Journal of Construction and Engineering Technology
Journal homepage: www.journal.fstu.uz

COMPARATIVE ANALYSIS OF CFD MODELING METHANE COMBUSTION IN A JET USING VARIOUS TURBULENCE MODELS

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Abstract

The article investigates the modeling of the turbulent diffusion combustion process of a methane–air jet using the COMSOL Multiphysics software package. This software is highly effective for simulating coupled phenomena involving the interaction of multiple physical processes, such as combustion. To model turbulent diffusion combustion, the interactions between turbulent flow, species mixing, chemical reactions, and heat transfer in fluids were taken into account. The k–ω, k–ε, and k–ω (SST) turbulence models were employed to simulate fluid flow, while the eddy dissipation model (EDM) was used to describe the combustion process. Methane combustion was represented by a two-step reaction mechanism involving the intermediate formation of carbon monoxide. The obtained temperature distribution results were compared with available experimental data.

Keywords: Turbulent diffusion combustion, methane-air combustion, k-ω turbulent model, EDM model, COMSOL Multiphysics, carbon monoxide, CFD modeling.

1. Introduction

Methane–air combustion is of considerable importance in a wide range of engineering applications, including internal combustion engines and combined heat and power systems. Numerical simulation of combustion phenomena serves as an essential tool for predicting key characteristics such as flame propagation behavior, heat generation, and the formation of reaction products. Nevertheless, the modeling of combustion processes continues to represent a challenging multi-physics problem due to the complex interaction of physical and chemical mechanisms. Among the major challenges in the numerical analysis of turbulent non-premixed flames is the accurate determination of the chemical reaction rate. This challenge stems primarily from the intricate coupling between turbulent transport processes and chemical reaction zones [1]. In non-premixed configurations, combustion is localized at the fuel–oxidizer interface, and thus the rate of chemical transformation is predominantly governed by the turbulent mixing rate [2]. Spalding [3] demonstrated that the effective reaction rate is dictated by the mixing timescale associated with the larger turbulent eddies, which can be represented by the ratio of the turbulent kinetic energy (k) to its dissipation rate (ε).

Turbulence is generally regarded as a key factor influencing combustion processes, frequently enhancing mixing efficiency and supporting flame stabilization. In contrast, under non-premixed combustion conditions, elevated turbulence levels may adversely affect the flame by encouraging quenching and extinction phenomena. At intermediate turbulence intensities, effective interaction between the oxidizer and fuel streams promotes sustained combustion. Nevertheless, when turbulence exceeds a certain critical level, intensified fluctuations can destabilize the flame structure, weaken reaction regions, and ultimately result in flame extinction. This phenomenon is theoretically attributed to the competition between diffusive transport of heat and species and the rate of chemical reaction, a balance extensively discussed in classical combustion theory [4]. When turbulence intensity is sufficiently high, the fuel–oxidizer interface becomes increasingly fragmented and chaotic, which suppresses the formation of a coherent reaction front. As a result, combustion can occur intermittently, with local reaction zones coexisting alongside regions of extinction, as described in the distributed reaction zone

Received: 23 May 2026
Revised: 17 August 2026
Accepted: 16 September 2026
https://doi.org/10.67846/jcet.2026.42114

regime [5]. A robust theoretical framework for analyzing this interplay requires reliable formulations that capture the coupled effects of turbulence, heat transfer, and mass diffusion on flame stability and extinction limits [6].

Magnussen and co-workers developed several approaches to describe the interaction between turbulent mixing and chemical reactions [1, 7]. Among these, the most widely applied and well-established formulation is the Eddy Dissipation Model (EDM), which represents an extension of Spalding's original eddy-breakup concept [3, 8]. The central premise of the EDM is to circumvent the explicit treatment of detailed chemical kinetics by substituting the chemical timescale of a representative single-step reaction with a turbulence-controlled timescale, expressed as the ratio of the turbulent kinetic energy to its dissipation rate (k/ε). Within this framework, the mixing of reactants and products is assumed to be the controlling factor for the overall reaction rate in turbulent flows [5].

