Analysis of carbon chemistry in numerical simulations of vortex flame interaction *

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Recent progress in simulation methodologies and new, high-performance parallel architectures have made it is possible to perform detailed simulations of time-dependent multidimensional combustion phenomena using comprehensive kinetics mechanisms. However, as simulation complexity increases, it becomes more difficult to extract meaningful quantitative information about the flame from the numerical solution, particularly regarding the details of chemical processes. Consequently, there is a need to develop new diagnostic tools that can be applied to interrogate numerical simulation data to extract information about the chemical processes occuring in the flow.

In this paper we discuss the application of a new diagnostic tool for analysis of flame simulations. This methologogy is based on following specific chemical elements, e.g., carbon or nitrogen, as they move through the system. From this perspective an "atom" is a component of a molecule that is being transported through the simulation domain by advection and diffusion. Reactions cause the atom to shift from one species to another with the subsequent transport of the atom determined by the movement of the new species.

Simulation Methodology

The specific problem we consider here is the interaction of a vortex with a premixed methane flame. This problem has been considered both experimentally and computationally by a number of authors, see [1] for a discussion of the literature in this area. Our motivation in performing simulations of this type was to investigate the ability of GRI-Mech 3.0 to capture the chemical detail observed experimentally by Nguyen and Paul [2]. We consider a flat flame interacting with a vortex pair as illustrated schematically in Fig. 1. We model the system using a low Mach number approximation in an unconfined domain ignoring Dufour and Soret effect, radiation and assuming a mixture model for species diffusion. Detailed simulations of this flow were performed for a range of stoichiometries on a 1.2×4.8 cm two-dimensional domain using an adaptive

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projection methodology. See Day and Bell [3] for a detailed discussion of the low Mach number model and the computational approach.

Conventional 2-d plots of the resulting species concentrations reveals a number of interesting changes in the predicted mole fractions of several species as the vortex distorts the flame. Here we will focus on CH. The computed behavior of CH mole fraction for equivalence ratios ϕ of 0.8 and 1.2 is depicted in Fig. 2.

Diagnostic Algorithm

Our basic approach to analyzing the carbon chemistry in the flame is to track carbon atoms as they move through the system. To achieve this goal we must translate our heuristic picture of how atoms behave to a mathematical model that is consistent with the governing flow equations. Here, we sketch the basic ideas of the algorithm. The reader is referred to [4] for a more detailed discussion.

We begin with the species equations cast in Lagrangian form

$$\frac{D\,Y_k}{D\,t} = \frac{\partial Y_k}{\partial t} + u \cdot \nabla Y_k = \frac{1}{\rho} \nabla \cdot \rho D_k \nabla Y_k + \omega_k \,.$$

These equations provide a Lagrangian view of molecules of species k reacting and diffusing while being transported along particle paths. We can now interpret this equation from the perspective of atoms in the system. For an atom A that is currently part of a molecule of species k the location x_A of A can be described by the stochastic differential equation

$$dx_A = u(x_A, t)dt + dW_k(x_A, t)$$

where dW_k denotes a generalized Wiener measure that determines a suitable Brownian motion with properties chosen to represent the differential diffusion of species k. To incorporate reactions into this type of probabilistic framework we note that over a small time interval, the reaction network can be recast as a Markov process representing transitions of the atom A from one molecule to another. Combining a discrete version of the stochastic differential equation with the Markov process to represent chemical reactions defines a probabilistic algorithm for computing the tracjectory an atom A through the simulated flame along with its chemical history. To analyze a numerical simulation, we generate an ensemble of trajectories and examine their statistics.

Computational Results

To apply the stochastic particle algorithm to the analysis of carbon chemistry in vortex flame interaction, we "release" 300,000 carbon particles on the left and right sides of the flame at $t = 0$ as indicated in Fig. 1 and track their behavior using the probabilistic model described above. We select, from each group of trajectories, those that enter the flame after 7 milliseconds and within two mm of the (left or right) boundary. Tabulating the chemical transitions for particles going through the unperturbed side of the flame we obtain the reaction path diagrams shown in Fig. 3 for $\phi = 0.8$ and 1.2. We note that these reaction path diagrams are essentially identical to those obtain for the steady flat flame (computed analytically from a PREMIX solution). As expected, the reaction path diagrams show a dramatic increase in the $CH_3 \rightarrow C_2H_6$ pathway for the richer flame along with a corresponding decrease in the $CH_3 \rightarrow CH_2(S)$, $CH_3 \rightarrow CH_2O$ and $CH_3 \rightarrow CO$ pathways.

The analogous reaction path diagrams from the right side of the flame are shown in Fig. 4. For the lean flame, we actually see only minor shifts in the carbon chemistry, as expected since we see little variation in the flame structure as evidenced by the CH profiles in Fig. 2. For the rich flame we see the $CH_3 \rightarrow C_2H_6$ pathway is enhanced relative to the unperturbed flame as is the $CH_3 \rightarrow CH_3O$ pathway. While these pathways are enhanced, the $CH_3 \rightarrow CH_2(S)$ and $CH_3 \rightarrow CH_2O$ are dramatically reduced. In particular, the as the vortex interacts with the flame, the fraction of the carbon reacting along the $CH_3 \rightarrow CH_2(S)$ pathway is reduced from 18% to 10%. This reduction is enhanced along the reaction chain resulting in an almost threefold reduction in CH as the vortex stretches the flame.

