

## SUPERSONIC COMBUSTION SIMULATIONS USING REDUCED CHEMICAL KINETIC MECHANISMS AND ISAT

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### ABSTRACT

Reduced chemical kinetic mechanisms for hydrogen and ethylene combustion, created using the CARM (Computer Aided Reduction Method) software have been implemented into the Vulcan CFD code and used for simulations of a supersonic jet flame. CFD simulations using reduced chemical kinetic mechanisms for hydrogen/air combustion show better agreement with detailed chemistry simulations and with experiments than existing models using the same number of species, indicating the importance of kinetic effects retained by the CARM-produced model. The CPU cost of using the CARM-produced models directly prompted the use of an *In Situ* Adaptive Tabulation (ISAT) algorithm. For a 20-species ethylene mechanism, the total CPU cost was cut by a factor of 42. Using ISAT, CFD simulations using a reduced mechanism for supersonic ethylene combustion demonstrate the ability of reduced mechanisms to implement realistic hydrocarbon combustion chemistry models into CFD.

### INTRODUCTION

Accurate CFD simulation of ignition, flame stabilization, combustion efficiency, and pollutant formation requires that significant chemical kinetic detail be retained in reacting flow models. Detailed chemical kinetic descriptions of large hydrocarbon combustion require the tracking of hundreds of chemical species and thousands of reaction steps. For the foreseeable future, CPU time and computer memory limitations will prohibit implementation of fully detailed descriptions of combustion chemistry into CFD simulations of practical devices. Within CFD simulations, memory use and CPU time increase

with the number of chemical species tracked. Methods that minimize this number while retaining essential features of the detailed chemistry are thus of great importance. Reduced chemical kinetic mechanisms that can represent important aspects of detailed chemistry using few enough scalars that they can be implemented into CFD simulations offer large potential improvement in the modeling of aviation combustors.

In this paper we report implementation of reduced mechanisms for hydrogen and ethylene into simulations of supersonic combustion. Reduced mechanisms for hydrogen and ethylene, combustion have been created and tested against measurements and detailed chemistry. These reduced mechanisms have been implemented into Vulcan<sup>1</sup>, a specialized CFD code for analysis of high-speed turbulent reacting flows, and used for simulating supersonic combustion.

In this work we have used the CARM (Computer Assisted Reduction Method)<sup>2</sup>, software that automates the reduction procedure, allowing large, detailed mechanisms to be reduced quickly. CARM reduces mechanisms by employing quasi-steady-state (QSS) assumptions for a number of species from the detailed mechanism.

The CARM-produced reduced mechanism may, however, require a great deal of CPU time to perform the iterative calculations for the QSS species concentrations. Very significant CPU time can be saved by speeding up the evaluation of the chemical source terms. In this study, an *In Situ* Adaptive Tabulation (ISAT) algorithm<sup>3,4</sup> was applied to reduce the cost of the reduced mechanisms. ISAT is based on the observation that the accessed region of the composition space, defined as the set of all compositions occurring during a calculation, is much smaller than the realizable region. It is sufficient to tabulate only the accessed region, rather than the whole realizable region. The table is built up during the reactive flow calculation, which is referred as *in situ* tabulation.

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When first introduced, ISAT was used to tabulate the species concentrations after integration over a certain time step. In our implementation, the species reaction rate source terms are tabulated directly. The ISAT subroutine receives an inquiry vector (concentrations of species, temperature, and pressure), uses an error criterion to determine whether to perform a direct calculation of the chemical source terms, or to interpolate from the table, then returns the reaction rates vector as well as the Jacobian matrix of the chemical source terms. A binary tree is used to store the table entries, providing a fast search for a close entry to the inquiry vector.

## RESULTS AND DISCUSSION

### Automated Mechanism Reduction

Formulation of a reduced chemical kinetic mechanism requires four basic steps: 1) Identification of the appropriate detailed mechanism containing the essential species and elementary reaction steps, 2) Identification of appropriate QSS approximations, 3) Elimination of reactions through use of the algebraic relations obtained in step 2, and 4) Solution of the coupled and nonlinear set of algebraic equations obtained in the previous steps to find the QSS species concentrations and reaction rates of the remaining species. CARM automates steps 2-4, producing source code for the calculation of the chemical source terms defined by the reduced mechanism. The subroutine produced by CARM contains code that iteratively solves the coupled, nonlinear set of algebraic equations giving the concentrations of the QSS species. These concentrations are used along with the rates of the elementary reactions from the detailed mechanism to calculate the chemical source terms for the non-QSS species.

### Reduced Mechanism for Hydrogen-Air Combustion

Using the automatic mechanism reduction software CARM, a reduced mechanism designed to model hydrogen combustion was created. The reduced mechanism is based on  $H_2$ - $O_2$  reactions extracted from a large hydrocarbon mechanism<sup>5</sup>. The reduced mechanism reduces the number of species from nine in the detailed mechanism to seven, by assuming that OH and  $H_2O_2$ , are in QSS. This reduced mechanism has been tested against detailed chemistry in constant pressure ignition delay calculations conditions of interest. The 7-species reduced mechanism shows excellent agreement with detailed chemistry and was selected for initial implementation into Vulcan. Reduction from nine to seven species is not a large reduction, but allows the Vulcan implementation to be

tested on a relatively simple case for which experimental data exists.

