

Implementation of Automatically Simplified Chemical Kinetics through Intrinsic Low-Dimensional Manifolds for Gaseous HMX*

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ABSTRACT

An automated method to generate, validate, and implement an intrinsic low-dimensional manifold (ILDm) has been developed. This method has been applied to a detailed mechanism for gaseous HMX that contains 44 species and 232 reactions. The resulting ILDM tracked detailed chemistry based on enthalpy, pressure, and mass fraction of N_2 . A one-dimensional BYU combustion program has been used to compare the ILDM with the detailed mechanism. Simulations show that the ILDM is an adequate representation of detailed kinetics away from the reacting surface ($> 100 \mu\text{m}$). An advantage of the ILDM method is that computational time is reduced by an order of magnitude. However, this advantage can be offset by the development time required to create and implement the ILDM method.

INTRODUCTION

Modeling of reacting flows is a computational challenge even for the world's largest supercomputers (1). This challenge is being explored by DOE's ASCI (Accelerated Strategic Computing Initiative) program. Part of the program is delegated to the University of Utah through C-SAFE (Center for Accidental Fires and Explosions). This initiative seeks to simulate a large jet-fuel pool fire. A canister filled with PBX is included in the simulation in the pool fire. As the canister is subjected to heat from the fire, the contents will begin to react. C-SAFE's goal is to simulate this situation from after the ignition of the pool fire, up to the rupture of the canister.

Performing the simulation with detailed kinetics is computationally prohibitive. To assist in this computational effort, a method for reducing chemical kinetics has been applied through the method of intrinsic low-dimensional manifolds (ILDm). The purpose of this project has been to automate a system for generating, validating, and implementing an ILDM for gaseous HMX.

OVERVIEW OF THE ILDM METHOD

Reduced Mechanism Methods

Traditionally, when chemical kinetic mechanisms were constructed manually, it required the technical expertise of someone familiar with the reaction mechanism (1). This person selected components and reactions that would be important under given conditions. In the pre-computer era, the chemical expert would apply the steady-state or partial-equilibrium approximation to various elementary reactions in the mechanism to come up with an analytic solution. Because analytical solutions were necessary, this limited the size of the kinetic mechanisms.

With the development of faster computers, it became possible to model complex chemical reactions with detailed kinetics. Though possible, it was still very expensive to calculate the kinetics with detailed mechanisms. To reduce the cost of computing, the chemical expert

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would systematically reduce the complex mechanisms into skeletal mechanisms. The drawbacks to this method are that it requires substantial knowledge of a detailed mechanism to generate a reduced mechanism. In addition, this method only works for a limited range of temperature, pressure, and composition.

Other Tools for Reducing Chemical Kinetics

A sensitivity analysis or principal component analysis is one of the tools to reduce complex chemical kinetics (1). The sensitivity analysis identifies reactions that have little effect on the overall reaction by measuring a normalized local sensitivity. After a reduced mechanism is achieved, the number of reactions can still be too great to implement the mechanism into a practical combustion code. Lumping procedures can be used to reduce the reaction system to a lower-dimensional system of equations (1). The CSP technique is a formal way to apply partial-equilibrium approximations on an *a priori* basis (4). The procedure begins by evaluating time scales of reactions and ordering them from fastest to slowest. The entire chemistry calculation proceeds with a time scale of the fastest reaction.

Intrinsic Low-Dimensional Manifold (ILDm)

Many of the previously mentioned methods for reducing chemistry rely on steady-state or partial-equilibrium approximations to reduce chemical kinetics. However, these approximations are generally limited to a range of temperature, pressure, or concentration (i.e. state space). Outside of this defined state space, large errors can occur.

To overcome this shortcoming, Mass and Pope proposed a new method for reducing chemical kinetics based on Intrinsic Low-Dimensional Manifolds (ILDm) (5,6). Their original work proposed a method to automatically apply the steady-state and partial-equilibrium approximations over the entire state space. The basic idea is that a thermochemical system is characterized by fast and slow reactions. The reactions that are the fastest can be decoupled from the slow ones. The fast reactions can be ignored while those with slow time scales are tracked using progress variables. By this means, a limited number of progress variables can be used to characterize the entire thermochemical system. For example, for a particular mechanism, three variables (e.g. enthalpy, pressure, and mass fraction of N₂) are selected as the progress variables. Once these variables are calculated, all other mass fractions of chemical species, temperature, entropy, and reaction rates are known from lookup tables. Since the progress variables completely describe the system, only these variables must be calculated. This leads to a dramatic reduction of CPU time for solving the chemistry in a laminar or turbulent reacting flow calculation. Some of the main ideas of a manifold along with results are presented below.

The Equations

The composition vector (ϕ) is composed of all intensive variables that define the thermochemical state of a system. It includes enthalpy (h) and all species mass fractions (Y_i , $i=1,2,\dots,n_s$) and is written as $\phi = (h, Y_1, Y_2, \dots, Y_{n_s})$. The descriptive equations for the composition ϕ include (1)

$$\frac{d\phi(x,t)}{dt} = S[\phi(x,t)] + \Gamma(x,t) \quad (1)$$

where S is the rate of change due to reactions (for enthalpy $S = 0$) and Γ is the rate of change due to transport effects (convection, diffusion, etc).

Chemical and Physical Process Time Scales

Chemical reactions typically have a much larger range of time scales than necessary for an accurate calculation of the system. Reaction time scales are on the order of 10^{-9} seconds (e.g. some radical reactions) to 10^2 seconds (e.g. NO formation in coal combustion) in reactions important to chemical combustion. On the other hand, the time scales necessary to model physical processes are on the order of 10^{-4} to 10^{-2} seconds. Figure 1 illustrates these ranges (6).

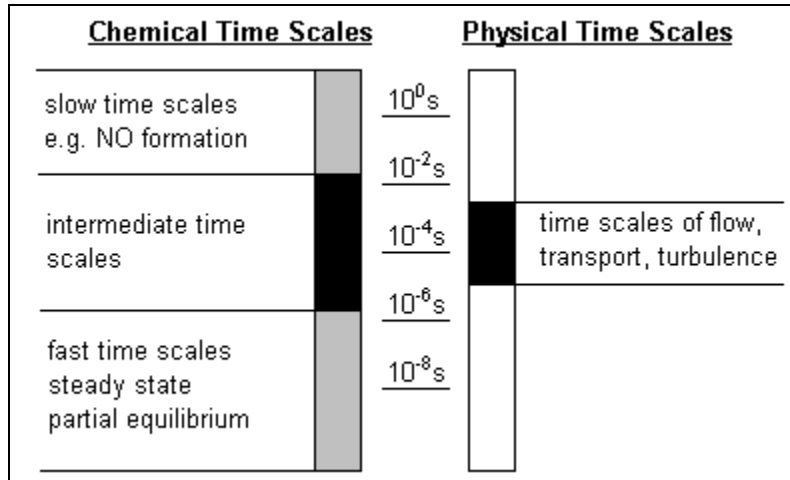


Figure 1—Time Scales Important to Reacting Flow

Those chemical reactions that happen much faster than the physical processes can be decoupled from the equations. Decoupling the species associated with fast time scales globally reduces the dimension of the composition space (2).

