VERIFICATION OF REDUCED METHANE KINETIC MECHANISM UNDER LAMINAR CONDITIONS USING A LOW DIMENSIONAL MODELING APPROACH

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ABSTRACT

Reduced/Skeletal kinetic mechanisms are of great interest to the research community, as these mechanism reduce the computational cost significantly. The study presented here considered a reduced kinetic mechanism under laminar flow conditions and resolves the full range length and time scales by solving governing equations for mass, momentum and energy. The reduced mechanism published in the literature is derived from the original GRI mechanism of methane gas and the simulations are performed with both original and reduced order mechanisms. The combustion of H_2 gas at elevated temperature is considered and the spatial and temporal resolutions are identified to be 1e-6 m and 2e-7 seconds respectively. Spatial profiles of reactants, product and temperature, from both simulations, are compared and quantitatively the profiles are in good agreement indicating the mechanism can be employed in the place of original GRI mechanism for some problems, reducing the computational cost significantly.

INTRODUCTION

Combustion devices of practical interest include internal combustion engines, stationary and aircraft gas-turbine combustors, and industrial burners. Combustion systems need to be operated such that the combustion reactions are brought to completion with a minimum of pollutants being formed [1]. An accurate prediction of the essential physical and chemical properties of the combusting systems is important to achieve the two main objectives, optimization of combustion efficiency and the reduction of pollutants. Most practical combusting systems are turbulent in nature and involve many phenomena and processes, such as turbulence, mixing, mass and heat transfer, radiation, and multiphase flow phenomena, which strongly interact. In many combustion processes chemical reaction controls the rate of combustion, and, in essentially all combustion processes, chemical rates determine pollutant formation and destruction. Ignition and flame extinction are intimately related to chemical processes.

The study of the elementary reactions and their rates, chemical kinetics, is a specialized field of physical chemistry. Much progress has been made in understanding the combustion because the

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chemists have been able to define the detailed chemical pathways (for simple fuels) leading from reactants to products, and to measure or calculate their associated rates [2-3].

Significant progress has also been made in coupling the kinetic mechanisms with Computational Fluid Dynamics (CFD) simulation tools [4] to optimize the designs of combusting systems. Many researchers have contributed to this area and chemistry representation ranges anywhere from equilibrium chemistry implementation to including the detailed kinetic reactions. The computational resource requirement scales accordingly. When detailed kinetics are considered the simulation cost exponentially grows as many species equations have to be solved and the source term computation includes resolving the elementary reactions. Scientists are actively looking for mechanisms with reduced number of species and reactions, compared to the original mechanism, and still capable of providing the same level of accuracy and detail related to the chemistry computation.

The work considered here verifies the performance of a reduced order reaction mechanism against the original reaction mechanism, by performing simulations, where reaction mechanisms are coupled with conservation equations for mass, momentum and energy, under laminar flow conditions. The paper is organized as follows, first the original and reduced order mechanisms are introduced followed by the description of simulation configuration and details. Results from both simulations are compared and the qualitative and quantitative agreement is analyzed.

REACTION MECHANISM

Typically any reaction mechanism includes a list of elementary reactions and associated rate constant expressions. GRI 3.0 mechanism developed by a group of researchers includes 53 species and 325 elementary reactions [5-6]. If such large mechanism is employed to resolve the kinetics in turbulent flow field (computing the source term in individual species equation) the computational resources requirement becomes intractable.

Slavinskaya et al. [7] have used KINLAC package tools to identify the redundant species and reactions in the original mechanism when applied to reproduce the laminar flame speed measurements under fuel lean conditions. Authors have performed extensive sensitivity and rate of production analysis to derive the reduced mechanism. The parameter of interest is the flame speed, and through analysis it has been identified that the rate coefficients of two reactions need to be modified to match the prediction of original mechanism. While different reduced mechanisms are derived and presented, in this work main focus is on the reduced mechanism including 19 species and 86 reactions. The species considered here include, H_2, H, O, O_2, OH, H_2O, HO_2, CH_2, CH_3, CH_4, CO, CO_2, HCO, CH_2O, CH_2OH, CH_3O, CH_3OH, N_2 and Ar.

SIMULATION DETAILS

The simulation tool considered for the current work solves the coupled mass, momentum and energy equations on a one-dimensional domain. Pressure is explicitly solved using the equation of state and mass conservation is enforced using the continuity equation. Full description of the model is not presented here, however for those interested, complete derivation of the equations is available here [8]. The constitutive relationships for the flux terms appearing in the governing equations are also defined based on the general principles. The tool in the current form resolves detailed kinetics and full range of diffusive-reactive length and time scales are maintained. Neumann boundary conditions are defined for momentum equations and Dirichlet boundary conditions are defined for mass and energy equations. Computational domain of 2 cm considered for the simulation, with 1e-6 m spatial resolution, and the solution marched in time at 2e-7 s steps. The selected 1D domain is represented as *y* and the initial conditions are defined as follows,

- At t=0, uniform velocity profile is defined with a value of 0.2 m/s over the entire domain
- At t=0, mass fraction of the fuel species, H_2 is 0.023 over the entire domain.
- At t=0, mass fraction of the oxidizer species, O_2 is 0.23 over the entire domain.
- At t=0, mass fraction of the N_2 species is 0.747 over the entire domain.
- All the remaining species are assigned zero value over the entire domain.