### Reduced Mechanisms for Ethylene-Air Combustion

Increasing in complexity beyond hydrogen, we turn to ethylene ( $C_2H_4$ ), a small hydrocarbon which has been used previously in combustor simulations as a scramjet fuel<sup>6</sup>.

Calculations were performed to compare the ability of two detailed chemical kinetic mechanisms<sup>7,8</sup> to compute ignition delay of ethylene-oxygen mixtures as compared to experiments<sup>9,10</sup>. Three of the cases measured by Baker & Skinner<sup>9</sup> were modeled. The initial pressure in all of these cases was 3 atm. The gas mixture for these cases consisted of 1% (by moles) ethylene with 3, 1.5, or 6%  $O_2$  and the balance argon. These cases correspond to equivalence ratios of 1.0, 2.0, and 0.5, respectively. Baker & Skinner<sup>9</sup> report only Arrhenius-form expressions fit to their data so individual data points can't be plotted. Figure 1 compares Baker & Skinner's measurements with calculations using the two detailed mechanisms and a 20-species reduced mechanism. Three cases measured by Colket et al.<sup>10</sup> were also compared to predictions of the detailed chemical kinetic mechanisms (not shown). These measurements have 0.7% ethylene with  $O_2$  mole fractions of 4.2%, 2.8%, and 2.1% with the balance argon. This gives equivalence ratios of 0.5, 0.75, and 1.0, respectively. The initial pressures range from 5.27-7.89 atm.

Both detailed mechanisms give reasonable agreement to the measurements. However, the Wang et al. mechanism<sup>7</sup> is noticeably superior for all of the measurements simulated. The Wang et al. mechanism also has the advantage of containing fewer species: 75 species and 529 reactions vs. 155 species and 689 reactions in the Marinov et al. mechanism<sup>8</sup>. Fewer species and reactions mean that the reduced mechanism is likely to exhibit better numerical behavior and agreement with the detailed mechanism using fewer non-QSS species.

Based on the results of the ethylene detailed mechanism comparisons, reduced mechanisms were created and tested based on the Wang et al. mechanism<sup>12</sup>. A reduced mechanism with 20 species (cf. 75 in the detailed mechanism) gives excellent agreement with detailed chemistry and experimental results (see Figure 1). A 15-species reduced mechanism did not perform satisfactorily. The 20-species reduced mechanism has been implemented into Vulcan to further evaluate the numerical accuracy and robustness of the implementation.

The non-QSS species in this mechanism are H<sub>2</sub>, H, O, O<sub>2</sub>, OH, H<sub>2</sub>O, HO<sub>2</sub>, CH<sub>3</sub>, CH<sub>4</sub>, CO, CO<sub>2</sub>, HCO, CH<sub>2</sub>O, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>3</sub>, C<sub>2</sub>H<sub>4</sub>, HCCO, CH<sub>2</sub>CO, CH<sub>3</sub>CHO, and N<sub>2</sub>. This new reduced mechanism is an improvement on previously published reduced mechanisms for ethylene combustion<sup>11</sup>.

#### Implementation of QSS Reduced Mechanisms

The main modification needed for use of CARM-produced reduced mechanisms in Vulcan was the addition of a numerical Jacobian matrix capability. This was necessary to allow Vulcan to use the non-analytical form chemical source terms from the reduced mechanism subroutines. CARM produces a FORTRAN subroutine that iteratively calculates chemical source terms for a given set of conditions, rather than Arrhenius rate coefficients. The numerical Jacobian routine has been implemented into Vulcan including both the species and temperature derivative contributions. The reduced mechanisms for hydrogen, and ethylene oxidation created by CARM have been implemented into Vulcan and tested for numerical accuracy and robustness. As a first case, the seven species hydrogen-air model was tested. High-speed diffusion flame cases have been run with the reduced mechanisms for hydrogen and ethylene combustion using Vulcan.

#### In Situ Adaptive Tabulation (ISAT)

The ISAT algorithm<sup>3,4</sup> builds a table of chemical source terms as the calculation proceeds. On receipt of a query, the ISAT subroutine checks first if the query conditions lie within the ellipsoid of accuracy of an existing table entry. If not, a new entry is generated containing the chemical source terms for the current composition and temperature. The Jacobian matrix of the source terms is also stored for use in future interpolations. A cutting plane is generated to divide the composition space into two parts. In our implementation, the cutting plane is defined as the plane perpendicular to the vector connecting the new entry with the existing nearby table point for which the accuracy was insufficient.

