n,j}^{(1)} x_n, \quad j = 1, \dots, U_1$$

$$\boldsymbol{a}(\boldsymbol{v}) = \boldsymbol{ReLU}(\boldsymbol{v}) = \boldsymbol{max}(\boldsymbol{0}, \boldsymbol{v})$$

$$f_j^{(2)}(\boldsymbol{x}) = a\left(w_{0,j}^{(2)} + \sum_{i=1}^{U_1} w_{i,j}^{(2)} f_i^{(1)}(\boldsymbol{x})\right)$$

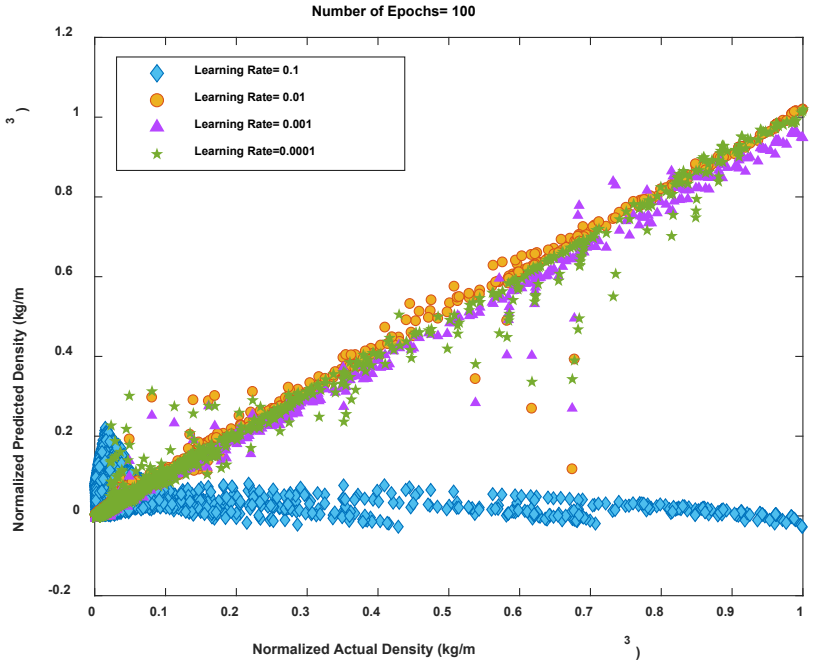
$$f_j^{(L)}(\boldsymbol{x}) = a\left(w_{0,j}^{(L)} + \sum_{i=1}^{U_{L-1}} w_{i,j}^{(L)} f_i^{(L-1)}(\boldsymbol{x})\right)$$

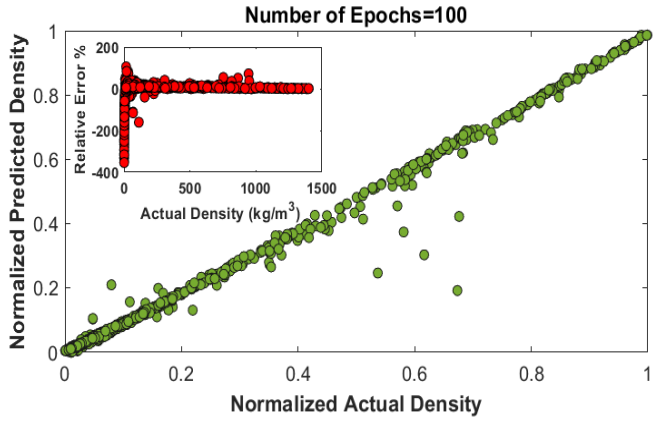
Neural Network algorithm (Python)

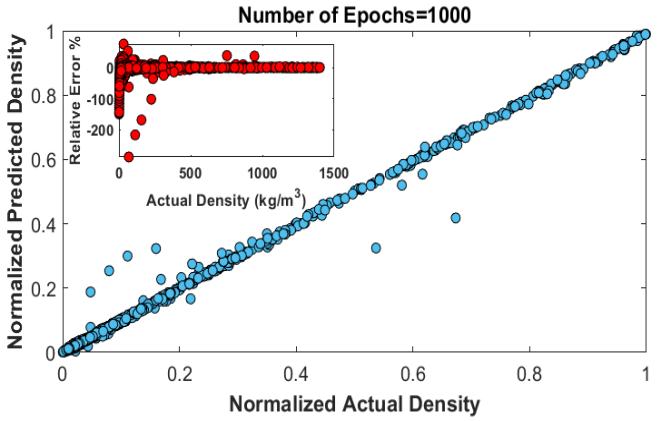
```python
#Import Numpy and Pandas libraries as dependencies
import numpy as np
import pandas as pd

#Read data from a csv file
df = pd.read_csv('file.csv')

#Choose inputs and outputs from imported data
X = df.drop(['variable1'....'variable n'], axis=1)
y = df.drop(['variable1'....'variable n'], axis=1)

#Split train and test dataset, 80 percent as the trainset and 20 pecent as the testset
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=0)

#Transform the output data of train and test dataset
y_test=np.log(y_test)
y_train=np.log(y_train)

#Scale the input and the output data between 0 and 1
from sklearn.preprocessing import MinMaxScaler
Xscaler=MinMaxScaler(feature_range=(0,1))
X_train=Xscaler.fit_transform(X_train)
X_test=Xscaler.transform(X_test)
Yscaler = MinMaxScaler(feature_range=(0,1))
y_train=Yscaler.fit_transform(y_train)
y_test=Yscaler.transform(y_test)
```

