A Fundamentally-Based Stochastic Mixing Model Method for Predicting NO and Soot Emissions from Direct Injection Diesel Engines

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Abstract—A Two-Step Approach for calculating slow and complex chemistry in inhomogeneous turbulent reactive flows, specifically in a direct injection (DI) diesel engine, was evaluated. The first step in this approach is to complete a Multi-Dimensional Model (MDM) solution of the unsteady reactive flow. This was accomplished for a DI diesel engine using the KIVA computer code developed at the Los Alamos National Laboratory. The output of this solution was used to define zones within the flow and to calculate zone processes and mass flow between zones. A Stochastic Mixing Model (SMM) computer code was developed to recalculate turbulent mixing and chemistry using the KIVA output. The SMM generates distributions of the turbulent properties within each zone which are required to calculate the slow emissions chemistry. This approach was evaluated by analyzing zone property distributions, the effect of changing zone boundaries, the effect of increasing the number of zones and the variance of SMM results over multiple stochastic runs. Predictions were compared to experimental results obtained under various engine operating conditions. This Two-Step Approach is an efficient and accurate method for calculating slow and complex chemistry in turbulent reactive flows.

Keywords: Combustion, emissions, stochastic, diesels.

INTRODUCTION

Reactive flows encountered in diesel engines are turbulent, unsteady and three-dimensional. Reaction rates governing the production of soot and NOx in diesel engines are much slower than those for combustion and have time scales of the same order as the turbulent fluctuations. The distribution of properties about the mean due to turbulent fluctuations is critical to slow-chemistry processes, therefore multi-dimensional models of diesel combustion, such as KIVA (Amsden et al., 1985), cannot accurately predict emissions. At present, the simultaneous consideration of flow details and slow chemistry in such flows is computationally unmanageable. In this paper we describe an approach which first uses the results of a multi-dimensional model calculation to predict the important details of the flow, and then computes the flow emissions-chemistry using a stochastic mixing model.

Stochastic mixing models have gained broad acceptance for modeling turbulent mixing and combustion in various types of chemical reactors. The fundamental concept of these models is coalescence/dispersion micromixing (Curl, 1963). The solution is typically accomplished using a Monte Carlo simulation. In its simplest form, initially segregated equal-mass elements (reactants) are fed into a reactor. Randomly selected pairs of elements within the reactor are instantaneously mixed on a molecular level (coalesced) according to a prescribed mixing rate and then separated again into two elements of equal average intensive properties (dispersed). Finite-rate batch-chemistry proceeds in each element during the time interval between mixings. Elements within the reactor acquire a distribution of properties which control the overall reaction rates. There is no spatial resolution within the reactor: each element is equally likely to be picked for mixing.
In previous study at MIT, Mansouri et al. (1981) used a stochastic mixing model to predict emissions in a divided-chamber (IDI) diesel engine. In this type of engine, the fuel is injected into a highly-turbulent prechamber where mixing occurs rapidly before combustion and expansion into the engine cylinder. Unlike the IDI process, DI diesel combustion is not well-mixed. The spatial distribution of the fuel spray within the combustion-chamber geometry is important to the DI diesel process. Our research attempts to answer the question: "Can the SMM method be used to calculate slow chemistry in DI diesel engines and other inhomogeneous turbulent reactive flows where flow details are likely to be critical to the calculation?"

We have developed a Two-Step Approach to this problem. The first step is to complete a Multi-Dimensional Model (MDM) solution of the reactive flow. The output of this solution is used to define zones within the flow by total fuel mass fraction limits. A typical four-zone schematic for a DI diesel engine is illustrated in Figures 1 and 2. These zones are not fixed in space, but are dependent on the constantly changing distribution of fuel and burned fuel within the flow. Total mass, species mass, volume, chemical heat release, mass of fuel burned, mass of fuel evaporated, wall heat transfer and turbulent intensity are calculated for each zone at each MDM timestep. The net flow of total mass, liquid fuel, unburned fuel vapor, and burned fuel between each zone is calculated from the MDM data using conservation of mass and species.

![Diagram of fuel spray in a divided-chamber diesel engine]

**FIGURE 1** Cylinder top view showing typical 4-zone arrangement in a direct injection diesel spray. Zones are specified by total fuel mass fraction (TFMF) limits.

