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on

Numerical Investigation of Ignition Delay Time and Flame Speed Validation of 70-Species Diesel Surrogate Mechanism Using OpenFOAM

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Abstract

This case study focuses on the numerical validation of a diesel 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 chemical mechanism comprising 70 species with 220 reactions was selected to accurately represent the surrogate diesel fuel blend containing n-decane, iso-octane, methylcyclohexane (MCH), and toluene. The Laminar flame speed simulations were performed using the reactingFoam solver within a 1D domain at a set of fuel to air mass fractions, with the resulting flame speeds post-processed in ParaView. The numerical results were benchmarked and plotted against established experimental data for both IDT and laminar flame speed. This comparison assesses the accuracy of the decoupling methodology mechanism and evaluates the reliability of the OpenFOAM numerical setup for predictive combustion modelling.

Keywords: Diesel surrogate fuel; reactingFoam; chemFoam; OpenFOAM

1. Introduction

1.1 Background of the Topic

As the world pushes toward cleaner and more efficient engines, researchers have increasingly turned to computational fluid dynamics (CFD) to better understand how combustion actually works. In diesel engines especially, what happens during combustion, how quickly fuel ignites, how the flame spreads, how much heat is released, and what pollutants form all comes down to the underlying chemistry of fuel oxidation. Getting that chemistry right in simulations is what makes the difference between a useful prediction and a misleading one. The problem is that real diesel fuel is incredibly complex. It contains hundreds of different hydrocarbon compounds spanning multiple chemical families from n-paraffins and iso-paraffins to cycloalkanes and aromatics. Trying to model all of that chemistry directly in a CFD simulation is not just difficult; it's largely impractical given current computing constraints. This is why surrogate fuels have become such a useful tool. Instead of modelling every component of real diesel, researchers define a small set of representative compounds that collectively capture the key combustion behaviour without the enormous computational overhead.

Alongside surrogate fuel development, there has been steady progress in creating skeletal chemical kinetic mechanisms. These are streamlined versions of detailed reaction mechanisms that keep the most important reaction pathways while cutting down significantly on the number of species and reactions involved. The reduced mechanism proposed by Chang et al. contains 70 chemical species and 220 elementary reactions to represent diesel surrogate combustion. Despite its relatively compact size, it has shown strong performance across a broad range of operating conditions.

1.2 Motivation of the Study

Two combustion properties sit at the heart of this work: accurate prediction of ignition delay time (IDT) and laminar flame speed (LFS) is essential for understanding the combustion behaviour of diesel surrogate fuels. Detailed chemical mechanisms can predict these properties with high accuracy, but their sheer size makes them too computationally expensive for most engineering simulations.

Skeletal mechanisms exist precisely to bridge this gap. They reduce the computational burden while holding onto the core chemistry that actually matters. That said, a mechanism can't simply be assumed to work well just because it's been published, it needs to be tested and validated against reliable experimental and numerical data before it can be trusted in real applications. That's what drives this study. The objective of this study is to evaluate the performance of a 70-species diesel surrogate mechanism implemented in OpenFOAM by validating its predictions of ignition delay time and laminar flame speed. If it holds up under validation, it opens the door to using this mechanism confidently in more complex diesel combustion and engine simulations down the line.

1.3 Problem Statement

Reduced and skeletal mechanisms for diesel surrogates have been developed by various research groups over the years, but implementing them in open-source CFD platforms like OpenFOAM and properly validating their performance is still an area that needs more work. Before any mechanism can be applied to practical combustion problems, its predictions for fundamental properties like ignition delay and flame speed need to be checked against known data.

This study takes on that task directly. The 70-species, 220-reaction skeletal diesel surrogate mechanism is implemented in OpenFOAM v2412, and two sets of simulations are carried out. First, ignition delay times for n-decane are calculated using chemFoam across a range of pressure conditions. Second, laminar flame speeds for Surrogate B are simulated using reactingFoam over varying fuel-air ratios. The results from both sets of simulations are then compared against published literature to judge how reliably the mechanism captures the combustion behaviour of diesel surrogates.

1.4 Literature Review

Significant research efforts have been directed toward the development of surrogate fuel formulations and reduced chemical kinetic mechanisms for diesel combustion modelling. Pitz and Mueller (2011) demonstrated that multi-component surrogate fuels are capable of reproducing both the physical and chemical behaviour of real diesel more accurately than single-component fuels. Narayanaswamy et al. (2014) subsequently showed that skeletal kinetic mechanisms obtained through systematic reduction techniques can accurately predict combustion properties such as ignition delay time and laminar flame speed while significantly lowering computational cost.