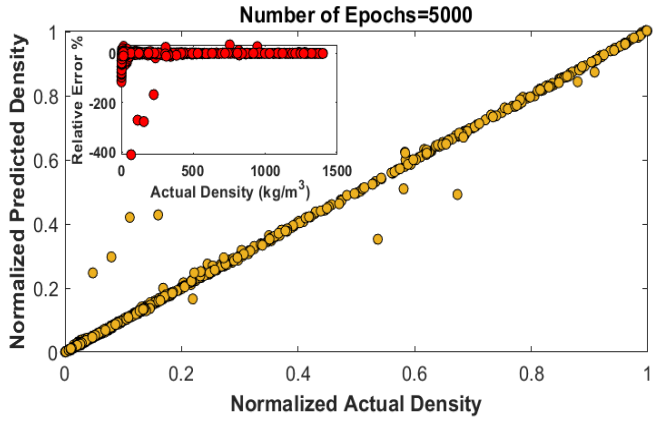
```python

#Import tensorflow and keras libraries, and specify the prefered hyperparameters
import tensorflow as tf
import keras
from keras.models import Sequential
from keras.layers import Dense
model = Sequential()
model.add(Dense(100, input_dim=3, activation='relu'))
model.add(Dense(100, activation='relu'))
model.add(Dense(1, activation='linear'))

#Keras optimization and the model compilation
lr_schedule = tf.keras.optimizers.schedules.ExponentialDecay(
    initial_learning_rate=0.0015,
    decay_steps=10000,
    decay_rate=0.9)
opt = keras.optimizers.Adam(learning_rate=lr_schedule)
model.compile(loss='mse', optimizer=opt, metrics=['mae'])

#Model fit with specification of the number of epochs and the batch size
history = model.fit(X_train, y_train,validation_data = (X_test, y_test), epochs=1000, batch_size=256)
```