The second step is to model each of these zones as a stochastic mixing zone. The flow and process information calculated by the MDM is used to specify flows between mixing zones, evaporation, heat transfer and mixing within the zones.
Information is transferred only from the MDM to the SMM. Using this information the flow mixing and chemistry are recalculated by the SMM resulting in species and temperature distributions for each zone as a function of time. In this way the distribution of turbulent properties throughout the combustion chamber is considered in the calculation of slow chemistry.

![Diagram showing a 4-zone Stochastic Mixing Model (SMM) simulation.](image)

**FIGURE 2** Schematic of a 4-zone Stochastic Mixing Model (SMM) simulation.

The goal of our research was to demonstrate the feasibility of the this Two-Step Approach for calculating slow and more complex chemistry in turbulent reactive flows. Our specific objectives were:

1. To develop a computer code based on this Two-Step Approach for calculating emissions formation in a DI diesel engine.
2. To evaluate the SMM approach for consistency by analyzing zone distributions, the effect of changing zone boundaries, the effect of increasing the number of zones, and the sensitivity to various physical and model parameters.
3. To evaluate the SMM accuracy by comparing predicted NO histories to experimental results.

The submodels included in our SMM are not intended to be unique. Each was developed to be consistent with the random selection principles fundamental to the method and the physical process being modeled, but valid arguments could be made for other schemes. Our intent is to illustrate and evaluate one example of how this approach might be applied.

**ASSUMPTIONS**

The basic assumption underlying this approach is that an inhomogeneous reacting flow, such as in a DI diesel engine, can be broken down into zones which individually may be modeled as stochastic mixing zones. It is further assumed that these zones are simply connected in series with a single flow in or out from the preceding zone and a single flow in or out to the next zone (see Figure 2). Total fuel mass fraction (TFMF, burned plus unburned fuel) is used to define these zones.
These zones are not fixed in space, but constantly change as the TFDF distribution within the cylinder changes. There is no spatial resolution within the zones and each zone is considered to be perfectly macromixed. Output from a multidimensional model solution is used to define the zones, to specify the flow between zones and to constrain certain processes within the zones. It is assumed that the slower emissions chemistry does not produce or use significant energy and is therefore only a perturbation of the major combustion and flow dynamics which are correctly modeled by the MDM.

MODEL OVERVIEW AND STRUCTURE

Prior to the start of injection only the air zone exists. As liquid fuel begins to evaporate and mix with the surrounding air, other zones are created. The MDM specifies the flows into and out of these zones. These flows are updated in the SMM with data from the MDM at specific update times. Evaporation, heat transfer, mixing intensity and zone volume in the SMM are also specified by the MDM data. Mass in the SMM is broken up into equal mass units called elements. Each elements consists of two primary components, unburned fuel vapor and burned gas. The burned gas fraction (BGFR) includes air and burned products. The BRGFR is assumed to be in equilibrium for a given temperature, pressure and burned fuel fraction (FR). Zone mixing occurs by random selection of two elements within a mixing zone, coalescence of these two elements into a single element and separation back into two elements with equal intensive properties. When combustion criteria are met in a specific element, all of the unburned fuel vapor in that element (1-BGFR) is instantaneously converted to burned gas and a new equilibrium is calculated to include the additional burned fuel fraction. The SMM includes submodels for updating thermodynamic properties, composition, evaporation, heat transfer and volume.

Figure 3 illustrates the model's basic structure. The primary inputs to the SMM are equilibrium data derived from the NASA equilibrium code (Svehla and McBride, 1973), MDM data from the KIVA output, and simulation control parameters. The equilibrium data and control parameters are input at the start of the simulation. The Main Program updates the simulation time and initiates the mixing events. When it is time for an MDM update, the Main Program calls the Stochastic Mixing Zone (SMZ) model. The SMZ model first completes the previous MDM timestep for each zone by updating the heat transfer, updating the chemical properties and conserving volume. It then reads the MDM data for the next MDM timestep and uses it to specify the flow between zones and to update evaporation. It also calculates a new mixing time for each zone. The smallest of these mixing times is used in the Main Program as the basic simulation time increment. Once these updates have been made, control returns to the Main Program and mixing continues until the next update.

Our basic approach requires that the individual zones be modeled as stochastic mixing zones. Pratt (1975) provides an excellent summary of this method and our paper adheres to the same conventions for terminology. Each mixing zone is perfectly macromixed with the degree of micromixing determined by the mixing intensity calculated in the MDM. The method used for mixing is coalescence/dispersion.

