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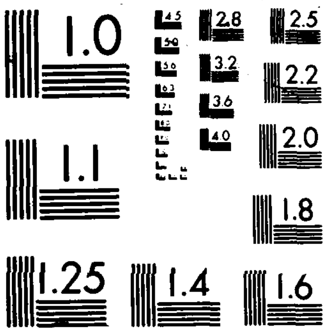

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A STOCHASTIC MIXING MODEL FOR PREDICTING EMISSIONS IN A DIRECT INJECTION DIESEL ENGINE

by

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B.S. Massachusetts Institute of Technology
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EMISSIONS IN A DIRECT INJECTION DIESEL ENGINE

by

ALAN JEFFREY BROWN

Submitted to the Department of Ocean Engineering
on September 1, 1986 in partial fulfillment
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Doctor of Philosophy in Combustion and Marine Systems Engineering

ABSTRACT

A Two-Step Approach for calculating slow and complex chemistry in inhomogeneous turbulent reactive flows, specifically in a direct injection diesel engine, was developed and evaluated. The first step in this approach is to complete a Multi-Dimensional Model (MDM) solution of the reactive flow. This was accomplished for a direct-injection diesel using the KIVA computer code developed at the Los Alamos National Laboratory. The output of this solution is 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 MDM information. The SMM generates distributions of turbulent properties within each zone which are necessary to calculate slow emissions chemistry. The submodels included in the SMM are not intended to be unique, but only to represent one example of how this approach might be applied.

This approach was evaluated for consistency 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. The standard deviation of pressure, soot and Nitric Oxide (NO) decreased and meann values and distributions approached asymptotic limits with more elements and more zones. These results are consistent with the structure of the stochastic model. The approach was evaluated for accuracy by comparison to experimental results with different engine operating conditions. The NO calculations were not calibrated in any way to the experimental results and provided the best indicator for honestly evaluating the model's ability to predict slow chemistry. NO predictions and trends showed good agreement with the experimental data.

The Two-Step Approach shows great promise for calculating slow and complex chemistry in turbulent reactive flows. Limitations in our application were due primarily to deficiencies in the MDM solution and to externally-imposed economies on KIVA computer time.

Thesis Supervisor: Prof. John B. Heywood
Title: Director, Sloan Automotive Laboratory

TABLE OF CONTENTS

LIST OF TABLES

✓

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A-1

LIST OF FIGURES

CHAPTER ONE

INTRODUCTION

1.1 Overview

Effective emissions control requires the simultaneous reduction of more than one pollutant. A trade-off exists in diesel engines between the reduction of soot and the reduction of Nitrogen Oxides (NO_x-mostly Nitric Oxide with some Nitrogen Dioxide). NO_x is a product of hot lean combustion and soot is a product of cooler rich combustion. Reducing one normally results in increasing the other, but their mechanisms are complex and influenced by many variables. Ultimately they depend on local composition and temperature which are controlled by engine variables such as compression ratio, intake air temperature and pressure, exhaust gas recirculation (EGR), cylinder geometry, engine speed, load, swirl, injection timing, fuel jet characteristics, and type of fuel. These mechanisms are very difficult to study empirically. A mathematical model of the diesel combustion process would allow its parameters to be varied independently to examine their effects on NO_x and soot. Past models have not given satisfactory results or have been limited to a narrow range of applications. Few have even considered the problem of calculating slow emissions chemistry simultaneously with flow details in a turbulent reactive flow. Such calculations must consider turbulent distributions of temperature and species concentration, but this is a formidable task in an already cumbersome unsteady, three-dimensional flow calculation. This research evaluates the feasibility of using a two-step modeling approach. A multi-dimensional model (MDM) solution to the reactive flow conservation equations is used to define zones within the engine cylinder, to specify the flow between these zones and to calculate evaporation, heat transfer and mixing intensity within the zones. A stochastic mixing model (SMM) uses this information to predict emissions.

1.2 Background

A description of direct-injection diesel combustion provides necessary insight into the complexity of this problem. Direct injection of fuel into the engine cylinder is used in medium and low speed diesel applications. Low speed diesels have flat or slightly concave pistons and relatively little initial air motion (quiescent). Medium speed diesels, which will be considered here, have deeper bowls inset into the piston. They depend on generating significant air flow and turbulence to achieve rapid and complete combustion.