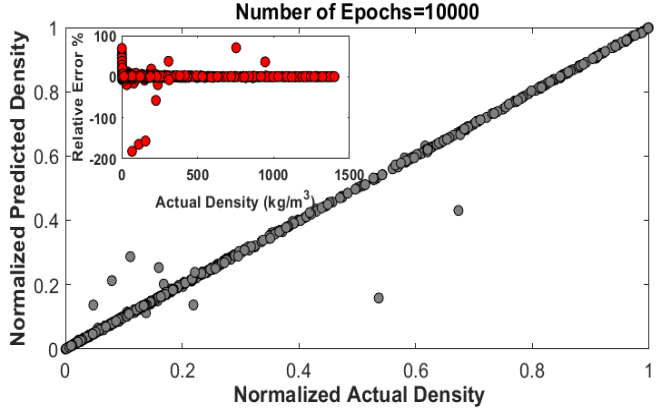
Hyperparameters Importance



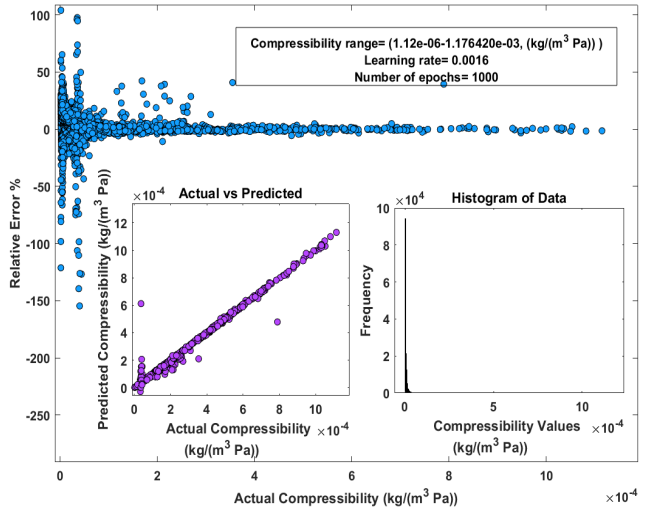


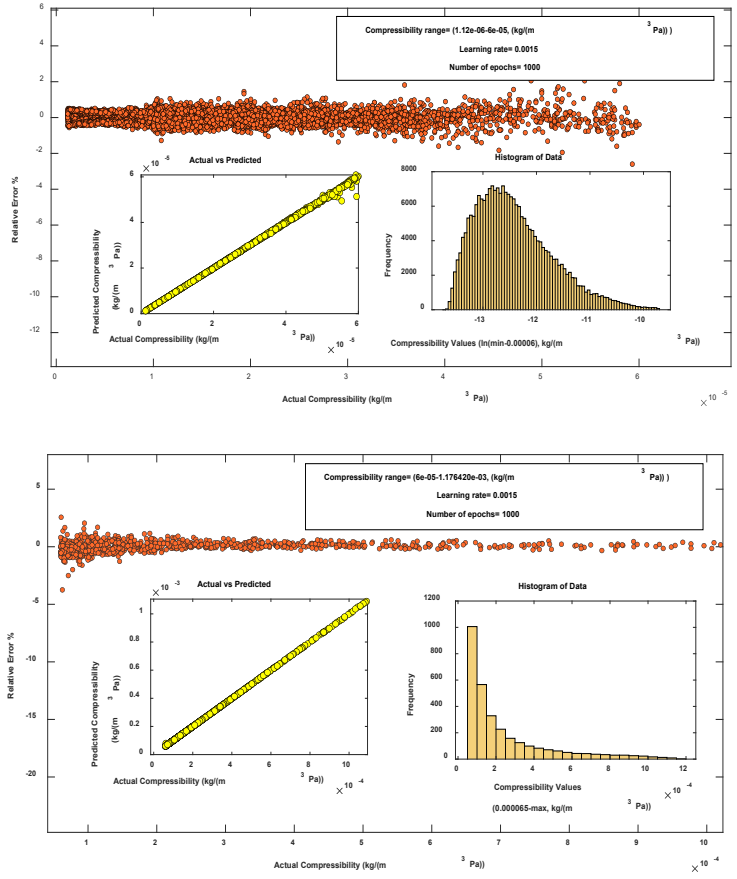


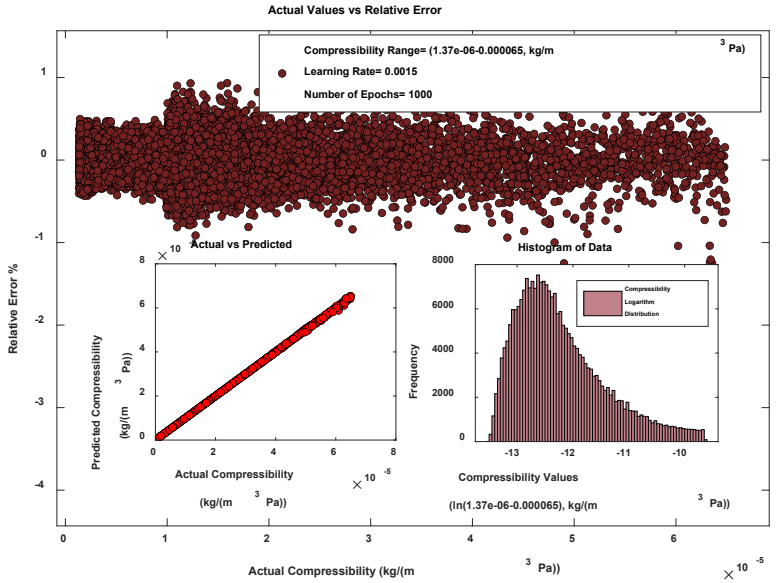




Compressibility Final Training Result

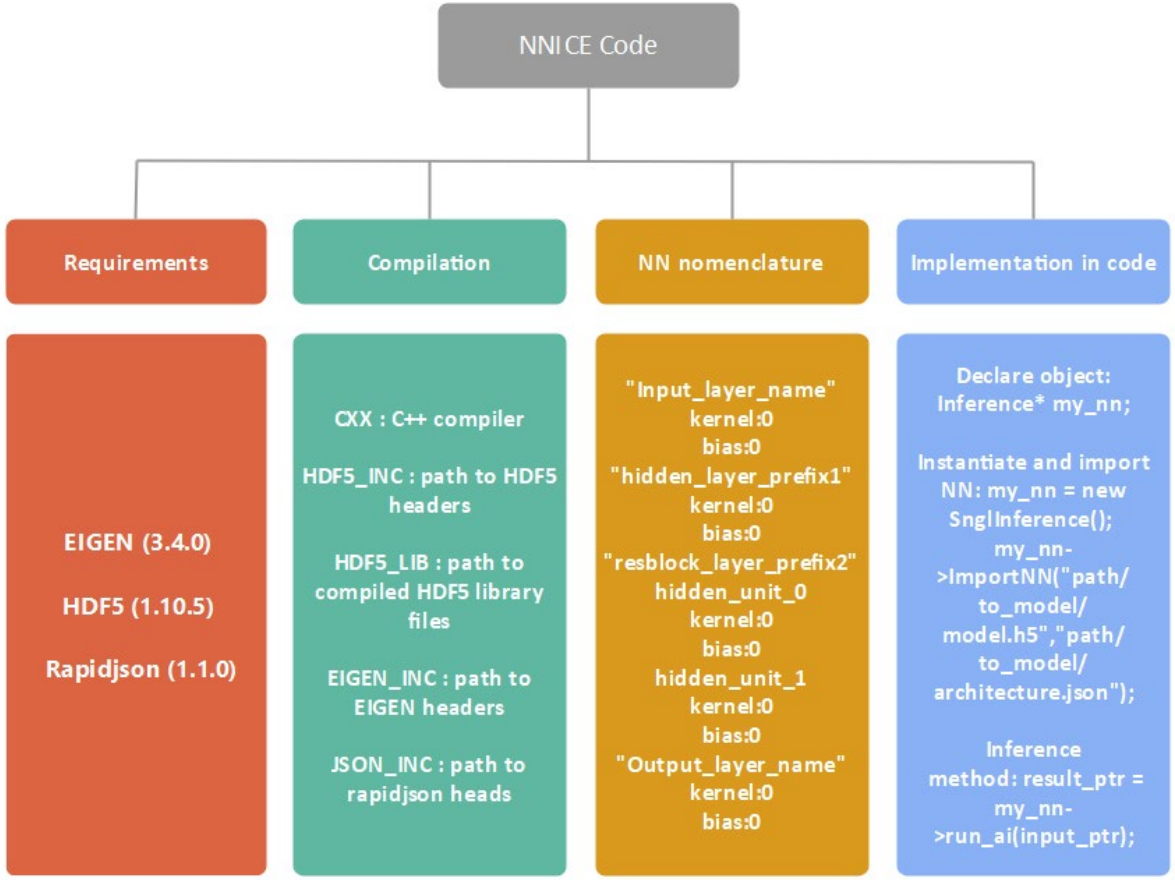


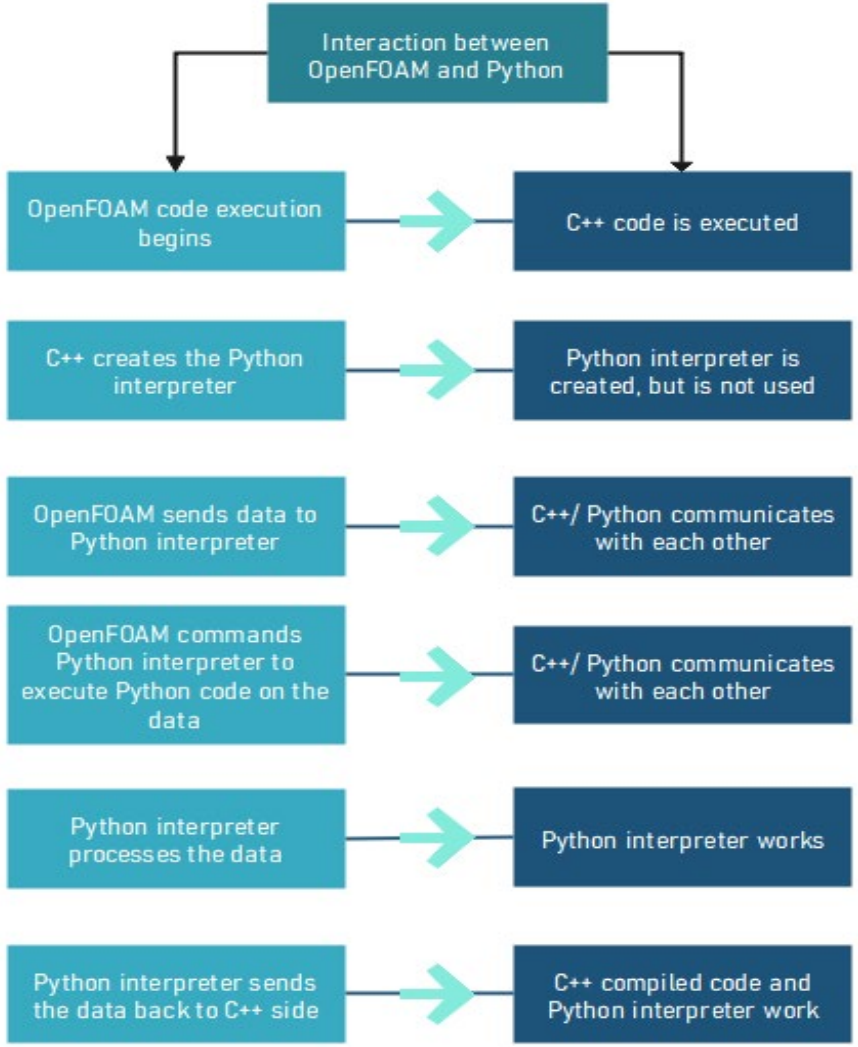