The Eddy Dissipation Model (EDM) has long been employed in the simulation of gas diffusion flames, with extensive evidence supporting its robustness in predicting key flame characteristics [9-11]. For instance, the study presented in [12] investigated turbulent premixed combustion over bluff bodies using the Eddy Dissipation Concept (EDC) model. A RANS-based finite-volume solver coupled with a standard k–ε turbulence closure was applied to analyze the downstream flame field. Similarly, Achim et al. [13] implemented an EDM-based computational framework to simulate coal combustion in a full-scale tangentially fired boiler, achieving results in close agreement with experimental heat flux measurements at the furnace walls. In another investigation [14], EDM in conjunction with the standard k–ε model was used to simulate a turbulent methane jet diffusion flame, focusing on the influence of fuel inlet excitation on NO and soot formation. The model successfully reproduced experimental trends in flame temperature, mixture fraction, and soot volume fraction. Furthermore, methane jet combustion has also been explored with EDM coupled to a novel two-fluid turbulence model [15, 16], providing additional validation of EDM's applicability across diverse combustion configurations Consequently, EDM remains a valuable engineering model for non-premixed methane–air CFD provided its assumptions (mixing-limited chemistry, appropriate turbulence model, and calibrated model constants) are carefully considered and, where necessary, complemented by higher-fidelity simulations or experimental validation [17-19].

COMSOL Multiphysics is a powerful simulation software used by engineers, researchers, and scientists to model a wide range of physical phenomena. It is particularly well suited for problems that require the interaction of multiple physical processes. COMSOL Multiphysics excels at modeling coupled phenomena, where multiple physical processes interact with each other. This eliminates the need to use multiple software packages for different aspects of the simulation, simplifying the workflow and increasing accuracy [20]. COMSOL Multiphysics uses the finite element method (FEM), a well-established numerical modeling technique that provides robust and accurate solutions. The software includes a wide range of solvers and discretization methods, allowing users to choose the most appropriate approach for their specific problem. The results obtained in COMSOL Multiphysics will be compared with experimental results [21].

2. Materials and Methods

2.1. Subsection

2.1.1. The k-ε Turbulence Model

The k–ε model is one of the most widely used turbulence closures in engineering CFD owing to its balance between computational efficiency and predictive capability. Originally developed by Launder and Spalding (1972) [22], the model introduces two additional transport equations: one for the turbulent kinetic energy (k), which quantifies the intensity of turbulence, and another for the rate of its dissipation (ε), which represents the scale at which turbulent energy is converted into thermal energy by viscous action. Closure of the Reynolds-averaged Navier–Stokes (RANS) equations is achieved through the Boussinesq eddy viscosity hypothesis, in which the Reynolds stresses are related to the mean strain rate using a turbulent viscosity expressed as a function of k and ε.

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{1}$$

Where Cμ is a model constant
The transport equations for k and ε reads:

$$\begin{cases} \rho\dfrac{\partial k}{\partial t} + \rho u \cdot \nabla k = \nabla \cdot \left(\left(\mu + \dfrac{\mu_t}{\sigma_k} \right) \nabla k \right) + P_k - \rho\varepsilon, \\ \rho\dfrac{\partial \varepsilon}{\partial t} + \rho u \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \dfrac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \dfrac{\varepsilon}{k} P_k - . \\ -C_{\varepsilon 2} \rho \dfrac{\varepsilon^2}{k} \end{cases} \tag{2}$$

In this expression the production term is:

$$P_k = \mu_t \left(\nabla u : \left(\nabla u + (\nabla u)^T \right) - \frac{2}{3} (\nabla \cdot u)^2 \right) - \frac{2}{3} \rho k \nabla \cdot u \quad (3)$$

Where

$$C_\mu = 0.09, C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92, \sigma_k = 1.0, \sigma_\varepsilon = 1.3.$$

2.1.2. The k-ω Turbulence Model

The standard k−ω turbulence model, originally formulated by Wilcox (1998) [23], is fundamentally an empirically derived framework. It is constructed around transport equations governing the turbulence kinetic energy (k) and the specific dissipation rate (ω), thereby providing a closure strategy for Reynolds-averaged Navier–Stokes (RANS) formulations.

$$\begin{cases} V \nabla k = \nabla \cdot \left[\left(\nu + \sigma^* \frac{\mu_t}{\rho} \right) \nabla k \right] + \tau_{ij} \nabla V - \beta^* \omega k, \\ V \nabla \omega = \nabla \cdot \left[\left(\nu + \sigma^* \frac{\mu_t}{\rho} \right) \nabla \omega \right] + \alpha \frac{\omega}{k} \tau_{ij} \nabla V - \\ -\beta \omega^2, \end{cases} \quad (4)$$

where $\mu_t = \alpha^* \frac{\rho k}{\omega}$ and $\varepsilon = \beta^* \omega k$.