Decoupling Fast Chemical Time Scales

Mass and Pope used an eigenvalue analysis to determine if a system is on a lower-dimensional manifold and is governed by slow chemistry. The eigenvalues are those of the Jacobian ($dS_i/d\phi_j$). A large negative eigenvalue associated with an elementary reaction means that the reaction is governed by fast chemistry and is in local equilibrium. Conserved variables (e.g. pressure in an isobaric system) create eigenvectors that have eigenvalues of zero.

Table 1—Eigenvalue Analysis

Eigenvalue (real part)	Response to Physical Perturbations
Positive	Perturbation will increase (instability)
Zero	Perturbation will not change with time (change of a conserved variable)
Negative	Perturbation will relax to zero

For every reacting flow calculation, there is a time scale for the flow (τ_{flow}) based on the resolution of the transport calculations. If the real part of an eigenvalue is greater than $-1/\tau_{\text{flow}}$, then the corresponding eigenvector is in the slow subspace (7). However, if the eigenvalue is less than $-1/\tau_{\text{flow}}$, then the corresponding eigenvector is in the fast subspace and can be decoupled from the reaction system. The number of reaction variables that cannot be decoupled form a reduced set. These are the only variables that must be tracked and calculated for the laminar or turbulent combustion calculation.

Manifold Dimension

The number of variables that are important for the calculation determines the dimension of the manifold. Since it is difficult to implement a variable-dimensional manifold into a CFD code, a constant parameterization should be used over the entire state space for the manifold calculation (2). This makes the implementation much less time consuming but also has some drawbacks. These drawbacks include:

- Calculation of the ILDM is attempted over the whole state space even though some domains of the state space are never accessed in practical applications.
- Fixed parameterization does not guarantee the uniqueness or existence of solutions and can yield ill-conditioned equation systems for the manifold.
- Higher dimensional manifolds may be required in some of the state space. This means that too few variables are tracked and calculated and could lead to errors typical of an invalid steady-state approximation.

Despite these drawbacks, a constant variable dimensional manifold is the only practical way to implement the ILDM method for combustion calculations at this time.

One-Dimensional Manifolds

Up to this point the manifolds have been described mathematically. Manifolds can also be observed through graphical techniques (8). The simplest case is a manifold plotted against one progress variable. Figure 2 shows the specific mole number of H_2O plotted against the specific mole number of CO_2 for a $CO-H_2$ -air system (6). Each starting point represents a starting point for the reaction. All points have the same elemental fractions but different species compositions. The trajectory represents the reaction progression and the square is the final equilibrium.

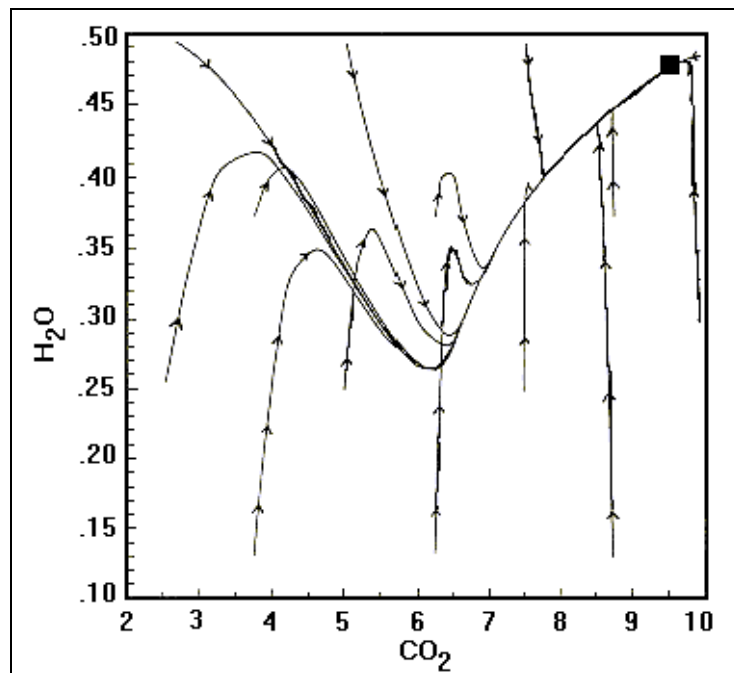


Figure 2—One-Dimensional Manifold

In this case, the specific mole number of CO_2 is the manifold coordinate. The projection or trajectory has the following properties (6):

- All approach one common point (equilibrium)
- All approach one common trajectory (manifold)
- On the manifold, only slow time scales govern the chemical reaction
- Once a thermochemical system is on the manifold, it will always remain on the manifold if there are no perturbations ($\Gamma = 0$).

Therefore, a thermochemical system is drawn to a unique manifold and progresses along it until the system is perturbed through physical processes (e.g. molecular diffusion, mixing, heat convection). If it is perturbed at a time scale slower than the fastest time scale of the manifold then the manifold is an accurate representation of the chemical dynamics. However, if the perturbations happen at a time scale that is faster than the existing manifold then a higher dimensional manifold should be employed (2). A higher dimensional manifold simply means that more variables must be added to the manifold to capture a larger number of time scales. This can dramatically increase the storage requirements for the manifold.

Two-Dimensional Manifolds

A two-dimensional manifold has the same characteristics as the one-dimensional manifold. The only difference is that two progress variables must be tabulated over the entire state space for the manifold lookup tables. Figure 3 is an example of a two-dimensional manifold (2).

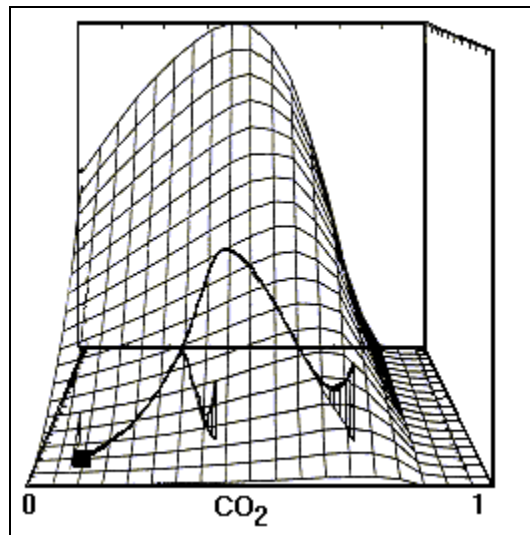


Figure 3—Two-Dimensional Manifold

The manifold is the grid surface. Each trajectory represents a starting point in the state space. Each trajectory relaxes to the grid surface quickly and stays on that surface until the thermochemical system reaches equilibrium.