- At t=0, temperature is defined using a Gaussian function [9] with assigned peak value of 1600 K, with 0.002 m width, at the center of the domain and rest of the domain assigned a value of 800 K.

RESULTS AND DISCUSSION

Figure 1 illustrates the spatial profiles of different quantities from the simulations performed using both original and reduced order mechanisms. Hydrogen fuel is highly reactive, in the presence of oxidizer, at elevated temperatures. Due to the presence of heat source in the center of the domain (1600 K) H_2 and O_2 species react together, as the time elapses, and the reaction front propagates in either direction from the center, consuming the fuel and oxidizer. Simultaneously the product species (H_2O) will start forming and the temperature will also rise. During such process, the intermediate species will be produced and consumed. Initially, at t=0, the mass fraction of H_2 species is at 0.023 and the O2 species composition is at 0.23, as the time progresses, both species composition at the center of the domain starts to decrease. After about 250 time steps, most of the fuel over 0.003 m domain is consumed.

The formation of OH radical species (flame indicator) can also be seen clearly at the corresponding time interval and the maximum mass fraction reaches 0.023. The temperature has a peak value of

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1600 K at the starting and it reaches ~2350 K, due to the strong combustion, at the simulation elapsed time of 5e-5 s. The formation of product species, in the form of H_2O can also be seen. The maximum values observed, for H_2O, corresponding to t=5e-5 s is 0.15. Small dip at the center location is also observed and at the same location OH exhibits a local maxima, indicating the reaction is not completed yet.

As the simulation progresses, more fuel in the computational domain is consumed and correspondingly the temperature increased. The domain over which the fuel species is consumed, the radical species and product species exists is much larger after 1125 time steps (t=2.25e-4 s), extends from 0.0035 to 0.0165 m. The maximum values observed for temperature, OH and H2O species are 2700 K, 0.018 and 0.18 respectively. It is interesting to note the location corresponding to the peak value observed for temperature, at this time interval, is where maximum fuel is also consumed.