Of direct relevance to the present work, Chang et al. (2015) reduced mechanism contains 70 chemical species and 220 elementary reactions and was generated using a decoupling-based reduction strategy. The mechanism is based on a four-component surrogate n-decane, iso-octane, methylcyclohexane, and toluene selected to represent the principal hydrocarbon classes of real diesel fuel. Validation against published experimental measurements confirmed good agreement over a broad range of pressures, temperatures, and equivalence ratios.

Despite these advances, the validation of the Chang et al. mechanism within open-source CFD platforms such as OpenFOAM remains insufficiently documented. The present study addresses this gap by implementing the 70-species skeletal mechanism in OpenFOAM v2412 and evaluating its predictive capability through ignition delay time and laminar flame speed simulations.

Table 1: Fuel composition

Compositions of diesel surrogate fuel	
Component	Mole Fraction (%)
n-Decane	26.67
Iso-octane	14.89
Methylcyclohexane	36.81
Toluene	21.64

The surrogate mechanism has been validated using shock tube and ignition delay measurements, jet-stirred reactor experiments, and laminar premixed flame investigations (Chang et al.).

2. Governing Equations

Combustion is modelled by solving the governing equations for fluid flow and species transport, which include the conservation of mass, momentum, energy, and chemical species, coupled with thermodynamic and chemical kinetic relations. The governing equations as implemented in OpenFOAM are presented in the following subsections.

2.1 Continuity Equation

Conservation of mass is expressed as:

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

where ρ represents the mixture density and $\mathbf{U}$ is the velocity vector.

2.2 Momentum Equation

The momentum conservation equation used in this study is

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

where p represents the thermodynamic pressure and $\boldsymbol{\tau}$ denotes the viscous stress tensor.

2.3 Energy Equation

The conservation of energy, expressed in terms of specific enthalpy, is written as:

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{U} h) = \nabla \cdot (k \nabla T) + \dot{\omega}_T$$

where h denotes the specific enthalpy, k is the thermal conductivity, T is the temperature, and $\dot{\omega}_T$ corresponds to volumetric heat release rate resulting from chemical reactions.

2.4 Species Transport Equation

The transport property of each chemical species is governed by:

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{U} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{\omega}_i$$

where Y_i indicates the mass fraction of species, the binary diffusion coefficient is denoted as D_i , and $\dot{\omega}_i$ is the total chemical production rate of species i due to all elementary reactions.

2.5 Equation of State

Thermodynamic closure is achieved through the ideal gas equation of state:

$$p = \rho RT$$

where R denotes the specific gas constant of the mixture.

2.6 Chemical Reaction Rate

The rate constant for each elementary reaction is evaluated using the modified Arrhenius expression:

$$k = AT^n \exp\left(-\frac{E_a}{RT}\right)$$

where A is the pre-exponential factor, n is the temperature exponent, and E_a is the activation energy. These parameters are specified for each reaction within the chemical kinetic mechanism.

2.7 Ignition Delay Time

The delay in ignition (IDT) was determined from the temperature–time histories obtained from simulation using *chemFoam* solver. Following standard practice in the combustion literature, the maximum rate of rise in temperature is defined as IDT

$$\tau_{\text{IDT}} = t \left(\frac{dT}{dt} \right)_{\text{max}}$$

Temperature histories were computed for n-decane at initial pressures of 13 atm, 50 atm, and 80 atm over an initial temperature range of 700–1200 K.

2.8 Laminar Flame Speed

The propagation of the flame front at a laminar flow regime is denoted as laminar flame speed (s_L). It is identified as the location of maximum temperature within the computational domain. The flame speed was computed from the temporal displacement of the flame front as:

$$S_L = \frac{x_2 - x_1}{t_2 - t_1}$$

where x_1 and x_2 denote the flame front positions at times t_1 and t_2 , respectively.

2.9 Fuel–Air Ratio

The fuel–air ratio employed in the laminar flame speed simulations is defined as:

$$F/A = \frac{m_f}{m_a}$$

where M_f and M_a are the mass of fuel and air, respectively. In the present study, the fuel–air ratio was systematically varied from 0.06 to 0.095 across eight simulation cases to characterise the dependence of laminar flame speed on mixture composition. In the present study both ignition delay time and laminar flame speed simulations were conducted under laminar flow condition. hence, Turbulence modelling was not employed.

3. Computational Domain

3.1 Geometry

A one-dimensional computational domain with a rectangular shape and having dimensions of $1\text{m} \times 0.1\text{m} \times 0.1\text{m}$ was employed for the laminar flame speed simulations, The channel with high axial aspect ratio ensured that flame propagation occurred predominantly along the streamwise direction, effectively suppressing transverse flow effects. The ignition delay time simulations were performed using the chemFoam solver, which represents a homogeneous zero-dimensional reactor and therefore does not require a physical spatial domain.

