



Direct numerical simulation of non-premixed syngas burning with detailed chemistry

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ABSTRACT

H₂/CO syngas non-premixed impinging jet flames were studied using three-dimensional direct numerical simulation (DNS) and flamelet generated manifolds (FGMs) based on detailed chemical kinetics. The computational domain employed has a size of four jet nozzle diameters in the streamwise direction and 12 jet nozzle diameters in the cross-streamwise direction. The results presented in this study were performed using a uniform Cartesian grid with 200 × 600 × 600 points. The Reynolds number used was Re = 2000, based on the reference quantities. The spatial discretisation was carried out using a sixth-order accurate compact finite difference scheme and the discretised equations were time-advanced using a third-order accurate fully explicit compact-storage Runge–Kutta scheme. Results show that the ratio of H₂ and CO in the syngas mixture significantly affects the flame characteristics including the near-wall flame structure. The high diffusivity of H₂-rich syngas flame leads to form weaker vortices and a thicker flame. In contrast, CO-rich syngas flame leads to form a thinner flame with strong wrinkles. Moreover, the DNS results suggest that the preferential diffusion influences the local flame structure for the simulated low Reynolds number H₂ flame.

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1. Introduction

Coal is one of the most abundant natural resources, providing around a 29.6% of the world's total energy up from 26% 10 years ago [1]. For example, China itself consumed 48.2% of the world's coal and accounted for nearly two-thirds of the global consumption growth. Over the years, various investigations have been focused on coal combustion such as fluidized-bed combustion [2], co-firing of coal and biomass [3], development of coal combustion technology in response to environmental challenges [4], as well as achieving improvements in the efficiency of pulverised coal combustion [5]. However, as one of the unclean fuels, coal use accounts for a significant proportion of greenhouse gas emissions in a global level with the world's 2300 coal-fired power stations contributing approximately 40% to all man-made emissions [6]. Although there is an urge to move to alternative energy sources, coal will still provide approximately 30% of the marketed energy [7] in the near future and there are challenges in utilising coal in a cleaner manner. Making coal power systems cleaner and more efficient contributes to the United Nations Kyoto Protocol of reducing carbon emissions [8].

Development of clean coal technology would allow continued use of coal without substantial emissions of greenhouse gases such as CO₂ [9]. Beyond that, it contributes to the balance between energy supply and demand, a strategic and necessary choice for realising the coordinated development of energy, environment and economy [10]. Such clean coal energy conversion technologies can rely on the combustion of gasified coal, referred to as synthesis gas or syngas, which is mainly a mixture of hydrogen (H₂) and carbon monoxide (CO) [11]. Coal is the predominant source of gasifier feedstock, supplying 55% of syngas worldwide in 2007 [12]. There is a considerable interest to produce H₂ from coal gasification processes and its consumption is expected to increase dramatically in the near future [13]. For example, in recent years significant progress has been made in the development of integrated gasification combined cycle (IGCC) technology to employ hydrogen and syngas fuels in gas turbines together with the potential for CO₂ capture for cleaner electric power production [14]. This integration of energy conversion processes provides more complete utilisation of energy resources, offering high efficiencies and ultra-low pollution levels [15]. Ultimately IGCC systems will be capable of reaching efficiencies of 60% with near-zero pollution. The unique advantages of IGCC systems have led to potential applications of gasification technologies in industry because gasification is the only technology that offers both

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upstream (feedstock flexibility) and downstream (product flexibility) advantages. Because they operate at higher efficiency levels than conventional fossil-fuelled power plants, IGCC systems emit less CO₂ per unit of energy. They are also well suited for the application of future technologies to capture and sequester CO₂ [16]. Investigations of H₂ and syngas production from various other applications including gas-to-liquid and biomass are also reported in the literature [17,18].

Unlike direct coal combustion, hydrogen combustion produces virtually no pollution or greenhouse gases while syngas produces much less emissions [11]. Therefore ongoing development of hydrogen and syngas combustion technology as an appropriate type of future energy source is playing an increasingly important role in the clean energy strategy. Particularly there is a growing interest in the combustion of hydrogen-enriched synthesis gas. There is a fair amount of experimental based research focused on the combustion of both non-premixed and premixed syngas applications in the past. Among them, investigations such as the scalar structure of CO/H₂/N₂ non-premixed flames [19], laminar flame speeds of H₂/CO/CO₂ premixed flames [20], effects of nitrogen dilution on flame stability of syngas mixtures [21], and global turbulent consumption speed of syngas H₂/CO mixtures [22] are notable. However, there are still lots of fundamental issues related to hydrogen and syngas combustion such as the effects of the high diffusivity of hydrogen-enriched fuels, especially the preferential diffusion, as well as the fuel variability of syngas fuels on the flame dynamics that have not been fully understood.