Figure 1-1 shows the basic events in a four-stroke diesel combustion process. Figure 1-2 illustrates a medium speed diesel cylinder and fuel spray geometry. During intake, air is drawn through the intake valve by the descending piston. Bulk motion of the intake charge is controlled by the shape of the intake passage. Typical of most medium speed diesels is a significant swirl motion as indicated in Figure 1-2. The intake valve closes shortly after bottom dead center (BDC). High temperature and pressure are generated as the piston compresses the air and residual gases. Before reaching top dead center (TDC) liquid fuel is injected into the cylinder. The fuel spray is atomized upon leaving the injector and immediately begins evaporating. As the fuel spray entrains and mixes with the hot gases a spray structure develops. This is characterized by a rich liquid core at the center of the spray surrounded by a progressively leaner distribution of fuel and air. Ignition occurs after a chemical ignition delay period. The combustion region spreads rapidly, often from multiple sites, until the fuel already mixed within combustible limits is burned. Following this premixed burning phase combustion becomes mixing controlled and proceeds more slowly. A typical heat release rate curve for this process is shown in Figure 1-3. As the piston passes TDC, the hot, high pressure gases drive the piston down, delivering useful work. Near TDC injection stops. Turbulent mixing and combustion continues until essentially all the fuel is burned. Since diesel combustion is overall very lean, most of the fuel's chemical energy is released. NO_x is produced in the hot, stoichiometric combustion regions. Soot is produced in the richer spray regions bordering the combustion zone. The quantity of soot reaches a maximum towards the end of injection, then decreases due to oxidation. Among the phenomena observed in the diesel combustion process are turbulent two-phase flow, moving boundaries, evaporation, turbulent mixing, ignition, combustion, slower emissions chemistry, convective heat transfer and radiation.

Despite its complexity, diesel combustion is still governed by the general equations for turbulent reactive flows, including conservation of mass, species, momentum and energy. Space and time resolution of this flow far exceeds present computer capabilities. The task is made manageable in state-of-the-art multi-dimensional models (MDM's) by considering only mean local properties with additional assumptions or equations to replace turbulent fluctuation terms. Chemical reaction rates are also expressed in terms of mean local properties. These general equations with boundary conditions and various submodels are then solved in time and space.

Because the reaction rates governing the production of soot and NO_x are much slower than those for combustion and have time scales of the same order as the turbulent fluctuations, the MDM cannot accurately predict emissions. The distribution of turbulent properties must be considered. In order to model more complex chemistry and consider the distribution of turbulent properties, compromises must be made in dealing with flow details. Otherwise, the solution becomes computationally unmanageable. 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. [1] Details of this method are provided in Appendix C. 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 or, in cases with a discharge, for removal from the reactor. This method has been applied to a divided chamber diesel [2] in a previous study at MIT. In this type of engine the fuel is injected into a highly-mixed prechamber for combustion and expansion into the engine cylinder. Unfortunately, direct injection diesel combustion cannot be described as well-mixed. The spatial distribution of the fuel spray and the cylinder geometry play important roles in this process. Ikegami and Shioji [53] use a stochastic single-zone method to calculate chemistry in a direct injection diesel, but their analysis assumes an initial distribution function for the fuel spray and requires a number of empirical parameters.

1.3 The Two-Step Approach

The purpose of a two-step approach to this problem is to provide a fundamentally-based method by which stochastic mixing model techniques may be applied to an inhomogeneous reactive flow such as a direct-injection diesel engine in which flow details are likely to be critical to the calculation. The first step in this approach is to complete a MDM solution of the engine reactive flow. The output of this solution is used to define zones within the engine cylinder according to total fuel mass fraction (burned plus unburned fuel). Four such zones are labeled in Figure 1-2. These zones are not fixed in space, but are dependent on the constantly changing distribution of total fuel within the cylinder. 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 timestep. Using conservation of mass and species, the net flow of total mass, liquid fuel, unburned fuel vapor, and burned fuel between each zone is calculated.

The second step is to model each of these zones as a stochastic mixing zone in a Stochastic Mixing Model (SMM). The flow and process information calculated by the MDM are used to specify flows between mixing zones and constrain 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 is 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 is considered in the calculation of slow chemistry. Figure 1-4 illustrates the flow of information between the MDM and the SMM. Tables 2-1 and 2-2 define the variables used.