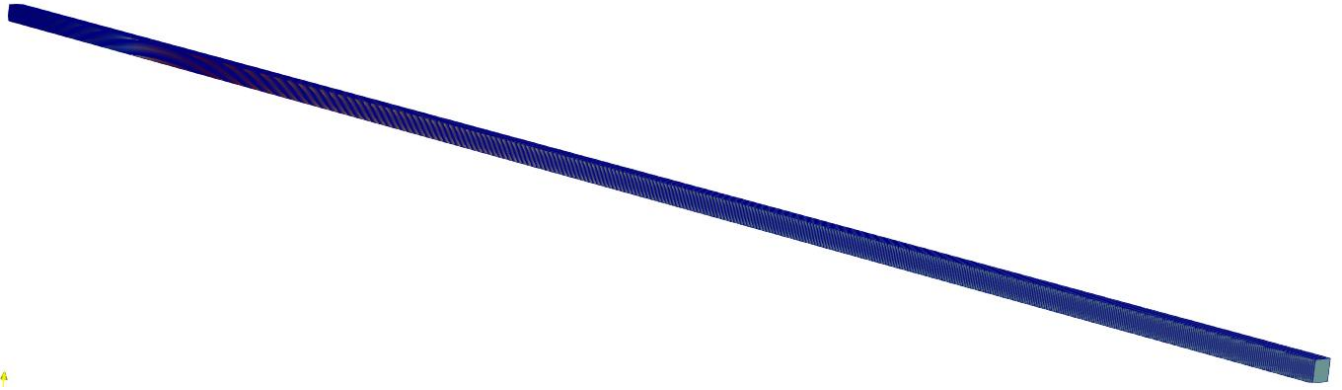


Fig 1 : 1D Isometric View of the channel with mesh generated (viewed in Parafoam v6.0.1)

3.2 Mesh

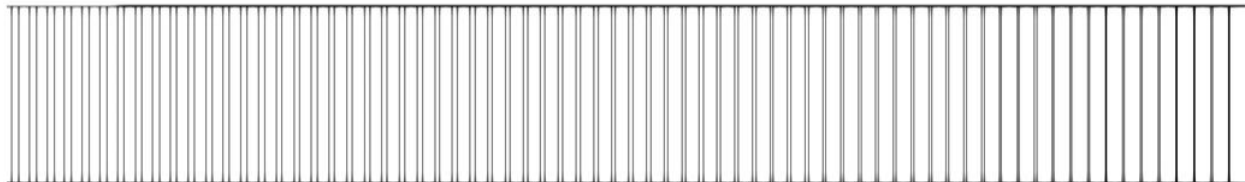
A structured hexahedral mesh was employed throughout the domain, The computational mesh was generated using the OpenFOAM blockMesh utility with 1000 uniformly distributed cells along the axial direction and a single cell in each transverse direction, yielding a total of 1000 cells. The resulting axial cell size was:

$$\Delta x = \frac{1}{1000} = 0.001 \text{ m}$$

The single-cell discretisation in the transverse directions enforced strictly one-dimensional flame propagation behaviour.

Table 2 : Mesh Parameters

Parameter	Value
Domain Length	1 m
Domain Width / Height	0.1 m
Cells in x-direction	1000
Cells in y / z-direction	1
Total Cells	1000

*Fig 2 Wireframe Front View of the channel with mesh generated (viewed in Parafoam v6.0.1)*

3.3 Boundary and Initial Conditions

The computational domain was initialised with a premixed unburned fuel–air mixture corresponding eight selected fuel–air ratios, which is ranging from 0.06 to 0.095. The fuel which is used in this simulation is Surrogate B, comprising n-decane, iso-octane, methylcyclohexane (MCH), and toluene, selected to represent the principal hydrocarbon classes present in real diesel fuel. The effect of fuel–air ratios was systematically analysed to characterise the dependence of laminar flame speed on mixture composition.

Combustion was initiated by introducing a localised high-temperature ignition patch near the inlet boundary by using `setFields` utility. A fixed temperature of 1500 K was prescribed within this ignition zone to provide sufficient thermal energy for chemical activation and flame kernel development. The remainder of the domain was initialised under unburned mixture conditions at the specified inlet temperature and pressure. Following successful ignition, the flame propagated freely through the premixed mixture in the axial direction of the domain. To enforce strictly one-dimensional flow behaviour, the **empty boundary** condition was applied to all transverse boundaries **top, bottom, front, and back faces**. This configuration ensures that the governing equations are solved exclusively in the axial direction, effectively eliminating any transverse velocity components or cross-flow effects, consistent with the one-dimensional nature of the laminar flame propagation study.