In recent decades, computational combustion has made remarkable advances due to its ability to deal with wide range of scales, complexity and almost unlimited access to data [23]. Direct numerical simulation (DNS), in which the complete spectrum of scales is resolved, is evolving as an extremely valuable computational tool from which much can be learned [24]. Early investigations include comprehensive simulations in two dimensions [25], as well as three-dimensional DNS of turbulent non-premixed flames including finite rate chemistry and heat release effects, e.g. [26]. Since then various DNS studies of non-premixed combustion have been performed to investigate a wide range of fundamental issues such as turbulence/chemistry interaction, flame stabilisation, local extinction and auto-ignition, e.g., the effects of flow strain on a hydrogen-air triple flame [27], scalar intermittency of CO/H₂ planer jet flame [28], flame stabilisation and structure of lifted hydrogen jet flame [29]. DNS studies of flame-wall interactions with one-step and multi-step chemical kinetics have been reported in the last two decades. For example, two-dimensional DNS of head-on quenching (HOQ) in a pseudo-turbulent reactive boundary layer [30] and three-dimensional HOQ of premixed propagating flame in constant density turbulent channel flow [31], side-wall effects on flame dynamics [32], one-dimensional simulation of hydrogen combustion interacting with an inert wall [33], three-dimensional DNS of sidewall quenching for v-shaped premixed flame [34] and turbulent flame-wall interaction using three-dimensional DNS and detailed chemical kinetics [35] were carried out. However, a complete understanding on certain aspects of the flame dynamics such as effects of fuel variability and preferential diffusion is still not available.

Since the next generation combustion system is rapidly shifting towards hydrogen and syngas fuels, there are a number of issues which need further investigations. For example, higher diffusivity and reactivity of hydrogen-enriched syngas combustion should lead to unconventional operating conditions, mixed-mode and therefore undiscovered turbulent-chemistry regimes. Furthermore, the application of hydrogen-enriched syngas to both internal and gas turbine combustion can likely develop undesirable flame flashback phenomenon, in which the flame propagates into the burner. Therefore, there is a growing interest in high fidelity simulation

techniques that could capture the fundamental fine scale turbulence-chemistry interactions, and especially flame dynamics with respect to fuel variability. For example, thermo-diffusive effects such as differences in the relative rates of mass diffusion with respect to syngas fuel variability may result in complex interactions that are not well understood. Also the effect of preferential diffusion, which depends on the amount of hydrogen in the syngas fuel mixture, is likely to further affect the flame dynamic behaviour. If the turbulence level is very low this effect may become significant in hydrogen-enriched syngas flames. The present investigation has two objectives: (1) to study the effects of fuel variability and flame dynamics of H₂/CO fuels, (2) to investigate the effect of preferential diffusion on hydrogen flame. Here we employed the DNS technique along with flamelet-generated manifold (FGM) approach. The detailed chemical kinetics has been employed through the FGM method [36], which not only uses complex chemistry, but also takes the most important transport processes into account. An impinging jet including buoyancy has been selected as the flow configuration to investigate, which not only provides details of flame dynamics in the primary jet shear layer but also information on the near-wall combustion which is a challenging topic that needs further investigations. In the following, the methods used in this study are presented first, including the governing equations, flame chemistry, and the numerical methods. The results and discussions are presented subsequently, mainly in terms of instantaneous flame characteristics. Finally conclusions are drawn.

2. DNS governing equations

In the present study, the three-dimensional unsteady compressible conservation equations of mass, momentum, energy, mixture fraction and transport equation for the progress variable in their original dimensional form are solved, which can be given as:

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial(\rho^* u_j^*)}{\partial x_j^*} = 0, \quad (1)$$

$$\frac{\partial(\rho^* u_j^*)}{\partial t^*} + \frac{\partial(\rho^* u_j^* u_k^* + p^* \delta_{jk})}{\partial x_k^*} - \frac{\partial \tau_{jk}^*}{\partial x_k^*} + (\rho_a^* - \rho^*) g_i^* = 0, \quad (2)$$

$$\frac{\partial \rho^* e^*}{\partial t^*} + \frac{\partial[(\rho^* e^* + p^*) u_k^*]}{\partial x_k^*} + \frac{\partial q_k^*}{\partial x_k^*} - \frac{\partial(u_j^* \tau_{jk}^*)}{\partial x_k^*} + (\rho_a^* - \rho^*) g_k^* u_k^* = 0, \quad (3)$$

$$\frac{\partial(\rho^* Y^*)}{\partial t^*} + \frac{\partial(\rho^* u_k^* Y^*)}{\partial x_k^*} - \frac{\partial}{\partial x_k^*} \left(\rho^* D_Y^* \frac{\partial Y^*}{\partial x_k^*} \right) - \omega_Y^* = 0, \quad (4)$$

$$\frac{\partial(\rho^* Z^*)}{\partial t^*} + \frac{\partial(\rho^* u_k^* Z^*)}{\partial x_k^*} - \frac{\partial}{\partial x_k^*} \left(\rho^* D_Z^* \frac{\partial Z^*}{\partial x_k^*} \right) = 0, \quad (5)$$

$$p^* = \rho^* R^* T^*. \quad (6)$$

In Eqs. (1)–(6), t stands for time, u_j is the velocity components in the x_j direction, e stands for total energy per unit mass, p stands for pressure, λ stands for heat conductivity, C_p stands for specific heat at constant pressure, μ stands for dynamic viscosity, γ is the ratio of specific heats, ω_Y is the source term of the progress variable, ρ is the density, subscript a stands for the ambient respectively. Here the superscript $*$ stands for dimensional quantities.

Viscous effects are represented by the stress tensor τ . The heat flux is given by

$$q_k^* = -\lambda^* \frac{\partial T^*}{\partial x_k^*} \quad (7)$$

In general, the transport coefficients are complicated functions of temperature and chemical composition of the mixture. In the

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