This analysis represents an illustration of the application of the stochastic particle algorithm to the analysis of combustion simulations with detailed kinetics. In the presentation we will present a more detailed description of the diagnostic algorithm and additional analysis of vortex-chemistry interaction including the examination of other chemical species exhibiting interesting behavior.

References

[1] Bell, J. B., Brown, N. J., Day, M. S., Frenklach, M., Grcar, J. F., and Tonse, S. R., *Proc. Comb. Inst.*, 28:1933–1939 (2000).

[2] Nguyen, Quang-Viet and Paul, Phillip H., *Twenty-Sixth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, Pennsylvania, 1996, pp. 357–364.

[3] Day, M. S. and Bell, J. B., *Combust. Theory Modelling*, 4:535–556 (2000).

[4] Bell, J. B., Day, M. S., and Grcar, J. F., "Stochastic algorithms for the analysis of numerical flame solutions," LBNL Technical Report No. LBNL-49326.
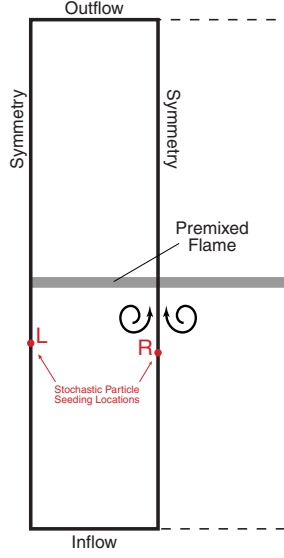
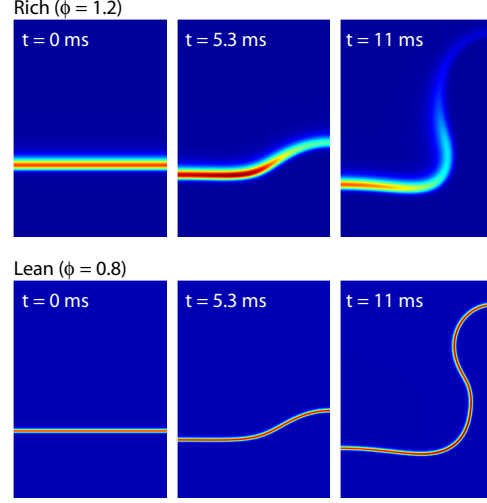Figure 1: V-flame configuration.

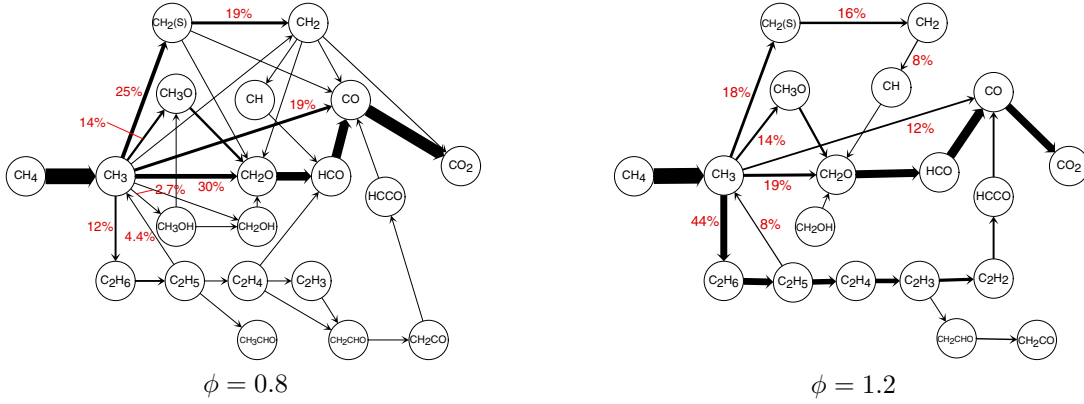Figure 2: CH mole fraction evolution for rich (top) and lean (bottom) flames.
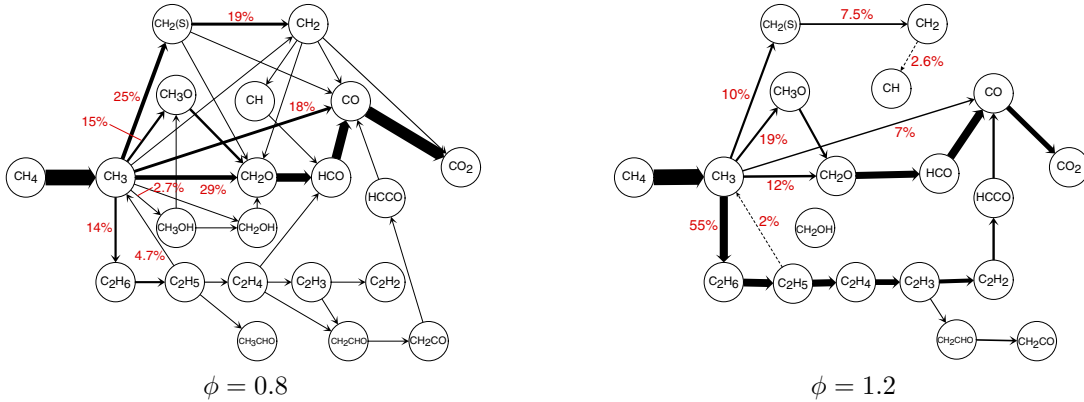

Figure 3: Reaction path diagrams for the unperturbed flame.

Figure 4: Reaction path diagrams for the strained flame.

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