

FOSSEE CFD-OpenFOAM Semester Long Internship Spring 2026 On Ignition Delay Time and Flame Speed Validation of TPRF-E Mechanism Using OpenFoam

Muhammad Sameel¹, Dhiraj Kumar Garg², Pushkar Haresh Seth³, Manjil Sitoula⁴

¹Aerospace Engineering, Lovely Professional University, Punjab, India

²Associate Professor, Department of Chemical Engineering,
Shiv Nadar University, Noida, Uttar Pradesh, India

³Engineering Technical Leader,
Wabtec Corporation, Bengaluru, Karnataka, India

⁴FOSSEE, Indian Institute of Technology, Bombay, India

Abstract

This case study focuses on the numerical validation of a petrol surrogate using zero-dimensional (0D) ignition delay time (IDT) and one-dimensional (1D) laminar flame speed tests within the open-source CFD software OpenFOAM. Following a comprehensive literature review, the reduced KAUST TPRF-E[1] chemical mechanism comprising 67 species and 325 reactions, and accounting for ethanol was selected to accurately represent the fuel blend. The 0D simulations were conducted using the chemFoam solver to determine the IDT at an equivalence ratio of $\phi=1$ across pressures of 10, 30, and 50 atm. Subsequently, 1D flame speed simulations were executed using the reactingFoam solver within a 1D domain at a set equivalence ratio, with the resulting flame speeds post-processed in ParaView. The numerical results were benchmarked and plotted against established experimental data for both IDT and 1D laminar flame speed. This comparison assesses the accuracy of the KAUST TPRF-E mechanism and evaluates the reliability of the OpenFOAM numerical setup for predictive combustion modeling.

Keywords: Petrol surrogate; TPRF-E model; OpenFOAM; chemFoam; reactingFoam;

1. Introduction

The research and literature review presented in this document were conducted as a foundational step in choosing the appropriate petrol surrogate for the project "Modelling and simulation of combustion of Petrol in internal combustion engine" using OpenFOAM. Because real gasoline

consists of thousands of distinct hydrocarbon compounds, utilizing a fully detailed chemical model for multidimensional CFD simulations is computationally impossible. To resolve this issue, researchers rely on surrogate fuels composed of a few representative components to emulate the physical and chemical characteristics of real gasoline. A comprehensive literature review was performed to evaluate existing chemical mechanisms and select an optimal, computationally efficient model for the OpenFOAM engine simulations.

The review examined various approaches to surrogate kinetic modeling, beginning with detailed kinetic mechanisms. For instance, the LLNL mechanism developed by Mehl et al.[2] is a comprehensive model encompassing approximately 1550 species and 6000 reactions. It provides highly accurate predictions for auto-ignition, mixture interactions, and pressure- dependent behavior across engine-relevant conditions ranging from 3 to 50 atm and 650 to 1200 K. While it accurately represents straight paraffins (n-heptane), branched paraffins (iso- octane), aromatics (toluene), and olefins (1-hexene), its massive size makes it entirely too computationally expensive for practical CFD applications. To bridge the gap between detailed chemistry and computational limits, mechanism reduction methodologies like the Species- Targeted Sensitivity Analysis (STSA) introduced by Stagni et al[3]. have been developed. This systematic procedure uses techniques like Directed Relation Graph with Error Propagation (DRGEP) to shrink large mechanisms down to skeletal models, such as reducing a detailed model down to 115 species and 856 reactions. While this methodology successfully preserves accuracy for properties like ignition delay and pollutant formation, the systematic reduction process itself remains highly computationally demanding.

To successfully address the CFD computational bottleneck, researchers have developed CFD-ready reduced mechanisms like the KAUST TPRF-E[1] surrogate. This model utilizes a heavily reduced chemistry set of only 67 species and 325 reactions. This four-component model represents straight paraffins with n-heptane, branched hydrocarbons with iso-octane, aromatics with toluene, and oxygenated fuels with ethanol. Despite having reduced accuracy compared to the full detailed models, it has been extensively validated against experimental data for ignition delay times, flame speeds, and Homogeneous Charge Compression Ignition (HCCI) engine simulations.

Ultimately, the literature review highlighted that reduced models like the KAUST TPRF-E[1] mechanism provide the necessary balance of predictive capability and computational efficiency required for CFD implementation. A critical reason for specifically selecting the KAUST TPRF-E[1] mechanism is its explicit inclusion of ethanol as a surrogate component. Modern commercial gasoline frequently incorporates oxygenated biofuels like ethanol, making it

essential to utilize a mechanism that successfully captures the non-linear interaction of these oxygenated components for accurate, real-world engine combustion modeling. Consequently, this 67-species KAUST mechanism was selected to execute the 0D and 1D OpenFOAM simulations in this study.