1.4 Goals and Objectives

The goal of this thesis is to demonstrate the feasibility of this two-step approach for calculating slow and complex chemistry in turbulent reactive flows. The specific objectives are:

1. To develop a Stochastic Mixing Model computer code based on this two-step approach for calculating emissions in a direct-injection diesel engine.
2. To evaluate the SMM for consistency by analyzing zone distributions, the effect of changing zone boundaries, the effect of increasing the number of zones, the sensitivity to various physical and model parameters and the variance of final results over multiple stochastic runs.
3. To evaluate the SMM by comparison to MDM results which are recalculated, but unconstrained in the SMM such as: pressure, zone burned fuel, zone fuel mass fraction and species flow.
4. To evaluate the SMM by comparing predicted NO histories to experimental results with primary emphasis given to trends as engine conditions are changed.

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

CHAPTER TWO

THE MULTI-DIMENSIONAL MODEL

2.1 Selecting a Multi-dimensional Model

Engine combustion modeling has received much attention in recent years. Models have been developed, reviewed, classified and discussed at all levels of the academic and professional communities. Heywood [4] provides the most widely accepted classification scheme for these models. These classifications include zero-dimensional, quasi-dimensional and multi-dimensional models. Zero-dimensional models do not consider spatial variations within the cylinder and are essentially a thermodynamic analysis. Heat transfer is modeled as bulk heat loss and the mass burning rate is specified by an empirical function. Quasi-dimensional models go a step further and attempt to predict the burning and mixing rates from more fundamental physical variables that describe the spatial structure in a parametric manner. Typically, phenomenalogical models are used for the fuel spray behavior, ignition and mixing.[5] For our application, spacial details of the flow are required to define zones and specify the flow between zones. Therefore, zero or quasi-dimensional models are not adequate. The necessary spatial details are provided only by multi-dimensional models.

Multi-dimensional models solve the fundamental mass, species, momentum and energy conservation equations in time and space. This requires mathematical descriptions or submodels for the fuel spray, ignition, combustion chemistry, heat transfer, and moving boundary surfaces. It requires a sophisticated numerical solution algorithm and a method for dealing with turbulent flow and combustion. This is a formidable task and computational fluid dynamics (CFD) with combustion is really only in its infancy. Our problem was to select a multi-dimensional model from existing computer codes, modify it to provide the particular data required for input to the Stochastic Mixing Model(SMM), and to run the code without major changes to its existing submodels. Codes with this level of sophistication cannot be used as a "black box". Running the code was challenging and educational. Among existing multi-dimensional models for internal combustion engine simulation, three stand out as being reasonably well-documented and as having solution algorithms and submodels which are "state-of-the-art" in their approach. These are:

1. PICALO (Piston-in-Cylinder Calculator) developed by CHAM of North America/Cummins Engine Co.
2. RPM (Reciprocating Piston Motion) developed at Imperial College, London by A.D. Gosman et al.
3. KIVA developed at Los Alamos National Laboratory by A.A.Amsden et al.

PICALO [6], working in conjunction with PHOENICS, a general-purpose flow analysis computer code, treats the two-phase flow as interpenetrating media using a continuum approach with coupling terms for mass, momentum and energy exchange between media. The conservative finite-difference numerical algorithm is fully implicit and iterative. A $k-\varepsilon$ model is used to model turbulence. Boundaries are treated as adiabatic and "no-slip". Instantaneous mixing-controlled chemical reaction is assumed.

The development and application of RPM has been well-documented for over a decade.[7,8,9,10,11,12] Most of the documented RPM versions use a curvilinear-orthogonal grid able to expand and contract in the axial direction. The conservative finite-difference numerical scheme is fully implicit and iterative. The most recent version uses a predictor/corrector algorithm in place of the iterative technique. All versions use a combination of upwind and central differencing for the discrete convection and diffusion terms. A $k-\varepsilon$ model is used to model turbulence. Boundaries are treated using a "law-of-the-wall" technique. Most of RPM's published applications have been for cold flow, but in the cases where combustion was included [8,9] a combination of an Arrhenius rate equation for the chemically controlled phase and an eddy mixing-model for the mixing controlled phase were used. A stochastic discrete-particle model is used to model the liquid spray. Although the RPM model was not selected for our use, the results presented in references [8] and [9] provide some interesting comparisons.

