15th Asia-Pacific Conference on Combustion
18 – 22 May 2025, Singapore

Development of a New OpenFOAM-based Framework for Simulations of Laminar Reacting Flows

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Abstract

Laminar reacting flows cannot be accurately simulated using the existing official versions of OpenFOAM (OF) due to the limitations of the Sutherland transport model and the simplified assumption of a unity Lewis number. This issue can be addressed by employing a detailed transport model, such as the Standard Kinetic Theory Transport Model (SKTTM). In this study, a new OF-based framework is developed for accurate and efficient simulations of laminar reacting flows with the SKTTM, providing a robust CFD tool for public use. Since the utilization of the SKTTM is relatively expensive, a program that allows the SKTTM to be replaced with third-order polynomial models using an orthogonal polynomial fitting algorithm is also developed. The developed code is then validated against benchmark data of NIST and reference data from CHEMKIN. The excellent agreement between the results of this study and the reference data confirms the proper implementation of the methodology and demonstrates that the developed code is well-suited for accurate laminar reacting flow simulations. Moreover, employing the polynomial fit model for dynamic viscosity and thermal conductivity reduces computational costs by 20% compared to direct property calculations with the SKTTM, while maintaining accuracy.

Keywords: Standard kinetic theory transport model; laminar flames; OpenFOAM; polynomial fit model.

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Information for Colloquium Chairs and Cochairs, Editors, and Reviewers

1) Novelty and Significance Statement

The laminar reacting flows cannot be captured accurately by the existing official versions of OpenFOAM (OF) due to the utilization of the simple transport models. Using a detailed transport model such as the Standard Kinetic Theory Transport model (SKTTM) can solve this problem. In this work, we develop a new OF-based framework for accurately and effectively simulating laminar reacting flows using the SKTTM. This work is significant because it can provide a robust open-source computational fluid dynamic tool for public use.

2) Author Contributions

- Danh Nam Nguyen: investigation, methodology, software, visualization, writing - original draft.
- Jae Hun Lee: investigation, methodology, software, validation, writing - review & editing.
- Chun Sang Yoo: Conceptualization, funding acquisition, methodology, project administration, resources, supervision, writing - review & editing.

3) Manuscript Length

- Four-page paper ☑
- Eight-page paper ☐

The four-page format was selected to highlight the key aspects of our research, delivering a concise presentation.

4) Colloquium Selection

- Colloquium topic 1: Numerical Combustion
- Colloquium topic 2: Flame Dynamics and Transport Processes

1. Introduction

Althogh the OpenFOAM (OF) [1], a robust computational fluid dynamics (CFD) tool, has been widely used to solve complex problems in fluid mechanics, it has limitations in simulating laminar flames. The official versions of OpenFOAM (OF) struggle to accurately model laminar reacting flows because they employ the Sutherland transport model and the simple unity Lewis number assumption [2]. A detailed transport model, such as the Standard Kinetic Theory Transport Model (SKTTM), can address this issue [2]. However, this model is not yet officially integrated into OpenFOAM (OF).

Therefore, the objective of this study is to develop a new OF-based framework for accurate and efficient simulation of laminar reacting flows using the SKTTM, offering a robust CFD tool for public use. To address the high computational cost of the SKTTM, a complementary program is also developed, enabling the SKTTM to be replaced with a third-order polynomial model through an orthogonal polynomial fitting algorithm. The developed code is validated against benchmark data from NIST [3] and CHEMKIN [4].

2. Theoretical modeling

Building upon the Standard Kinetic Theory, the dynamic viscosity μ and thermal conductivity λ of k-th species are given as [4]:

$$\eta_k = \frac{5}{16}\frac{\sqrt{\pi m_k k_B T}}{\pi \sigma_k^2 \Omega^{(2,2)*}}, \tag{1}$$

$$\lambda_k = \frac{\eta_k}{m_k}(f_{trans}C_{v,trans} + f_{rot}C_{v,rot} + f_{vib}C_{v,vib}), \tag{2}$$

where m_k is the molecular mass, k_B the Boltzmann constant, T the temperature, and σ_j the Lennard-Jones collision diameter. The collision integral $\Omega^{(2,2)*}$ is determined by a quadratic interpolation of the tabulated values derived from Stockmayer potentials [5]. The details of the coefficients in Eq. 2 can be found in [4]. The subscripts *trans*, *rot*, and *vib* represent the translational, rotational, and vibrational contributions, respectively.