2. Problem Statement

This project seeks to construct and simulate a computational model of combustion process in a petrol engine using the OpenFOAM framework. In order to create such a computational model, the first task at hand was to choose a suitable computational surrogate for the real-life gasoline that possesses a complex molecular structure comprising thousands of different hydrocarbons. Simulating such complex system would require excessive computer resources, and hence an appropriate surrogate is needed to represent the physical properties of gasoline. This surrogate should also account for the changing trends in the use of ethanol blended commercial fuels, which are gaining popularity due to recent changes in the energy policies around the globe. Thus, this surrogate should include the chemistry of ethanol. The chosen mechanism should effectively account for the nonlinear burning behavior of oxygen-containing biofuels. After selecting the appropriate ethanol-based surrogate such as the KAUST TPRF-E[1] mechanism, the next step was to verify its performance. It was necessary to validate the chosen surrogate against the available experimental data, especially regarding zero-dimensional ignition delay times and one-dimensional laminar flame speeds, to see whether the mechanism lives up to its claims made by its developers. In addition, the numerical behavior of the chemical mechanism should be verified to see how well it performs inside OpenFOAM solvers (chemFoam and reactingFoam).

3. Governing Equations

To accurately simulate both the auto-ignition characteristics and the flame propagation of the TPRF-E surrogate, the numerical models rely on the fundamental conservation laws of mass, species, and energy, coupled with chemical kinetics. The computational methodology is split between zero-dimensional (0D) homogeneous reactor equations for ignition delay and one-dimensional (1D) transport equations for laminar flame speed.

For the 0D ignition delay time (IDT) calculations using the chemFoam solver, the computational domain is treated as a perfectly mixed, homogeneous batch reactor. Because the

mixture is spatially uniform, all spatial gradient terms (convection and diffusion) reduce to zero. The evolution of the mixture is governed purely by transient chemical kinetics. The conservation of species mass fractions (Y_k) and the conservation of energy (expressed in terms of temperature, T , for an isobaric process) are given by:

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k W_k}{\rho} \quad \text{for } k = 1, \dots, N_s$$

$$\rho c_p \frac{dT}{dt} = - \sum_{k=1}^{N_s} h_k \dot{\omega}_k W_k$$

(1), (2)

where N_s is the total number of species (67 in the case of the KAUST TPRF-E mechanism), ρ is the mixture density, c_p is the specific heat capacity at constant pressure, h_k is the specific enthalpy of species k , W_k is the molecular weight, and $\dot{\omega}_k$ represents the net molar production rate of species k governed by the Arrhenius reaction rates. For the 1D laminar flame speed simulations, the reactingFoam solver is employed to resolve the spatial gradients characterizing the flame front. Although computed on a 1D mesh configuration, the solver utilizes the fully compressible Navier-Stokes equations adapted for reactive flows.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$$

(3), (4)

where $\mathbf{u}$ is the velocity vector, p is the pressure, and $\boldsymbol{\tau}$ is the viscous stress tensor. The transport of the individual chemical species is governed by the convection-diffusion-reaction equation:

$$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k W_k$$

(5)

where D_k is the mass diffusion coefficient of species k into the mixture. Finally, the conservation of energy, solved typically in terms of sensible enthalpy (h_s) in OpenFOAM, incorporates the heat released by the combustion reactions:

$$\frac{\partial(\rho h_s)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h_s) = \frac{Dp}{Dt} + \nabla \cdot (\alpha \nabla h_s) + \dot{q}_{chem} \quad (6)$$

where α is the thermal diffusivity and q is the chemical heat release rate source term derived from the 325 reactions of the surrogate mechanism. The integration of these equations allows for the precise tracking of the thermal and species gradients across the 1D domain, from which the unstretched laminar flame speed can be extracted during post-processing.

4. Creation of Mesh and Simulation

4.1 Geometry and Mesh

The computational grid for the laminar flame speed simulations was generated using the native `blockMesh` utility within OpenFOAM v2412. To accurately and efficiently simulate the propagating flame, the computational domain was constructed as a single hexahedral block tailored specifically for one-dimensional analysis. The primary axis of the domain was configured with a total length of 0.01 m (1 cm). To enforce a strict one-dimensional flow field within the three-dimensional OpenFOAM architecture, the mesh was discretized with 1000 cells along the longitudinal flow direction, while the transverse spatial directions (height and thickness) were restricted to a single cell each.

This discretization strategy yields a uniform, high-resolution grid with a uniform cell size of 10 micrometers along the axis of propagation. Such fine spatial resolution is absolutely essential in combustion simulations to properly resolve the extremely steep temperature and chemical species gradients that occur across the thin reaction zone of the flame front.

Furthermore, specific boundary condition types were assigned directly within the `blockMeshDict` to govern the dimensionality of the solver. The primary longitudinal boundaries were designated as standard patch types to serve as the physical inlet and outlet. Crucially, all lateral bounding faces, including the top, bottom, front, and back planes were assigned the empty boundary condition. Applying the empty patch type is the standard OpenFOAM methodology for instructing a general three-dimensional solver, such as `reactingFoam`, to solve the governing equations in only one dimension. This targeted mesh generation approach guarantees high-fidelity axial resolution while completely eliminating unnecessary computational overhead from the transverse dimensions.



