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CHEMICAL MODELING FOR LARGE EDDY SIMULATION OF TURBULENT COMBUSTION

Flow Physics and Computation Group
Department of Mechanical Engineering
Stanford University
Stanford, CA 94305-3030

1 STATUS OF EFFORT

This research program consists of two major efforts: (I) the development of improved turbulence/chemistry interaction models for large eddy simulations (LES), and (II) the development of reduced kinetic mechanisms for JP-8 surrogate fuels based on a component library approach.

With regard to part I, a new numerical method for solving the level set equation to understand the effect of numerical errors was developed. This method has interesting implications for turbulent burning velocity models and can be used potentially for error estimation in LES. With regard to part II, an efficient multi-stage approach for the reduction of large kinetic mechanisms was developed and validated.

2 TECHNICAL DISCUSSION

2.1 Combustion Models for LES

In a typical LES of a premixed flame, reaction zones exist on a sub-filter length-scale. Since these zones are not resolved, they can be treated effectively as interfaces. Such an approach is taken in the G-equation model, in which a level set is used to describe these interfaces. The G-equation model was the subject of prior work performed under AFOSR funding, and was used to simulate real premixed combustion cases successfully [1]. Throughout this work, however, the effects of numerical errors on level set transport were understood poorly. Accurate numerics are important in any type of computational simulation, but they are especially so when level sets are used. The level set equation is valid only on a two-dimensional surface of a three-dimensional space. As a result, a special filtering procedure must be used when deriving a level set formulation of a filtered interface for LES. Moreover, the level set field variable away from the front must be reinitialized to a smooth function periodically, which can alter the location of the front artificially.

Some standard test-cases exist, which can be used to check the accuracy of different numerical level set schemes. These test-cases include advecting Zalesak's disk, evolving a sphere in a deformation field, and releasing a drop of water under the influence of gravity. These tests assess how well a scheme performs some specific task, such as transporting sharp corners or conserving area. The results of these tests, however, cannot be used readily to assess the accuracy in real flow fields where turbulence and front propagation may occur.

To overcome this problem, an adaptive mesh refinement technique was adopted and applied to a turbulent flame.
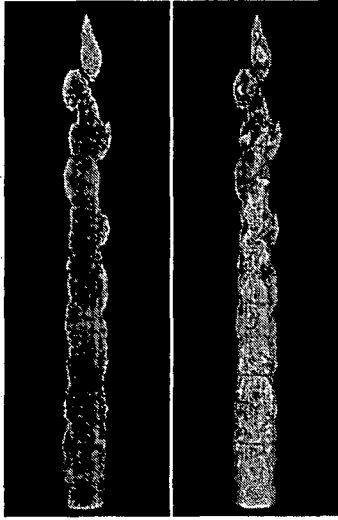
In this technique, which is called the Refined Level Set Grid (RLSG) approach, a computational mesh is created locally around the level set of interest. This mesh is created in addition to, and with more resolution than the mesh on which the flow is solved. The refined mesh adapts to the level set as it moves, and the level set is transported entirely on the refined mesh. Figure 1 demonstrates how this mesh is created around the flame front during the simulation of the F3 flame, the characterics of which were described in a previous report.

Because of the refinement, the RLSG approach effectively increases the order of accuracy of the schemes used for transport and reinitialization. Thus, the influence of numerical errors on flame location may be assessed by running with increasingly refined level set meshes. If the numerical errors that occur by solving the level set on the flow solver mesh are significant, then the more accurate, refined solutions should be different, and should also converge to the correct solution as resolution is increased.

To assess the effect of the numerical methods, the turbulent premixed F3 bunsen flame was computed using several different levels of refinement for the solution of the G-equation. For the spatial discretization, a 3rd order WENO scheme was used. The comparison of the results in Figure 2 shows that there are only minor differences between the results of the different simulations. Slight differences occur however, especially in the regions closer to the nozzle. At $x/D = 2.5$, the more refined mesh shows a wider distribution of the water profile, which is in better agreement with the experiments. This trend is to be expected, since the finer resolution should describe the turbulent motions of the front with better accuracy. Although the differences between the simulations are small, the trends also seem to indicate that the solution converges with increased refinement.