Higher-Dimensional Manifolds

Higher-dimensional manifolds can be visualized through lower-dimensional plots by taking slices of the full manifold. For example, a three-dimensional manifold of the CH₄-air system can be characterized by enthalpy, pressure, and mass fraction of CO₂. If the enthalpy is held constant then the manifold can be plotted as a two-dimensional manifold. Then the enthalpy can be held constant at another value and another two-dimensional manifold plot can be generated. In this way, a higher-dimensional manifold can be visualized and selected graphically.

Examples of Manifold Implementation

The ILDM method has been implemented successfully for laminar premixed CO-H₂-O₂-N₂ flames (8). The ILDM method tracks all species, including radicals, within 3% error. In addition, there is a speedup in chemistry by a factor of 10.

The ILDM method has also been implemented successfully in turbulent flame calculations. Three examples include:

- A numerical simulation of a turbulent non-premixed CH₄-H₂-air flame shows that the ILDM method models flames near extinction and near equilibrium (9).
- A piloted CO-H₂-N₂-air diffusion flame simulation shows that extinction can be predicted within 5% of the experimental value (10).
- A CH₄-air combustion system shows that the ILDM method is 1,500 times faster in computing chemistry than a skeletal mechanism (3).

Recent Improvements to the Manifold Method

New strategies have been developed to overcome some of the shortcomings to the original ILDM method. The drawbacks to the standard tabulation method are (3):

- The entire state space must be calculated for a fixed dimensional manifold.
- The resulting lookup table can be very large and increases dramatically for higher dimensional manifolds.
- For higher-dimensional manifolds, the work to retrieve information is not trivial.

To overcome these shortcomings, the method of *In Situ* Adaptive Tabulation in Principal Directions (ISAT) was created (3). The ISAT method operates under the same principals as the ILDM method but it calculates and stores the manifold during the reacting flow calculation. Thus, only areas of the state space that are accessed are included in the manifold. Storage and lookup requirements are kept to a minimum while a significant speedup in chemistry is still observed.

Another technique to overcome the drawbacks of the standard tabulation method is to store the manifold as a piecewise polynomial. As a polynomial, only the coefficients to the polynomial need to be stored. For a test case, this method reduces the storage requirements of the manifold by a factor of 100 compared with the storage requirements for individual points (11).

MANIFOLD GENERATION FOR GASEOUS HMX

One of the major challenges in the ILDM or ISAT has proved to be the application of the theory to actual systems. The developers of these methods have shown the success of the methods for laminar and turbulent flame calculations (3,5-8,10).

Manifold Generation

There are six steps to the generation of a fixed-dimensional manifold: selecting the dimension, choosing the parameterization, generating starting points in the composition space, tracking each starting point to equilibrium, identifying the manifold, and storing the manifold.

Dimension of the Manifold

The dimension of the manifold can be investigated through an eigenvalue analysis of the Jacobian. The number of eigenvalues that have a real portion greater than $-1/\tau_{\text{flow}}$ determines

the dimension of the manifold. Generally, as the dimension of the manifold increases, the storage requirement and accuracy increase. The dimension of the gaseous HMX manifold was arbitrarily fixed at three parameters.

Choice of Parameterization

Once the dimension of the manifold was determined, three parameters were chosen to track the system. For the one-dimensional laminar combustion code these three parameters were chosen as enthalpy, pressure, and a reaction progress variable. As explained previously, these three variables track the entire state space. Therefore, if these three parameters are known then all other species concentrations are also known.

Starting Points in the Composition Space

To generate starting points in the composition space, all but one of the parameters must be held constant. For the one-dimensional laminar combustion code, enthalpy and pressure were held constant. This was accomplished in a closed adiabatic reacting system of a Perfectly Stirred Reactor (PSR).

A PSR code was developed by Glarborg et. al. (12). This code was used to create realistic combustion gases that include radicals. These partially reacted gases were then mixed in proportions of 95%, 80%, 65%, 50%, and 35% unreacted HMX on a mass basis. The products of the PSR and unreacted HMX were mixed according to the following equation:

$$Y_j = Y_{PSR_j} (1 - y_{Reactants}) + Y_{Reactants_j} y_{Reactants} \quad (2)$$

where j is an index number for each species, Y is the mass fraction, Y_{PSR} is the mass fraction of PSR products, $Y_{Reactants}$ is the mass fraction of species in unreacted feed, and $y_{Reactants}$ is the mass fraction of unreacted feed that is mixed with the PSR products.

After the mass fractions are evaluated, the temperature of the new mixture is computed. Since the PSR is specified as an adiabatic reactor, the products of the PSR have the same enthalpy as unreacted HMX. Therefore, the mixture of PSR products and unreacted HMX have a known enthalpy. By this means, the temperature of the mixture can be solved iteratively. The secant method is used to find the temperature with the initial guess midway between the high temperature of the PSR products and the low temperature of the reactants. Generally, the temperature meets the 10^{-11} K convergence criteria in fewer than 10 iterations.

Reaction Progression

A file is written from the PSR code and is read into a batch reactor program. Figure 4 is an overview of the simulation sequence from the PSR to the batch reactor and finally to the creation of trajectories.

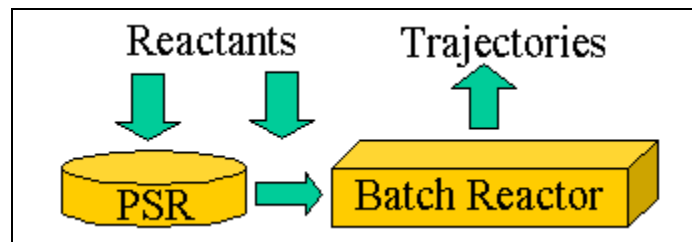


Figure 4—Reaction Path for Manifold Generation

The batch reactor receives the mixture of PSR products and reactants and simulates an adiabatic, premixed reactor. The mass fractions of the species, temperature, reaction rate of N_2 , entropy, and enthalpy are computed starting at the initial time and stepping forward until equilibrium is reached. The progression towards equilibrium forms a trajectory when plotted against time. Figure 5 shows CO_2 mass fraction plotted against time.

