Second-Order Moment Turbulent Combustion Model A Priori Test Postprint

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Abstract

This study performs a priori validation and evaluation of the second-order moment (SOM) combustion model using a compressible DNS database of isotropic turbulent combustion. The validation reveals that neglecting density fluctuations and third-order fluctuation correlations is feasible, effectively simplifying the reaction rate equation. Examination of the exact terms in the correlation transport equations indicates that the chemical reaction term makes the most significant contribution and requires accurate closure. Assessment of the modeled transport equations shows that while the modeling of some exact terms is unsatisfactory, the overall concept and methodology of the SOM combustion model are feasible and warrant further development.

Full Text

Preamble

A-priori Validation of a Second-order Moment Combustion Model

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Abstract: This paper presents an a-priori validation and evaluation of the Second-order Moment (SOM) combustion model using a compressible DNS database of isotropic turbulent combustion. The validation reveals that neglecting density fluctuations and third-order fluctuation correlation terms is feasible and effectively simplifies the reaction rate equation. By examining the exact terms in the transport equations for correlation quantities, the chemical reaction term is found to contribute most significantly and requires accurate closure. Validation of the modeled transport equations shows that while some exact terms are not ideally predicted, the overall SOM combustion model concept and methodology remain feasible and warrant further development.

Keywords: second-order moment; turbulent combustion model; direct numerical simulation; a-priori validation

0 Introduction

Turbulent combustion is widely applied in industrial sectors such as energy, metallurgy, chemical engineering, and transportation. Research on turbulent combustion enhances our understanding and application of combustion processes. With advances in turbulence research and computer technology, RANS, LES, and DNS have become important approaches for studying turbulent combustion, and various combustion models have been proposed and applied.

The primary challenge in turbulent combustion simulation lies in the closure of chemical reaction source terms. Scholars have proposed numerous turbulent combustion models, such as the EBU-Arrhenius model [1-3], Probability Density Function (PDF) models [4], flamelet models [5], transported PDF models [6-7], and Conditional Moment Closure (CMC) models [8-9]. However, these models were developed for specific combustion modes and struggle to simultaneously predict both premixed and diffusion flames. Meanwhile, DNS calculations have shown [10] that premixed and diffusion flames can coexist, posing a challenge to the aforementioned models. Consequently, developing models capable of simultaneously predicting different combustion modes has become a significant challenge in combustion modeling.

In recent years, the Second-order Moment (SOM) combustion model proposed by Zhou Lixing [11] has attempted to address this issue. The SOM combustion model is based on the Arrhenius equation for reaction rates, representing the nonlinear exponential function of temperature with a reaction rate coefficient K, then deriving transport equations for fluctuation correlations from fundamental transport equations, and subsequently closing these transport equations using methods similar to turbulence closure. Theoretically, the SOM combustion model has no restrictions on combustion modes and can therefore predict premixed flames, diffusion flames, and partially premixed flames effectively, while also capturing strong chemical reaction phenomena such as ignition and extinction. In studies by Zhou Lixing et al. [12], the EBU-Arrhenius model and simplified PDF models were considered theoretically flawed, with simulation results showing large discrepancies from experimental values. Meanwhile, transported PDF models, flamelet models, and CMC models are relatively complex, computationally expensive, and cannot simultaneously predict diffusion and premixed flames. Therefore, the relatively simple SOM combustion model based on reaction rate closure has become a promising turbulent combustion model for engineering simulations of turbulent combustion, as demonstrated in relevant literature [11-13].

Nevertheless, the SOM combustion model involves certain assumptions, including neglecting density fluctuations and third-order fluctuation correlations, and the modeling results require validation. Therefore, this paper employs a compressible DNS database to conduct an a-priori validation and evaluation of the SOM combustion model.

1 SOM Combustion Model

For a two-component single-step global reaction, the instantaneous reaction rate in Arrhenius form is:

$$\dot{w} = BY_{\text{fu}}Y_{\text{ox}}\exp\left(-\frac{E}{RT}\right)$$

where the subscript “fu” denotes fuel, “ox” denotes oxidizer, Y_{fu} and Y_{ox} represent the mass fractions of the two reactants, B is the pre-exponential factor, E is the activation energy, and R is the universal gas constant.

Applying Reynolds averaging to equation (1) and neglecting density fluctuations and third-order fluctuation correlations yields the mean reaction rate:

$$\bar{\dot{w}} = \bar{K}\bar{Y}_{\text{fu}}\bar{Y}_{\text{ox}} + \overline{Y'_{\text{fu}}Y'_{\text{ox}}}\bar{K} + \overline{Y'_{\text{fu}}K'}\bar{Y}_{\text{ox}} + \overline{Y'_{\text{ox}}K'}\bar{Y}_{\text{fu}}$$

where $K = B\exp(-E/RT)$ is the reaction rate coefficient. The concentration-concentration correlation $\overline{Y'_{\text{fu}}Y'_{\text{ox}}}$ and concentration-reaction rate coefficient correlations $\overline{Y'_{\text{ox}}K'}$, $\overline{Y'_{\text{fu}}K'}$ in equation (2) are obtained by solving their transport equations.