For the present example, the differences among the coarse and the fine simulations are much smaller than remaining differences of any of the simulations with experiments, which would indicate that even the coarsest resolution is appropriate. This observation, however, is not a general result. The solution depends on the numerical schemes used for the advection and reinitialization of the level set function. Further, the solution depends on the resolution of the flow solver mesh. In a turbulent combustion case, numerical errors are
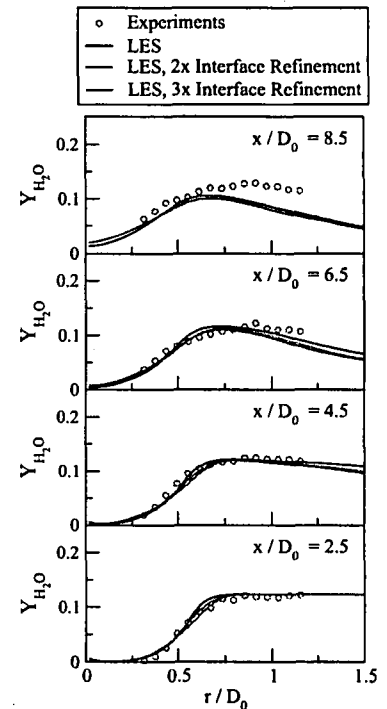

Figure 2: Water mass fraction results as a function of interface mesh refinement

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not important if the consumption of flame surface because of the numerical errors is small compared with the production of flame surface on the filter scale, which is caused by the turbulent energy transfer. Using the RLSG method, the level set equation can be solved simultaneously on two different levels of grid refinement. From this, an error can be estimated, which can be compared with the change of flame surface caused by physical phenomena. In the future, the RLSG method will be used to provide error estimates and the effect of numerical errors for test-cases that are more sensitive to the small-scale turbulent motions will be assessed. A good test-case will be a lifted turbulent jet flame.

2.2 Automatic Multi-stage Reduction of Large Chemical Kinetic Mechanisms

A new automatic multi-Stage approach for the reduction of large kinetic mechanisms was developed, that combines advantages of several techniques. The user needs to specify the detailed mechanism, some targets (e.g. ignition delay times, species profiles), an error tolerance and a domain of applicability in terms of temperatures, pressures or equivalence ratios. The first step explicitly removes negligible species and reactions through the Directed Relation Graph method with Error Propagation (DRGEP). The DRGEP method is based on path-dependent coefficients that estimate the error introduced in a target when other species are changed or removed. Although this technique is very efficient in removing minor chemical paths, resulting skeletal mechanisms are still too large for practical purposes.
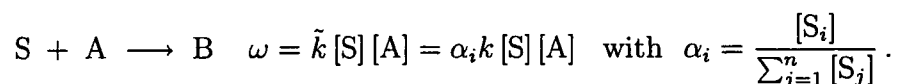
An important feature of hydrocarbon oxidation is that a large number of isomers of certain species are needed to represent oxidation correctly. A new lumping technique was designed to combine a number of isomers S_i, $i = 1..n$ into one single representative species S defined such that:

$$[S] = \sum_{i=1}^{n} [S_i].$$

where $[S_i]$ refers to the concentration of species S_i. This lumping reduces the size of the mechanism by $n - 1$ species. Each reaction involving S_i is modified to include only species S and the rate coefficients of the consumption reactions are reduced to account for the increase of the reactant's concentration (S instead of S_i).

$$S_i + A \longrightarrow B \quad \omega = k[S_i][A]$$

becomes

$$S + A \longrightarrow B \quad \omega = \tilde{k}[S][A] = \alpha_i k[S][A] \quad \text{with} \quad \alpha_i = \frac{[S_i]}{\sum_{j=1}^{n}[S_j]}.$$