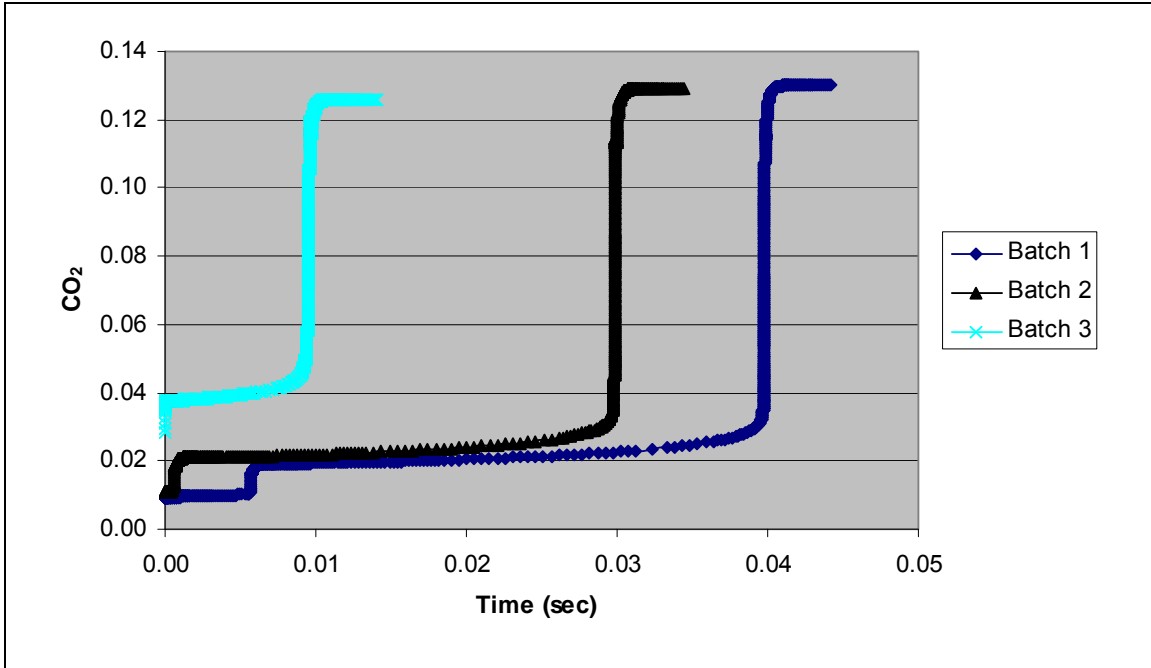


Figure 5—Batch Reactor Results

Each point on the graph represents a time where all of the state space was computed and recorded. Initially, the time step is small to account for fast reactions. Once the reaction time scale slows, larger time steps can be used. Initially, the batch reactor program only allowed for a constant time step equal to the smallest time step during the entire calculation. The batch reactor program was modified to allow for changing time scales. This modification sped up the calculation by many orders of magnitude.

Manifold Identification

The mixtures of unreacted and reacted HMX were imported to a batch reactor program. During the course of reaction simulation, the species, temperature, and reaction rate of N_2 were stored in data files.

Figure 6 shows an example of the graphical method for identifying the lower dimensional manifold.

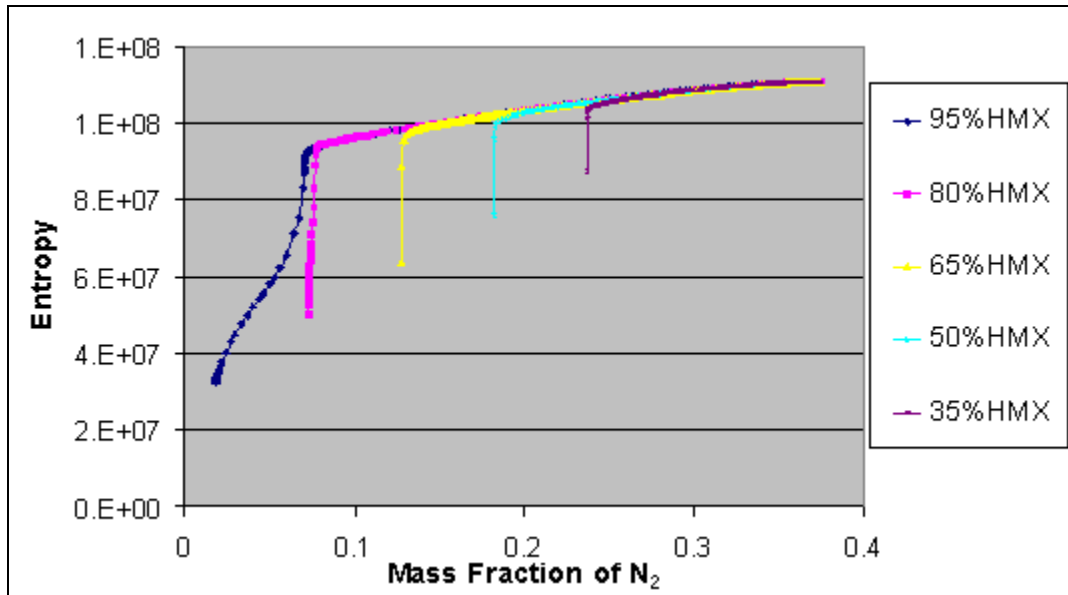


Figure 6—Portion of HMX Manifold

In this case, entropy is plotted against the mass fraction of N_2 . Each trajectory represents a separate simulation performed in the adiabatic batch reactor. Each starting point represents a different percentage of unreacted HMX mixed with products of HMX combustion from a PSR. The initial conditions of the unreacted HMX are arbitrarily set at 127 °C and 20 atm. All the trajectories are attracted towards the manifold and end at the point that represents equilibrium.

Since the HMX manifold is calculated with three dimensions, the pressure and enthalpy are varied over a range necessitated by the state space of the combustion system that will employ the manifold. For example, a manifold for a pressurization simulation would include batch reactor results across the entire range of pressures.

Manifold Storage and Retrieval

Once the manifold was identified, it was stored in a data file for future use in a combustion code. Because the project uses multiple operating systems, the files were stored in the ASCII format.

At runtime, the data files are loaded into arrays within the combustion application. A multivariable linear interpolator looks up values in the tables based on enthalpy and mass fraction of N_2 . For mass fractions of N_2 below the manifold values, a linear extrapolation between the lowest available value and the initial concentration is used (2).

MANIFOLD IMPLEMENTATION WITH 1-D LAMINAR SIMULATION

In order to validate the effectiveness of the HMX manifold, results from a detailed mechanism and a manifold approach were compared in a one-dimensional combustion code. The code that is used to test the manifold includes a condensed phase and a gas phase (13). Since the gas phase calculation typically required more than 99% of the CPU time, the manifold was only used to simplify gas-phase reactions.

Direct Substitution

A quick check to see how well the manifold follows the detailed kinetics is to substitute manifold values into every node using the solution of enthalpy and mass fraction of N₂ from the detailed kinetics calculation. Figure 7 shows the concentration of CO₂ versus distance from the surface.