3.4 Laminar Flame Speed Simulations

At the inlet boundary, a fixed velocity of 0.1 m/s and a fixed temperature of **443 K** were prescribed, along with fixed species mass fractions corresponding to the specified fuel–air ratio. A zero-gradient condition was applied to pressure at the inlet. At the outlet, a fixed pressure of **101,325 Pa** was imposed, with **zero-gradient** conditions applied to velocity, temperature, and species mass fractions. The side boundaries were assigned the empty boundary condition to enforce one-dimensional flow behaviour consistent with the mesh configuration. The computational domain was initialised with a temperature of **443 K**, a pressure of **101,325 Pa**, and an inlet velocity of 0.1 m/s, with **Surrogate B** over a fuel–air ratio range of **0.06–0.095**. Flame ignition was initiated through a localised high-temperature patch, the temperature of which was determined individually for each fuel–air ratio case based on preliminary simulation results.

3.5 Ignition Delay Time Simulations

Ignition delay calculations were performed using chemFoam under homogeneous, adiabatic, **constant-volume** conditions for n-decane at an equivalence ratio of 0.5. Simulations were conducted over an initial temperature range of **700–1200 K** at three pressure conditions: 13 atm, 50 atm, and 80 atm.

3.6 Discretization Schemes

OpenFOAM v2412 uses the finite volume method to discretize the governing equations. The Spatial and temporal discretization schemes were selected to provide numerical stability while accurately resolving flame propagation and chemical reaction processes.

3.7 Gradient Schemes

Spatial gradients were evaluated using the Gauss linear scheme, which provides second-order spatial accuracy and is widely used for reacting flow simulations. Linear interpolation schemes were used for face-value reconstruction, while corrected surface-normal gradient schemes were employed to maintain consistency between cell-centred and face-centred quantities.

3.8 Solver Selection

Two OpenFOAM solvers were employed in this study. The chemFoam solver was used for ignition delay calculations, directly integrating the chemical kinetic mechanism under constant-volume conditions to yield temperature and species evolution histories. The reactingFoam solver was employed for laminar flame speed simulations, solving the compressible reacting flow equations coupled with species transport and energy conservation, making it well-suited for premixed flame propagation modelling.

4. Simulation Parameters

The ignition delay simulations were executed in serial mode using chemFoam, while the laminar flame speed simulations were performed in parallel across 8 processors. An adjustable time-stepping strategy was employed throughout to maintain numerical stability by controlling the Courant number within prescribed limits.

Table 3 : Simulation Parameters

Parameter	IDT Simulations	Flame Speed Simulations
Fuel	n-Decane	Surrogate B
Temperature Range	700–1200 K	443 K
Pressure	13, 50, 80 atm	1 atm
Equivalence Ratio / F-A Ratio	0.5	0.06–0.095
Number of processors	—	8
Solver	chemFoam	reactingFoam
Execution	Serial	Parallel

5. Chemistry Configuration

Chemical kinetics calculations were enabled through the `chemistryProperties` dictionary. The skeletal diesel surrogate mechanism was converted from CHEMKIN format using the `chemkinToFoam` utility and subsequently integrated into OpenFOAM. The chemistry model employed an ODE-based chemistry solver for the integration of reaction rates and species source terms. The simulations included 70 chemical species and 220 elementary reactions.

The reacting flow simulations utilized the `hePsiThermo` thermodynamic package together with the perfect gas equation of state. Thermodynamic properties were evaluated using JANAF polynomial coefficients, while sensible enthalpy was selected as the energy variable. These models provide accurate representation of temperature-dependent thermodynamic properties required for combustion calculations.

6. Results

6.1 Ignition Delay Time Validation

Ignition delay time (IDT) simulations were carried out using the *chemFoam* solver in OpenFOAM to assess the capability of the 70-species skeletal diesel surrogate mechanism in predicting the autoignition characteristics of n-decane. Computations were performed at an equivalence ratio of 0.5 over an initial temperature range of 700–1200 K and at three pressure conditions — 13 atm, 50 atm, and 80 atm. The ignition delay time was extracted from the simulated temperature history using the maximum rate of temperature rise as the defining criterion.

6.2 Ignition Delay at 13 atm

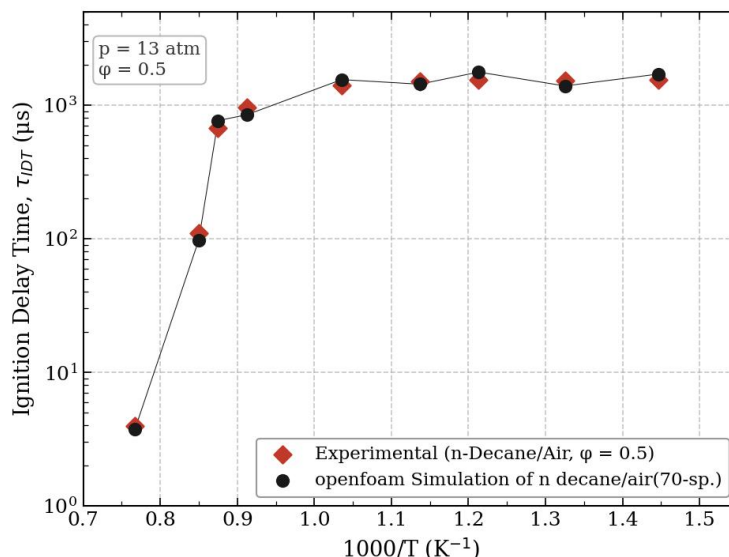


Figure 6.1 compares the ignition delay time predicted by *chemFoam* as a function of inverse temperature for the n-decane/air mixture at 13 atm[1].