The implicit solution method used in Vulcan requires the evaluation of the Jacobian matrix of the chemical source term, which has been stored in the ISAT table. Significant CPU time is saved when the ISAT subroutine returns not only the reaction rate vector, but the Jacobian matrix. The only additional cost introduced by ISAT is that of traversing the binary tree data structure to find an entry close to the inquiry vector. The cost of this operation is very small compared to direct evaluation of the reaction rates and associated Jacobian matrix. An existing ISAT table can

be used for a new case with the same chemistry but different boundary conditions.

The memory,  $M$ , occupied by the ISAT table can be estimated as  $M = 8N(n^2 + 6n + 14)$  bytes, where  $n$  is the number of species, and  $N$  is number of table entries. For a 20-species mechanism and a table size of 50,000, the memory occupied by the table is about 214MB. In the Vulcan simulations, we found that the ISAT table size increases rapidly in the early stages of the simulation due to the fast changes in species concentrations and temperature. Many of these early table entries are rarely used in the later time steps. A tree-trimming method was developed to control the table size. An upper limit is set for the size of binary tree. Once the limit is reached, table entries that have not been accessed during the most recent few time steps are removed from the table.

#### Supersonic Reacting Test Case

The case considered is the coaxial jet flow experiment conducted by Evans et al.<sup>12</sup>. The experiment consisted of coaxial injection of a cold, Mach 2, hydrogen jet at matched pressure into a hot, Mach 1.9, vitiated air stream. Figure 2 is a schematic of this experiment. The fuel nozzle was conical with a five degree exit half-angle. The computational domain extended seven jet diameters ( $d = 0.009525$  m) upstream of the nozzle exit to capture the flow angularity at the inner nozzle exit and to include a boundary layer in the exit profiles. Modeling the flow upstream of the jet exit was found to yield better agreement with the experimental data. The computational domain also extended 30 diameters downstream of the nozzle exit and two diameters in the transverse direction. The modeled flow conditions are given in Table 1. The computational grid downstream of the nozzle exit plane that was used for the majority of the calculations was discretized with 120 and 68 cells in the streamwise and transverse directions, respectively. Calculations were performed with grids containing 240×136 and 60×34 cells to assess grid sensitivity in the results. Complete grid independence was not obtained, but differences between the solutions on the medium and fine grids were minor. The results shown in the succeeding figures were obtained on the medium grid (120×68).

**Table 1. Conditions for supersonic jet flame simulations.**

Specified condition	Fuel jet	Outer jet
Mach number	---	1.9
Temperature (K)	---	1495
Pressure, $p$ (bar)	---	1.0
Total temperature (K)	452	---
Total pressure (bar)	8.6068	---
O <sub>2</sub> mass frac.	0.0	0.241
N <sub>2</sub> mass frac.	0.0	0.478
H <sub>2</sub> O mass frac.	0.0	0.281
Fuel mass frac.	1.0	0.0

Turbulence was modeled with the Menter BSL (Baseline) two-equation turbulence model<sup>13</sup>. The Menter BSL model couples the standard forms of the  $k$ - $\omega$  and  $k$ - $\epsilon$  models. The BSL model invokes the  $k$ - $\omega$  model near solid surfaces and smoothly transitions to the  $k$ - $\epsilon$  model in the outer portion of the boundary layer and in regions of free shear. At solid surfaces, the wall matching procedure of Wilcox<sup>14</sup> was employed. Also, the compressibility correction of Wilcox<sup>15</sup> was used to model the reduction in mixing associated with high convective Mach numbers.

Solutions were obtained in three steps. First, flow upstream of the jet nozzle exit plane was calculated. The resulting solution was used as the inflow boundary condition for the flow calculation downstream of nozzle exit plane. A no-slip, adiabatic boundary condition was applied at the injector lip, a symmetry boundary condition was applied along the centerline and zeroth order extrapolation was used at the outflow boundary and at the upper domain boundary. Secondly, the coaxial jet flow field calculation was advanced with reactions disabled. Finally, the calculation was continued with the reactions enabled. Comparable convergence was observed with the CARM-produced reduced kinetics models as with Arrhenius-form finite rate models.

#### Supersonic Hydrogen Flame Simulations

Solutions were obtained for both reduced and detailed H<sub>2</sub>-air kinetics models. The detailed model used in Vulcan is a subset of the GRI-Mech3.0 mechanism<sup>16</sup>. The mechanism included the nine species H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, OH, O, H, HO<sub>2</sub>, H<sub>2</sub>O<sub>2</sub> and N<sub>2</sub>. All of the reactions involving these species were included except one, which was omitted because pressure-dependent reactions are currently not supported by Vulcan. The resulting mechanism had 27 reactions.

Two reduced kinetic mechanisms were employed. The first is the CARM-produced reduced kinetic

mechanism using the seven species H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, O, H, HO<sub>2</sub> and N<sub>2</sub>. The second is a reduced model obtained by eliminating HO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> from the mechanism of Jachimowski<sup>17</sup>, which yields a 7-step, 7-species Arrhenius-form global mechanism which we refer to in the following as the 7×7 mechanism.

