DIRECT NUMERICAL SIMULATION OF WET-CO COMBUSTION.

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Summary $CO/H_2/H_2O$-air and $CO/CH_4/H_2O$-air premixed flames were studied computationally and a skeletal mechanism suitable for dry and wet Blast Furnace Gas (BFG) combustion was derived and validated. Two-dimensional Direct Numerical Simulations (DNS) were conducted for a dry and a wet mixture using this skeletal mechanism. The two mixtures despite having approximately equal turbulence parameters, exhibit major differences in terms of the flame structure.

INTRODUCTION

The fossil fuel reserves are projected to be decreasing, and stringent emission regulations require the use of environmentally friendly fuels. Currently, the main fuel source for industrial gas turbines is natural gas when more efficient use could be made of Blast Furnace Gas (BFG). BFG is produced in large quantities in the steel industry and released into the atmosphere; instead it could be exploited as an alternative fuel for power generation. Thus, one needs to study the combustion characteristics of BFG and to validate/derive appropriate combustion models for industrial applications. The main challenge with BFG is that it has a low calorific value since the H_2 and CH_4 content is low, and the CO and CO_2 content is high [1]. Hence, BFG is mixed with other gases to improve its fuel quality. H_2O may be used for this purpose: it has long been known [2, 3, 4] that H_2O vapour addition to dry CO mixtures increases the flame speed and the heat release rate. Hence, H_2O (a relatively cheap and abundant species) may be used to improve the combustion characteristics of BFG.

The effect of H_2O in $CO/H_2, CH_4$-air mixtures

Fig.1(a) shows flame speeds of $CO/H_2/H_2O$-air mixtures for different ratios f_{H_2}=X_{H_2}/X_{CO} and H_2O% by volume. The calculations were performed using Cosilab [5] with GRI Mech 3.0 [6]. Fig.1(b) shows the results for $CO/CH_4/H_2O$-air mixtures. The composition studied is typical of BFG after CO_2 capture. It is clear that there is a non-monotonic variation of the flame speed with H_2O%. It was found that as H_2O% increases, the OH radical production rate increases with CO consumed mainly through $CO + OH <=> CO_2 + H$, consistent with [2, 3, 4]. For increasing f_{H_2} or f_{CH_4}, the positive chemical effect of H_2O is reduced and the increase in the flame speed is not as pronounced. To explain this, flame speed sensitivity analysis was conducted for both mixtures and a 38-reaction 15-species skeletal mechanism was derived to accurately predict the flame speeds. By examining the reaction rates for a dry and wet mixture this trend was explained, more details of this will be discussed in the presentation.

DNS of $CO/H_2/CH_4/H_2O/CO_2$-air mixtures.

The DNS was conducted using Senga2 [7] with the skeletal mechanism developed. A fully compressible formulation was used, with 4th order 5-step Runge Kutta scheme for time stepping and a 10th order finite difference scheme for spatial differencing. The domain size was L_x=L_y=10 mm with 520x520 grid points. The run was initialized using 1D steady-state solutions obtained using PREMIX [8]. Two cases were considered as in Table 1 with about the same turbulence attributes. The composition is typical of BFG for case A but with a smaller amount of CO_2 to reduce the computational time (typically in BFG f_{CO_2}=$X_{CO_2}/X_{CO} \simeq 1$). Case B is the same as case A but with 14% (by volume) of H_2O added. Figs. 2 and 3 show a comparison of the flame structure between the two cases in terms of the CO consumption rate at t^+=$t/(L_x/u_{in})$=1.4. By comparing Figs. 2(a) and 3(a) it is clear that in the wet case the CO consumption rate is increased and that the flame is more wrinkled and less thickened by the turbulence. By comparing Figs. 2(b) and 3(b) it is clear that the trend of the scatter plot is in better agreement with the laminar flame result (red line) for the wet case, while for the dry case the trend is worse: there are significant deviations especially in the range $0.5 \leq c=(T - T_u)/(T_b - T_u) \leq 1.0$. This implies that H_2O addition not only increases the CO consumption rate and thus the turbulent flame speed, but also produces a more flamelet-like flame. Further results will be presented during the conference.