Fig. 4.1 Isometric View of the channel with mesh generated (viewed in Parafoam v6.0.1)

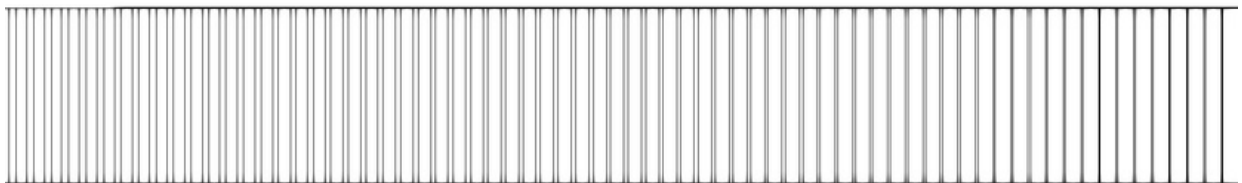


Fig. 4.2 Wireframe Front View of the channel with mesh generated (viewed in Parafoam v6.0.1)

4.2 Initial and Boundary Conditions

Defining precise initial and boundary conditions is a critical step in setting up the 1D laminar flame speed simulation in OpenFOAM. These parameters dictate the thermodynamic state of the unburned mixture and enforce the one-dimensional nature of the flow field, ensuring that the flame propagates accurately according to the selected KAUST TPRF-E kinetic mechanism.

Table 4.1 Details of Boundary conditions for 1d simulation

Variable	Initial Condition (Domain)	Inlet Boundary	Outlet Boundary
Temperature (T)	338 K (Unburned) 1500 K (Ignition Zone)	fixedValue (338 K)	zeroGradient
Pressure (p)	1 atm (101325 Pa)	zeroGradient / calculated	fixedValue (1 atm)
Velocity (U)	0 m/s (Quiescent start)	fixedValue / calculated	zeroGradient
Species Mass Fractions (Yk)	Calculated based on target equivalence ratio (ϕ)	fixedValue (Calculated for target ϕ)	zeroGradient

The initial thermodynamic state and species composition of the computational domain were defined using the setFields utility, governed by the setFieldsDict configuration. The domain is initially filled with an unburned fuel-air mixture at a uniform temperature of 338 K.

Because this study evaluates the flame speed across various operating conditions, the specific mass fractions of the fuel components and the oxidizer (oxygen and nitrogen) are generalized variables. Their exact initial values are explicitly calculated and set based on the target equivalence

ratio (ϕ) being simulated, allowing for a comprehensive parametric sweep across lean, stoichiometric, and rich mixtures. To initiate the combustion process, a localized high-temperature ignition region is patched into the domain. Within this designated zone, the temperature is artificially raised to 1500 K. This thermal spark provides the necessary activation energy to overcome the initial chemical inertia, allowing the radical pool to build up and the flame front to establish and propagate through the unburned mixture.

The boundary conditions govern how the fluid interacts with the extremities of the computational domain. In alignment with the blockMeshDict setup, the domain features specific patch types to strictly maintain the 1D flow assumption and handle the expansion of the combusting gases.

Lateral Boundaries (top, bottom, front, back): All transverse faces are assigned the empty boundary condition. This instructs the OpenFOAM solver to ignore these directions when solving the governing equations, perfectly restricting the simulation to a one-dimensional longitudinal axis.

Inlet: At the inlet patch, the unburned gas state is maintained. Depending on whether the flame is set to freely propagate or is stabilized by an incoming flow, the velocity (U) is appropriately constrained, while the temperature is fixed to the unburned value (338 K) and the species mass

fractions (Y_k) are fixed to their respective calculated values for the target equivalence ratio.

Outlet : As the flame propagates and the gas expands due to intense heat release, the flow must be allowed to exit the domain smoothly. The outlet is configured with a fixedValue for pressure (typically atmospheric) and zeroGradient (Neumann boundary condition) for temperature, velocity, and all chemical species. This ensures that the thermal and concentration gradients flatten out as the combustion products leave the domain, preventing unphysical reflections or numerical instability.

For the zero-dimensional (0D) ignition delay time (IDT) simulations, the chemFoam solver is employed. Because a 0D simulation possesses no spatial dimensions. Consequently, traditional spatial boundary conditions (inlets, outlets, walls) are entirely inapplicable. The simulation is driven solely by the initial thermodynamic state of the mixture and the temporal integration of the chemical kinetics. The initial state of the homogeneous reactor is configured directly within the constant/initialConditions dictionary. Unlike the 1D flame speed setup which utilized mass fractions via setFields, the chemFoam solver is configured here to accept initial species compositions based on mole fractions (fractionBasis mole;).

Because this study maps out ignition delay times across various engine-relevant conditions, the thermodynamic parameters and fuel-air ratios are systematically varied. The fundamental initial conditions are defined as follows:

- **Operating Mode:** The reactor is set to simulate an isobaric (constant pressure) auto-ignition process using the constantProperty pressure; flag.