The computed results show good agreement with the experimental measurements across the full temperature range investigated.

At elevated temperatures corresponding to low values of $1000/T$ — the ignition delay is short, as the accelerated chemical kinetics drive rapid fuel oxidation and early autoignition. With decreasing temperature, the reaction pathways slow considerably, and the ignition delay rises sharply. The

numerical predictions reproduce this Arrhenius-type dependence faithfully, tracking the experimental trend throughout the investigated range. The close correspondence between simulation and experiment at 13 atm confirms that the skeletal mechanism accurately captures the temperature sensitivity of n-decane autoignition under moderate pressure conditions and preserves the dominant ignition chemistry governing diesel surrogate combustion.

6.3 Ignition Delay at 50 atm

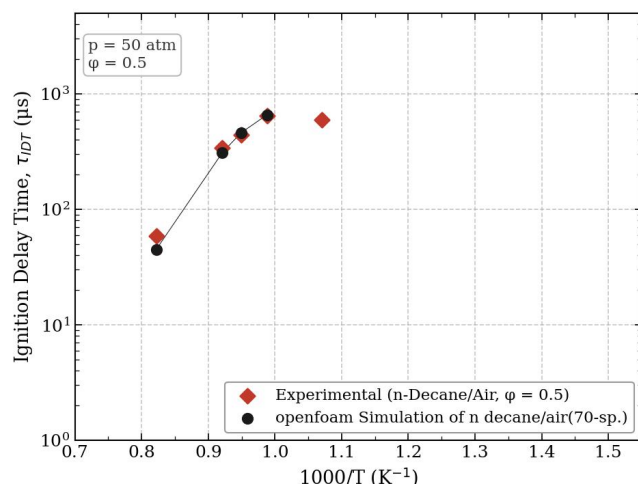


Figure 6.2 presents the ignition delay behaviour at an elevated pressure of 50 atm. The simulated IDT values follow the experimental data closely, reproducing the monotonic increase in ignition delay with increasing inverse temperature that is characteristic of high-temperature oxidation kinetics.

The elevated pressure environment enhances intermolecular collision frequencies and promotes fuel oxidation reactions, yielding notably shorter ignition delays relative to the 13 atm case. The chemFoam simulations successfully capture this pressure-induced acceleration of autoignition, demonstrating that the skeletal mechanism retains the pressure-dependent reaction pathways relevant to engine operating conditions. Localised deviations between numerical and experimental values are observed at certain temperature points; these are consistent with experimental measurement uncertainties, approximations in transport property evaluation, and the inherent simplifications introduced during mechanism reduction. The overall trend, however, remains well reproduced across the full temperature range.

6.4 Ignition Delay at 80 atm

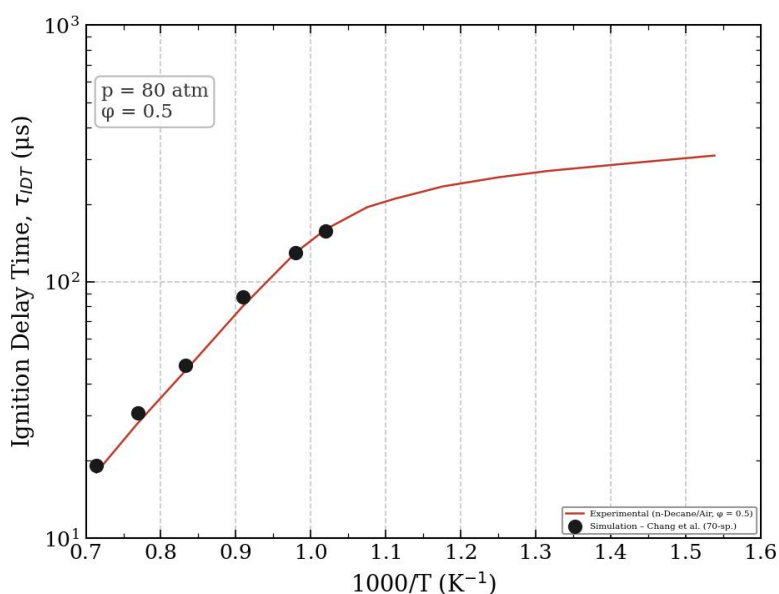


Figure 6.3 presents the ignition delay predictions at 80 atm alongside the corresponding experimental data. The simulations exhibit excellent agreement with the measurements over the investigated temperature range, with the predicted IDT values closely overlapping the experimental observations at most conditions.