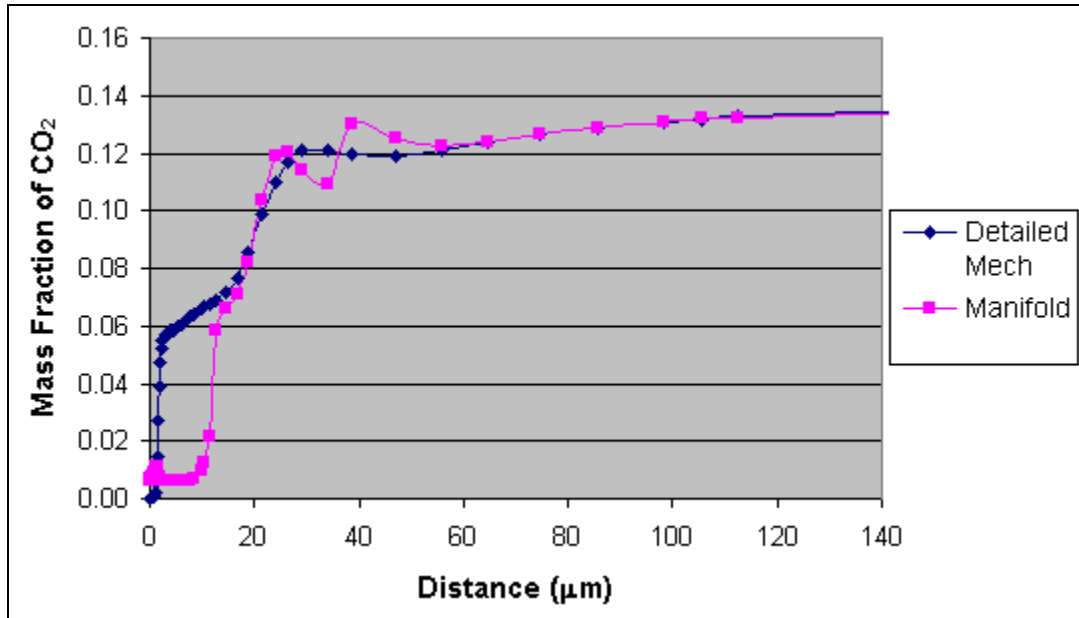


Figure 7—Detailed Mechanism versus Manifold

Near the surface (0 to 60 μm) the manifold does not agree with the detailed kinetics while further from the surface (60 μm to infinity) the two are exactly equal. This is due to the varying time scales along the temperature profile. The time scale of the one-dimensional flow is computed by the following equation:

$$\tau_{flow} = \frac{\Delta distance}{velocity} \quad (3)$$

Figure 8 shows the calculated time scale versus distance.

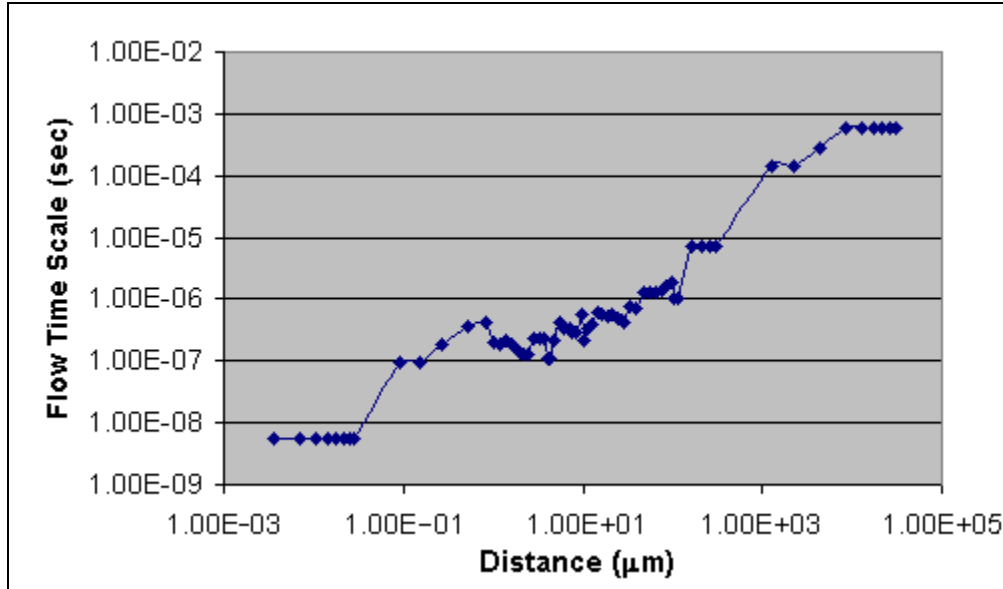


Figure 8—Flow Time Scale

Because the time scale is so small near the surface, a higher dimensional manifold should be used to get accurate results. As long as the correct dimension of the manifold is used, the manifold should accurately represent the detailed kinetics.

Implementing the Manifold with the Control Volume Approach

The Equations

Since the HMX manifold is only a function of enthalpy and mass fraction of N_2 , the equations that must be solved are the energy equation in the enthalpy form and the continuity equation for N_2 . These two equations are

$$n_{mass} \frac{dH}{dx} = \frac{d}{dx} k \frac{dT}{dx} \quad (4)$$

for enthalpy (where H is enthalpy, n_{mass} is the mass flux, k is the thermal conductivity, and T is the temperature) and

$$n_{mass} \frac{d}{dx} Y_{N_2} = \omega_{N_2} W_{N_2} \quad (5)$$

for N_2 (where Y_{N_2} is the mass fraction of N_2 , ω_{N_2} is the reaction rate of N_2 , and W_{N_2} is the molecular weight of N_2).

Discretization of the Equations

The enthalpy equation and N_2 conservation equations were discretized using the control volume layout as shown in Figure 9.

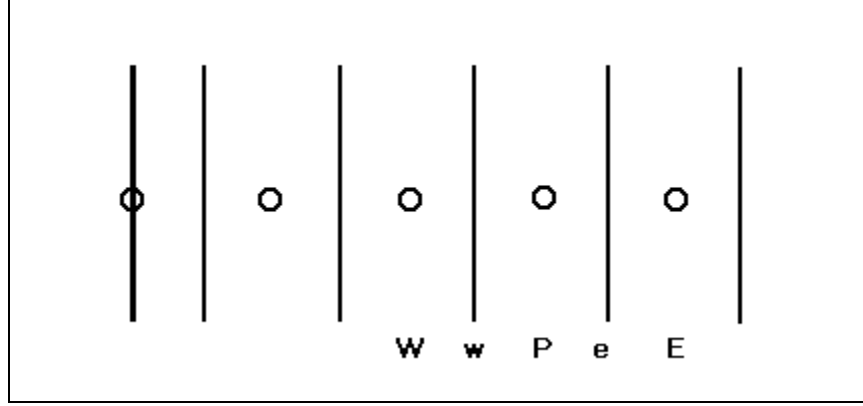


Figure 9—Control Volume Layout

The control volume approach integrates the differential equations over a distance from e (east) to w (west). Using the control volume approach and integrating between the control surfaces for P, the energy equation becomes

$$n_{mass} (H_e - H_w) = k_e \left(\frac{dT}{dx} \right)_e - k_w \left(\frac{dT}{dx} \right)_w \quad (6)$$

and the N₂ conservation equation becomes

$$n_{mass} (Y_{N_2_e} - Y_{N_2_w}) = \omega_P W_P \Delta x_P \quad (7)$$

where Δx_P is the distance across the control volume for P from e to w.