The viscosity and thermal conductivity of a mixture are determined based on a mixture averaged model as [4]:

$$\eta = \sum_{k=1}^{K} \frac{X_k \eta_k}{\sum_{j=1}^{K} X_j \Phi_{kj}}, \tag{3}$$

$$\lambda = \frac{1}{2}\left(\sum_{k=1}^{K} X_k \lambda_k + \frac{1}{\sum_{k=1}^{K} X_k/\lambda_k}\right), \tag{4}$$

where η_k, λ_k, and X_k are the dynamic viscosity, thermal conductivity, and mole fraction of k-th species in the mixture. The coefficient Φ_{kj} in Eq. 3 is calculated by:

$$\Phi_{kj} = \frac{1}{\sqrt{8}}\left(1 + \frac{m_k}{m_j}\right)^{-\frac{1}{2}}\left(1 + (\frac{\eta_k}{\eta_j})^{\frac{1}{2}}(\frac{m_j}{m_k})^{\frac{1}{4}}\right)^2 \tag{5}$$

The mixture diffusion coefficient is also calculated based on the mixture averaged model as [4]:

$$D_{km} = \frac{1 - Y_k}{\sum_{j\neq k}^{K} X_j/D_{jk}}, \tag{6}$$

where the binary diffusion coefficients D_{jk} are calculated as:

$$D_{jk} = \frac{3}{16}\frac{\left(\frac{2\pi k_B^3 T^3}{m_{jk}}\right)^{\frac{1}{2}}}{P\pi\sigma_{jk}^2\Omega^{(1,1)*}}, \tag{7}$$

where P is pressure. The collision integral $\Omega^{(1,1)*}$ is also determined by the quadratic interpolation of the tabulated values given in [5].

For ideal gas problems, employing a polynomial fit model can significantly reduce computational costs because direct property calculations with the SKTTM are computationally intensive [4]. In this study, a third-order polynomial fit model is implemented for the dynamic viscosity and thermal conductivity of each species [4]:

$$\ln \eta_k = \sum_{n=1}^{N} a_{n,k} (\ln T)^{n-1}, \tag{8}$$

$$\ln \lambda_k = \sum_{n=1}^{N} b_{n,k} (\ln T)^{n-1}, \tag{9}$$

where coefficient a_n and b_n are evaluated using an orthogonal polynomial fitting algorithm [4] based on the transport properties calculated by the SKTTM in a preprocessing step.

3. A new developed framework

Building upon the implementation approach described in [6] for a new thermophysical model with a complex mixing rule, we developed a new framework for simulating laminar reacting flows in OF-8. This framework incorporates the SKTTM, polynomial fit transport model, and a new solver which solves the same governing equations in *realFluidReactingFoam* [6].

4. Results and discussions

To validate the implementation of the SKTTM, the dynamic viscosity and thermal conductivity of major species are calculated using the developed framework. The numerical predictions are then compared with benchmark data from NIST [3], results from CHEMKIN [4], and predictions from the original OF

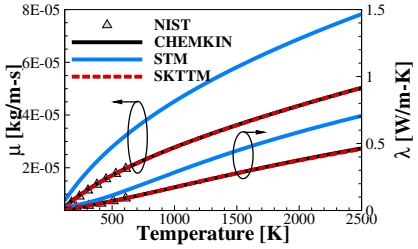

Fig. 1: The variations of the dynamic viscosity (left) and thermal conductivity (right) of pure methane as a function of temperature. Symbols: NIST data, black lines: data obtained from CHEMKIN, blue lines: predicted data by original OF with the STM, red lines: predicted data by the developed framework with the SKTTM.

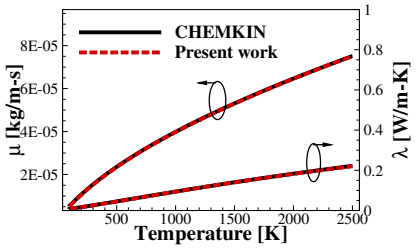

Fig. 2: Variations in the dynamic viscosity (left) and thermal conductivity (right) of a mixture as a function of temperature. Black lines: data obtained from CHEMKIN [4], dashed red lines: predicted data by the developed framework using SKTTM.

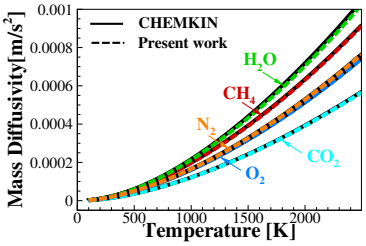

Fig. 3: Variations in the diffusion coefficient of a mixture as a function of temperature. Black lines: data obtained from CHEMKIN [4], dashed color lines: predictions by the developed framework using SKTTM.

employing the Sutherland transport model (STM). Fig. 1 shows the comparison for CH_4 species (results of other species are not shown here for the sake of brevity). The predicted data from our framework with the SKTTM matches perfectly with the benchmark data from NIST and CHEMKIN, whereas the predictions from the original OF with the STM show significant uncertainty. This discrepancy demonstrates why the original OF struggles to accurately predict laminar flames.

To further validate the implementation, the transport properties of a mixture containing CH_4/CO_2/H_2O/N_2/O_2 in equal proportions (20% by volume for each species) were calculated. Figs. 2 and 3 present the dynamic viscosity, thermal conductivity, and diffusivity of the mixture as evaluated by the developed framework, compared to calculations from CHEMKIN at 1 atm over a wide temperature range. The results demonstrate that the transport properties predicted by the developed framework are in perfect agreement with those from CHEMKIN, confirming the accuracy of the SKTTM implementation. Additionally, the fitted SKTTM was validated, showing a deviation of less than 1% compared to the SKTTM [4]. For brevity, these results are not shown here. With these validations, the implemented models are now ready for use in reacting flow simulations.