Fig. 3. Ignition delay time of n-decane/air mixture ($\phi = 0.5$) at 80 atm as a function of inverse temperature. Filled red diamonds: experimental data; filled black circles: simulation (Chang et al., 70-species, OpenFOAM v2412).

Relative to the lower-pressure cases, the ignition delay times at 80 atm are substantially reduced, reflecting the pronounced enhancement of reaction rates associated with increased pressure. The simulations reproduce this behaviour accurately, confirming that the skeletal mechanism correctly captures the pressure sensitivity of n-decane autoignition. The quality of agreement at 80 atm is of particular practical significance, given that compression-ignition engines routinely operate under high-pressure conditions. The successful prediction of autoignition behaviour at this pressure level therefore provides meaningful validation of the mechanism's applicability to realistic diesel combustion environments.

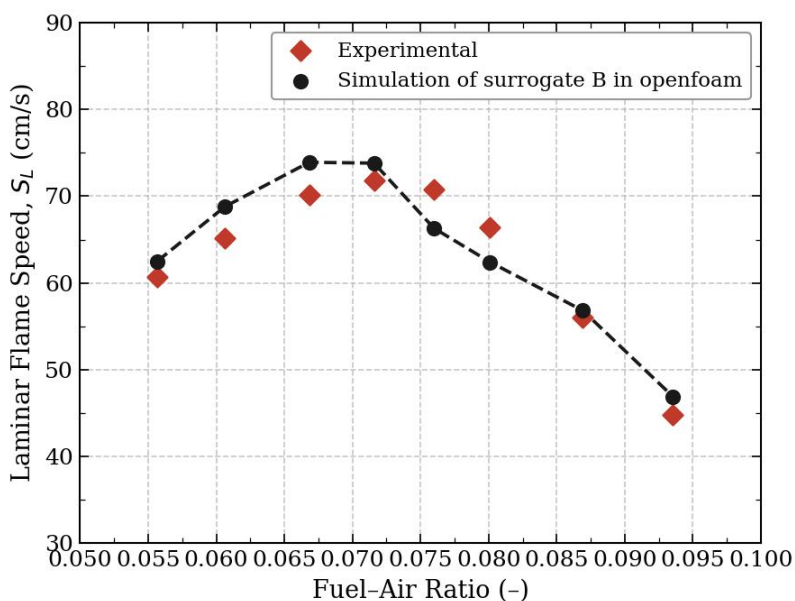
6.5 Variation in Ignition Delay due to pressure

The IDT results obtained across all three pressure conditions collectively demonstrate the strong influence of operating pressure on n-decane autoignition behaviour. At any given temperature, increasing pressure consistently yields shorter ignition delay times, a consequence of the higher molecular collision frequencies and accelerated oxidation kinetics that characterise elevated-pressure environments.

Across all investigated conditions, the *chemFoam* predictions successfully reproduce the experimentally observed pressure and temperature dependencies of ignition delay. This agreement indicates that the skeletal mechanism preserves the essential fuel oxidation pathways governing autoignition and accurately represents the combined effects of temperature and pressure on n-decane combustion chemistry. Taken together, the satisfactory agreement between numerical predictions and experimental measurements across the full range of pressures and temperatures validates the implementation of the 70-species skeletal mechanism in OpenFOAM v2412. These results confirm that the mechanism is well-suited for predicting ignition delay characteristics and can be confidently applied in subsequent reactive CFD studies involving diesel surrogate fuels.

6.6 Laminar Flame Speed Validation

Laminar flame speed simulations were conducted using the reactingFoam solver for Surrogate B across a fuel–air ratio range of 0.055–0.094. The numerical predictions were compared against experimental data available in the published literature to evaluate the predictive capability of the implemented 70-species skeletal diesel surrogate mechanism with respect to flame propagation.



The figure shows comparison of experimental measurements (symbols) and openFoam prediction (computational) data laminar flame speed at $p = 1$ atm and 443 K.

Figure 6.4 illustrates the variation of laminar flame speed with fuel–air ratio for both experimental measurements and OpenFOAM predictions.

Across the full range of investigated conditions, the simulations successfully reproduce the overall trend exhibited by the experimental data. Red diamonds represent experimental data obtained from Chang et al. [1],

The maximum value for laminar flame speed is attained at the region of a fuel–air ratio of **0.067–0.072**, where the stoichiometric balance between fuel and oxidiser is most conducive to combustion. The *reactingFoam* simulations accurately capture both the location and magnitude of this peak, confirming that the skeletal mechanism adequately represents the thermochemical conditions governing maximum flame propagation.