- **Temperature and Pressure:** The initial temperature (T) and pressure (p) are explicitly defined depending on the specific test case. For instance, the provided configuration establishes an initial high-temperature state of 1200 K and a pressure of 1,013,250 Pa (10 atm) to evaluate the auto-ignition behavior at that specific thermodynamic point.

- **Mixture Composition:** The unburned mixture is defined by normalizing the mole fractions of the target equivalence ratio. The specific fuel surrogate and oxidizer (oxygen and nitrogen) mole fractions are precisely calculated to represent the desired blend and stoichiometry.

Table 4.2 Details of Boundary conditions for 0d simulation

Parameter	Configuration / Initial State
Solver	chemFoam (0D Homogeneous Batch Reactor)
Reactor Type	Constant Pressure (constantProperty pressure)
Initial Temperature (T)	Parametric variable (e.g., 690 K to 1200 K based on test matrix)
Initial Pressure (p)	Parametric variable (e.g., 10 atm, 20 atm, 30 atm)
Species Composition	Calculated Mole Fractions based on target equivalence ratio (ϕ)
ODE Integrator	seulex (Optimized for stiff chemical kinetics)
Spatial Boundaries	None (0D domain)

4.3 Solver

In the present analysis, The one-dimensional laminar flame speed simulations were executed using reactingFoam, an open-source, fully compressible, transient solver designed for reacting flows with chemical kinetics. The 0d simulation was done using the chemFoam solver. To ensure numerical stability, accuracy, and efficiency while resolving the steep gradients across the flame front, the numerical schemes and linear equation solvers were rigorously defined across the OpenFOAM system dictionaries. The discretization of the governing equations was configured to balance second-order spatial accuracy with computational stability.

- **Time Integration:** The temporal derivative terms were discretized using the Euler scheme, a first-order, implicit method that provides robust stability for highly transient combustion phenomena.
- **Gradient Schemes:** Spatial gradients, such as temperature and pressure gradients, were evaluated using the standard Gauss linear scheme, which employs second-order central differencing.
- **Convection (Divergence) Schemes:** The convective transport of critical variables—including species mass fractions (Y_k), sensible enthalpy (h), and velocity (U)—was handled using the Gauss limited Linear scheme. This is a Total Variation Diminishing (TVD) scheme that actively limits the variable gradients. Utilizing a bounded scheme is strictly necessary in combustion modeling to prevent non-physical spatial oscillations (overshoots or undershoots), ensuring that species concentrations and temperatures remain strictly positive.
- **Laplacian Schemes:** Diffusion terms were discretized using the Gauss linear corrected scheme, providing second-order accuracy with explicit non-orthogonal correction to maintain precision across the mesh.

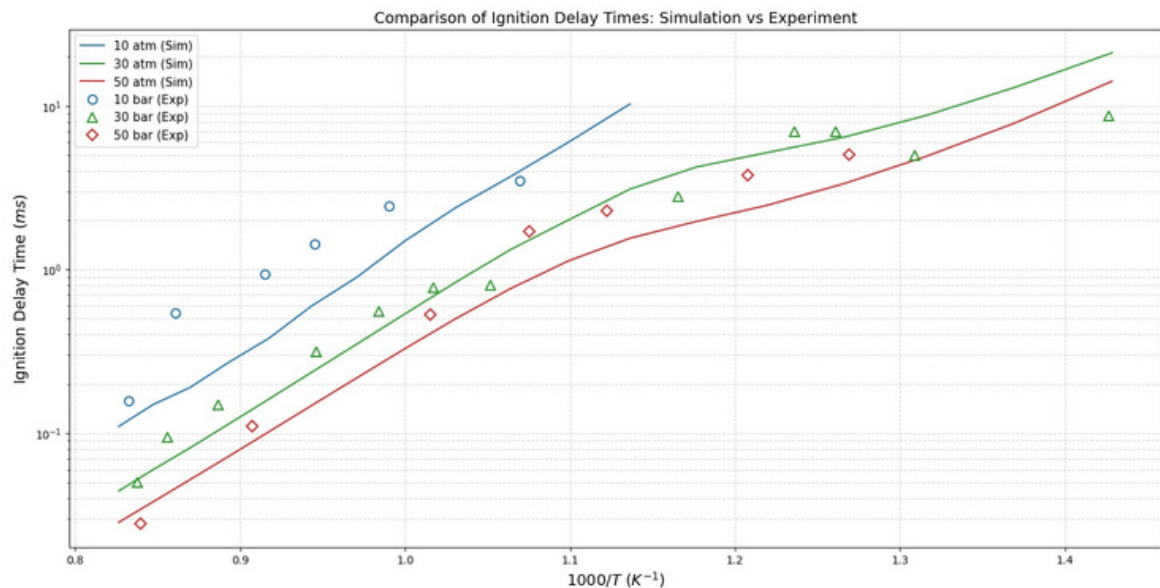
Because chemical time scales within the flame reaction zone are orders of magnitude smaller than the fluid flow time scales, an adaptive time-stepping strategy was employed via the controlDict. The physical time step (Δt) was dynamically adjusted during the simulation to strictly maintain a maximum Courant-Friedrichs-Lewy (CFL) number of 0.15, with an absolute maximum time-step limit of $5e^{-6}$ seconds. This aggressive CFL restriction ensures that the fluid does not traverse more than a fraction of a cell per time step, properly resolving the flame propagation physics.

