



# Impact of multi-component diffusion in turbulent combustion using direct numerical simulations



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## ABSTRACT

This paper presents the results of DNS of a partially premixed turbulent syngas/air flame at atmospheric pressure. The objective was to assess the importance and possible effects of molecular transport on flame behavior and structure. To this purpose DNS were performed at with two proprietary DNS codes and with three different molecular diffusion transport models: fully multi-component, mixture averaged, and imposing the Lewis number of all species to be unity.

Results indicate that

1. At the Reynolds numbers of the simulations ( $Re_{\text{turb}} = 600$ ,  $Re = 8000$ ) choice of molecular diffusion models affects significantly the temperature and concentration fields;
2. Assuming  $Le = 1$  for all species predicts temperatures up to 250 K higher than the physically realistic multi-component model;
3. Faster molecular transport of lighter species changes the local concentration field and affects reaction pathways and chemical kinetics.

A possible explanation for these observations is provided in terms of species diffusion velocity that is a strong function of gradients: thus, at sufficiently large Reynolds numbers, gradients and their effects tend to be large. The preliminary conclusion from these simulations seems to indicate molecular diffusion as the third important mechanism active in flames besides convective transport and kinetics. If confirmed by further DNS and measurements, molecular transport in high intensity turbulent flames will have to be realistically modeled to accurately predict emissions (gaseous and particulates) and other combustor performance metrics.

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## 1. Introduction

Commonly thought unimportant, molecular diffusion effects in turbulent flames are attracting the attention of combustion researchers. In fact, molecular transport is driven by the same collisional physics as chemical kinetics and is the last step preceding reaction, suggesting that at the scale where kinetics takes place diffusion should also have some significant role.

Measurements and simulations of turbulent flames indicate that diffusion of light species (e.g.,  $H_2$ , H, OH and  $H_2O$ ) may significantly influence species distribution and thus local temperature and emissions. That preferential (faster) diffusion of lighter species may be responsible for locally faster flame propagation was realized by Zel'dovich in his 'active centers' theory [1]. Measurements in premixed  $H_2$ /air and stratified  $CH_4$ /air flames showing effects of diffusion have been reported [2–9]. In jet- and coaxial burner flames these

effects have been reported to decrease with the distance from the fuel injector and with increasing Reynolds number. However, that molecular diffusion may be important in turbulent combustion is the conclusion in reviews of this effect [8]; Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) results cited in [10] by [11–16] suggest molecular diffusion is significant even in flames at Reynolds numbers ( $Re$ ) of order  $10^4$ .

Although many of the references cited infer or suggest preferential diffusion is present in turbulent flames, measurements in [6,7,17] and [18] were the first to purposely address this issue. They included species concentrations, equivalence ratio ( $\varphi$ ) and carbon to hydrogen (C/H) ratio in a vertical laminar  $CH_4$ /air flame, plotted vs. local temperature, and measurements of the same quantities in a turbulent bluff-body burner up to  $Re \sim 10000$ . In both flames measurements were compared to predictions obtained with detailed kinetics using the zero dimensional CHEMKIN code and for the same flame in the laminar regime. (Since CHEMKIN cannot predict spatial profiles, results were reported as a function of temperature instead of, radial or axial distance across the burner.) Just as the laminar flame results were in agreement with CHEMKIN and showed the known

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effect of preferential diffusion [19] to manifest itself in locally non conserved H atoms and C/H ratios, a similar effect was observed in the turbulent measurements; however, agreement with CHEMKIN was poor. Accordingly, the authors concluded that significant preferential diffusion was present also in the turbulent flame. Contributing to this conclusion was the observed enrichment of CO<sub>2</sub> in the bluff-body recirculation region, plausibly explained by the preferential e.g., faster, emigration of lighter species such as H<sub>2</sub>O, H<sub>2</sub> and H away from regions of high concentration, therefore modifying local  $\varphi$  and C/H ratio. The magnitude of this effect in turbulent flame was ascribed to sharper concentration gradients due to flame stretch which also increases with increasing Reynolds numbers. These measurements [7] and [17] also indicate that H<sub>2</sub> concentration and local H/C and equivalence ratios (ER) in lean and rich *premixed* methane/air atmospheric flames differ by up to 10–15% from those calculated with detailed kinetics. These results have been supported by LES calculations of equivalence ratio and C/H ratio using mixture-averaged diffusion modeling [19]. A recent summary of questions on this issue, for both premixed and non-premixed flames, is in [20].

These findings are intriguing because (i) they are observed in turbulent flames; (ii) effects are not negligible; (iii) they are observed in both experiments and DNS, and (iv) they are not only observed in hydrogen flames but also in hydrocarbon flames [8]. Molecular transport is only one of many extant questions about LES; however, the role of diffusion lends itself to be scrutinized more easily than, say, the two-way coupling between turbulence and chemical kinetics. In fact, exploring the impact of molecular diffusion matches current interest by industry and government organizations in improving the physical accuracy of LES; were the experimental results in [6,7,17] to be confirmed by DNS, it would help in convincing the combustion community of the importance of diffusion and of the need to account for it to enable predictive simulations. Moreover, the fact those spatial profiles measured in [6,17] were compared only to CHEMKIN calculations were and still is a source of skepticism. This motivated the present authors to perform full DNS of a turbulent combustion test case focusing on the impact of molecular diffusion. Accordingly, the main goal of the present investigation is to quantitatively assess the impact of molecular diffusion in turbulent flames, at Reynolds numbers not too far from those of industrial interest and by means of DNS containing different diffusion models, with a linked goal to compare them and assess their performance.