Conservation of mass is used to calculate the net mass flow, fuel vapor mass flow, and burned fuel mass flow between zones for each MDM timestep. These
flows represent convection, turbulent diffusion and rezoning of MDM cells to richer or leaner zones due to changes in their TFMF. The flow between zones in the SMM must be accomplished within the model structure. This means exchanging elements between two ensembles of elements. It is necessary that elements be kept intact and that the selection of elements adhere to the basic random selection criteria to the greatest extent possible. The exchange of elements must also transfer the correct net total mass and species mass. The resulting overall distribution of elements according to TFMF should be continuous at zone boundaries and should converge to a single distribution as the number of zones and elements increases. This mass exchange was accomplished by grouping elements according to fuel mass fraction and randomly selecting elements from TFMF subgroups to achieve the required total mass flow, fuel vapor mass flow and burned fuel mass flow.

FIGURE 3  Flow diagram showing the Stochastic Mixing Model (SMM) basic structure.
The amount of fuel evaporated in each zone during an MDM timestep is input with the MDM data at the start of the timestep. Pure vapor elements are added to the zones by mixing with zone elements. Mass and enthalpy are conserved.

Combustion is accomplished by testing elements to determine if they contain fuel vapor within combustible limits and if the element history satisfies the ignition delay criteria. If an element satisfies the combustion criteria, the element is instantaneously burned at constant pressure to equilibrium products.

Wall heat transfer is updated at the end of each MDM timestep. The Heat Transfer Model distributes the zone heat transfer specified by KIVA among the zone elements. The heat transfer to element "i" is assumed to be proportional to its surface area and to the temperature difference between the element and the wall.

In addition to conservation of mass, species and energy, the total volume of all the elements must be equal to the actual cylinder volume. This constraint affects conservation of energy through the work term in the First Law. An iterative technique is used to calculate new element temperatures and a new cylinder pressure while satisfying the volume constraint.

The NO model uses the extended Zeldovich mechanism (Bowman, 1975) to calculate the time rate of change of NO. Equilibrium concentrations of species in these expressions are provided in the NASA equilibrium data as a function of temperature, pressure and equivalence ratio. The concentration of NO in each element is updated periodically and before mixing events.

Wang, Matula and Farmer (1981) studied soot formation for toluene behind reflected shock waves. Their results provide two correlations for predicting soot formation rates, one with oxygen in the mixture and one without. These correlations are used in our soot model. Occurring simultaneously with soot formation is soot oxidation. Park and Appleton (1973) have shown that the surface reaction rate for the oxidation of soot in a flame is nearly the same as that for pyrolytic graphite. The semi-empirical formula proposed by Nagle and Strickland-Constable (1962) for predicting the oxidation of pyrolytic graphite is used to predict soot oxidation in our model.

THE MULTI-DIMENSIONAL MODEL

Multi-dimensional models solve the fundamental mass, species, momentum and energy conservation equations in time and space. KIVA was selected for our application. KIVA is a finite-difference computer code for solving reactive fluid-flow problems in two or three dimensions. It is specifically designed to model the in-cylinder fluid dynamics of internal combustion engines including gas flow, liquid fuel injection, spray dynamics, evaporation, heat transfer, combustion, species transport, and mixing. KIVA was written specifically for the CRI Cray-1 computer. Run times for an axisymmetric simulation from -90 degrees to 80 degrees ATDC were approximately 18 minutes on a CRAY X-MP/12 computer. An axisymmetric grid (Figure 4) was used for all computations to conserve computer time.

EXPERIMENTAL DATA

In order to evaluate the SMM it was necessary to obtain or generate test data. The NO calculation includes no calibrating constants and is an unbiased indicator of how well the SMM method is predicting slow chemistry. The SMM provides
cylinder averaged NO mass fraction as a function of crank angle. An experimental technique that provides similar data is to dump and quench the cylinder contents for chemical analysis at various crank angles. The University of Wisconsin-Madison has had an ongoing study using this technique and their results were used in our analysis (Chan, 1982). Test engine specifications are provided in Table I. All test cases used an equivalence ratio of 0.5, an eight-hole injector, and an engine speed of 1000 RPM.