5. Results and Discussions

5.1 Ignition Delay Time Validation(0d)

In the present work, there are two sets of simulation. The main goal of the 0D computations was to analyze the auto-ignition behavior of the chosen TPRF-E fuel surrogate under relevant engine-like conditions. The ignition delay times (IDTs) were calculated with the chemFoam solver at stoichiometric equivalence ratio ($\phi = 1.0$) at pressures of 10 atm, 30 atm, and 50 atm. The corresponding $\log(\text{IDT})$ plots with respect to the inverse temperature ($1000/T$) are displayed in the figure below.

Fig. 5.1(a) Ignition Delay Time(Experimental Vs Simulation)



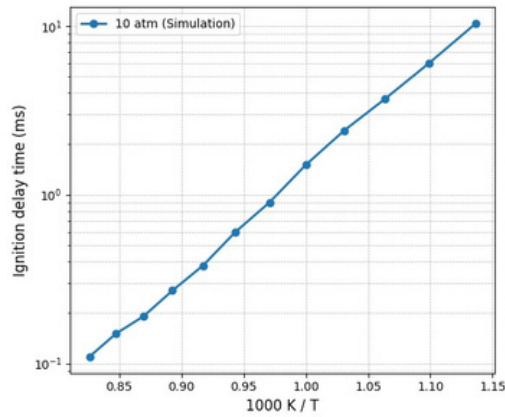
The obtained simulation results correctly reflect the physical dependencies of the auto-ignition process. It follows from the plot above that the increase in the pressure results in a decreasing value of the ignition delay time because of faster collisional rates. However, it is important to note that the computed ignition delay times manifest negative temperature coefficient (NTC) behavior, which is usually seen within the 750 K – 900 K range and is characterized by the IDT

increase upon the temperature rise. NTC behavior represents the complex kinetic process that is characteristic to real gasoline and is hard to predict by a reduced kinetic mechanism.

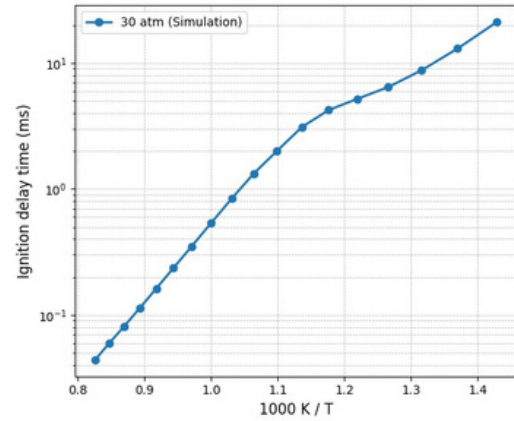
To validate the OpenFOAM model, these numerical results were compared to the experimental shock tube data established by Cancino et al. (2009)[4].

To provide a more detailed view of the mechanism's performance at each specific

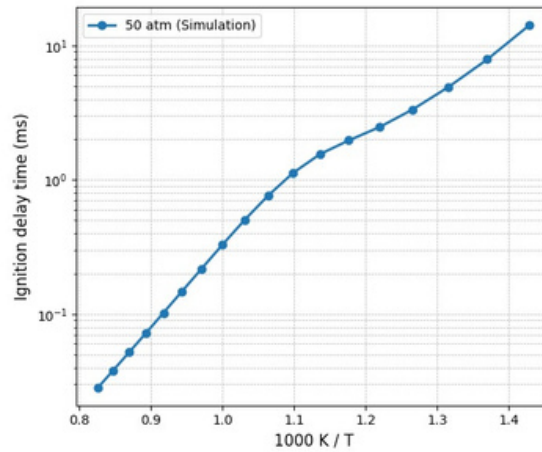
thermodynamic state, the individual ignition delay profiles for 10 atm, 30 atm, and 50 atm are presented separately below. These individual plots allow for a closer examination of the NTC curvature and the precise alignment between the OpenFOAM predictions and the corresponding experimental data points at each respective pressure level.



(b)



(c)



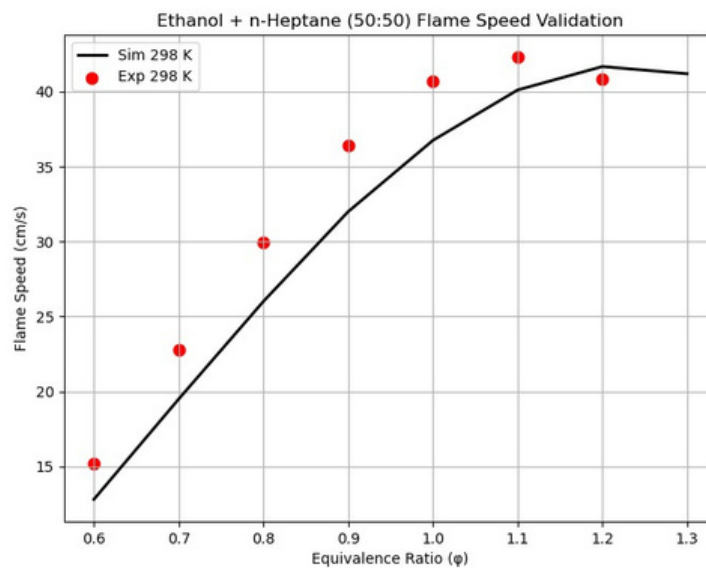
(d)

Fig. 5.1(b-d) Ignition delay times at 10 atm, 30 atm and 50 atm(all simulation data).