In addition, the Wilcox turbulence model has the following empirical constants

$$\alpha = \frac{5}{9}, \ \beta = \frac{3}{40}, \beta^* = \frac{9}{100}, \sigma = \sigma^* = \frac{1}{2}.$$

2.1.3. The k-ω (SST) Turbulence Model

The Shear Stress Transport (k−ω SST) model, introduced by Menter (1994) [24], represents a hybrid approach that combines features of the k−ε and k−ω formulations. In this framework, the standard k−ε model is reformulated in terms of k−ω, after which a blending function is employed to ensure a smooth transition between the two models. This blending function assumes a value of unity in the near-wall region, thereby activating the k−ω formulation, while in the outer flow region it approaches zero, effectively switching to the k−ε formulation expressed in k−ω terms.

2.2. Modeling of combustion

In this paper, the two-step reduced reaction mechanism of methane air combustion is modeled, taking into account the formation and oxidation of carbon monoxide.

$$CH_4 + 3/2\, O_2 = CO + 2H_2O$$
$$CO + 1/2\, O_2 = CO_2$$

Using symmetry, a two-dimensional model is solved using a cylindrical coordinate system.

Using the turbulence model in the reacting flow interface, the formation rate (SI unit: kg/(m^3 s)) of species i resulting from reaction j is modeled as a minimum of the average closure reaction rate and the eddy scattering model rate.

$$R_{ij} = \nu_{ij} M_i \cdot \min\left[r_{MVC,j}, r_{ED,j} \right] \quad (5)$$

The mean closure rate is the kinetic rate of reaction expressed using average mass fractions. It corresponds to the characteristic reaction rate for reactions that are slow relative to turbulent mixing, or the reaction rate in regions with negligible levels of turbulence.

Reaction rate determined by the eddy-dissipation model (EDM).

$$r_{ED} = \frac{\alpha_j}{\tau_T} \rho \cdot \min\left[\min\left(\frac{\omega_r}{\nu_{rj} M_r} \right), \beta \sum_p \left(\frac{\omega_p}{\nu_{pj} M_p} \right) \right] \quad (6)$$

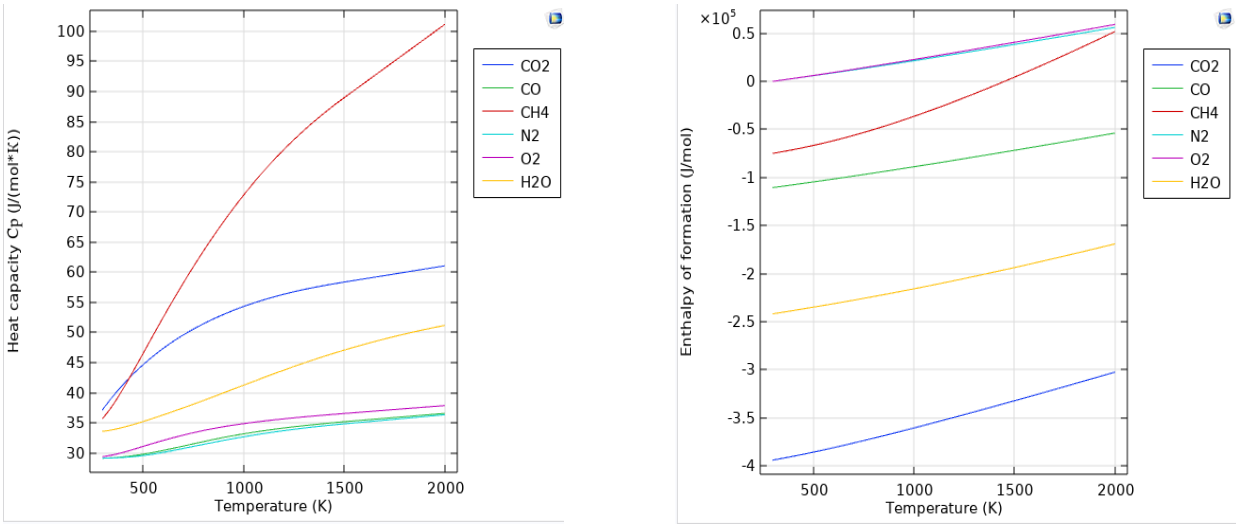
where τ_T - (SI unit: s) is the turbulence mixing time scale, ρ - is the mixture density (SI unit: kg/m^3), ω - is the mass fraction of particles, ν - denotes the stoichiometric coefficients, and M - is the molar mass (SI unit: kg/mol). The properties of the reactants of the reaction are denoted by the subscript "r", and the properties of the products are denoted by the subscript "p".