Contours of the Mach number, temperature, fuel-air equivalence ratio, and the ratio of turbulent-to-laminar viscosity from the solution with the CARM 7-species reduced model are shown in Fig. 3. The hydrogen jet expanded from sonic conditions to a nominal Mach number of 2.0 at the nozzle exit. Further expansion elevated the Mach number to a maximum of 2.72. The hydrogen jet turned back toward the centerline at  $x/D \sim 1.0$ , recompressing the jet. The wake behind the lip generated a mixing layer between the hydrogen jet and the vitiated airstream. The minimum Mach number at the exit of the domain ( $x/D = 30$ ) was 1.26. The wake also generated relatively high levels of turbulent kinetic energy, and thus, high eddy viscosity values, which were convected downstream. The fuel-air equivalence ratios indicate a thin surface of approximately stoichiometric proportions along the outer edge of the shear layer that formed between the two streams. Ignition was observed at  $x/D \sim 2$ . The flame occurred at the stoichiometric surface. Contours of the O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub> mass fractions from the same solution are shown in Fig. 4.

Oxygen penetrated into the fuel-rich region upstream of the flame surface. This oxygen diffuses and reacts. Downstream of ignition, little oxygen penetrated through the flame zone. N<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub> diffuse in the region below the flame surface. Contours of H<sub>2</sub>O reveal that little diffusion occurs above the shear layer due to low values of turbulent viscosity at the outer edge of the shear layer.

Profiles of the mass fraction of the major species O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub> are compared for the solutions with three kinetics models and the experimental data in Fig. 5. Experimental data for other species and for the temperature were not available. As reflected in the N<sub>2</sub> profiles, near the centerline, the shear layer mixing is slightly underpredicted at the first measurement station but predicted well at the succeeding three stations. However, the extent of mixing near the edge of the shear layer ( $x/d \sim 0.7$ ) is greater in the calculations than in the experimental data. The measured values for O<sub>2</sub> and H<sub>2</sub>O in the vitiated stream ( $x/d > 1.2$ ) are observed to deviate from their nominal values. As seen in Fig. 4, oxygen penetrated into the fuel rich region and positive values of oxygen mass

fraction are predicted below the flame at  $x/d = 8.26$ . Each of the kinetics models predicted more oxygen than was observed in the measurements with the CARM reduced model predicting the least oxygen and the 7×7 model the most. Both the CARM reduced mechanism and the GRI-Mech 3.0 model predicted negligible  $O_2$  at the last three stations in accord with the measurements, while the 7×7 model predicted significant levels of  $O_2$ . This demonstrates the presence of kinetic effects retained in the CARM model and detailed chemistry, but absent from the 7×7 mechanism.

### Supersonic Ethylene Flame Simulations

Calculations using the same geometry and boundary conditions were repeated with ethylene ( $C_2H_4$ ) as the fuel using the 20-species reduced mechanism described previously. The total pressure and temperature of the  $C_2H_4$  jet were the same as for the  $H_2$  jet to again produce matched pressure conditions. No numerical stability problems were encountered. Shown in Fig. 6 are contours of the temperature and the mass fractions of  $O_2$ ,  $N_2$ ,  $CO_2$  and  $C_2H_4$ . The standoff flame distance has increased from  $x/d \sim 2.0$  to  $x/d \sim 17.0$ . The calculation demonstrates the capability for modeling high speed combustion problems using hydrocarbon fuels with CARM-produced kinetic mechanisms in a state-of-the-art CFD solver. Unfortunately, very little experimental data is available for supersonic hydrocarbon flames.

The error tolerance for ISAT for both cases was set to 0.02, with a maximum table size of 50,000 entries. After several hundred iterations, the table size stabilized at around 30,000. The number of new entries added to the table at each time step is less than 10. The average CPU time per time step for the mechanism is listed in Table 2. For the hydrogen flame, the CPU cost of the reacting flow simulation with directly evaluated reaction rates was only 1.8 times that of the nonreacting case. Still, a speed-up factor of 1.34 was achieved with ISAT. For the ethylene flame case, the CPU cost of the reacting flow simulation without ISAT is about 82 times that of nonreacting flow. Numerically evaluating the reaction rate Jacobian matrix is extremely expensive for the CARM-produced reduced mechanisms. More than 98% of total CPU time was consumed by the reduced mechanism subroutine. Using ISAT, the total CPU time was cut by a factor of 42, making the reacting flow comparable in CPU time to the nonreacting flow simulation.

