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A COMPARISON BETWEEN THE PERFORMANCE OF TWO EXTENDED MECHANISMS IN PREDICTING POLLUTANTS OF A METHANE-AIR JET DIFFUSION FLAME

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ABSTRACT

The present paper deals with the influence of the extended chemical kinetics mechanism on the accuracy of the thermo-chemical quantities in reacting flows. Two extended mechanisms, namely the GRI-Mech3 and the Konnov mechanisms are used to simulate Methan-Air opposed jet flow. Results show that GRI-Mech3 better predicts CO and H_2 species than the Konnov mechanism. However, the Konnov mechanism is superior in predicting heavier hydrocarbons such as C_2H_2 and C_2H_4. Results for pollutant species show that the Konnov mechanism predicts NO to a very good degree of accuracy. As to the computational economy, GRI-Mech3 stands higher than the Konnov mechanism, as it has less species and reactions.

INTRODUCTION

Combustion-generated pollution of the environment requires intense research on the fluid mechanics, as well as the chemistry of combustion phenomena. One of the least understood aspects of combustion is the underlying chemical reaction itself, even for relatively simple fuels like natural gas. In part, this is due to the restrictions on experimental methods imposed by the harsh conditions under which combustion proceeds, and also due to the inherent chemical complexity of combustion. In addition to these obstacles, inadequate information about the elementary chemical reactions responsible both for the main chemistry and for the side reactions that lead to undesirable pollutants such as oxides of nitrogen and sulfur makes the study of combustion processes a serious challenge. The Gas Research Institute (GRI) initiated an extensive research program for the optimization of the chemical scheme regarding natural gas. Precise details of the optimization scheme in that program are discussed in detail by Bowman et al. [1]. At temperatures above 1000 K, combustion of simple fuels, such as hydrogen, can be calculated using an eight-step reaction mechanism for which the reaction rate data is known with confidence, see Dixon-Lewis et al. [2]. However, complex hydrocarbon fuels, such as kerosene, require more than 1000 reaction steps with over 200 species; see Dagaut et al. [3]. Hence, as all the reaction rate data is not well known, there is a high degree of uncertainty in the results obtained using these large detailed reaction mechanisms. We note that various methods have been proposed to find a set of reaction rate parameters that gives the best fit to a given set of experimental data. However, for complex hydrocarbon fuels, the object function is usually highly structured. The reaction mechanisms of reactive species are generally fall into three categories. The first one deals with extensive mechanisms, where many species and reactions are considered for the chemical kinetics. The second category makes use of the reduced mechanisms to mimic the prevailing chemical kinetics of the reactions. The third category of reaction mechanisms are global reactions, mostly one- and two-step reactions. We briefly explain these categories next.

EXTENDED MECHANISM

This type of mechanisms considers many species and reactions for modelling of the chemical kinetics. Extended Mechanism gives accurate results, but is computationally expensive. Two of the most common extensive mechanisms are the GRI-MECH3 and the Konnov mechanism [4].
The GRI-MECH3 mechanism includes 53 species and 325 reactions. The base of this mechanism is combustion of natural gas that includes methane and ethane. So this mechanism is

able to model up to C_3 species and this is the bottle-neck of GRI mechanism, because for modelling of some pollutants, we need higher hydrocarbons in the chemical reaction mechanism. For example, we need to consider species C_4H_6, C_4H_2, C_6H_6 for modeling of soot [5] and GRI-MECH3 mechanism cannot predict these species in combustion mechanism.
The Konnov mechanism includes 121 species and 1027 reactions and covers the reaction of heavy hydrocarbons up to C_6. This mechanism includes higher range of species, and can be used to predict pollutants and heavier hydrocarbons. However, the calculations with this mechanism requires more time for modeling combustion processes, because it has more reaction and species than GRI-MECH3.

Wang et al. [6] suggested a detailed reaction mechanism which consists of 527 reactions and 99 chemical species. It is partly based on GRI-MECH 1.2 [7] and extended to describe acetylene and ethylene oxidation, because the GRI-MECH was optimized for natural-gas combustion.

REDUCED MECHANISMS

This type of mechanisms is very popular with the CFD community as far as the computational work and computational economy is concerned. However, the accuracy of reduced mechanisms is less than the extensive mechanism.

One of these mechanisms presented with Sung et al. [8] that have a 12-step, 16-species reduced reaction mechanism. This mechanism contains species up to C_2.

GLOBAL MECHANISM

The third category of reaction mechanisms are global reactions. These mechanisms are very rough, and are used as a first approximate to reaction problems [9]. For example, equation (1) is a one-step reaction of methane oxidation:

CH4 + 2O2 ===> CO2 +2 H2O (1)

THE PRESENT STUDY

The present study aims to compare the performance of the GRI-MECH3 and the Konnov mechanisms in simulating a non-premixed Methane-air flame. The OPPDIF code [10] is used to assess the aforementioned mechanisms in simulating an opposed jet diffusion flame (Figure 1). The comparison is made for two different temperature of the air-inlet as shown in table(1).