The exact transport equations for correlation quantities are derived from species and energy equations. The exact equation for concentration-concentration correlation is:

$$\frac{\partial\overline{Y'_{\text{fu}}Y'_{\text{ox}}}}{\partial t}+\bar{u}_j\frac{\partial\overline{Y'_{\text{fu}}Y'_{\text{ox}}}}{\partial x_j} = -\overline{u'_jY'_{\text{ox}}}\frac{\partial\bar{Y}_{\text{fu}}}{\partial x_j}-\overline{u'_jY'_{\text{fu}}}\frac{\partial\bar{Y}_{\text{ox}}}{\partial x_j}+\frac{\partial}{\partial x_j}\left(D\frac{\partial\overline{Y'_{\text{fu}}Y'_{\text{ox}}}}{\partial x_j}\right)-2D\overline{\frac{\partial Y'_{\text{fu}}}{\partial x_j}\frac{\partial Y'_{\text{ox}}}{\partial x_j}}+\overline{Y'_{\text{fu}}\dot{w}'_{\text{ox}}}+\overline{Y'_{\text{ox}}\dot{w}'_{\text{fu}}}$$

The right-hand side terms represent: (1) turbulent diffusion, (2) production due to mean concentration gradients, (3) laminar diffusion, (4) molecular dissipation, and (5) chemical reaction source terms, all requiring closure. The closed form becomes:

$$\frac{\partial\overline{Y'_{\text{fu}}Y'_{\text{ox}}}}{\partial t}+\bar{u}_j\frac{\partial\overline{Y'_{\text{fu}}Y'_{\text{ox}}}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(C_{g1}\frac{k}{\varepsilon}\overline{u'_ju'_k}\frac{\partial\overline{Y'_{\text{fu}}Y'_{\text{ox}}}}{\partial x_k}\right)-C_{g2}\frac{\varepsilon}{k}\overline{Y'_{\text{fu}}Y'_{\text{ox}}}-C_{g3}\frac{\varepsilon}{k}\overline{Y'_{\text{fu}}Y'_{\text{ox}}}+C_{g4}\frac{1}{\tau_c}\overline{Y'_{\text{fu}}Y'_{\text{ox}}}$$

The right-hand side terms represent: (1) diffusion, (2) production, (3) dissipation, and (4) chemical reaction. Here, C_{g1}, C_{g2}, and C_{g3} are empirical coefficients, τ_T and τ_c are turbulent diffusion time and chemical reaction time, defined as:

$$\tau_T = \frac{k}{\varepsilon}, \quad \tau_c = \frac{1}{\bar{K}}$$

Similarly, the exact equation for concentration-reaction rate coefficient correlation is:

$$\frac{\partial \overline{K'Y'_{\mathrm{fu}}}}{\partial t} + \bar{u}_j \frac{\partial \overline{K'Y'_{\mathrm{fu}}}}{\partial x_j} = -\overline{u'_j Y'_{\mathrm{fu}}} \frac{\partial \bar{K}}{\partial x_j} - \overline{u'_j K'} \frac{\partial \bar{Y}_{\mathrm{fu}}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(D \frac{\partial \overline{K'Y'_{\mathrm{fu}}}}{\partial x_j}\right) - 2D \overline{\frac{\partial K'}{\partial x_j}\frac{\partial Y'_{\mathrm{fu}}}{\partial x_j}} + \overline{K'\dot{w}'_{\mathrm{fu}}} + \overline{Y'_{\mathrm{fu}}\dot{w}'_K}$$

Like the concentration-concentration equation, the right-hand side terms include: (1) and (2) diffusion, (3) production, (4) dissipation, and (5)-(8) chemical reaction source terms. Using a similar closure approach, the modeled equation becomes:

$$\frac{\partial \overline{K'Y'_{\mathrm{fu}}}}{\partial t} + \bar{u}_j \frac{\partial \overline{K'Y'_{\mathrm{fu}}}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(C_{k1} \frac{k}{\varepsilon} \overline{u'_j u'_k} \frac{\partial \overline{K'Y'_{\mathrm{fu}}}}{\partial x_k}\right) - C_{k2} \frac{\varepsilon}{k} \overline{K'Y'_{\mathrm{fu}}} - C_{k3} \frac{\varepsilon}{k} \overline{K'Y'_{\mathrm{fu}}} + C_{k4} \frac{1}{\tau_c} \overline{K'Y'_{\mathrm{fu}}}$$

Similarly, the right-hand side terms represent: (1) diffusion, (2) production, (3) dissipation, and (4) chemical reaction.