**Table 2. Average CPU time for a single time step for the jet flame simulations.**

Mechanism	7-spe. $H_2$	20-spe. $C_2H_4$
CPU, nonreacting	0.35 sec.	0.93 sec.
CPU, reacting, direct	0.63 sec.	76.4 sec.
CPU, reacting, ISAT	0.47 sec.	1.8 sec.
ISAT speed-up factor	1.34	42.4

Calculations of the Evans et al.<sup>12</sup> diffusion flame case have been repeated for comparison to other ethylene kinetic models. A solution was obtained with a 6-species, 3-reaction ethylene mechanism which has been used previously in scramjet combustor simulations<sup>6</sup>. This model represents the computational effort that is available for 3D scramjet simulations. The CPU time compared to the 20-species ethylene reduced kinetics model with and without the use of ISAT is shown in Table 3. The timings were obtained on a single Compaq SC-45 processor for each of the three calculations. The benefits of using ISAT are apparent.

**Table 3. CPU times for calculations performed on one processor.**

Mechanism	Sec. per iteration
$C_2H_4$ (6×3)	0.54
$C_2H_4$ (reduced 20 spe.)	76.4
$C_2H_4$ (red. 20 spe.) +ISAT	1.8

### Parallelization

Further calculations were performed using the 20-species  $C_2H_4$  reduced mechanism and ISAT, but using multiple processors on a Compaq SC-45. The results of the timings are shown in Table 4. The relatively poor speedup is due to the small grid employed (121×69) and the consequent large relative ratio of communication to computation, which increases as the number of processors increases.

**Table 4. CPU times for 2-D ethylene jet flame calculations (with ISAT) on multiple processors.**

Processors	Sec. per iteration	Speedup
1	1.8	---
2	1.1	1.6
4	0.7	2.6
8	0.5	3.5
12	0.5	3.6
24	0.8	2.3

No convergence problems were encountered using multiple processors. However, discrepancies were initially observed among solutions obtained using different numbers of processors. The calculation was repeated with four processors and with the ISAT error tolerance tightened from 0.05 to 0.01. The solution with the tighter error tolerance became indistinguishable from the solution obtained without ISAT.

We believe that the solution differences seen using ISAT and multiple processors are due to the fact that a separate ISAT table is generated for each processor. Differences among the tables will require a tighter overall tolerance on the ISAT interpolation to achieve the same results. Reducing the error tolerance caused the CPU time to increase from 0.7 seconds/iteration to 1.2 seconds/iteration.

Finally, a three-dimensional grid was used to further evaluate the parallel speedup of the ISAT routine. The 3D grid was derived from the axisymmetric grid by sweeping 180 degrees in 36 intervals, resulting in a 121×69×37 grid. The CPU timings for the ISAT routine on the three-dimensional grid are given in Table 5. Note that for the parallel computations both the axisymmetric and three-dimensional grids were split in the axial direction.

**Table 5. CPU times for calculations performed on multiple processors using a three-dimensional grid.**

Processors	Sec. per iteration	Speedup
1	73.6	---
2	41.1	1.8
4	25.1	2.9
8	16.2	4.5
12	11.3	6.5
24	8.63	8.5

### CONCLUSIONS

Reduced chemical kinetic mechanisms for hydrogen and ethylene combustion have been created using the CARM (Computer Aided Reduction Method) software. These reduced mechanisms were tested against measurements and detailed chemistry and found to give good agreement. The reduced mechanisms have been implemented into the Vulcan CFD code and used for simulations of a supersonic jet flame. CFD simulations using reduced chemical kinetic mechanisms for hydrogen/air combustion show better agreement with detailed chemistry simulations and with experiments than existing models using the

same number of species, indicating the importance of kinetic effects retained by the CARM-produced reduced mechanism. High speed CFD simulations using a reduced mechanism for ethylene/air combustion demonstrate the ability of reduced mechanisms to implement realistic hydrocarbon chemistry models into CFD.

The ISAT tabulation method was successfully implemented to reduce the CPU cost associated with CARM-created reduced mechanisms. The speed-up factor of the simulation of a supersonic ethylene jet flame was approximately 26. The reuse of the Jacobian matrix evaluated in the ISAT table greatly improved the efficiency. The CPU time of a reacting flow simulation with ISAT is comparable with the nonreacting flow simulation. These techniques have been demonstrated using multiple processors.

### FUTURE WORK

Future work will include extension to realistic 3D scramjet combustor geometries, and CFD implementation of reduced mechanisms for larger hydrocarbon fuels, such as *n*-heptane reduced mechanisms based on the mechanism of Held et al.<sup>18</sup> and JP-8 surrogates, using existing<sup>19</sup> or new reduced mechanisms based on detailed mechanisms such as those by Mawid et al.<sup>20</sup> or Violi et al.<sup>21</sup>.