KIVA was selected for our application. A description of KIVA will be presented in the next section. The primary reasons for selecting KIVA were availability, excellent documentation, its ability to calculate multi-component chemistry, its extensive use of vector calculations and its computational efficiency at low Mach number.

2.2 Description of KIVA

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 uses an arbitrary-Lagrangian-Eulerian (ALE) mesh which facilitates calculations with curved and changing boundaries. The species and chemical reactions that can be represented in KIVA are not limited. The documentation for KIVA [13,14] is excellent and contains an extensive list of references and more detail than will be presented here.

2.2.1 KIVA Nomenclature

A	Scaling constant of order .05
a_{mr}, b_{mr}	stoichiometric coefficients for species m in reaction r; a for reactants, b for products
a'_{mr}, b'_{mr}	order of reaction for species m in reaction r
D	species diffusivity (same all species)
∇	vector operator $\underset{\sim}{\nabla} = \underset{\sim}{i} \frac{\partial}{\partial x} + \underset{\sim}{j} \frac{\partial}{\partial y} + \underset{\sim}{k} \frac{\partial}{\partial z}$
δ_{ij}	Kronecker delta
f	drop distribution function
$\dot{f}_{coll}$	rate of change in f due to drop collisions
$\underset{\sim}{F}$	drop acceleration
$\underset{\sim}{F}_S$	momentum transfered from spray droplets
h_m	specific enthalpy of species m (datum at absolute zero)

I	specific internal energy (datum at absolute zero)
$\underset{\sim}{J}$	heat flux vector
k_{fr}, k_{br}	forward and backward rate coefficients for reaction r
K	thermal conductivity
K_c^s	Equilibrium constant for reaction s
μ_{air}	air viscosity
μ_t	turbulent viscosity
ν_o	background kinematic viscosity
p	pressure
Pr	Prandtl number
q	subgrid-scale specific turbulent kinetic-energy (cm^2/sec^2)
$\dot{Q}_c$	rate of chemical heat release
$\dot{Q}_S$	spray energy source rate
q_r	heat of reaction r
$\dot{Q}_T$	turbulent disipation source rate
$\dot{R}$	rate of change in drop radius
ρ	total mass density (g/cc)
ρ_1	fuel(ex: diesel) density
ρ_m	species m mass density (g/cc)

$\dot{\rho}_m^C$	change in ρ_m due to chemical reaction
$\dot{\rho}_S$	change in fuel density (ρ_1) due to evaporation
Sc	Schmidt number
$\underset{\approx}{\sigma}$	viscous stress tensor
t	time (s)
T	absolute temperature (K)
$\dot{T}_d$	rate of change in drop temperature
$\underset{\sim}{u}$	fluid velocity (cm/s) $\underset{\sim}{u} = u\underset{\sim}{i} + v\underset{\sim}{j} + w\underset{\sim}{k}$
$\dot{\underset{\sim}{u}}'$	rate of change in drop gas turbulence velocity
$\dot{\omega}_r$	kinetic progress rate for reaction r
W_m	molecular weight of species m
χ_m	mole of species m

2.2.2 The Basic Equations

The conservation equations for mass, species, momentum and energy as expressed in KIVA are:

$$\frac{\partial \rho}{\partial t} + \underset{\sim}{\nabla}\cdot(\rho\underset{\sim}{u}) = \dot{\rho}_S \tag{2.1}$$

$$\frac{\partial \rho_m}{\partial t} + \underset{\sim}{\nabla}\cdot(\rho_m\underset{\sim}{u}) = \underset{\sim}{\nabla}\cdot[\rho D\underset{\sim}{\nabla}(\rho_m/\rho)] + \dot{\rho}_m^C + \dot{\rho}_S\delta_{m1} \tag{2.2}$$

$$\frac{\partial}{\partial t}(\rho\underset{\sim}{u}) + \underset{\sim}{\nabla}\cdot(\rho\underset{\sim}{u}\underset{\sim}{u}) = -\underset{\sim}{\nabla}p + \underset{\sim}{\nabla}\cdot\underset{\approx}{\sigma} + \underset{\sim}{F}_S \tag{2.3}$$

$$\frac{\partial}{\partial t}(\rho I) + \underset{\sim}{\nabla}\cdot(\rho I\underset{\sim}{u}) = -p\underset{\sim}{\nabla}\cdot\underset{\sim}{u} + \underset{\approx}{\sigma}:\underset{\sim}{\nabla}\underset{\sim}{u} - \underset{\sim}{\nabla}\cdot\underset{\sim}{J} + \dot{Q}_C + \dot{Q}_S + \dot{Q}_T \tag{2.4}$$

where:

$$\underset{\sim}{J} = -K\underset{\sim}{\nabla}T - \rho D \sum_m h_m \underset{\sim}{\nabla}(\rho_m/\rho) \qquad (2.5)$$