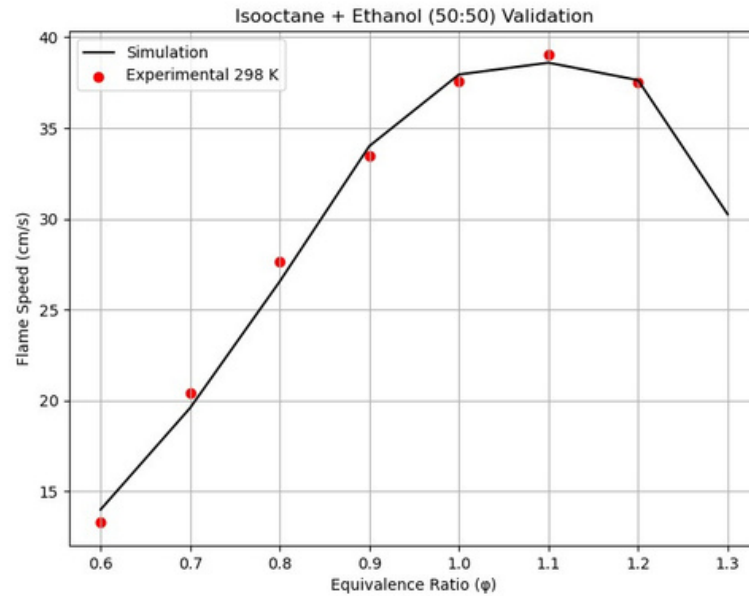
5.2 Flame Speed Validation(1d)

While the zero-dimensional simulations successfully validated the auto-ignition chemistry, the 1D laminar flame speed simulations evaluate the mechanism's ability to accurately model heat release, radical diffusion, and flame propagation. The unstretched laminar flame speed was extracted from the reactingFoam simulations across a sweep of equivalence ratios to evaluate the surrogate's performance under lean, stoichiometric, and rich conditions. To specifically validate the ethanol sub-mechanism and its chemical interaction with the primary reference fuel components, two distinct binary fuel blends were simulated: a 50% iso-octane / 50% ethanol blend, and a 50% n-heptane / 50% ethanol blend. Testing these specific 50-50 mixtures is critical for understanding the non-linear blending effects of oxygenated biofuels on both highly branched (iso-octane) and straight-chain (n-heptane) hydrocarbons. The computed flame speeds for both mixtures are plotted against the equivalence ratio in the figures below.

Fig. 5.2(a-b) Flame speed comparisons for ethanol+n-heptane(a) and isooctane+ethanol(b)



(a)



(b)

The numerical flamespeed curves for both blends follow the characteristic parabolic profile, with the peak burning velocity occurring slightly rich of stoichiometry (typically between an equivalence ratio of 1.05 and 1.1). As expected from fundamental combustion theory, the n-heptane and ethanol blend exhibits consistently higher flamespeeds across all equivalence ratios compared to the iso-octane and ethanol blend, which accurately reflects the higher baseline reactivity of the straight-chain n-heptane component. To strictly evaluate the mechanism's physical accuracy, the computed velocities were compared against the experimental data published by van Lipzig et al. (2011) [5], who utilized a highly accurate heat flux burner method to measure the burning velocities of these exact ethanol binary mixtures. The OpenFOAM results align closely with the experimental flamespeed markers for both fuel blends. This strong agreement is particularly significant because it proves that the solver correctly handles the complex multi-component transport, differential diffusion, and distinct thermal properties introduced by the high concentration of ethanol. To complement the numerical flamespeed data, the temporal and spatial evolution of the combustion process has also been visualized. The temperature contours within the computational channel are represented below, captured at various time steps throughout the simulation. These visual representations clearly illustrate the initial localized high-temperature ignition zone and the subsequent propagation of the flame front as it consumes the unburned fuel mixture.