Figure 1 includes data from both the simulations, and most profiles presented here are in good agreement. Both qualitatively and quantitatively the reduced mechanism reproduced the original mechanism behavior. For OH species, at t=2.25e-4, minor differences are observed (refer to figure 1D). In most research efforts, OH species is treated as a flame indicator and high reaction rates are associated with the species. The differences observed are due to the fact that reduced mechanism didn't take in to account all the species and elementary reactions. Author verified most of the major species profiles (such CO_2, CO) and found no differences. In summary, the reduced mechanism includes less number of species (19 vs 53) and elementary reactions (86 vs 325) compared to the original GRI 3.0 mechanism, and the results presented here indicate that the hydrogen fuel combustion can be accurately represented by the reduced mechanism.
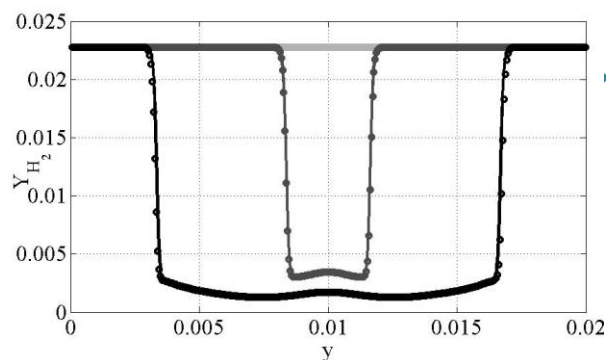
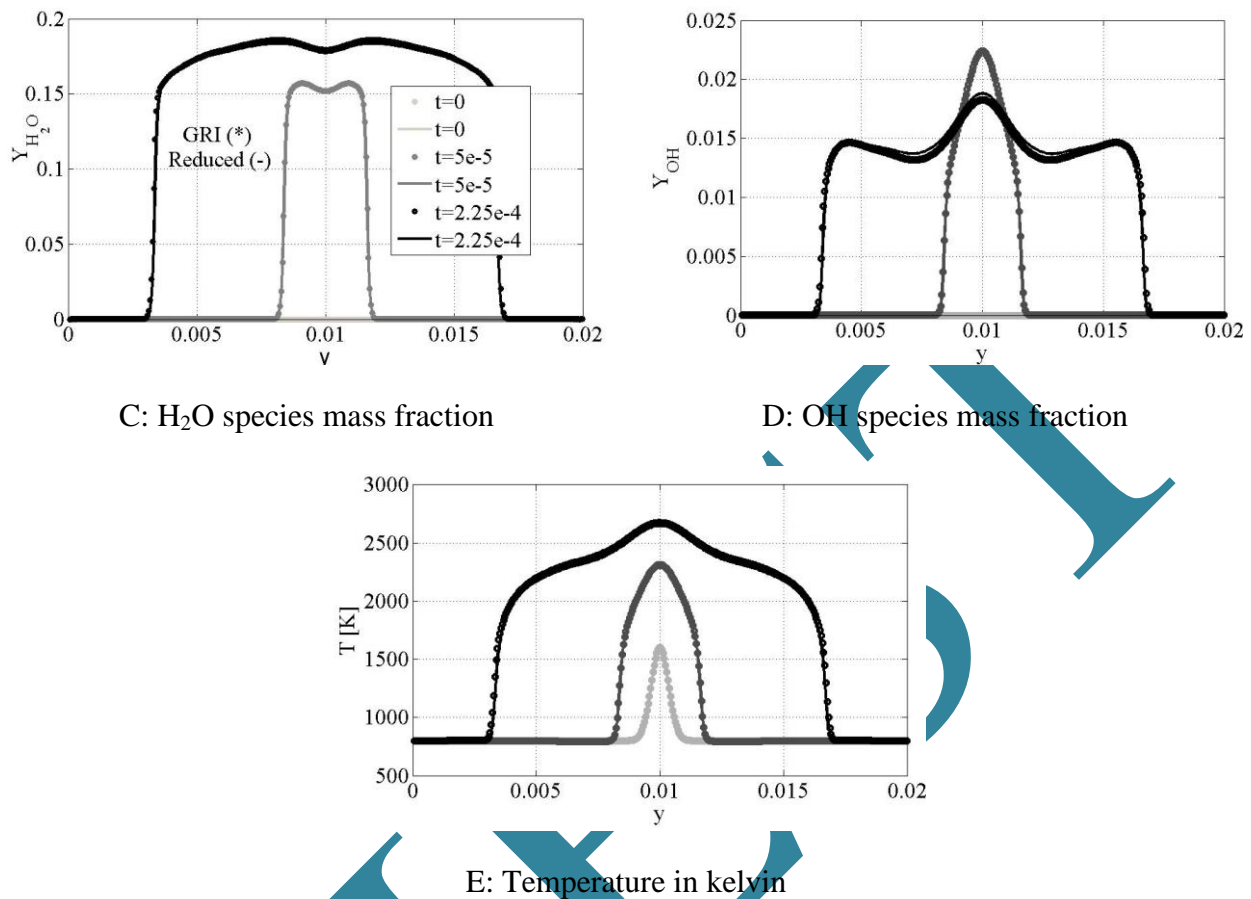A: H_2 species mass fraction   B: O_2 species mass fraction

C: H₂O species mass fraction   D: OH species mass fraction
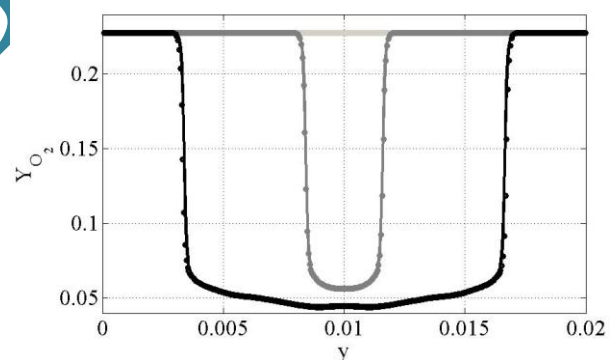
E: Temperature in kelvin

Figure 1: Spatial profiles of reactants (H₂, O₂), product (H₂O), intermediate species (OH) and temperature at three different time intervals. Light gray: initial, Medium gray: 5e-5 s and Dark gray: 2.25e-4 s. Dots represent the original GRI 3.0 mechanism and line represents the reduced mechanism.

CONCLUSIONS

In this work, 1D simulations are performed to verify the reduced order mechanism against the original GRI mechanism. Hydrogen species combustion characteristics are studied and the spatial and temporal resolutions are fixed at 1e-6 m and 2e-7 s respectively. Spatial profiles of different species and also temperature, from both simulations, are compared at different time intervals. The comparison indicates that the reduced mechanism reproduces the original mechanism performance. Quantitatively minor differences are observed in the OH species profile. Due to the accurate reproduction of the original mechanism behavior, the reduced mechanism can be utilized in performing simulations, to design combusting systems to improve the performance, and the author's future efforts will be focused in that direction.

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