State relations are for an ideal gas mixture. Chemical reactions are represented by:

$$\sum_m a_{mr}\chi_m \rightleftarrows \sum_m b_{mr}\chi_m \qquad (2.6)$$

The chemical source term in the species continuity equation is then given by:

$$\dot{\rho}_m^C = \hat{W}_m \sum_r (b_{mr} - a_{mr})\dot{\omega}_r + \hat{W}_m \sum_s (b_{ms} - a_{ms})\dot{\omega}_s \qquad (2.7)$$

and the chemical heat release in the energy equation by:

$$\dot{Q}_C = \sum_r q_r\dot{\omega}_r + \sum_s q_s\dot{\omega}_s \qquad (2.8)$$

Fast reactions are assumed to be in equilibrium. Slower reactions are advanced kinetically. Kinetic reaction rates are computed using:

$$\dot{\omega}_r = k_{fr} \prod_m (\rho_m/W_m)^{a'_{mr}} - k_{br} \prod_m (\rho_m/W_m)^{b'_{mr}} \qquad (2.9)$$

where:

$$k_{fr} = A_{fr}T^{\zeta_{fr}}\exp(-E^+_{fr}/T) \qquad (2.10)$$

$$k_{br} = A_{br}T^{\zeta_{br}}\exp(-E^+_{br}/T) \qquad (2.11)$$

Equilibrium reaction rates are implicitly determined from the equilibrium constraints:

$$\prod_m (\rho_m/W_m)^{b_{ms}-a_{ms}} = K_c^s(T) \qquad (2.12)$$

where:

$$K_c^s = \exp(A_s \ln T_A + B_s/T_A + C_s + D_s T_A + E_s T_A^2)$$

$$T_A = T/1000$$

Complete space and time resolution of a turbulent flow far exceeds present computer capabilities. KIVA assumes a Reynold's decomposition with mass or Favre averaging and applies the same conservation equations (2.1 thru 2.5) in terms of local mean properties to the turbulent flow. Reynold's decomposition expresses dependent variables as the sum of mean and fluctuating components. For an unsteady cyclic process this mean represents an ensemble mean or average over many cycles at a particular time in the cycle. Ensemble averaging of the decomposed conservation equations results in similar equations using local mean properties, but with additional terms containing products of the fluctuating components. There are more unknowns than equations. This is the turbulent closure problem. The most common closure scheme is to model these additional terms as a turbulent gradient flux and to replace the molecular transport coefficients with turbulent ones. The turbulent coefficients are then calculated using additional algebraic or partial differential equations to describe the turbulence. KIVA follows this scheme and calculates turbulent viscosity using a subgrid-scale turbulence model (SGS) with a single partial differential equation for subgrid turbulent kinetic energy:

$$\mu_t = A\rho L q^{1/2} \qquad \mu = \rho\nu_0 + \mu_{air} + \mu_t$$

$$K = \mu c_p/Pr \qquad D = \mu/(\rho Sc) \tag{2.13}$$

$$\frac{\partial}{\partial t}(\rho q) + \underset{\sim}{\nabla}\cdot(\rho q \underset{\sim}{u}) = -\frac{2}{3}\rho q \nabla\cdot\underset{\sim}{u} + \underset{\approx}{\sigma}:\underset{\sim}{\nabla}\underset{\sim}{u} + \nabla\cdot(\mu\underset{\sim}{\nabla}q) - D\rho L^{-1}q^{3/2} + \dot{W}_S \qquad (2.14)$$

KIVA also replaces temperature and concentrations in the chemical equations with local mean values assuming that the chemical reactions are fast enough not to be effected by turbulent fluctuations. This is not valid for the slower emissions chemistry. The rational for including the effects of turbulent fluctuations on slower chemistry is developed in Appendix C.

