1B12: TABULATION OF NO_x CHEMISTRY FOR LARGE-EDDY SIMULATION OF NON-PREMIXED TURBULENT FLAMES.

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You defined the progress variable from a linear combination of major species and nitrogen oxides having distinctly different time scales. What is the motivation for combining these species into a single progress variable rather than using two variables to characterize the fast chemical reactions and slow NO_x formation separately?

In a recent work [1], in addition to a reaction progress variable defined from major species, enthalpy was used to account for heat loss effects. It was found that by accounting for radiative heat loss effects that occur on time scales comparable with NO-formation and the consideration of unsteady flamelet effects, this model [1] leads to improved predictions for the NO-formation. What is the significance of radiation in the experimental configuration you investigated, and can the over-prediction of NO predicted with your model potentially be attributed to the neglect of heat loss effects?

Reference:

[1] M. Ihme, H. Pitsch, *Phys. Fluids* 20, 055110 (2008).

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As already discussed by Nafe and Maas [1] NO_x can be accounted for without increasing the overall dimension of low-dimensional manifold tabulations (e.g. using a single progress of reaction). In particular, NO_x prompt chemistry, which is one of the objectives of this work, is coupled with hydrocarbon oxidation in the reference detailed mechanisms that has been tabulated. It is shown in the paper that the choices made allow for exactly reproducing NO_x levels (both prompt and thermal) in laminar combustion model problems, when compared with their corresponding fully detailed chemistry solutions. For NO_x slow chemistry (thermal part), the key point is to have a progress of reaction that is still evolving with NO_x in burnt gases when most of the species have reached their equilibrium. In addition, the one-to- one correspondence between progress of reaction and all tabulated species (even NO_x) was thoroughly investigated. Notice also that a separate balance equation is solved for NO_x mass fraction.

Radiative heat transfer is indeed an important aspect of SGS modeling for closed combustion chambers and furnaces. In open flames it can also play some role, usually it is less crucial even though it would be nice, indeed, to have it in the modeling loop for the flame we simulated. The quality of Large-Eddy Simulation depends on many ingredients, as the accuracy of numerics, the mesh and combustion modeling.

Unfortunately, errors sometimes compensate to bring LES results close to measurements. So far, the modeling of radiative heat loss was quite basic when introduced in LES. Hence, having better predictions after including it does not always mean that this results from an improved description of the physics and we think that it is difficult to draw definitive conclusion now. More discussions on the introduction of radiative heat transfer in LES may be found in Goncalves dos Santos et al. [2]. Fiorina et al. [2] have also completed the introduction of generic non-adiabatic flame behavior in the modeling used in the present paper, which is then ready for coupling with radiative heat transfer observed in furnaces, to complete eventual NO_x prediction with radiation.

References:

[1] Nafe, Maas, *Proc. Combust. Inst*. 29 (1) (2002) 1379–1385.
[2] Goncalves dos Santos et al., *Combust. Flame* 152 (3) (2008) 387–400.
[3] Fiorina et al., *Proc. Combust Inst*. 30 (1) (2005) 867–874.