The model parameter β indicates that the reaction requires a product, modeling the activation energy. For gaseous non-premixed combustion, the model parameters were found to be $\alpha = 4, \ \beta = 0.5$.

2.3. Thermophysical properties

In this simulation, a thermodynamic system is set up that includes all the species present. The system is used to determine the species as well as the properties of the mixture depending on the temperature and composition. When connecting the Chemistry interface to the Thermodynamic system, all the necessary thermodynamic and transport properties are automatically determined.

The two important thermal properties are the heat of reaction and the heat capacity of the mixture. Figure 1 shows the change in the enthalpy of formation with temperature for all individual species. It is evident that the enthalpy of formation increases with temperature for all species, and accurate results will be obtained by taking into account the temperature dependence. Since the heat of formation of the products is lower than that of the reactants, both reactions are exothermic and proceed with the release of heat.



(**a**) (**b**)

Figure 1. a – specific molar heat capacity and b – enthalpy of formation of gases in the COMSOL Multiphysics software.

$$\Delta H_r = \sum_p \Delta H_{f,298K} - \sum_r \Delta H_{f,298K} \quad (7)$$

3. Problem statement

This paper studies the axisymmetric combustion of methane in an air flow. Methane is injected through a 4 mm diameter jet nozzle, concentric inside a 1 m long annular burner. The flame configuration is shown in Figure 2. The mass flow rate of methane is $1.72\times10^{-4}\,kg/s$, the air flow rate is $118\times10^{-4}\,kg/s$ at a temperature of 300ºK. At such mass flows, the velocities of methane and air are U_{jet}=20.3m/s and U_{cof}=0.45m/s, respectively. The Reynolds number at the exit from the nozzle is 5000 [21].

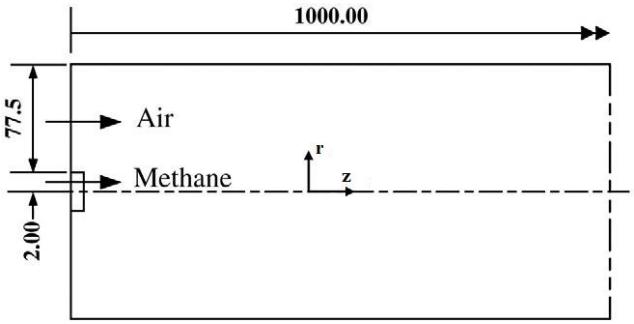


Figure 2. Flame configuration. Dimensions in mm.

4. Results

Figure 3 shows the dependence of the dimensionless axial temperature on the distance to the nozzle. Figures 4-6 illustrates the profiles of the dimensionless longitudinal temperature at a distance of 150 mm, 200 mm and 300 mm from the nozzle, respectively.

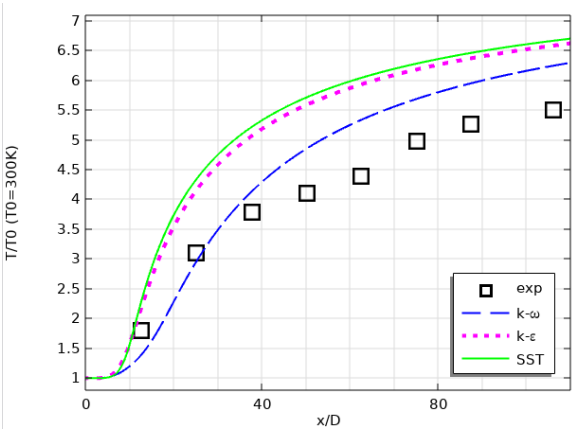


Figure 3. Temperature along the axis from the distance to the nozzle.