The fuel spray is modeled using a Monte Carlo discrete-particle technique. Discrete computational particles represent groups of droplets of similar physical properties. A drop distribution function, f, is used to specify these properties including location, velocity, radii, temperature and gas turbulence velocity. The gas turbulence velocity is added to the local mean gas velocity when calculating drag and vaporization rate. Drops may collide resulting in either coalescence or an exchange of momentum. The time evolution of f is given by the spray equation:

$$\frac{\partial f}{\partial t} + \underset{\sim}{\nabla}\cdot(f\underset{\sim}{v}) + \underset{\sim}{\nabla}_v\cdot(f\underset{\sim}{F}) + \frac{\partial}{\partial r}(fR) + \frac{\partial}{\partial T_d}(f\dot{T}_d) + \underset{\sim}{\nabla}_{u'}\cdot(f\dot{\underset{\sim}{u}}') = \dot{f}_{coll} \qquad (2.15)$$

The droplet acceleration, F, is calculated from gas flow velocities using a drag coefficient. The rate of droplet radius change is calculated using the Frossling correlation. Heat conduction to the droplet is given by the Ranz-Marshall correlation. This set of coupled equations is solved to generate a time-dependent, spacially-resolved description of the particle motion. Exchange functions for mass, momentum and energy are calculated from this description of the spray and included as source terms in the gas flow conservation equations.

2.2.3 Numerical Solution

The basic equations are reformulated in integral form so that schemes explicitly conserving mass, species, momentum and energy may be implemented. The temporal difference scheme is explicit using an acoustic subcycling method at low Mach numbers. Spacial differencing is on an arbitrary Lagrangian /Eulerian grid (ALE). Spatial difference approximations use a control volume approach to conserve local properties.

Quantities are advanced one cycle, from time t^n to time t^{n+1}, in three phases. Phase A considers terms in the basic equations other than pressure and convection. Phase B is a Lagrangian sub-cycling calculation considering acoustic terms (pressure,work,spray particle drag) in which the vertices of the volume elements are assumed to move with the local fluid velocity. Phase C is the rezone phhase, in which convective transport associated with moving the vertices from their Phase B locations to their final locations is calculated. Timesteps are adjusted each cycle based on minimum stability requirements.

The general structure of the code is shown in Figure 2-1. The code was written specifically for the CRI Cray-1 computer.

2.3 Modifications to KIVA

Six types of modifications were made to the documented version of KIVA [13] for our application:

1. Modifications for compatibility with the VAX/CRAY System at the Navy Research Lab, Washington, where most of

the KIVA runs were made.

2. Modifications for calculating data for input to the Stochastic Mixing Model(SMM).

3. Modifications for using the MIT "standard" diesel fuel.

4. Modifications to increase diffusivity and the rate of combustion on the expansion stroke.

5. Other minor modifications adapting the code to this application.

6. Los Alamos National Lab(LANL) KIVA update 092085/1435. [15]

The update decks for these changes are listed in Appendix E.

Subroutine MDMOUT calculates zone properties for output to the SMM. KIVA computational cells are sorted by total fuel mass fraction (TFMF) into ten zones. Properties for each of these zones are calculated and written to an output file for subsequent post-processing and input to the SMM. These properties are listed in Table 2-1 and their relationship to the SMM illustrated in Figure 1-4.

The documented version of KIVA includes data for octane combustion. Specifying a different fuel in the input data requires changes to data statements in Subroutine RINPUT. This data includes fuel enthalpy, latent heat, and vapor pressure. The fuel used in our calculations is a multicomponent "standard" diesel fuel, $C_{10.8}H_{18.7}$. Coefficients used for calculating fuel enthalpy are from Reference [16]. Latent heat and vapor pressure values used are for dodecane [17].

The requirement to increase diffusivity on the expansion stroke will be discussed in Section 2.5. This was accomplished by gradually increasing variables ATKE, RPR and RSC after top dead center.

Originally, the law-of-the-wall heat transfer model predicted only

7-8 per cent of the total heat release as heat loss to the wall. This was substantially lower than the 12-15 per cent expected. In order to compensate for this discrepancy the constant C_W in the following heat flux equation was increased from 1.125 to 2.0:

$$J_w = C_w\,(\tau/U)c_p(T - T_w) \tag{2.16}$$

A similar change was reported in constant volume bomb simulations using KIVA at Purdue University [18].