The above constitutes the fundamental concept of the second-order moment combustion model, whose assumptions and modeling methods require validation. Wang Fang et al. [14] validated the SOM combustion model using direct numerical simulation of incompressible isothermal reactive flow in a channel. This paper conducts an a-priori validation and evaluation of this conceptual approach using a compressible DNS database provided by the State Key Laboratory of Clean Energy Utilization at Zhejiang University.

2 Description of the DNS Database

The DNS database used in this study was generated by Wang Haiou et al. [15], who performed direct numerical simulation of spray combustion in isotropic turbulence using a single-step irreversible reaction mechanism. The computational domain measures $2\pi \times 2\pi \times 2\pi$ mm in the x, y, and z directions with a grid resolution of 128^3 and a mesh size of 49μm. Initially, droplets were randomly distributed within a layer between $3\pi/8$ and $5\pi/8$, after which they evaporated, ignited, and burned, diffusing along the x-axis toward both sides. At the selected time instant, all droplets have completely evaporated, and the combustion can be considered purely gas-phase. Detailed information can be found in relevant literature [15-16].

The chemical reaction mechanism used is:

$$\mathrm{C_7H_{16}} + 11\mathrm{O_2} \rightarrow 7\mathrm{CO_2} + 8\mathrm{H_2O}$$

The reaction rate follows the Arrhenius law, with parameters selected based on Westbrook' s research [17]. The pre-exponential factor is $5.1 \times 10^{13}\mathrm{cm}^{0.75}\mathrm{mol}^{-0.75}\mathrm{s}^{-1}$, and the activation energy is 30.0Kcal/mol. The exponents for heptane and oxygen mass fractions are 0.25 and 1.5, respectively. The specific Arrhenius expression is:

$$\dot{w} = A \exp\left(-\frac{E}{RT}\right) Y_{\mathrm{C7H_{16}}}^{0.25} Y_{\mathrm{O2}}^{1.5}$$

where A is the pre-exponential factor, E is the activation energy, W is the molar mass of species, ν is the stoichiometric coefficient, and m and n are species exponents, with $A = A_0 W_{\mathrm{C7H_{16}}}^{-0.25} W_{\mathrm{O2}}^{-1.5} \nu_{\mathrm{C7H_{16}}}^{0.25} \nu_{\mathrm{O2}}^{1.5}$.

[Figure 1: see original paper] shows the distribution of mean temperature and species mass fractions at the selected time instant. As can be seen, the central region is a high-temperature reaction zone where both reactants $\mathrm{C_7H_{16}}$ and $\mathrm{O_2}$ exist in large quantities. The left and right sides are flame fronts, representing the interface between fresh and burned gases, with flames diffusing from the center toward both sides. This database is used to conduct an a-priori validation of the SOM combustion model, with all averaged data being local statistical averages, i.e., the statistical average over the yz plane serves as the local value at position x.

3 Validation Results of the SOM Combustion Model

3.1 Validation of Assumptions

Based on the second-order moment concept, we validated equation (2) and the modeled equations (4) and (7). The derivation of equation (2) employed the assumptions of neglecting density fluctuations and third-order fluctuation correlations, which we now examine.

[Figure 2: see original paper] compares the calculated values when neglecting density fluctuations, neglecting fluctuation correlations, and neglecting both simultaneously, against the exact values. The figure clearly shows that all three curves agree well with the exact values, with maximum errors within 40%. This indicates that in the second-order moment method, neglecting density fluctuations and third-order fluctuation correlations is feasible and can effectively simplify the model. However, it is noteworthy that the density used in this validation is the local mean density, which exhibits density gradients in the

x direction. Using a constant-density incompressible assumption would significantly affect the results, necessitating the derivation of correlation transport equations under compressible conditions.

By comparing the magnitudes of terms on the right-hand side of the exact mean reaction rate expansion, we find that the mean value product $\bar{K}\bar{Y}_{\mathrm{fu}}\bar{Y}_{\mathrm{ox}}$ is the dominant term determining the direction and magnitude of the reaction rate. The correlation quantities containing fluctuations have relatively small variations in the reaction zone and exhibit certain peaks at the two flame fronts, which cannot be neglected. Third-order correlation quantities, however, are negligible except for minor fluctuations at the flame fronts. Therefore, the SOM combustion model' s assumption of neglecting third-order fluctuation correlations is acceptable, while second-order fluctuation correlations require accurate modeling.