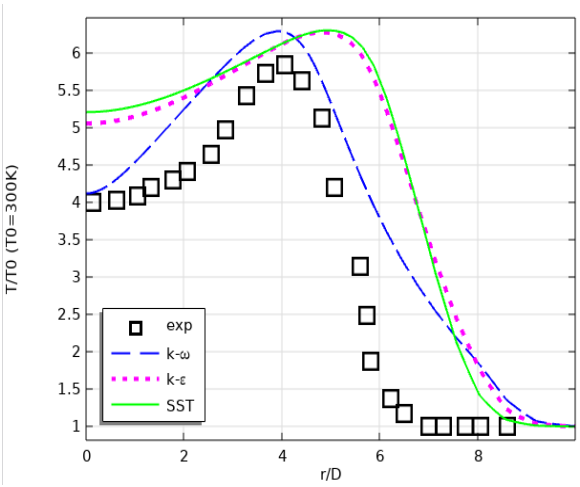


Figure 4. Temperature profile at a distance of 150 mm from the nozzle.

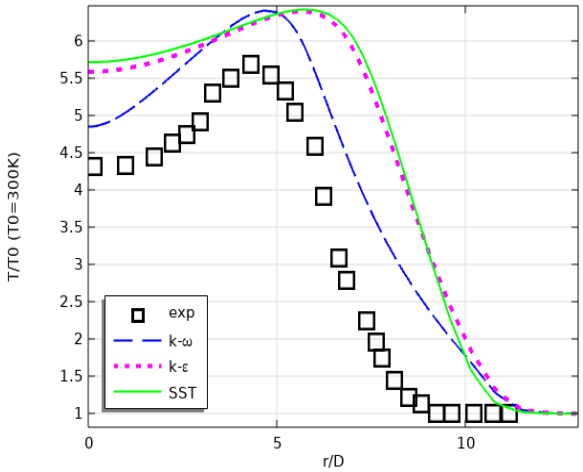


Figure 5. Temperature profile at a distance of 200 mm from the nozzle.

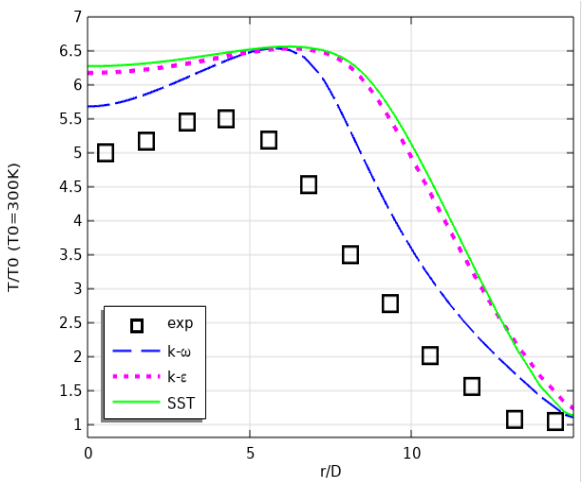


Figure 6. Temperature profile at a distance of 300 mm from the nozzle.

5. Discussion

It is evident from the figures that modeling of diffusion combustion in the COMSOL Multiphysics environment gives results close to the experiment. The obtained results of temperature distribution along the axis show that the k-e model gives values close to the experimental ones. the maximum temperature values in the radial direction are the same for all models, but in the k-e model it coincides with the radial distance of the maximum temperature in the experiment, although it gives an overestimated value.

5. Conclusions

The paper presents numerical results of methane combustion in a jet based on the k-ω, k-ε and k-ω (SST) turbulence model obtained in the CFD package of COMSOL Multiphysics programs. The obtained numerical results are compared with known experimental data. It is shown that the results of the k-ω model are close to the experimental data than other two. The SST and k-ε turbulence model demonstrated predictive capability, yielding temperature distributions that showed satisfactory agreement with the corresponding experimental measurements. Thus, in the CFD package of COMSOL Multiphysics programs, combining various physics, it is possible to model and obtain an adequate solution to more complex problems, such as the process of turbulent combustion.

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