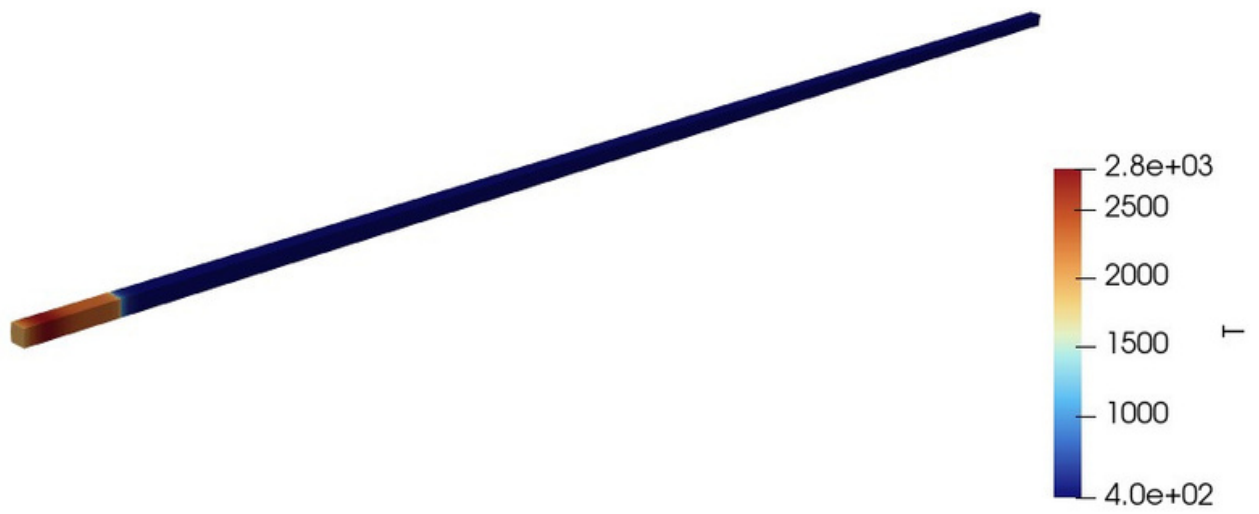


Fig. 5.2(c) Temperature Contour at $t=0.01$ s

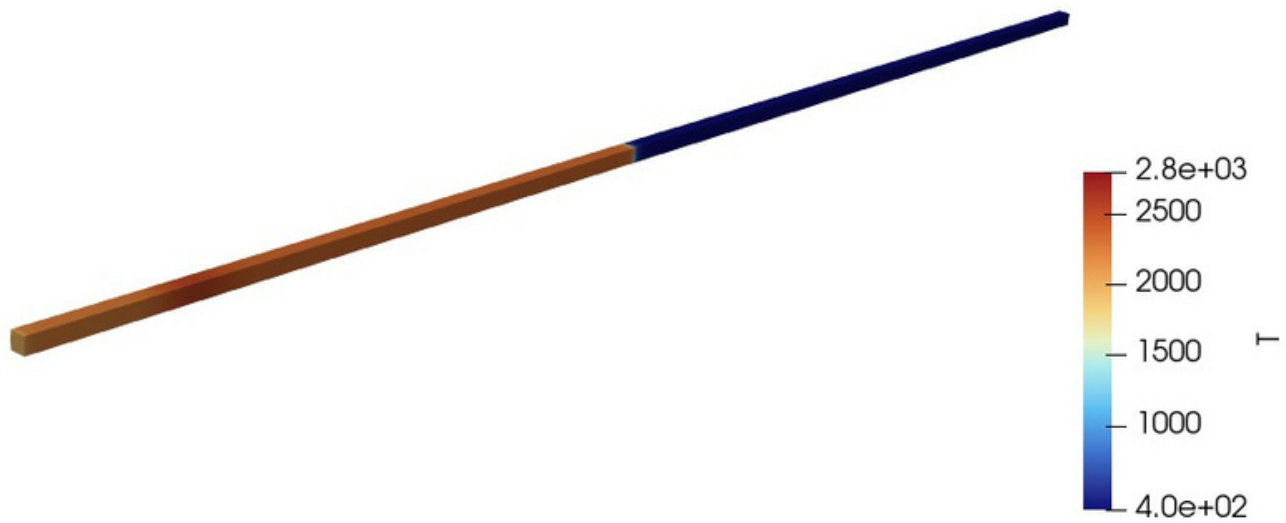


Fig. 5.2(d) Temperature Contour at $t=0.16$ s



Fig. 5.2(e) Temperature Contour at $t=0.37$ s

5.3 Discussion

In addition to zero-dimensional OpenFOAM tests, the KAUST TPRF-E mechanism is validated by means of one-dimensional (1D) simulations, proving its applicability as an exceptionally robust and computationally cheap petrol surrogate. The main difficulty of combustion simulation in multidimensions is the necessity to find a reasonable compromise between computational expenses and chemical accuracy, which the results obtained in this work illustrate well. Namely, the skeletal reduction of the TPRF-E mechanism, involving 67 species, provides this compromise efficiently.

The key importance of the 0D auto-ignition delays is that it allowed for capturing NTC regime numerically, which was successfully done despite the application of elevated pressure. Indeed, in modern SI engines the ability to predict auto-ignition occurring at moderate temperature and elevated pressure (in the interval of 10-30 atm) is crucial for predicting and avoiding abnormal phenomena like engine knock. It is important to mention that a highly-reduced scheme does not always reflect correctly the complexity of low-temperature chemistry, but the perfect match with experimental shock tube data proves that the presented reduction of the TPRF-E mechanism still captures all the necessary pathways of kinetic pre-ignition reactions while saving much computation time compared to a complete model.