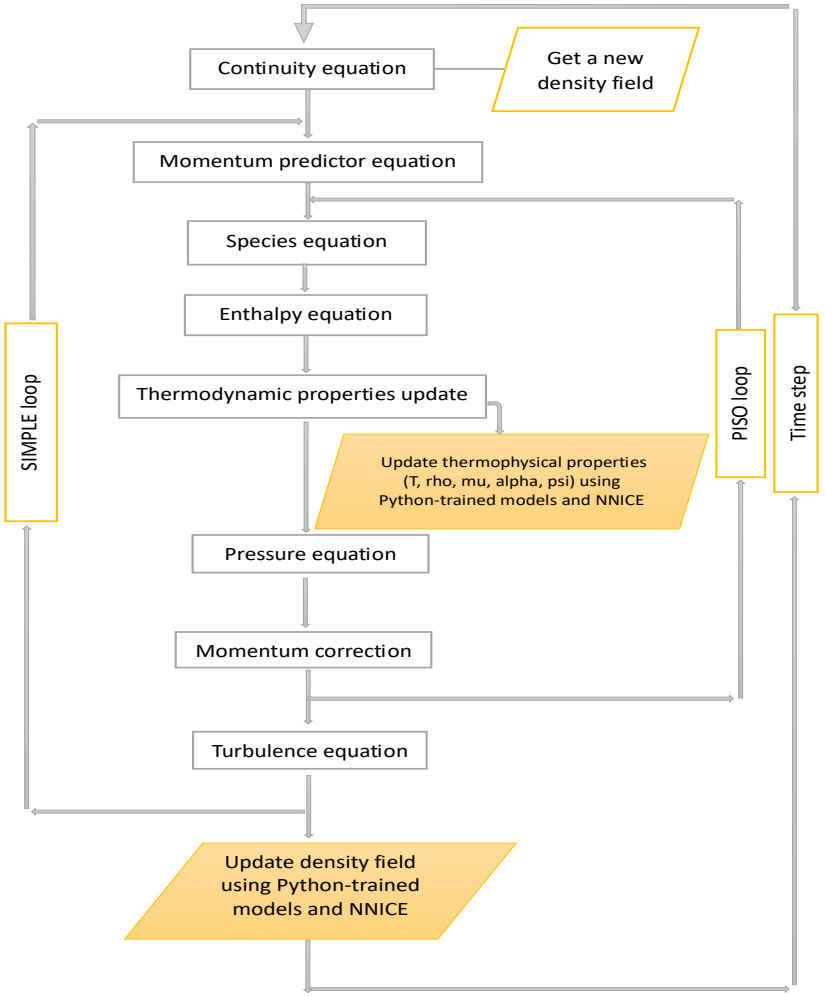
Output (applied min-max-scalar)	Inputs (applied min-max-scalar)	Hidden layer size	Activation function	Solver	Learning-rate-init	Loss metrics	epochs	batch-size
$rho, mu, alpha, he, psi,$	Y_{H2}, T, p	100 × 100	ReLU	ADAM	0.0015	MSE	1000	256
T	Y_{H2}, p, he	100 × 100	ReLU	ADAM	0.0015	MSE	1000	256