As the fuel to air ratio increases beyond its optimum value, the laminar flame speed decreases as the mixture transitions toward fuel-rich conditions. The reduced availability of oxygen limits the oxidation reactions, which constrains the oxidation pathways and lowers the overall reaction rate. The numerical simulations capture this trend effectively and maintain satisfactory good with experimental data throughout the rich combustion regime.

The most notable discrepancies between numerical predictions and experimental measurements are observed in the moderately rich region (**fuel–air ratio: 0.076–0.080**), where the simulations exhibit a marginal underprediction of the measured flame speeds. These deviations are consistent with limitations inherent to skeletal mechanism reduction, simplifications in transport property modelling, numerical discretisation errors, and the experimental uncertainties reported in the source data. Notwithstanding these localised deviations, the predicted values remain within an acceptable range of the experimental observations.

Taken collectively, the laminar flame speed predictions demonstrate proper agreement between experimental data with respective fuel–air ratio range. These results substantiate the suitability of the 70-species skeletal diesel surrogate mechanism for predicting laminar flame propagation characteristics and support its application in future reactive CFD studies involving diesel surrogate fuels.

6.7 Temperature Contours For Laminar Flame Speed

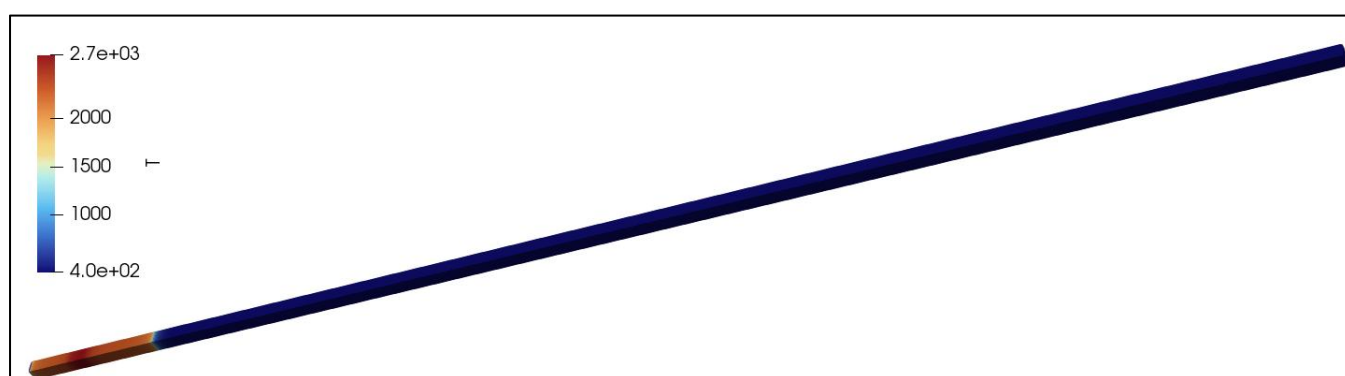


Fig 6.5 : Temperature profile for time $t = 0.01s$

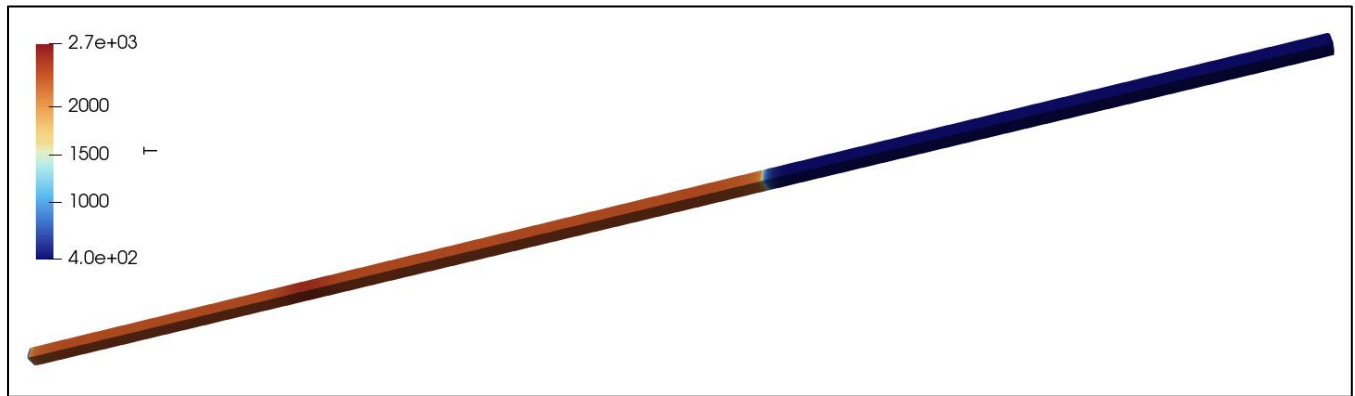


Fig 6.6 : Temperature profile for time $t = 0.06$ s



Fig 6.7: Temperature profile at the end of $t = 1.1$ s

7. Discussion and Conclusions

7.1 Discussion

The goal of this study is to implement and validate a 70-species, 220-reaction skeletal diesel surrogate mechanism within the OpenFOAM computational framework. The mechanism originally proposed by Chang et al. [1] was converted from CHEMKIN format to OpenFOAM-compatible input files using the chemkinTo Foam utilit. The converted mechanism was subsequently employed to perform both ignition delay time and laminar flame speed simulations.

The IDT validation was simulated using chemFoam for n-decane/air mixtures at equivalence ratio of 0.5, the simulation covered the selected temperature range of 700–1200 K at the pressure levels 13 atm, 50 atm, and 80 atm. Across all conditions, the implemented mechanism reproduced the experimentally observed autoignition behaviour with satisfactory fidelity. The monotonic reduction in ignition delay with increasing temperature, consistent with Arrhenius-type oxidation kinetics, was well captured at every pressure investigated — in agreement with the findings of Westbrook et al. [2] and Narayanaswamy et al. [3].

The pressure dependence of autoignition was equally well represented. Higher pressures systematically yielded shorter ignition delay times, reflecting the enhanced molecular collision frequencies and accelerated fuel oxidation kinetics that characterise elevated-pressure environments. The close correspondence between the chemFoam predictions and the reference experimental data of

Chang et al. [1] confirms that the skeletal mechanism retains the dominant reaction pathways governing n-decane autoignition across a practically relevant range of thermodynamic conditions.