This transformation is exact if α_i is a known function of time and space. Unfortunately, this function is most often unknown and a closed form has to be assumed. Here, rather than specifying α_i as a function of physical space and time, α_i will be expressed as a function of the state space

$$\alpha_i = \alpha_i\left(T, [S_j]_{j=1..N-n+1}\right),$$

where $[S_j]_{j=1..N-n+1}$ are the concentrations of all species remaining in the system. α_i can then be determined as the conditional average over all conditions used for the reduction validation. This method surely would provide quite accurate results. However, if the dependence on the entire state space is retained, the resulting mechanism cannot easily be used in standard

chemistry packages, such as the Chemkin libraries. For this reason, only the temperature dependence of α_i is considered, which, if expressed in Arrhenius form, can be absorbed into the Arrhenius parameters of the involved reactions. The basis function for representing the temperature

$$\alpha_i(T) = \beta T^\gamma e^{-\frac{\delta}{RT}} \ .$$

The various coefficients β, γ, and δ are fitted from the detailed solutions. The quality of the fit determines the quality of the lumping. Figure 3 shows an example of a fit obtained for the lumping of the $C_7H_{15}O_4$ isomers.

The last step of the reduction procedure is the introduction of quasi steady-state assumptions. The Level of Importance (LOI) criteria developed by Løvas et al. [2] was found to be an efficient way of automatically selecting species for which steady-state assumptions can be applied. Here, DRGEP coefficients for the targets, $R_{T,i}$, were used as sensitivity coefficients. The LOI index is given by

$$\mathrm{LOI}_i = -R_{T,i}c_i \left[\frac{\partial \omega_i}{\partial c_i}\right]^{-1}$$

where c_i is the concentration and ω_i is the production rate of species S_i.

This combined reduction procedure was applied to the LLNL mechanism for n-heptane autoignition and oxidation. The mechanism was reduced from 558 species to only 58 species and 36 steady-state species, while the error introduced on the targets had a maximum value of 25% around the NTC region and an average value of less than 14%. Ignition delay times for stoichiometric mixtures of n-heptane and air are shown in Figure 4 for different pressures. It is obvious that the error introduced by the mechanism reduction is much smaller than the error of the original mechanism compared with experimental data.
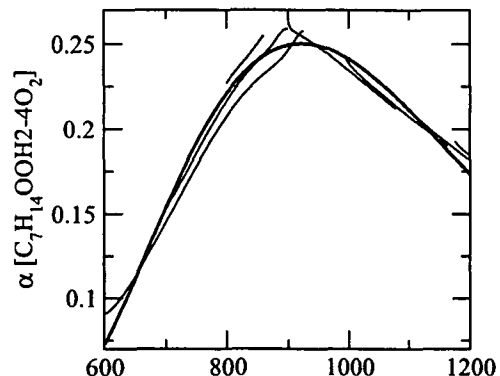

Figure 3: α_i for one $C_7H_{15}O_4$ isomer plotted as function of the temperature. Comparison between exact (thin lines) and fitting (bold line) functions.
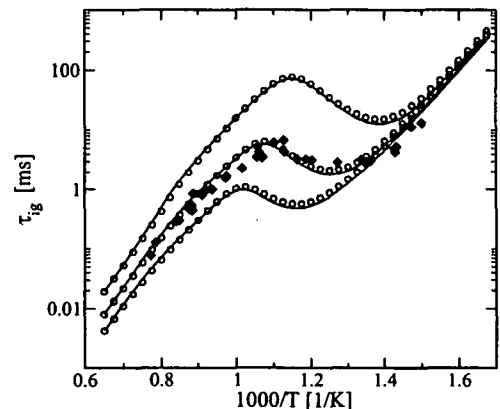

Figure 4: Ignition delay times for a stoichiometric mixture of n-heptane and air at $p = 3.2$, 13 and 42 bar. Comparison between experiments (filled symbols), detailed (solid line) and 58 species reduced (symbols) mechanisms.

References

[1] H. Pitsch and L. Duchamp de Lageneste. Large-eddy simulation of premixed turbulent combustion using a level-set approach. *Proc. Combust. Inst.*, 29:2001–2008, 2002.

[2] T. Lovas, P. Amneus, F. Mauss, and E. Mastorakos. Comparison of automatic reduction procedures for ignition chemistry. *Proc. Combust. Inst.*, 29:1387–1393, 2002.