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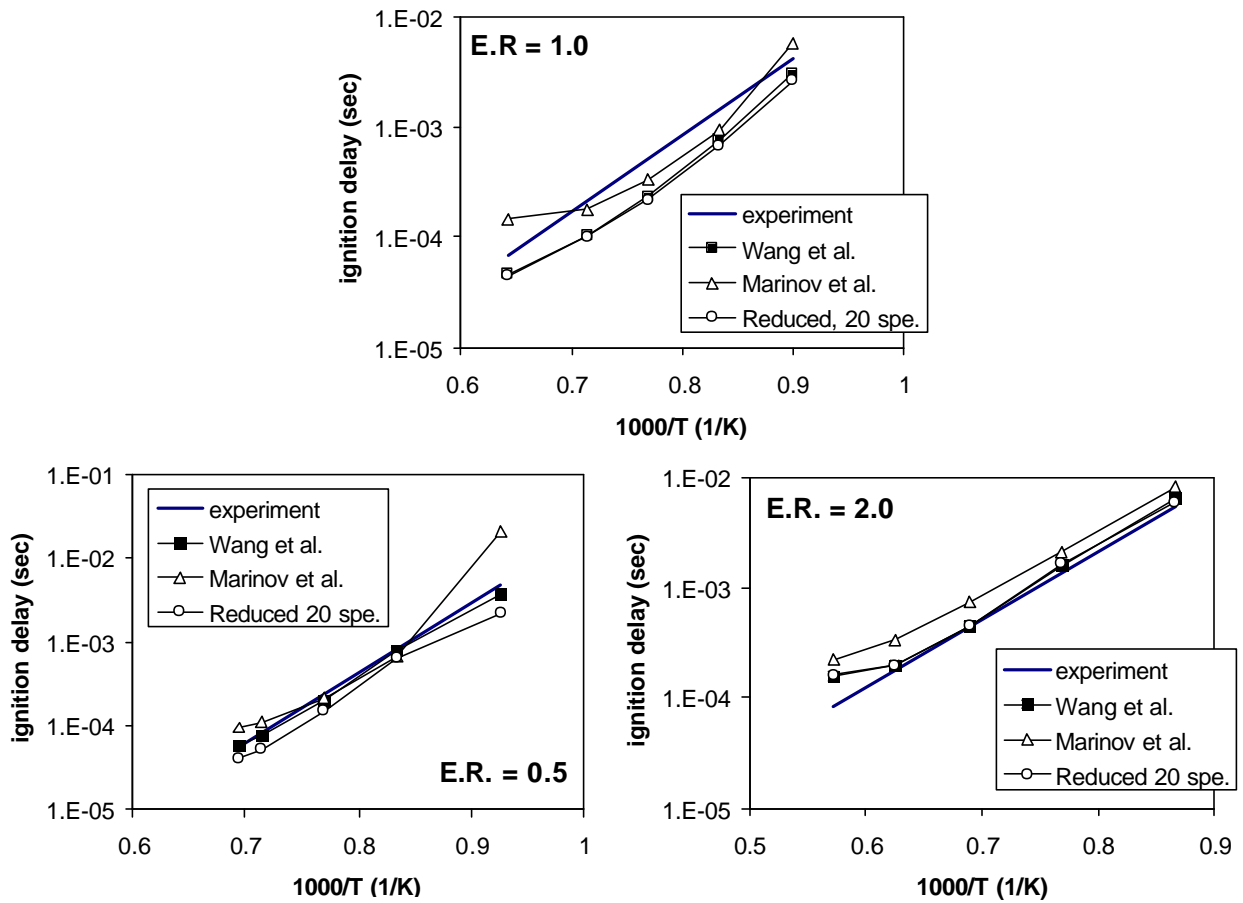


Figure 1. Comparison of ignition delay as a function of temperature for experiments<sup>9</sup>, detailed chemistry<sup>7,8</sup> and the reduced mechanism for ethylene-air mixtures at equivalence ratios of 0.5, 1.0, and 2.0.

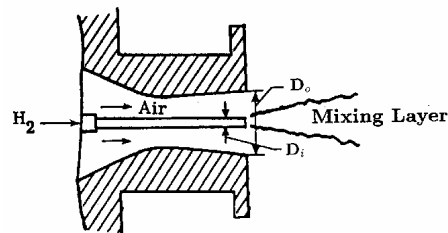


Figure 2. Schematic of the supersonic diffusion flame experiment of Evans et al.<sup>12</sup>.