Table 1: condition of problem [11]

T_{air}(K)	T_f (K)	V_{air} (cm/s)	V_f (cm/s)
300	300	70	70
560	300	70	70

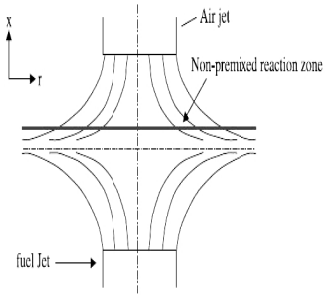

Figure 1: Schematic of the counterflow nonpremixed flame simulated in the present study.

The governing equations for a one-dimensional, incompressible, steady flow may be written as [15]:

Continuity:

$$\frac{d(\rho v)}{dy} + (j+1)\rho U = 0 \qquad (2)$$

Momentum:

$$\rho v \frac{dU}{dy} = -\rho U^2 + P + \frac{d}{dy}\left(\mu \frac{dU}{dy}\right) \qquad (3)$$

Mixture fraction:

$$\rho v \frac{dZ}{dy} = \frac{d}{dy}\left(\rho D \frac{dZ}{dy}\right) \qquad (4)$$

Species mass fractions:

$$\rho v \frac{dY_i}{dy} = \frac{d}{dy}\left(\rho D_i \frac{dY_i}{dy}\right) + \dot{\omega}_i \qquad (5)$$

where the axial pressure gradient may be expressed as:

$$P = \rho_\infty a^2 \qquad (6)$$

In the above equations, j=0 represents the plane-flow, and j=1 is used for the axi-symmetric flow. Variables U and v are used for velocity components in x-direction, and y-direction, respectively. The rate of strain on the fluid elements is represented by a in the above equations. Parameter Z is used to denote the mixture fraction, and Y_i refers to the i^{th} species. Subscript ∞ refers to conditions far from the nozzles.
The boundary conditions to close the above set of equations are:

$$y \to \infty: \quad v_\infty = -ay, \quad U_\infty = a, \quad Z = 0 \qquad (7)$$

$$y \to -\infty \quad v_{-\infty} = -(\rho_\infty / \rho_{-\infty})^{1/2} ay, \quad U_{-\infty} = a\rho_\infty / \rho_{-\infty}, \quad Z = 1 \qquad (8)$$

In this work we investigate the CH_4-air flame where the operating conditions are shown in Table 1. We use GRI database [1] for thermodynamic data and transport data and for Konnov mechanism, we use Konnov database [4].

RESULTS AND DISCUSSION

We first compare the computational time for these two mechanisms. The computations are performed on a Pentium IV computer with 1 Gigabyte RAM. Both simulations are done on the same computer in the same system conditions. The Konnov mechanism requires 228 min time to converge, whereas the GRI mechanism only needs 6 min to converge to the solution. Such a great difference in the computational time indicates that the GRI mechanism may be preferred whenever possible.

Next, the impact of the reaction mechanism on the major and minor species is studied. Figures 2 and 3 show such a comparison for CH_4 and CO_2 as the major species. As appears in these figures, there is practically no difference between the predictions of these mechanisms for major species. Good agreement exists between the numerical predictions and experimental data.

The numerical prediction results for intermediate species are shown in figures 4-8. While the GRI mechanism shows better agreement with the experimental data for H_2 and CO, the Konnov mechanism is equally good or much better for the rest of predictions. The reason that H_2 prediction of GRI mechanism is better than that of Konnov mechanism is due to the over-prediction of GRI mechanism for C_2H_2 and C_2H_4, which consumes H atoms and leaves a lower concentration of H2 as compared to the Konnov mechanism. It should be noted that both mechanisms fail in predicting the location of maxima in the intermediate C_2 species profiles. However, the Konnov mechanism gives surprisingly good results for NO, while the GRI mechanism is known to over-predict NO profile as appears in the present study.

The temperature profiles are shown in Fig.9. As appears in this figure, the GRI mechanism predicts slightly better results for the case of low temperature air-inlet, but both the mechanisms are of the same order of accuracy for the high-temperature air-inlet case.

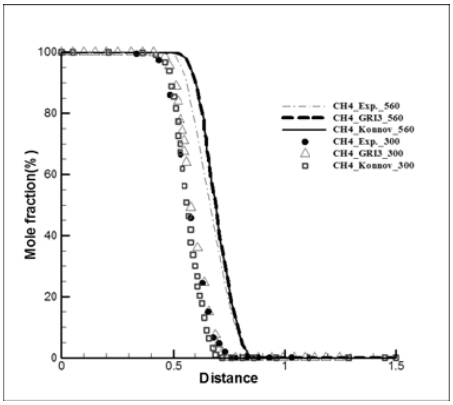

Figure 2: Comparison of the result of CH4 mole fraction of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