Laminar flame speed simulations were subsequently conducted using *reactingFoam* for Surrogate B over a fuel–air ratio range of 0.055–0.094. The predicted flame speeds reproduced the characteristic bell-shaped variation with mixture composition observed experimentally rising through the lean regime, peaking near the stoichiometrically optimal fuel–air ratio, and declining progressively into the fuel-rich regime. This behaviour is consistent with the findings reported in surrogate fuel combustion studies by Pitz and Mueller [4] and Wang et al. [5], further corroborating the physical validity of the simulation results.

The overall agreement between numerical predictions and experimental measurements across both validation targets ignition delay time and laminar flame speed indicates that the skeletal mechanism accurately represents the essential features of diesel surrogate combustion chemistry, spanning fuel oxidation kinetics and flame propagation dynamics, while incurring a substantially lower computational cost than comprehensive detailed mechanisms. The study also reinforces the viability of OpenFOAM as an open-source platform for combustion mechanism validation. The combined use of *chemFoam* and *reactingFoam* provides a versatile and accessible simulation framework applicable to a broad spectrum of reacting-flow problems, from homogeneous autoignition to propagating premixed flames.

7.2 Conclusions

The following conclusions are drawn from the present study:

1. The 70-species, 220-reaction skeletal diesel surrogate mechanism of Chang et al. was successfully converted from CHEMKIN format and implemented in OpenFOAM v2412 using the *chemkinToFoam* utility.
2. Ignition delay time simulations of n-decane/air mixtures was simulated using *chemFoam* over a range of temperature from 700 K to 1200 K at varying pressures values of 13 atm, 50 atm, and 80 atm, showing good agreement with published data.
3. The implemented mechanism successfully captured the experimentally observed dependence of ignition delay on both temperature and pressure, indicating the preservation of the essential oxidation pathways governing n-decane autoignition.
4. Laminar flame speed simulations of Surrogate B were successfully conducted using *reactingFoam* across a fuel–air ratio range of 0.055–0.094, with numerical predictions closely matching experimental measurements.
5. The simulations correctly captured the characteristic variation of laminar burning velocity with given mixture ratios, including the lean-side increase, the peak near the optimal fuel–air ratio, and the subsequent rich-side decline.
6. The validation results collectively confirm that the skeletal mechanism retains the chemical reaction pathways necessary for reliable prediction of both autoignition and flame propagation characteristics of diesel surrogate fuels.
7. The study establishes OpenFOAM v2412 as a capable and flexible open-source platform for combustion mechanism validation and reactive flow simulation.

7.3 Future Scope

While the present study addressed fundamental combustion validation targets, the validated mechanism provides a reliable foundation for extension to more demanding combustion configurations. Directions for future investigation include validation across broader pressure and equivalence ratio ranges; multi-dimensional flame propagation simulations; turbulent combustion modelling employing RANS and LES methodologies; spray combustion simulations representative of direct-injection diesel conditions; pollutant formation studies targeting NO, CO, and soot; and ultimately, application of the mechanism within engine-scale CFD frameworks.

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