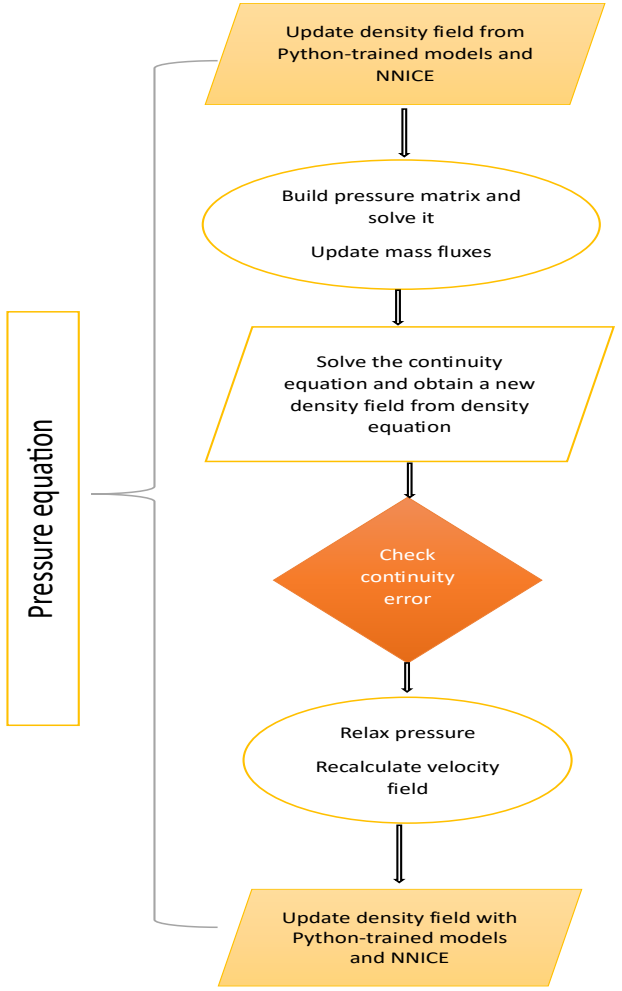
NNICE and PythonFOAM Implementations



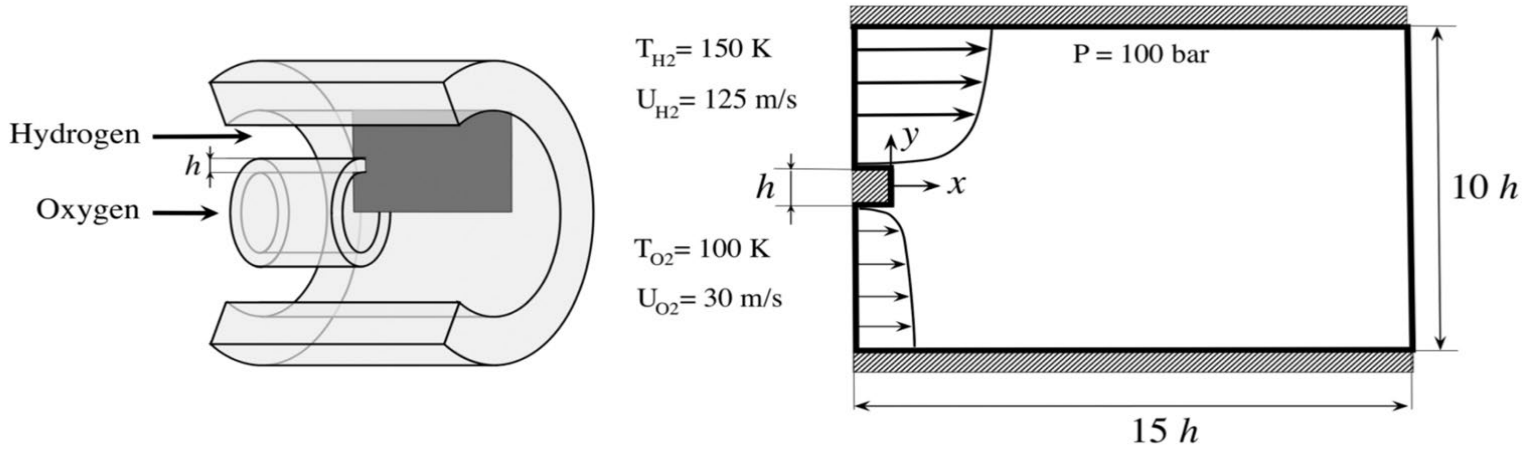


Implementation of the NN models within the PIMPLE loop





GH2-LOX test case: operating condition

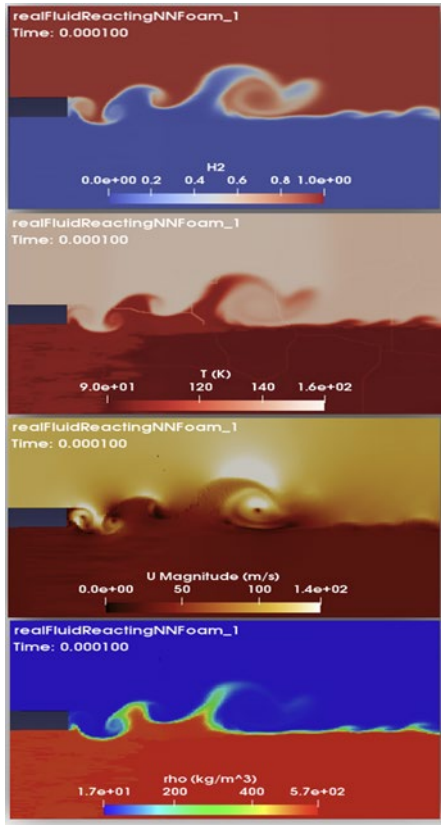


- we analyze a **two-dimensional mixing layer** with an injector lip that divides streams of liquid oxygen **(LOX)** and gaseous hydrogen **(GH2),** both at **supercritical pressure**.
- The simulation setup involves an injector lip with a height **(h) of 0.5 mm**, segregating high-speed gaseous hydrogen (GH2) in the surroundings from dense liquid oxygen (LOX) in the center.
- The area of interest of the computational domain spans **15h** along the axial direction and **10h** in the transversal direction.
- a relatively coarse mesh is employed with a uniform grid spacing of Δ**x/h = Δy/h = 20.**
- At the injector lip, we implement an **adiabatic no-slip** wall condition, while the top and bottom boundaries are treated as **adiabatic slip walls**. Furthermore, we apply a **Dirichlet pressure boundary condition** at the outlet.

