The effects of turbulence and differential diffusion on autoignition delay time in a H2/N2 jet flame with a vitiated coflow using Linear Eddy Model

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The autoignition of a fuel jet into a hot turbulent coflow is of great theoretical and practical interest, since the influence of turbulence on ignition delay typifies the fundamental interactions among chemical reactions, molecular diffusion, and turbulent transport. The main objectives of the current work are to investigate numerically the effect of turbulent mixing and differential diffusion on ignition delay, τ_{ign}, under atmospheric pressure and elevated pressure conditions. With a homogeneous reactor model, a 'most reactive' mixture fraction, ξ_{MR}, can be determined around which a mixture is most likely to autoignite at low scalar dissipation rates. The ignition delay at ξ_{MR} provides a reference autoignition delay time, $\tau_{ign,ref}$. Previous studies have suggested two distinct regimes where turbulence may or may not impact the autoignition time by comparing $\tau_{ign,ref}$ to the turbulent time scale, τ_{lo}. When $\tau_{ign,ref} \leq \tau_{lo}$, the chemical kinetics dominates the autoignition delay time with little effects from turbulence. When $\tau_{ign,ref} > \tau_{lo}$, turbulent mixing may have a strong impact on the autoignition delay.

Previous studies have also suggested that differential diffusion can alter the calculated τ_{ign} by a factor of two or three for hydrogen combustion. Therefore equal diffusivity as well as differential diffusion calculations are performed for different turbulence Reynolds numbers, Re_t. The differences between the two transport models are observed under the influence of turbulence and they are useful for understanding the importance of differential diffusion. The 1-D Linear Eddy Model (LEM) is used to simulate the autoignition phenomenon in a vitiated coflow burner. Specifically, the LEM is used for isolating the effects of turbulence and diffusion models on chemical reactions. The molecular diffusion and the chemical reactions are solved exactly by the corresponding species and energy equations. The grid is spatially resolved below 1/6 of the Kolmogorov scale. LEM uses a 'triplet mapping' to model turbulent mixing, which is a stochastic process. The triplet mapping mimics the turbulent stirring events by rearranging the concentration field leading to stiffer concentration gradients. The molecular diffusion process is modeled by a simple transport model with unity and variable Lewis numbers as well as by a mixture-averaged multicomponent diffusion model. Both ξ_{MR} and $\tau_{ign,ref}$ are calculated with initial homogeneous mixtures based on properties of fuel and oxidizer streams. The fuel consists of 30% H_2 with 70 % N_2 by volume at 300K. The coflow is a simulated premixed flame at 1045K with associated species concentrations.

In the case of laminar diffusion processes, the LEM domain is initially described by cold fuel (ξ = 1) and hot oxidizer (ξ = 0) regions. The interface between these two regions is characterized by the mixing layer thickness, δ. The calculated effect of δ on τ_{ign} is shown in Figure 1 using both equal diffusivity and differential diffusion models. When δ is sufficiently

large such that little diffusion occurs across the layer before autoignition, both results approach the homogeneous limit, $\tau_{ign,ref}$. When δ is small, the effect of δ on τ_{ign} is different depending on the diffusion model used. With the equal diffusion model, τ_{ign}increases with decreasing δ. The opposite trend is seen when differential diffusion model is used. Most importantly, in comparison to equal diffusivity results and $\tau_{ign,ref}$, differential diffusion leads to shorter delays when the mixing layer is thin. Since turbulent stirring increases local concentration gradients by compressing local mixing layers, one expects that turbulence will shorten the ignition delay in the present coflow burner under the influence of differential diffusion.

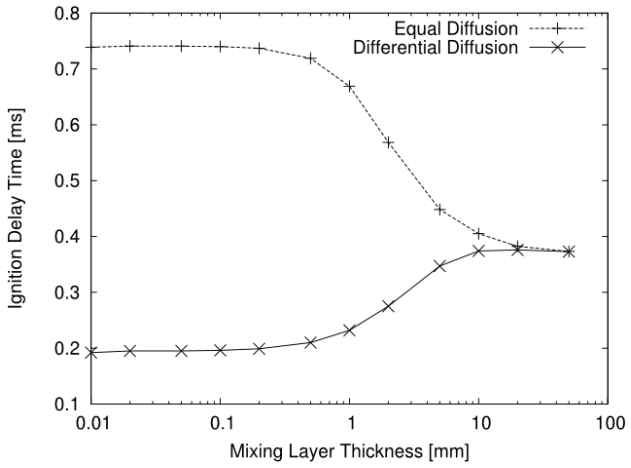

Figure 1: Laminar results demonstrating importance of mixing width on autoignition delays. Thin initial mixing layers lead to shorter delays under the influence of differential diffusion.

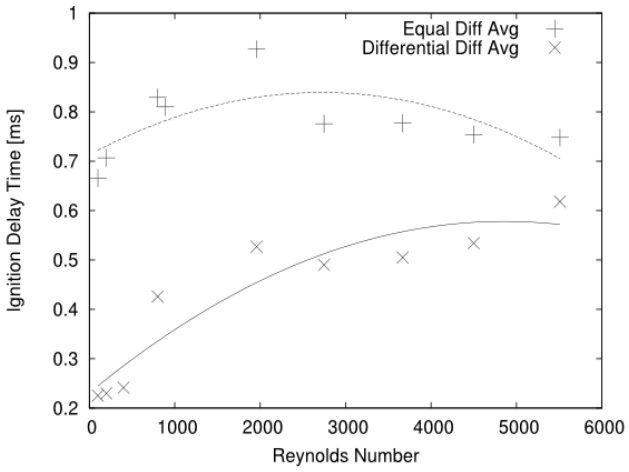

Figure 2: Turbulent results for $\tau_{ign,ref} > \tau_{lo}$ reveal faster ignition with differential diffusion.

Next, we consider the turbulence cases when $\tau_{ign,ref} > \tau_{lo}$. In the LEM simulations, the integral length scale, l_o, is kept constant, thus the turbulence time scale $\tau_{lo} = l_o / u'$ decreases with increasing Re_t. Figure 2 displays computed average values for τ_{ign} vs. Re_t at atmospheric pressure based on several runs for each Re_t due to the stochastic nature of the calculation. Both transport models show that at low Re_t, τ_{ign} asymptotes to those values presented in Figure 1. When Re_t is very high, the intense mixing causes the differences between the mixing models to diminish. Interestingly, for all simulations performed, the results with differential diffusion transport always ignite faster than those with the equal diffusivity model. This trend is consistent with the observation seen in the laminar case. The high penetration of light H_2 species into the hot oxidizer where radical production is facilitated has been identified as the main reason for reducing τ_{ign}. Preliminary results for the turbulence cases when $\tau_{ign,ref} \le \tau_{lo}$ have been obtained revealing little effect of turbulence on autoignition delay. Some simulations at high pressure have been conducted indicated strong pressure effects on τ_{ign}.