## 2. Molecular diffusion

The quantity characterizing molecular diffusion is the statistical diffusion velocity  $\mathbf{V}_i$  of the  $i$ th species.  $\mathbf{V}_i$  appears in the  $ns$  species transport Eq. (1) present in the set of reactive Navier–Stokes equations (NSE), and obtained by integrating and statistically averaging the Boltzmann equation [21].

$$\frac{DY_i}{Dt} = -\frac{1}{\rho} \nabla \cdot (\rho Y_i \mathbf{V}_i) + \frac{w_i}{\rho} \quad [i = 1, 2, \dots, ns] \quad (1)$$

Neglecting approximations like Fick's law, valid only in two-component mixtures, physically accurate  $\mathbf{V}_i$  may be obtained either from kinetic theory, or derived from non-equilibrium thermodynamics. A convenient but less accurate diffusion model is that assuming each species " $i$ " is characterized by a Lewis number  $Le_i$  constant in time and space. A brief description of  $\mathbf{V}_i$  models is presented in Appendix A.

## 3. Simulation strategy

To assess the impact of molecular diffusion in turbulent reacting flows, DNS were performed of a test case with the mixture-averaged diffusion (MAD), multi-component diffusion (MCD) and with constant Lewis number models and results were compared and analyzed.

DNS eliminates the uncertainty due to turbulence closures and models invariably present in RANS and LES. However, computational burden of DNS significantly restricts the turbulent Reynolds number,  $Re_t$ , and the scale of the test case. Ideally, both should be close to conditions representative of real combustion applications. Such flows are characterized by intense shear, mixing between air, fuel and partial reaction products, and high temperatures/pressures; all of which may impact the magnitude of molecular diffusion and mixing. DNS also limits the kinetics complexity and therefore the type of fuel that can be economically simulated. In spite of these difficulties, DNS has been performed at a moderate turbulent Reynolds number using moderately complex chemical kinetics to highlight the impact of molecular diffusion models.

### 3.1. Test case, initial conditions and kinetics model

The setup considered here is a temporally evolving jet/shear layer at atmospheric pressure (101325 Pa). The initial condition corresponds to a central rectangular syngas/air jet of height  $H = 2.56$  mm with an equivalence ratio  $\varphi$  varying from 2 in the center to 1 in the outer region and flowing from left to right (see Fig. 1b). This jet is sandwiched between two symmetrical rectangular jets formed by combustion products at  $\varphi \sim 1.0$  from a syngas/air mixture, thus creating a partially premixed flame. Note the burnt products are situated slightly outside the shear layer (separation distance =  $5.12$  mm =  $2H$ ). Inside the rich, unburnt central jet the equivalence ratio varies within the inner  $1H$  region (see Fig. 2). Figure 1 shows also the contour map of the O<sub>2</sub> mass fraction.

A freely propagating, laminar premixed flame simulation using CHEMKIN–PREMIX, at equivalence ratio 1.0 initializes the reacted jets. The temperature in the central reactant jet is set to be 900 K. Syngas ( $0.675$  H<sub>2</sub> +  $0.225$  CO +  $0.1$  N<sub>2</sub>, molar) is the fuel used in the present investigation since it can be argued that it is representative of the reactants composition following initial pyrolysis of hydrocarbon fuels; a small amount of nitrogen was added to moderate combustion temperature and its spatial gradients, and thus to limit mesh fineness. Syngas oxidation kinetics was modeled by a skeletal mechanism including 29 reactions and 12 species (H<sub>2</sub>, H, O, OH, H<sub>2</sub>O, O<sub>2</sub>, HO<sub>2</sub>, H<sub>2</sub>O<sub>2</sub>, CO, CO<sub>2</sub>, HCO and N<sub>2</sub>) [22] derived from the C1 mechanism in [23]. The first five species are the lightest and most impacted by preferential diffusion. Initial conditions for the streamwise velocity are approximated using a hyperbolic tangent profile (peak velocity 312 m/s) with turbulent fluctuations superimposed to all three velocity components corresponding to 7.5% turbulence intensity. The bulk Reynolds number based on the jet height,  $H$ , jet velocity,  $U$ , and viscosity at the initial jet temperature is  $Re_{\text{bulk}} = \rho U H / \mu = 8000$ . Based on turbulence intensity, the initial turbulent Reynolds number imposed is  $Re_{\text{Turb}} = \rho u' H / \mu = 600$  and  $Re_{\lambda} = 110$ , where  $Re_{\lambda}$  is the Taylor scale Reynolds number.

Figure 2 shows the initialized profiles on the mid-plane as a function of the transverse coordinate. It is important to notice the unique initialization used in this study since it may have some implications on the results reported later in this paper. The two premixed flames are initialized slightly outside the shear layer (flat temperature region); composition and temperature of these two flames correspond to those of a stoichiometric mixture. The equivalence ratio ( $\varphi$ ) is initialized within the inner  $1H$  region inside the unburnt portion of the flames as shown in Fig. 2 (right). Similarly, turbulent fluctuations were imposed only in the unburnt portion of the flame, to ensure that turbulence interacts with the flame only after fluctuations develop into realistic turbulence.

### 3.2. Domain, grid size and boundary conditions

The extent of the domain is  $5H$  in the streamwise ( $x$ ) direction,  $10H$  in the cross-stream/transverse ( $y$ ) direction and  $3H$  in the

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