Assuming a linear temperature profile between nodes, using an under-relaxation parameter ($\alpha < 1$) to ensure the stability of the solver, and using an upwind scheme (valid for high Peclet numbers) the enthalpy equation becomes

$$H_{P,i} = H_{P,i-1} + \alpha \left[\frac{\left(n_{mass} H_{W,i} + \left(k_e \frac{T_E - T_P}{\delta x_e} - k_w \frac{T_P - T_W}{\delta x_w} \right) \right)}{\frac{n_{mass}}{\alpha}} - H_{P,i-1} \right] \quad (8)$$

and the N₂ conservation equation becomes

$$Y_{N_2_{P,i}} = Y_{N_2_{P,i-1}} + \alpha \left[\frac{\left(n_{mass} Y_{N_2_{W,i}} + (\omega_P W_P \Delta x_P)_{i-1} \right)}{\frac{n_{mass}}{\alpha}} - Y_{N_2_{P,i-1}} \right] \quad (9)$$

where the subscript (i) denotes the current iteration value and the subscript (i-1) denotes the value from the previous iteration.

Iterative Solving Routine

Both of the discretized equations are explicit in time and distance yet the solving routine is still iterative. The global scheme is iterative because the manifold is a function of enthalpy and the mass fraction of N_2 . Once the enthalpy is solved, the mass fraction of N_2 is solved. This iterative step repeats until the solution converges. An interesting characteristic of the manifold solution is that the mass fraction of N_2 and enthalpy continue to oscillate slightly around a solution but never converge. This is due to the discontinuities in the reaction trajectories in the fast reaction zone. The oscillations appear because a higher dimension manifold should be used. Figure 10 shows the temperature profile at the last iteration versus the temperature averaged over the last 100 iterations.

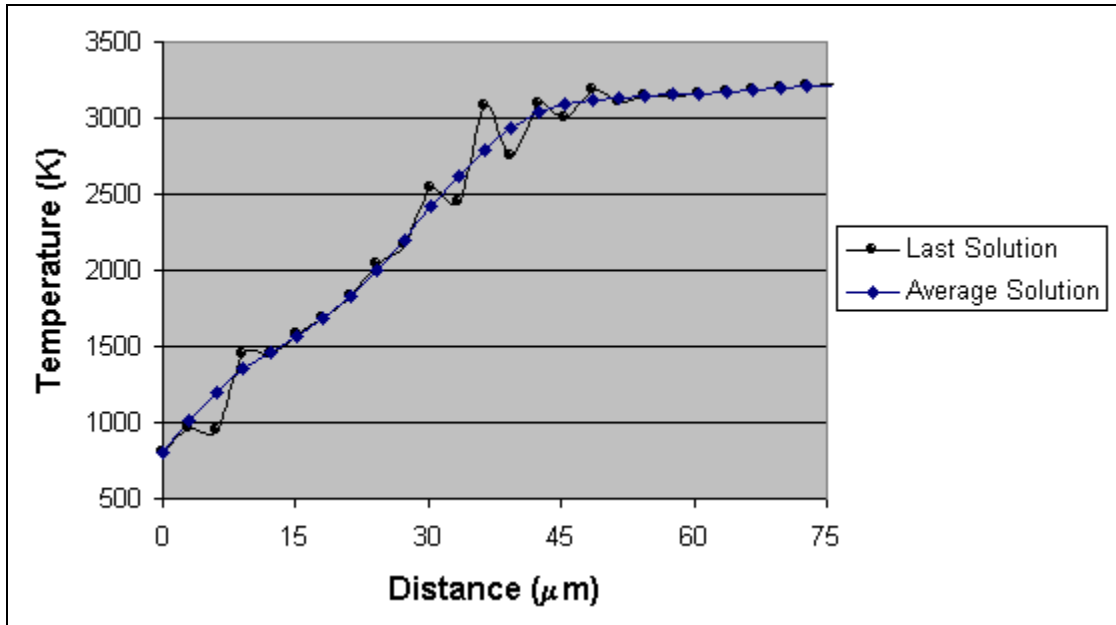


Figure 10—Oscillations in the Final Solution

The averaged solution over the last 100 iterations is used to ensure physically realistic results and smooth out the oscillations.

Grid Independent Study

An important aspect of numerical analysis is a grid independent study. Generally, a numerical solution becomes more accurate as more nodes are used. However, using additional nodes also increases the required computer memory and computational time. The appropriate number of nodes can be determined by increasing the number of nodes until the numerical solution changes by less than a specified tolerance. Figure 11 shows temperature versus distance for the grid independent study.