Ignition crank angle is specified as an input to the calculation. The code was modified to delay all chemistry until ignition at which point chemical reaction proceeded spontaneously. Spark ignition was not required.

A spray model update developed at LANL, but not included in the documented update, was used. In this update the spray turbulent kinetic energy is calculated independent of the flow turbulent kinetic energy and the particle diffusion algorithm is modified for spray turbulent correlation times smaller than the computational time step. These changes were required to achieve reasonable spray penetration without artificially changing the values of the input spray parameters.

2.4 Selecting Model Parameters and Running KIVA

Complete KIVA input for the five test cases is listed in Appendix A. The following parameters required particular consideration for this application:

NX	Number of radial cells. 22 for all runs.
NY	Number of azimuthal cells. Set to 1 for this axisymmetric calculation. Although KIVA is capable of 3-D calculations, an axisymmetric geometry was chosen to conserve computer time.

NZ	Number of axial cells. 18 for all runs. Grid points along the piston bowl were laid out on graph paper. Eleven planes were chosen for the squish region at the start of the run (-90° ATDC). Approximately 400 total cells were desired. Actual indices for the piston bowl are input variables KPO, RPO and ZPO. Figure 2-2 shows the resulting grid layout at -90° ATDC and TDC.
LWALL	+1 selects law-of-the-wall boundary conditions which were used for all calculations.
NCHOP	KIVA uses a CHOP routine to reduce the number of planes in the squish region as the piston approaches TDC. A minimum thickness of 3 cells in the squish region was chosen for all calculations. NCHOP=3. See Figure 2-2.
STROKE, SQUISH, RPM, CONROD, SWIRL, CA1INJ, CA2INJ, TSPMAS	Values for engine parameters were taken directly from the engine test data. [19]
CONE, DCONE	A hollow cone spray pattern must be used with an axisymmetric geometry to simulate the actual 8-hole spray pattern With moderate swirl and 8 holes this is a reasonable approximation. The injection angle used was from the engine test data. A spray included angle of 15 degrees was used for all runs.

TEMPI RHO1-12	Initial charge temperature and composition were specified at -90° ATDC using the data supplied in the test results and the NASA equilibrium code to calculate burned composition. The initial charge includes air, water vapor, residual fraction, and EGR.
A0,B0	These parameters were set to 0 and 1 respectively. This results in a weighted average between centered and upwind differencing for evaluating cell-faced quantities. The weighting factor is calculated each timestep for marginal stability. This is KIVA's least numerically diffusive differencing scheme.
UVFREE	Set to 1.0 for all runs. Allows the velocities along flat vertical and horizontal walls to "float". Momentum loss for vertices one cell away from the wall is calculated using the law-of-the-wall. Velocities along walls where UVFREE=1.0 are then calculated as if the wall were not there. No-slip boundaries were found to be over-restrictive on the flow. This remains a problem on curved surfaces.
ADIA, TWALL	A constant wall temperature (ADIA=0.,TWALL=400.) was used for all runs.
CA1IGN	Crank angle at ignition was specified as input. Its value was determined from the experimental pressure trace Chemistry is not allowed to occur until ignition.
TKEI, DTKE, ATKE	Various values for the turbulent parameters were tried in the preliminary runs. Those specified in the KIVA documentation were found to work well.
RPR,RSC	Prandtl and Schmidt numbers of approximately 0.9 were used for all calculations. This differs from the value of 1/3 used in the documented KIVA test case.

SMR	Reference [20] provides an excellent overview of modeling and measuring engine fuel sprays. A review of the engine spray literature indicates a broad range of predicted and measured Sauter Mean Radius. 9.5 μm represents a typical initial SMR for $\Delta p_{inj}=21$ MPa. This value was used for all KIVA runs.
VELINJ	An initial injector velocity of 166 m/s was calculated for $\Delta p_{inj}=21$ MPa and $C_D=0.76$. This value was used for all KIVA runs.
MW1, HTF1, CF1,AM1, BM1	Input chemical reaction properties were modified for burning diesel fuel vice octane.

Run times for an axisymmetric simulation from -90° to 80° ATDC were approximately 18 minutes on a CRAY X-MP/12 computer. Contour plots of the KIVA results were obtained by post-processing KIVA output data using Program KIVAPP.