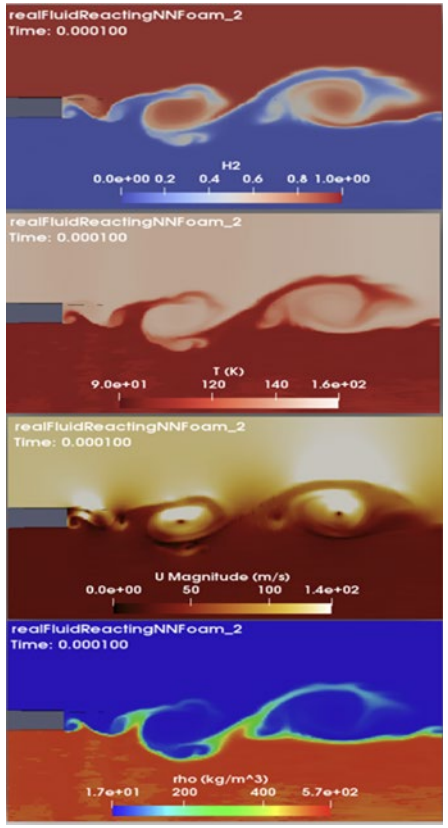
Rahantamialisoa F.N.Z, Pandal A., Ningegowda B.M., Jacopo Z., Nasrin S., H. Jasak, Hong G. Im, Battistoni M., ICLASS 2021.