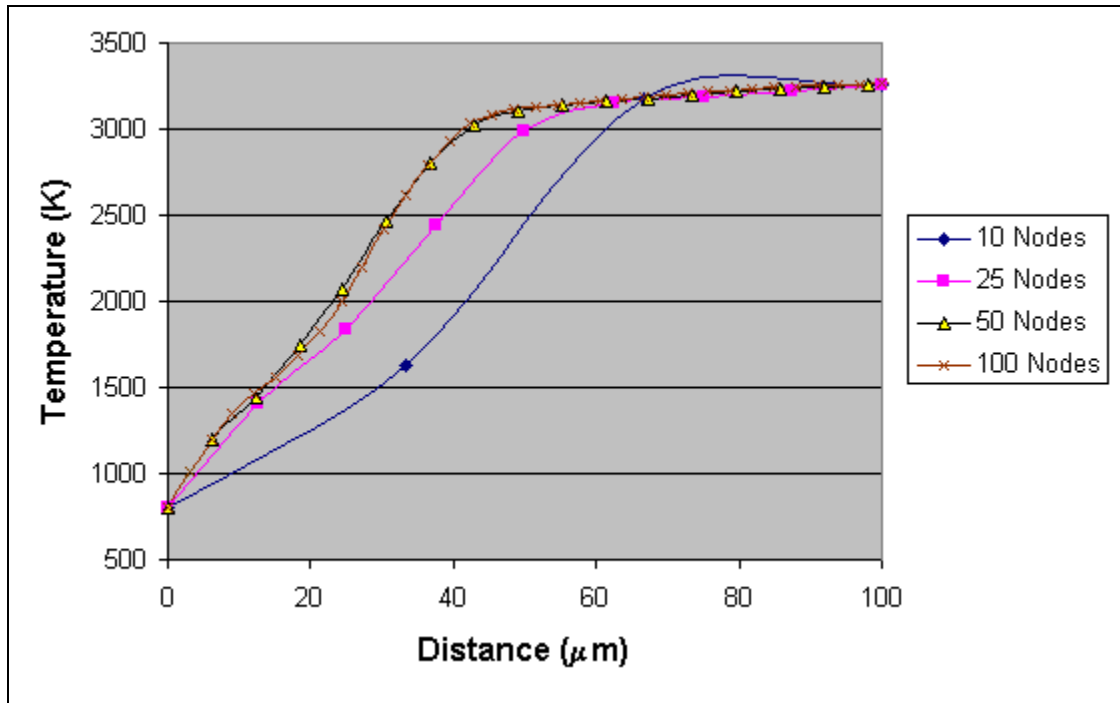


Figure 11—Grid Independent Study

The total computational distance is selected as 300 μm . Therefore, using 50 nodes, the grid spacing is 6 μm . The solutions at 50 and 100 nodes are within a 0.5%. Therefore, grid spacing less than 6 μm gives a grid independent solution.

There is also a minimum grid spacing requirement due to the oscillations during the iterations. For 500 nodes the grid spacing is 0.6 μm . With this grid spacing, the enthalpy solution oscillates because of jumps in the temperature with a magnitude of up to 500K. Because the node spacing is small, this leads to a large numerical temperature derivative and a large increase or decrease in enthalpy. The solver handles this big step in enthalpy by decreasing the under-relaxation parameter (α) and attempting to solve the equation again. However, with such a large step the under-relaxation parameter decreases to the point that the solution requires many more iterations to reach a converged solution. With 1000 iterations the solution is still dependent on the initial guess. Increasing the number of iterations until a converged solution is found would be very computationally expensive. Figure 12 shows the enthalpy curves for a grid spacing of 3 μm (100 Nodes) versus 0.6 μm (500 Nodes).

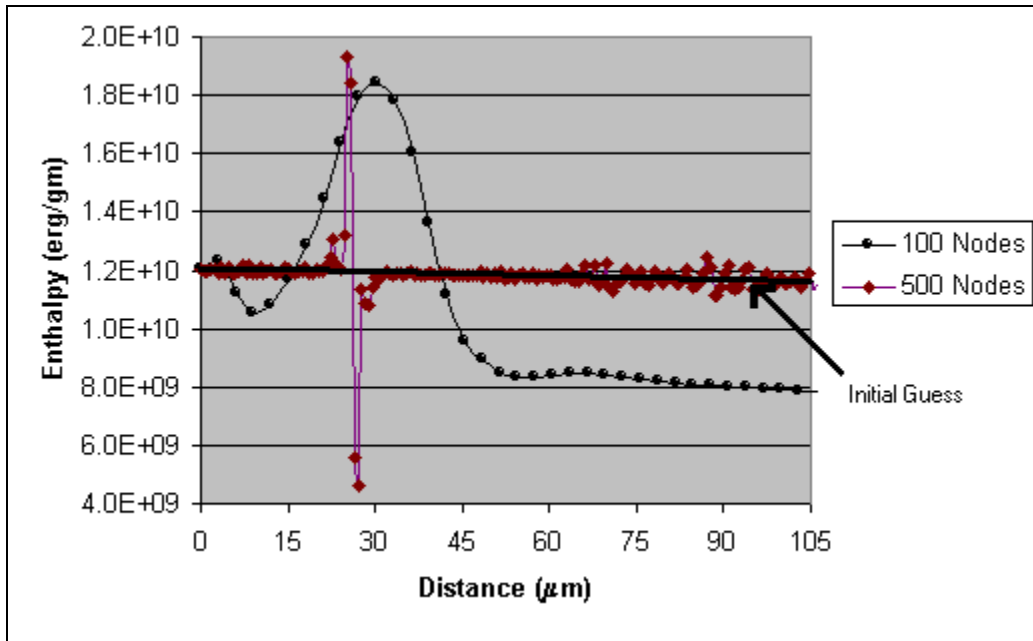


Figure 12—Grid Independent Study

After 1000 iterations the final value of the under-relaxation parameter for grid spacing of $3.0 \mu\text{m}$ is 0.125 whereas for a grid spacing of $0.6 \mu\text{m}$ the under-relaxation parameter is 6.9×10^{-18} for the enthalpy equation.

For the purposes of the grid independent study, any grid spacing less than $6 \mu\text{m}$ will yield a grid independent solution. Any grid spacing less than $0.6 \mu\text{m}$ will also give an accurate solution but the computational time will be prohibitive. A grid spacing of $3 \mu\text{m}$ is recommended for HMX manifold one-dimensional calculations.

Results

One of the advantages to using the ILDM approach over reduced mechanisms is that all of the species profiles, even the minor radicals, are calculated. To illustrate the capabilities of the ILDM approach, the species profiles of NO, CO₂, H₂O, and the temperature profile for the manifold and full kinetic mechanism are shown in Figures 13-16.