CONCLUSIONS

$CO/H_2/H_2O$-air and $CO/CH_4/H_2O$-air premixed flames were computationally studied, and a skeletal chemical mechanism was derived for $CO/H_2/CH_4/H_2O$ mixtures. 2D DNS was performed using this skeletal mechanism for a dry and a wet mixture with composition similar to that of BFG. It is found that the wet mixture exhibits a higher CO consumption rate and a more flamelet-like behaviour. Further analysis results will be discussed at the conference.

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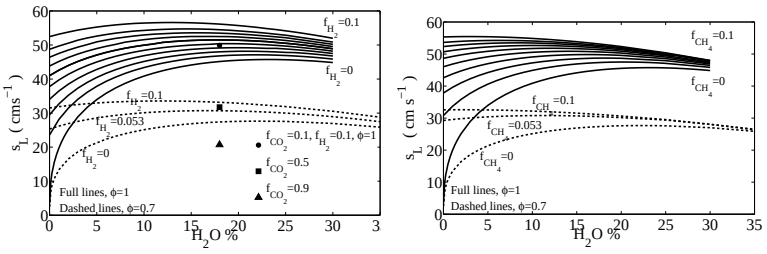
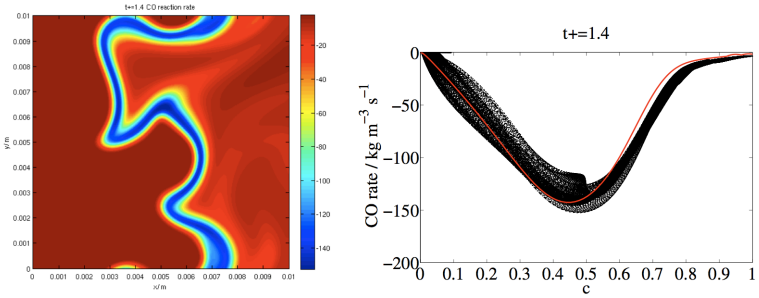
Case	ϕ	X_{H_2}/X_{CO}	X_{CH_4}/X_{CO}	X_{CO_2}/X_{CO}	$H_2O\%$	δ_{ol}	s_{ol}	u_{rms}/s_{ol}	l_{int}/δ_{ol}
A	1	0.025	0.01	0.3	0%	0.98mm	$1.84ms^{-1}$	3.85	13.18
B	1	0.025	0.01	0.3	14%	0.73mm	$2.24ms^{-1}$	3.16	15.77

Table 1: Turbulent flame parameters.



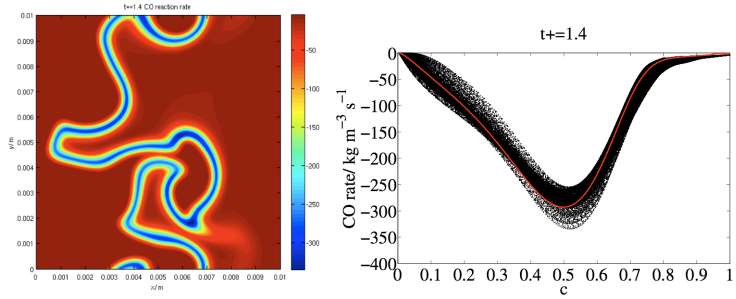
(a) (b)

Figure 1: (a) Flame speeds of $CO/H_2/H_2O$-air mixtures with T_u=323 K, p=1 atm, for ϕ=1,0.7. For $\phi = 1$, f_{H_2} steps are: 0.1, 0.083, 0.073, 0.063, 0.053, 0.043, 0.033, 0.023, 0.013, 0.0. (b) Same as (a) for $CO/CH_4/H_2O$-air mixtures.



(a) (b)

Figure 2: (a) CO consumption rate at t^+=1.4 for dry mixture. (b) Scatter plot of CO consumption rate at t^+=1.4 for dry mixture. Red line indicates unstrained flame result.



(a) (b)

Figure 3: (a) As in Fig. 2(a) for wet mixture. (b) As in Fig. 2(b) for wet mixture.

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