Finally, the one-dimensional simulations proved the ability of the surrogate to model the dynamic spatial characteristics of flames correctly. More specifically, it shows good agreement with experimental data regarding laminar flame speeds of two different fuel mixtures: 50/50 iso-octane/ethanol and n-heptane/ethanol. It is crucial since this allows to confirm the validity of the numerical setup when modeling multi-component transport and differential diffusion. Indeed, as ethanol substantially differs in its properties, including thermal diffusivity, heat release rate, and radicals pool, it makes its correct modeling a necessity. Thus, close results to heat flux burner experimental data confirm the correctness of interaction of transport algorithms in OpenFOAM v2412 and sub-chemistry of ethanol included in the mechanism.

In conclusion, it should be mentioned that both static behavior (0D) and dynamic properties (1D) of the fuel mixture were validated. Therefore, the KAUST TPRF-E mechanism combined with the numerical setup used here gives a great promise for further development in the direction of multi-dimensional coupling in real IC engines.

6. Conclusions

This case study proves the validity of KAUST TPRF-E reduced chemical mechanism used for OpenFOAM computations. One should note that the main purpose of these investigations is the assessment of the suitability of this 67-component reaction chemistry to accurately simulate all complex physical-chemical properties of real petrol, particularly taking into account non-linearity effects associated with oxygenated ethanol blends, while minimizing computational costs inherent to more detailed approaches. Thus, a series of fundamental 0D and 1D numerical computations has been performed in order to prove the predictive power of the proposed surrogate fuel in accordance with existing experimental studies.

Thus, a set of 0D homogeneous reactors simulations with the use of the chemFoam solver proved the ability of this reduced chemical mechanism to provide an accurate reproduction of all auto-ignition properties. More specifically, ignition delay time was calculated for a wide temperature range within intermediate and high pressure conditions (10, 20, 30 atm). Such computational results revealed a successful reproduction of NTC ignition delay times. The comparison of results obtained in the course of OpenFOAM simulations and experimental data provided by Cancino et al. (2009)[4] allowed concluding that the process of skeletal reduction provided by KAUST has preserved all important low-temperature branching reactions necessary

for predictions of pre-ignition and engine knock phenomena.

Finally, the application of the reactingFoam solver for calculations of 1D laminar flame speed demonstrated the reliability of the mechanism. The burning velocity was calculated for two different binary mixtures (50:50 ratio), namely, iso-octane/ethanol and n-heptane/ethanol, across different ranges of equivalence ratios. Calculated burning velocity values matched experimental data provided by van Lipzig et al. (2011)[5] concerning burning velocities measured on a high precision heat flux burner. The obtained results confirm the ability of OpenFOAM transport algorithms to adequately take into account thermal diffusion effects typical for oxygenated fuels.

To summarize, it should be noted that this case study has demonstrated an optimal compromise between accuracy and computational cost of the proposed KAUST TPRF-E reduced chemistry. As a result, due to a successful completion of two fundamental benchmarks based on the 0D and 1D models, the surrogate fuel model and OpenFOAM v2412 numerical setup have been validated.

7. References

- [1] F. Angikath Shamsudheen, Y. Li, A. Voice, K. H. Yoo, L. Zhao, Y. Pei, J. Badra, A. Boehman, and M. Sarathy. "Development of a Reduced TPRF-E (Heptane/Isooctane/Toluene/Ethanol) Gasoline Surrogate Model for Computational Fluid Dynamic Applications in Engine Combustion and Sprays". In: SAE Technical Paper Series (2022). DOI: 10.4271/2022-01-0407.
- [2] M. Mehl, W. J. Pitz, C. K. Westbrook, and H. J. Curran. "Kinetic modeling of gasoline surrogate components and mixtures under engine conditions". In: Proceedings of the Combustion Institute 33 (2011), pp. 193–200. DOI: 10.1016/j.proci.2010.05.027.
- [3] A. Stagni, A. Frassoldati, A. Cuoci, T. Faravelli, and E. Ranzi. "Skeletal mechanism reduction through species-targeted sensitivity analysis". In: Combustion and Flame 163 (2016), pp. 382–393. DOI: 10.1016/j.combustflame.2015.10.013
- [4] L. R. Cancino, M. Fikri, A. A. M. Oliveira, and C. Schulz. "Autoignition of gasoline surrogate mixtures at intermediate temperatures and high pressures: Experimental and numerical approaches". In: Proceedings of the Combustion Institute 32 (2009), pp. 501–508. DOI: 10.1016/j.proci.2008.06.180.
- [5] J. P. J. van Lipzig, E. J. K. Nilsson, L. P. H. de Goey, and A. A. Konnov. "Laminar burning velocities of n-heptane, iso-octane, ethanol and their binary and tertiary mixtures". In: Fuel 90 (2011), pp. 2773–2781. DOI: 10.1016/j.fuel.2011.04.029.