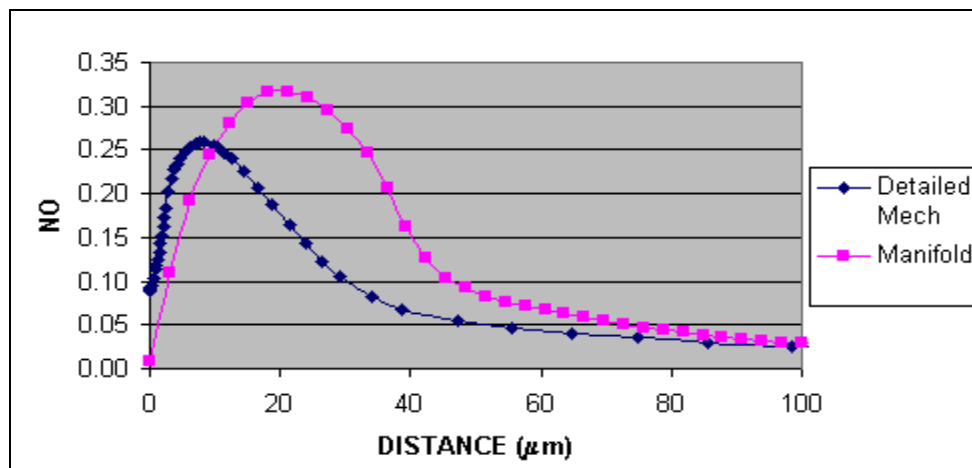


Figure 13—Results of One-Dimensional, Steady-State Simulation

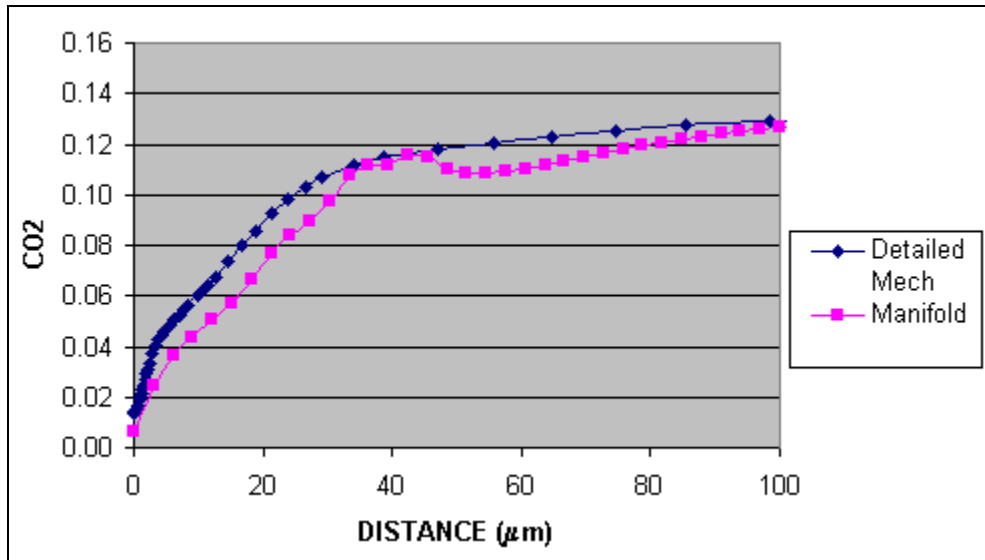


Figure 14—Results of One-Dimensional, Steady-State Simulation

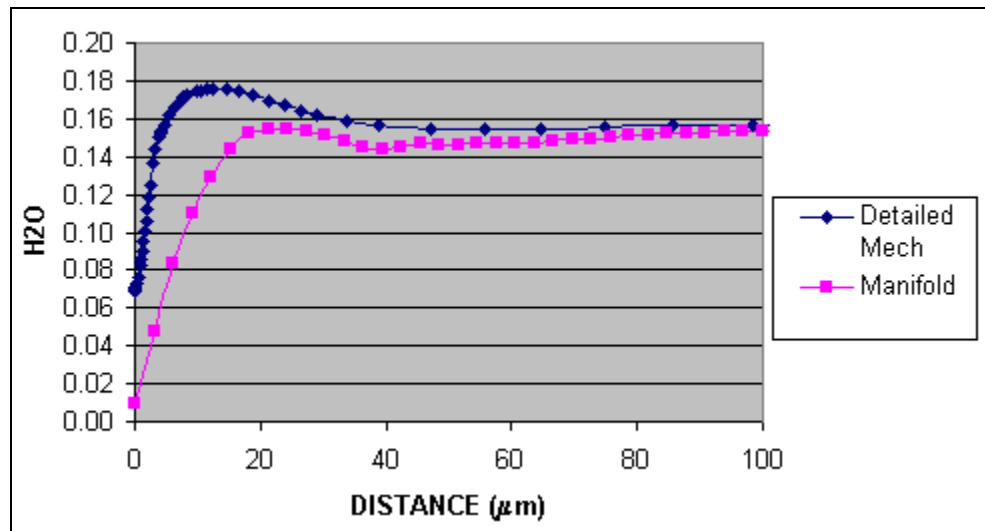


Figure 15—Results of One-Dimensional, Steady-State Simulation

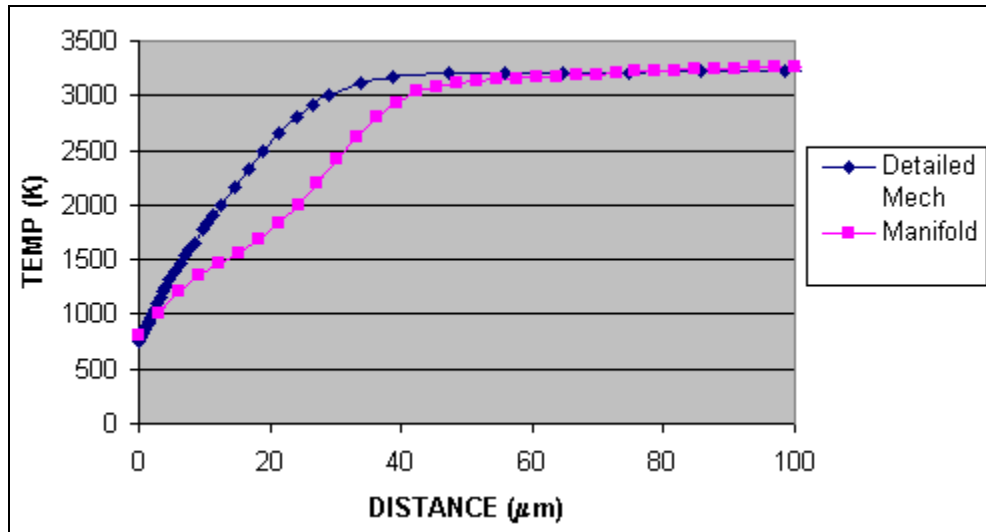


Figure 16—Results of One-Dimensional, Steady-State Simulation

The manifold lags the detailed mechanism in the formation of the major product species. This is due to a dark zone where NO is the dominant species near the surface. One method to overcome this lag is to include another tracking species in the manifold, such as NO.

CONCLUSIONS

One of the major obstacles to manifold implementation has been the lack of automation for manifold generation and implementation. This project automates the manifold process. This is done through the Chemkin paradigm of interchangeable reaction mechanisms. As new detailed mechanisms are developed for HMX or as other solid propellants are modeled, a new manifold can be generated simply by switching out mechanism files.

This project also provides an example of using the ILDM method for combustion of solid propellants. Up to this point, the only applications of the ILDM method have been with simple combustion reactants such as short-chained hydrocarbons, H₂, and O₂. This project is the first attempt to use the manifold method for a complex reactant molecule such as HMX.

There are large errors near the surface of the burning HMX (< 100 μm) and good agreement beyond that. If coarse gridding is used in a simulation, as in the C-SAFE simulation, then the manifold method is sufficient. With the manifold method, only a limited number of differential equations must be solved. This speeds up the convergence by eliminating much of the stiffness in the differential equations. For this project, computational savings were an order of magnitude less for the ILDM method.

Another possible use for the manifold method is to use it as an initial guess for a detailed mechanism simulation. BYU's one-dimensional, steady-state code converges on the order of minutes instead of hours when good guess values are used. The manifold method could provide good guess values where initial guess values accelerate convergence.

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