To evaluate the capability of the developed framework for simulating laminar reacting flows, we performed a test case simulation of a two-dimensional (2-D) axisymmetric laminar non-premixed counterflow flame of CH_4 and O_2/CO_2, as described in [6]. The computational domain is 20 mm $\times$ 20 mm in the radial (r) and axial (z) directions, respectively, as shown in Fig. 4. The fuel is pure CH_4 issuing from the lower nozzle and the oxidizer is air (21% O_2 and 79% CO_2 by volume) from the upper nozzle. Plug-flow boundary conditions are applied at both nozzles. To describe the flow and flame behaviors, the global strain rate, defined as $a = 2(|U_F| + |U_O|)/L$, is adopted, where U is the axial velocity and L is the separation distance between the two nozzles. The subscripts F and O denote the fuel and oxidizer streams, respectively. In this test case, a is fixed to 100 s^{-1} and the fuel and oxidizer temperatures are set to 300 and 1000 K, respectively. The pressure is 1 atm.

To accurately resolve the flame thickness, the mesh size in the axial direction near the flame zone is refined to 20 μm. The PIMPLE algorithm is employed to solve the governing equations, and the GRI 3.0 mechanism [7] is utilized for chemistry calculations. The simulation is performed with the utilization of the SKTTM under the steady state condition. It is worth noting that the results of a 2-D counterflow flame can be approximated by a 1-D problem using similarity solutions [8]. In this study, 1-D profiles along the axial axis, extracted from the 2-D results, are validated against the 1-D numerical solution obtained using OPPDIF [8]. Fig. 5 shows the profiles of flame temperature, concentrations of major species and OH radical, as well as transport properties along the axial axis obtained using the developed framework. The corresponding solutions from OPPDIF [8] are also plotted for comparison purpose. The predicted data from the developed framework with the SKTTM show excellent agreement with benchmark data from OPPDIF, verifying the accurate implementation of the SKTTM. This confirms the reliability of the developed framework for simulating reacting flows in OF.

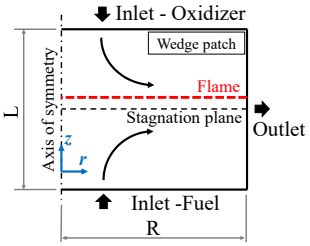

Fig. 4: The configuration of the counterflow non-premixed flame for testing cases

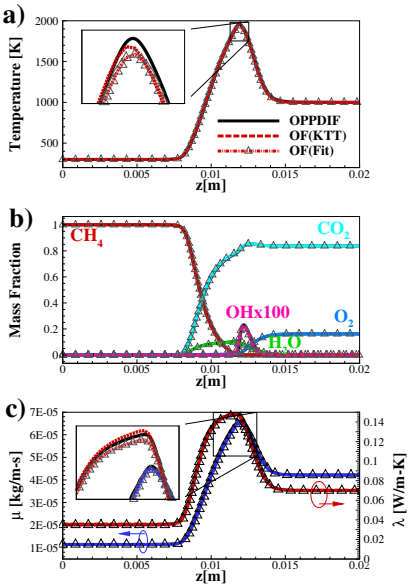

Fig. 5: The axial profiles of (a) temperature, (b) the mass fractions of major species and OH, and (c) viscosity and thermal conductivity of the steady laminar counterflow non-premixed flame of CH_4 versus O_2/CO_2 with the global strain rate of 100 s^{-1} at 1 atm. Black lines represent the results from OPPDIF; the colored dashed lines denote predictions of our framework using SKTTM; the colored dashed dotted lines with symbols denote predictions of our framework using polynomial fit model for μ and λ.

An additional simulation was performed using the polynomial fit model for dynamic viscosity and thermal conductivity to evaluate its efficiency in reducing computational time, as outlined in [4]. All other settings were identical to those in the previous simulation. The results were then compared to those obtained from direct property calculations with the SKTTM, as shown in Fig. 5. The comparison clearly demonstrates that the predictions from the polynomial fit model align perfectly with those from the detailed SKTTM, with fitting errors remaining below 1%. Furthermore, the use of the polynomial fit model reduced computational time by approximately 20% compared to the detailed SKTTM.

5. Conclusions

In this study, we successfully developed a new framework integrating the Standard Kinetic Theory Transport Model (SKTTM) and a polynomial fit transport model for simulating laminar reacting flows in OpenFOAM. The developed code was rigorously validated against benchmark data from NIST [3] and CHEMKIN [4], demonstrating excellent agreement with the reference data. These results confirm the accuracy and reliability of the developed code, making it well-suited for high-precision simulations of laminar reacting flows. Furthermore, employing the polynomial fit model for dynamic viscosity and thermal conductivity reduces computational costs by 20% compared to direct property calculations with the SKTTM, without compromising accuracy.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2024-00356149).

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