MODEL VALIDATION

The first step in evaluating the SMM approach was to consider its sensitivity to the values of important model and physical parameters and the variance in results for different stochastic runs with all other parameters held constant. To accomplish this we analyzed the effect of varying the total number of elements and the number and definition of the mixing zones.
TABLE I
Experimental engine specifications

<table>
<thead>
<tr>
<th>Engine type</th>
<th>Labeo Tacom single cylinder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>11.4 cm</td>
</tr>
<tr>
<td>Stroke</td>
<td>11.4 cm</td>
</tr>
<tr>
<td>Displacement</td>
<td>1173 cc</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>16.8:1</td>
</tr>
<tr>
<td>Conrod length</td>
<td>22.9 cm</td>
</tr>
<tr>
<td>Squish clearance</td>
<td>0.092 cm</td>
</tr>
<tr>
<td>IVC</td>
<td>−120° ATDC</td>
</tr>
<tr>
<td>EVO</td>
<td>+120° ATDC</td>
</tr>
<tr>
<td>Injector nozzle</td>
<td>8 holes</td>
</tr>
<tr>
<td></td>
<td>0.025 cm diam</td>
</tr>
<tr>
<td></td>
<td>157° injection angle</td>
</tr>
<tr>
<td>Opening pressure</td>
<td>21.0 MPa</td>
</tr>
<tr>
<td>Piston bowl</td>
<td>8.89 cm diam</td>
</tr>
<tr>
<td></td>
<td>1.27 cm max depth</td>
</tr>
<tr>
<td></td>
<td>74.3 cc volume</td>
</tr>
</tbody>
</table>

The total number of elements used in the SMM is a critical model parameter. The number of elements is determined by the individual element mass, specified as a model input parameter, and the total mass of the cylinder contents (fuel plus air plus residual). Included in the model input parameters is a random number seed which determines the series of random numbers selected by the random number generator for a particular run. A different random number seed will result in different element selection and a different solution. Output is averaged over a number of stochastic runs with different random number seeds. Figure 5 shows predicted maximum NO versus the total number of elements used in the runs. Each data point represents the mean of ten stochastic runs with different random number seeds. The vertical lines indicate the standard deviation and the tick marks indicate the 95 percent confidence interval for the mean value. Two important observations may be made from these data. First, the standard deviation decreases with more elements and, second, the mean value approaches an asymptotic limit with more elements. To achieve continuous distributions of properties within each zone requires a sufficient number of elements. As these distributions approach their limiting values they become less sensitive to further increases in the number of elements and to changes in the random number seed. Figure 6 shows the distribution of elements as a function of TFMF and the total number of elements. Distributions properly converge as the number of elements is increased.

Computer run time for an SMM run varies directly with the number of elements. For computational efficiency of a single run it is desirable to have fewer elements, but since standard deviation decreases with more elements, fewer runs are required with more elements for the same computational accuracy. A compromise number of 5750 elements and ten runs was selected for subsequent computations. Mean results using this number of elements and runs are within 5 percent of their asymptotic values and the 95 percent confidence factor range is less than plus or minus 5 percent of the mean value. Run time from start of injection to 40 degrees ATDC for one run on a VAX 750 is approximately 90 minutes.
FIGURE 5 Effect of the number of mass elements on the mean value and standard deviation of maximum NO for 10 SMM runs. The curve represents the calculated mean value, vertical lines represent standard deviation and tick marks represent the 95 percent confidence interval for the actual mean.

FIGURE 6 Effect of the number of mass elements on element total fuel mass fraction (TFMF) distribution.
We have assumed that an inhomogeneous flow may be broken down into a discrete number of zones which individually may be modeled as well-mixed. The validity of this hypothesis is dependent on local turbulent length scales and turbulent intensities. "Well-mixed" implies that any element within a zone is equally likely to mix with any other element in the same zone, however this is not valid if the zone is much larger than the typical turbulent length scale. Thus an evaluation of how the number and definition of mixing zones used in the SMM effects the results is most important. Increasing the number of zones and consequently decreasing their size should improve the validity of our hypothesis. As the number of zones is increased, the results should converge to a solution. Increasing the number of zones eventually becomes computationally unmanageable and other model hypotheses, such as having simply-connected zones, begin to break down. Our concern was that this might occur before the results converged to a solution.

Figure 7 shows the zone definitions used in our analysis. Figure 8 shows NO concentration histories for six different zone definitions. These curves show excellent convergence. Figure 9 shows the distribution of elements as a function of TFMF and zone definition. The larger zones in the 5 and 7 zone models show peaks around the zone mean TFMFs. This is much less evident with more zones as the fuel is forced into the proper TFMF interval and the distribution stabilizes. The distributions with more zones have more elements in the stoichiometric region. This results in higher mean temperatures, higher pressures, more NO and less soot. The distributions also converge with more zones.

FIGURE 7 Mixing zone definitions used in the model analysis. Zones defined by total fuel mass fraction (TFMF) limits.
FIGURE 8  Effect of zone definition on model predicted NO and comparison to test results.