GH2-LOX - Results and discussion: fields @ t = 0.1 ms

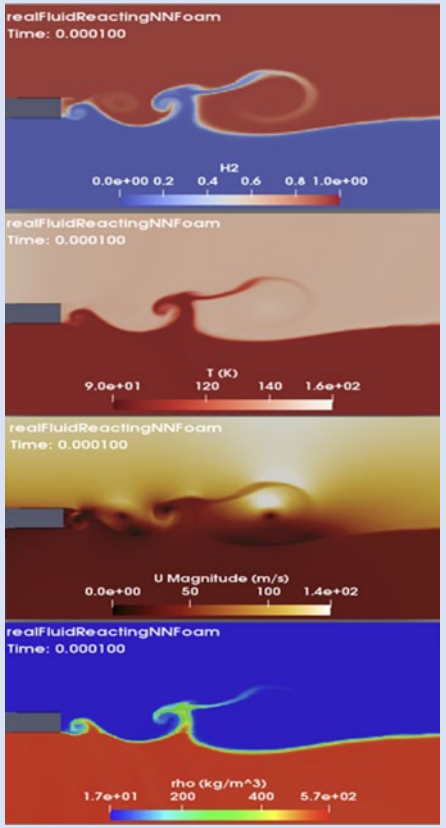
realFluidReactingNNFoam_1
NN_1



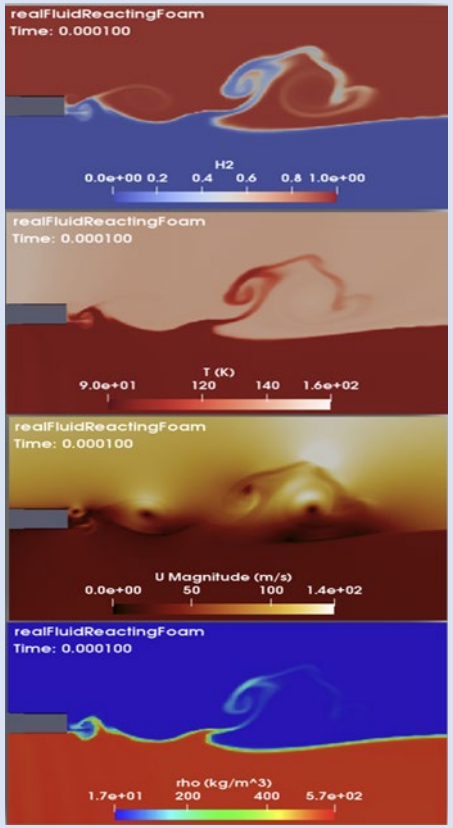
realFluidReactingNNFoam_2
NN_2



realFluidReactingNNFoam



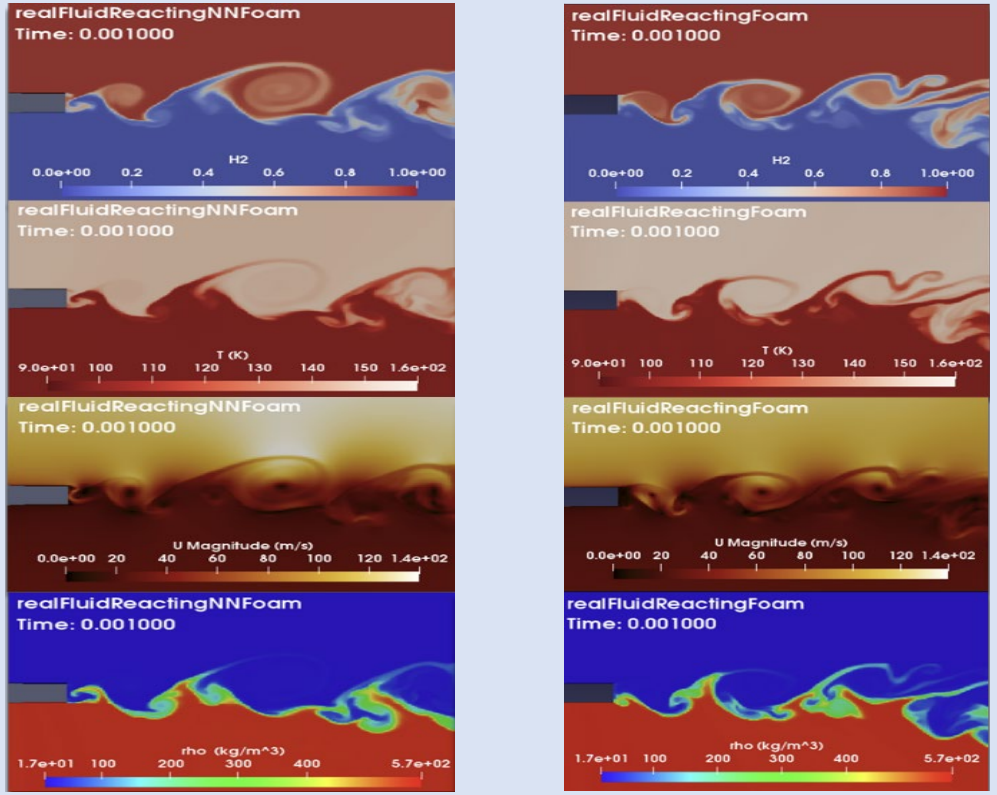
realFluidReactingFoam



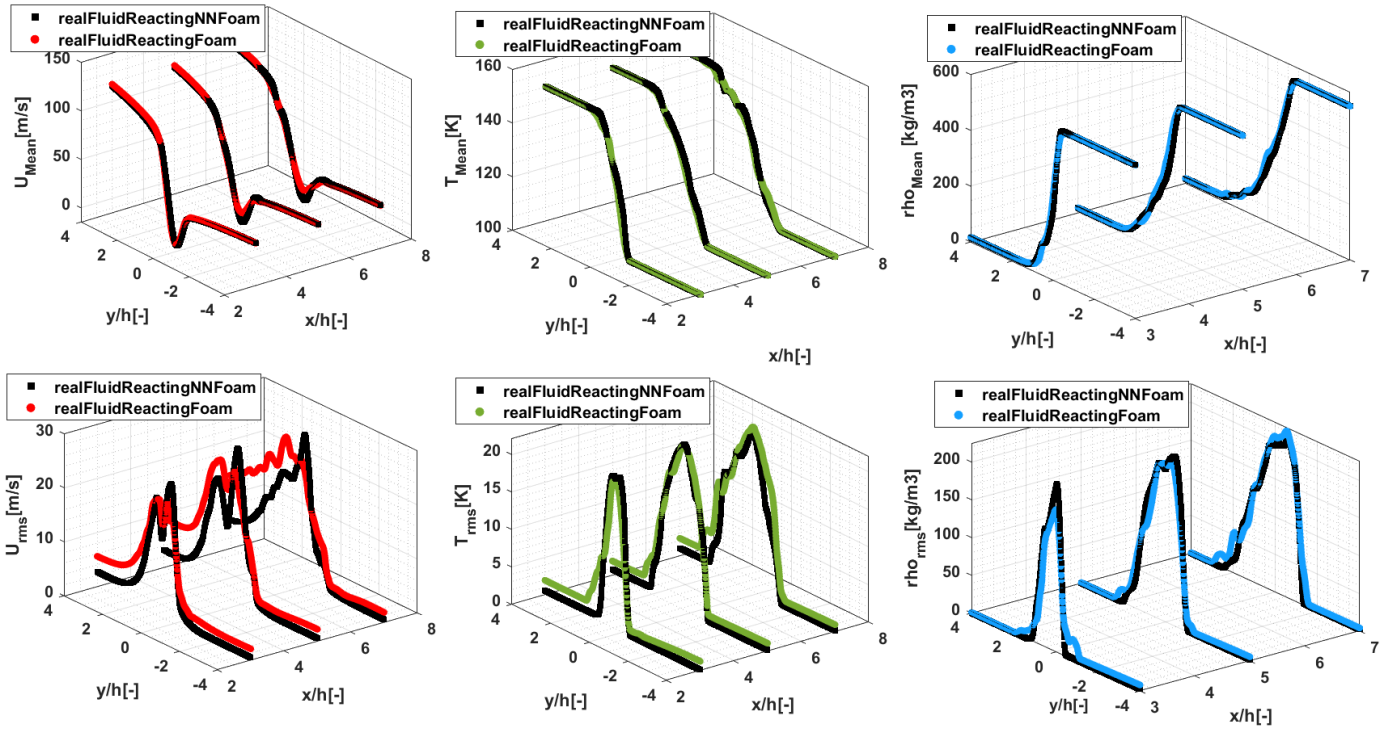
GH2-LOX - Results and discussion: fields @ t = 1 ms and time averages