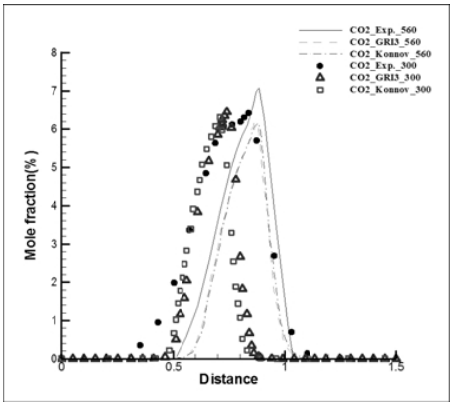

Figure 3: Comparison of the result of CO2 mole fraction of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

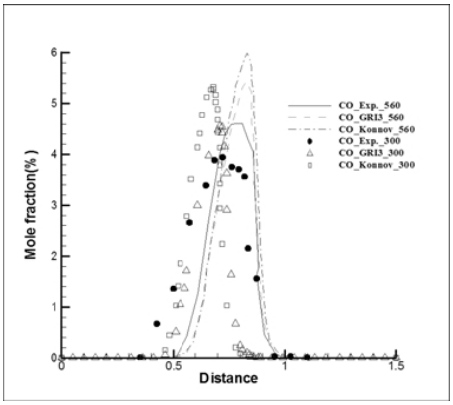

Figure 4: Comparison of the result of CO mole fraction of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

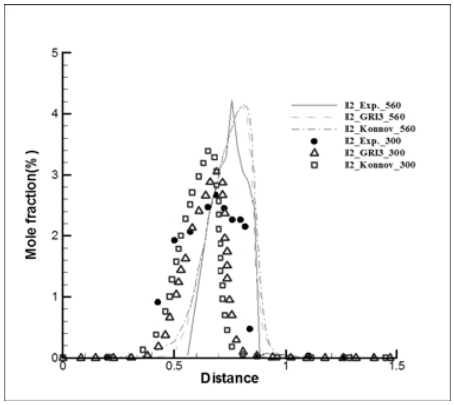

Figure 5: Comparison of the result of H2 mole fraction of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

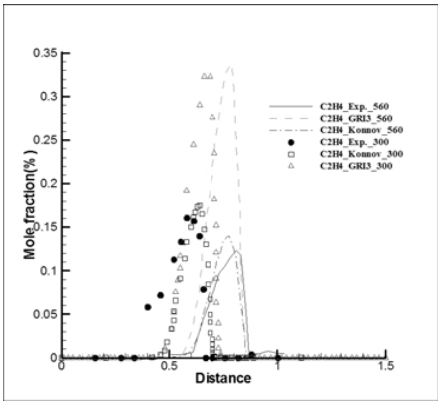

Figure 6: Comparison of the result of C2H4 mole fraction of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

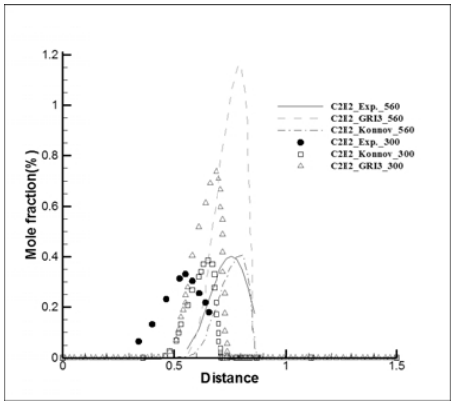

Figure 7: Comparison of the result of C2H2 mole fraction of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

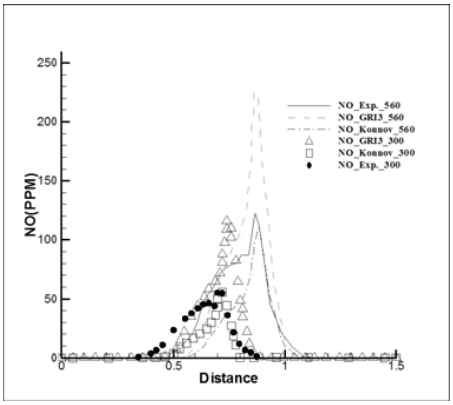

Figure 8: Comparison of the result of NO (PPM) of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

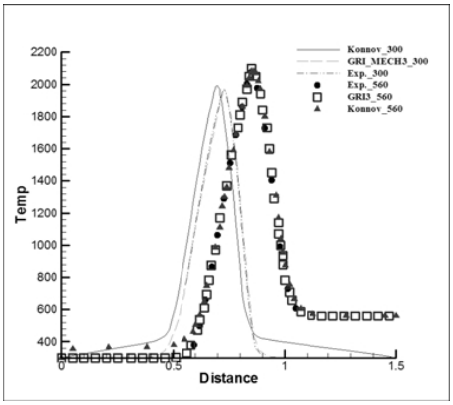

Figure 9: Comparison of the result of Temperature of GRI-MECH3 and Konnov mechanisms with experimental data at different distance from fuel nozzle in 300K and 560K air

CONCLUSION

It may be concluded from the present study that the GRI Mech3 may be suitable when only the mean temperature and the main species are of concern. For cases when the minor species concentrations, especially NO and heavier hydrocarbons are of concern, it is recommended that the Konnov mechanism is used. The computational work for the Konnov mechanism is much higher than that of the GRI-Mech3.

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