The transport equations for correlation quantities—namely the concentration-concentration correlation equation (3) and the concentration-reaction rate coefficient correlation equation (6)—require validation of their exact production, diffusion, dissipation, and chemical reaction terms. [Figure 3: see original paper] shows the relative magnitudes of these exact terms.

[Figure 3: see original paper] reveals that these four terms are of the same order of magnitude, with the reaction term being the largest, followed by the diffusion term, production term, and finally the dissipation term. Figure 3: see original paper clearly shows that the chemical reaction term contributes most significantly. Wang Fang et al.' s [14] incompressible DNS validation concluded that the chemical reaction source term contributed minimally to the right-hand side, which differs from our results. This discrepancy arises primarily from the different heat release rates in the selected databases. The heat release rate in Wang Fang et al.' s study is far smaller than that in our heptane combustion case—approximately two orders of magnitude difference, as evident from the temperature profiles in [Figure 1: see original paper] and reference [13]. Specifically, the channel reactive flow temperature used by Wang Fang et al. [13] is much lower than the heptane combustion temperature, resulting in relatively lower chemical reaction rates for all species and an underestimation of the chemical reaction source term contribution.

3.2 Validation of Modeled Terms

[Figure 4: see original paper] and [Figure 5: see original paper] show the validation results for modeled terms in the concentration-concentration fluctuation correlation and concentration-reaction rate coefficient fluctuation correlation equations, respectively. Figure 4: see original paper, 4(b), 5(a), and 5(b) demonstrate that the production and diffusion terms are modeled reasonably well, capturing the trends of the exact terms and resolving the two peaks at the flame fronts. The main limitation is that the modeled terms show strong dependence on coefficient selection, which requires improvement.

Figure 4: see original paper shows the dissipation term modeling for the concentration-concentration fluctuation correlation. While the modeled results follow the basic trend of the exact term, the exact term exhibits two peaks at the flame fronts whereas the modeled term shows only one. The two peaks in the exact term arise from species gradient fluctuations on both sides of the flame front, which are difficult to capture using dissipation closures based on species fluctuations and turbulent kinetic energy. Figure 5: see original paper shows the dissipation term modeling for the concentration-reaction rate coefficient fluctuation correlation, with similarly unsatisfactory results. However, since the dissipation term contributes relatively little to the transport equation, the modeling error is acceptable.

Figure 4: see original paper displays the reaction term modeling for the concentration-concentration correlation equation, revealing notably poor closure performance. The reason lies in the neglect of reaction rate coefficient K fluctuations—specifically temperature fluctuations—which significantly affect the results. Therefore, a new closure method for the chemical reaction term is necessary that incorporates fluctuations in the reaction rate coefficient. Conversely, the reaction term closure for the concentration-reaction rate coefficient correlation shows better performance, accurately capturing the exact values in the central reaction region but underestimating them at the two flame fronts. This occurs because in the modeled homogeneous isotropic turbulent reaction, temperature variations in the central combustion zone are not large and fluctuations are small, while at the flame fronts, sharp changes in species and temperature create large gradients that increase the reaction term. Thus, actual species and temperature gradients must be considered.

4 Conclusions

This study employs a compressible turbulent combustion DNS database to conduct an a-priori validation and evaluation of the second-order moment concept, yielding the following conclusions:

(1) The SOM combustion model neglects density fluctuations and third-order fluctuation correlations to simplify the reaction rate equation. The validation shows that density fluctuations and third-order fluctuation correlations have minimal impact on the reaction rate equation, making this assumption feasible. However, it is important to note that the local mean density was used in the validation, necessitating the derivation of compressible correlation transport equations. Additionally, since the reaction rate equation contains non-first-order concentration exponents, care must be taken during simplification.

(2) Examination of the exact terms in the concentration-concentration and concentration-reaction rate coefficient correlation transport equations reveals that the chemical reaction term contributes most significantly and requires accurate modeling.

(3) Validation of the production and diffusion terms shows good modeling performance, capturing the trends of exact terms, though numerical results show strong dependence on coefficient selection, which can be corrected using dynamic subgrid methods. The dissipation term is poorly modeled, but its small contribution makes the modeling error acceptable. For the chemical reaction term, the second-order moment method employs a chemical reaction time scale closure. The validation shows that reaction term modeling is not ideal for the concentration-concentration correlation, while for the concentration-reaction rate coefficient correlation, closure performs well in the central reaction zone but requires improvement at the flame fronts.

(4) Overall, the model’ s fundamental concept and methodology are feasible and provide a valuable reference. Future development of the SOM combustion model will proceed through theoretical and DNS validation, including treatment of strong shear jets and swirl in actual combustion processes, ultimately establishing the model as an important tool for engineering turbulent combustion simulations.

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