FIGURE 9  Effect of zone definition on element total fuel mass fraction (TFMF) distribution.
COMPARISON TO EXPERIMENTAL DATA

The next step in evaluating the SMM approach is the comparison of model results to experimental results. The NO histories for Test Case 17 using 10 zones (Figure 8), and for all test cases, show excellent agreement with the experimental data. Results for five test cases are summarized in Table II. Predicted NO trends agree with the experimental results in all test cases and the magnitude of predicted NO compared to the experimental values is excellent. The largest discrepancy occurs in Test Case 19 and is attributed to the inaccuracy of the model initial conditions and pre-ignition chemistry, which would both have their greatest effect in this early injection case.

<table>
<thead>
<tr>
<th>Run</th>
<th>Inject (*ATDC)</th>
<th>Swirl</th>
<th>ERG (%)</th>
<th>[NO]_{ppm}</th>
<th>Soot_{max} (C)</th>
<th>Soot_{avg} (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>17(SMM)</td>
<td>-15</td>
<td>2.46</td>
<td>0.0</td>
<td>841</td>
<td>11.3</td>
<td>0.016*</td>
</tr>
<tr>
<td>17(EXP)</td>
<td>-15</td>
<td>2.46</td>
<td>0.0</td>
<td>842</td>
<td>0.016</td>
<td></td>
</tr>
<tr>
<td>18(SMM)</td>
<td>-15</td>
<td>4.00</td>
<td>0.0</td>
<td>508</td>
<td>11.2</td>
<td>0.269</td>
</tr>
<tr>
<td>18(EXP)</td>
<td>-15</td>
<td>4.00</td>
<td>0.0</td>
<td>625</td>
<td>0.017</td>
<td></td>
</tr>
<tr>
<td>19(SMM)</td>
<td>-25</td>
<td>2.46</td>
<td>0.0</td>
<td>1100</td>
<td>7.36</td>
<td>0.013</td>
</tr>
<tr>
<td>19(EXP)</td>
<td>-25</td>
<td>2.46</td>
<td>0.0</td>
<td>1600</td>
<td>0.011</td>
<td></td>
</tr>
<tr>
<td>20(SMM)</td>
<td>-15</td>
<td>2.46</td>
<td>10.0</td>
<td>378</td>
<td>9.97</td>
<td>0.425</td>
</tr>
<tr>
<td>20(EXP)</td>
<td>-15</td>
<td>2.46</td>
<td>10.0</td>
<td>356</td>
<td>0.030</td>
<td></td>
</tr>
<tr>
<td>21(SMM)</td>
<td>-15</td>
<td>4.00</td>
<td>10.0</td>
<td>525</td>
<td>9.85</td>
<td>0.500</td>
</tr>
<tr>
<td>21(EXP)</td>
<td>-15</td>
<td>4.00</td>
<td>10.0</td>
<td>290</td>
<td>0.049</td>
<td></td>
</tr>
</tbody>
</table>

*Calibrated to match experimental value

SUMMARY AND CONCLUSIONS

This paper proposes and evaluates a Two-Step Approach for calculating slow and complex chemistry in inhomogeneous reactive flows, specifically in a DI diesel engine. The first step is to complete a MDM solution of the unsteady reactive flow. In the second step, a stochastic mixing model uses the results of the MDM solution to recalculate turbulent mixing and chemistry. The validity of this approach was evaluated by analyzing its sensitivity to mixing zone boundaries, to the number of mixing zones and to various physical and model parameters. Its accuracy was evaluated by comparison to experimental data.

Results noted in the DI diesel application of the SMM approach were:

1) The standard deviation of pressure, soot and NO decreased with more elements and their mean value approached an asymptotic limit with more elements. TFMF distributions converged with more elements.

2) Pressure, soot and NO histories converged as the number of mixing zones was increased. TFMF distributions also converged. Nine or ten zones were required for convergence in our application.
3) The SMM and experimental NO histories showed good agreement, both in magnitude and in trend, as the engine operating conditions were changed.

The Two-Step Approach shows great promise for calculating slow and complex chemistry in turbulent reactive flows. The KIVA code provided detailed information about the diesel reactive flow that could not be obtained by any other means. Our DI diesel application of this approach was remarkably successful in predicting NO histories working from basic principles with no model calibration of use of experimental data. Limitations in our application were due primarily to deficiencies in the MDM solution and to economies on CRAY computer time.

REFERENCES