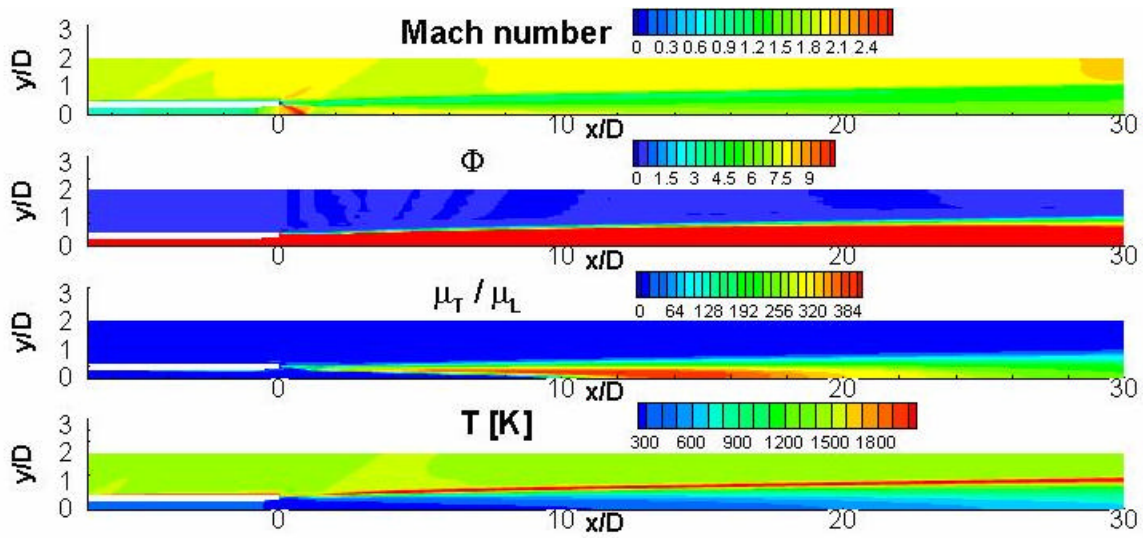


Figure 3. Contours of Mach number, fuel-air equivalence ratio, ratio of turbulent to laminar viscosity and temperature for the solution obtained with the CARM 7-species reduced chemical kinetic mechanism.

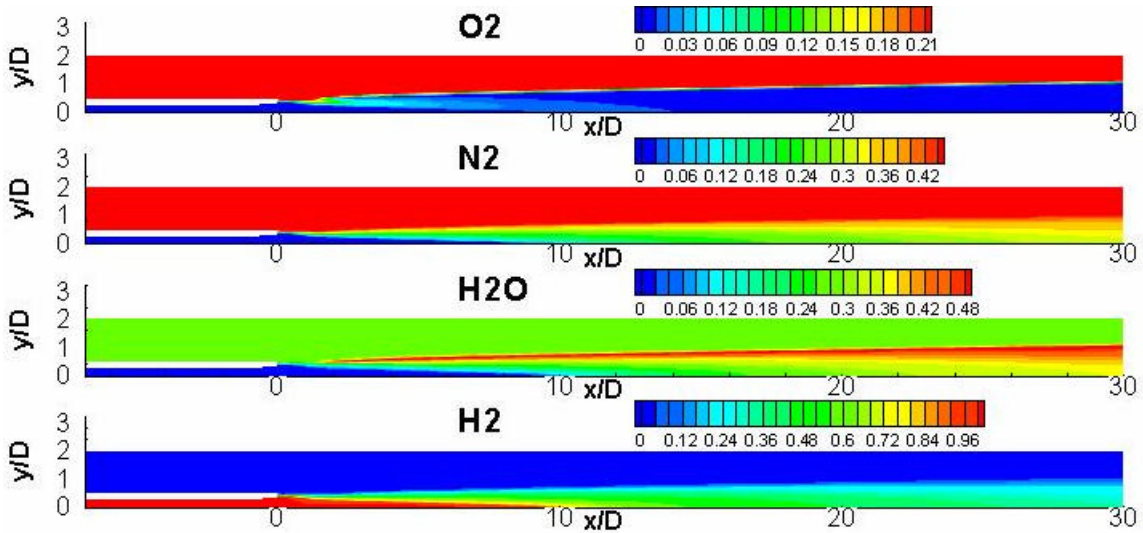


Figure 4. Contours of mass fraction of O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub> for the solution obtained with the CARM 7-species reduced chemical kinetic mechanism.