realFluidReactingNNFoam

realFluidReactingFoam



t = 1 ms



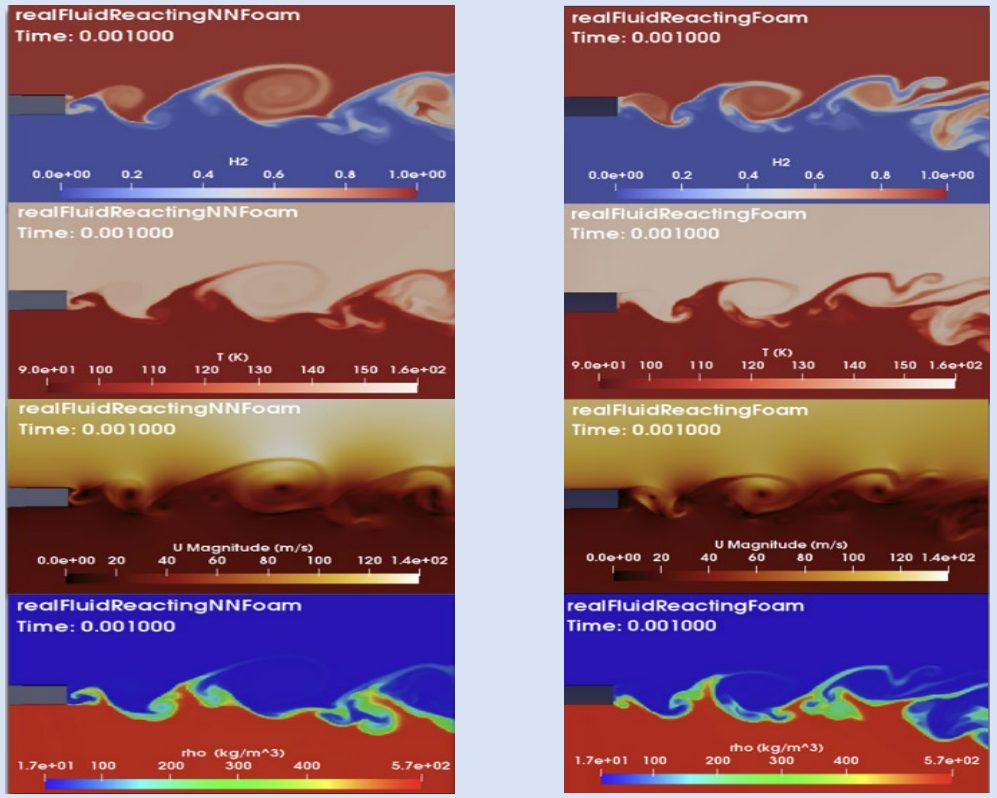
Averages over 4 FTT (1-1.2 ms)

N. Sahranavardfard, D. Aubagnac-Karkar, C. Habchi, G. Costante, F. N. Z. Rahantamialisoa, and M. Battistoni. “Computation of real-fluid thermophysical properties using a neural network approach implemented in OpenFOAM”, Fluids, MDPI, 2024

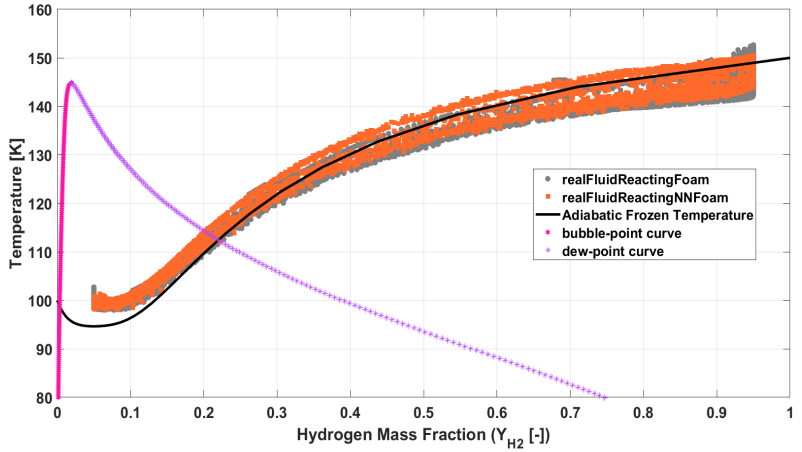
GH2-LOX - Results and discussion: fields @ t = 1 ms and time averages

realFluidReactingNNFoam

realFluidReactingFoam



t = 1 ms



Solver	Total execution			Iteration	
	Time (s)	Speed-up	Total number of Iterations	Time/Iter (s/Iter)	Speed-up
realFluidReactingFoam	511096	1	200550	2.548	1
realFluidReactingNNFoam	179317	2.850	523200	0.343	7.5

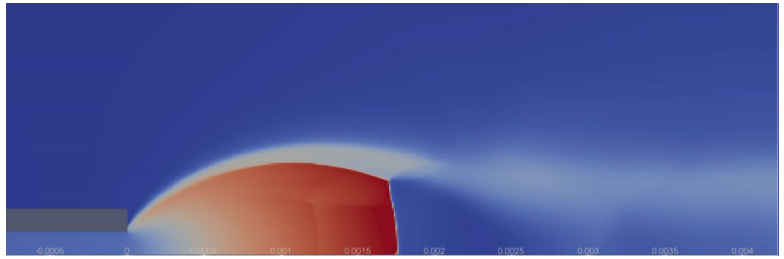
Conclusion: summary and future works

Summary:

- ✓ Exploration of the integration of NN models within the RFM approach for efficiently simulating complex thermodynamic functions in openFoam for a binary mixture under transcritical conditions.
- ✓ realFluidreactingFoam results indicates that the NN model outperforms the original approach in terms of execturion time at the same level of accuracy

Future work

- ✓ The study opens avenues for exploring the full potential of ML techniques in addressing complex problems related to multiphase flows also
- ✓ also with more than just two species
- ✓ or with other highly-volatile fuels (zero and low carbon fuels)



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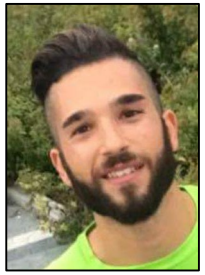

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Thank you