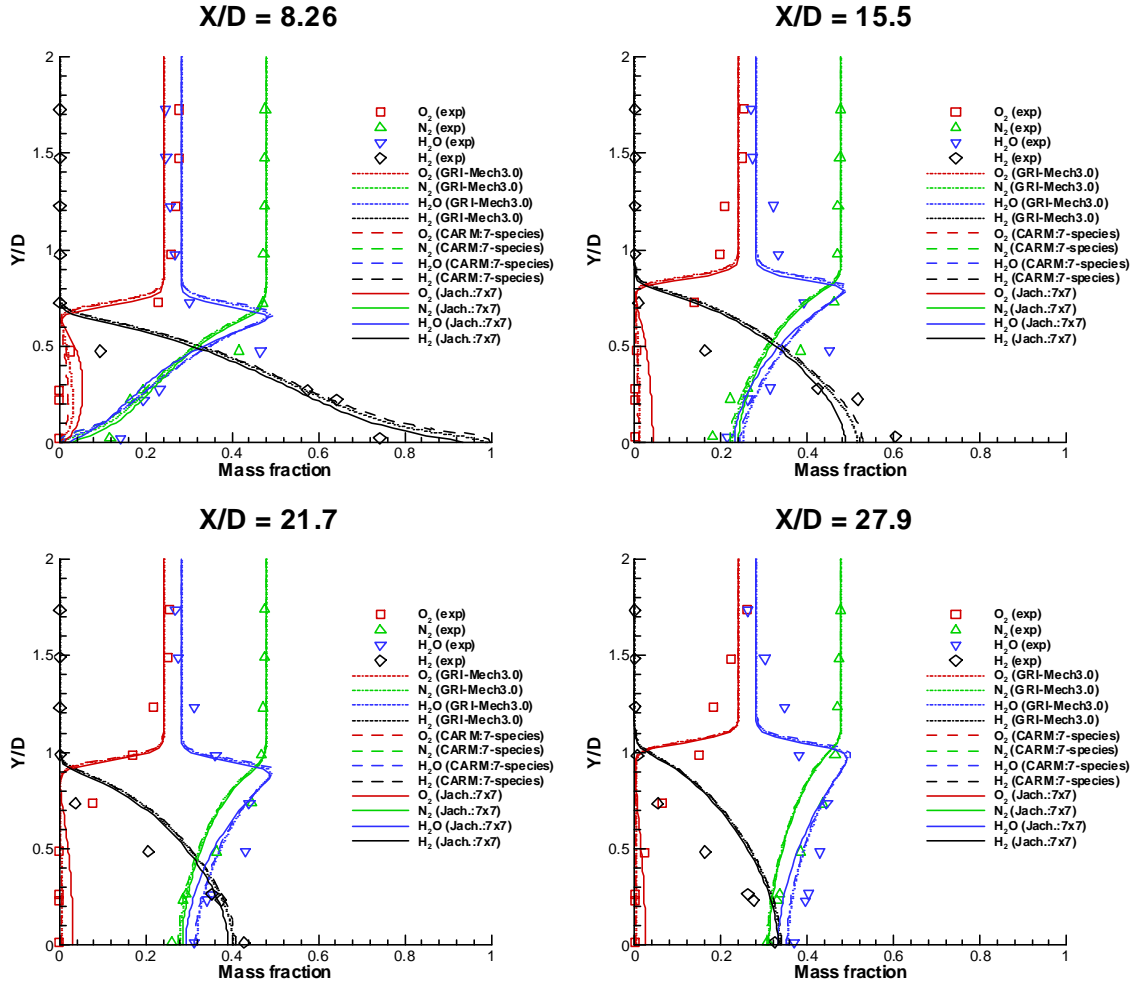
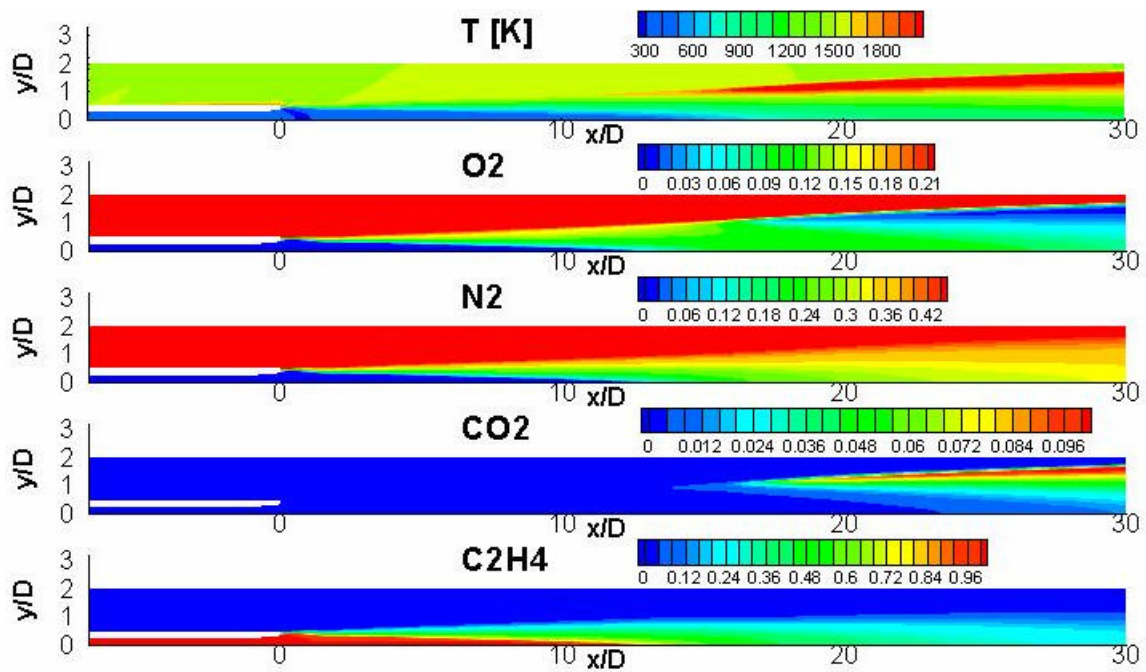


Figure 5. Comparison of species profiles between calculation and experiment.



**Figure 6. Contours of temperature and mass fraction of O<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub> and C<sub>2</sub>H<sub>4</sub> for the solution obtained with the 20-species C<sub>2</sub>H<sub>4</sub> reduced chemical kinetic mechanism.**