2.5 KIVA Results

In addition to the KIVA output to be processed and used by the SMM, contour and global property plots were generated in order to examine the multi-dimensional results more directly. This section will discuss the plots for Run 17 which is the basic retarded injection test case with an injection crank angle of -15°, swirl ratio of 2.46 and zero EGR. Figures 2-3 thru 2-7 are global plots of pressure, mass, and heat release rate versus crank angle. Figures 2-8 thru 2-20 are plots of velocity, spray particle distribution, total fuel mass fraction (TFMF), oxygen mass fraction, and temperature.

2.5.1 Pressure, Mass and Heat Release Rate

Figure 2-3 compares the KIVA pressure trace with the test results for Test Case 17 [19]. The rapid rise in the KIVA trace has two probable causes. The global chemistry scheme used by KIVA does not include any precursive chemistry. Once ignition is allowed to occur the premixed portion of the fuel vapor is burned very rapidly, dependent only on temperature and equivalence ratio. Furthermore, the coarse grid spacing is larger than the actual flame thickness so that the burned mass is discretized to elements larger than the actual burned amount. This results in excessive flame speeds and faster burning.

The experimental data used in our analysis was obtained from experiments conducted at the University of Wisconsin-Madison (Chapter 4). Using a dump and quench technique, average cylinder NO versus crank angle was measured in a direct-injection diesel engine. [19] This data is difficult to obtain and so far as we know it is the only time-resolved, cylinder-averaged NO data available for DI diesels. The NO data from these experiments is internally very consistent and the procedures thorough and well-documented. Unfortunately, the experimental pressure traces have some questionable features. This can be seen in the Test Case 17 results, Figure 2-3. Prior to ignition, which occurs at -7.8° ATDC, the experimental trace shows a slight loss in pressure below the motoring trace. Once ignition occurs, the pressure increase seems to "fizzle out" instead of following a more conventional shape. These discrepancies occur to a varying degree in four of the five test caces, but in Test Case 19 these problems are not apparent. See Figure 2-4. Case 19 is also the only test case in which the peak experimental pressure exceeds that predicted by KIVA. This variable pressure loss may result from leakage around the dumping diaphragm (see Section 4.1) which was replaced after each dumping event, accounting for different leakage from run to run. Another uncertainty in these traces is the problem of unburned fuel. The KIVA simulation did not achieve complete combustion in any of the test cases. Although hydrocarbons were not measured in the experiment it was observed that combustion was poor and a great deal of smoke was generated. The extent to which KIVA is accurately predicting this problem is not known. This unknown prevented accurate heat release analysis of the experimental pressure trace to determine if leakage was occuring.

Despite these discrepancies, the KIVA results provide a reasonable approximation to the experimental data and are consistent when compared to each other. This is an important characteristic when evaluating trends in the SMM results. Figure 2-5 compares the KIVA pressure traces for the 5 test cases. (Table 4-2) Maximum pressure for the early injection case, Test 19, is 10 to 15 atmospheres higher than the other runs and occurs earlier. Maximum pressure for the two retarded injection cases with EGR, Tests 20 and 21, is 2-3 atmospheres lower than the cases without EGR, Tests 17 and 18. Test 20 has the lowest peak pressure. These comparisons are the same for the KIVA results and the experimental results.

The heat release rate, Figure 2-6, has a typical profile for diesel combustion with a reasonably long ignition delay. The large premixed burning spike is followed by diffusion or mixing controlled burning. The noise in this trace is attributed to the relatively coarse grid where the burning of a single grid cell has a significant effect on the overall heat release.

Figure 2-7 shows mass of fuel injected, mass of fuel evaporated, and mass of fuel burned versus crank angle. Once ignition occurs, the mass evaporated trace shoots up much more quickly, closely following the mass of fuel injected. The problem with incomplete combustion is evident in the fuel mass burned plot. At approximately 20° ATDC there is a distinct elbow in the mass burned curve and by 80° only 85 per cent of the fuel has burned. This is attributed to a lack of large scale convective flow in the lower portion of the bowl and possibly to insufficient penetration of the fuel jet.

2.5.2 Mean Local Properties

Before analyzing the sequence of local property plots, a brief discussion of initial conditions is necessary. A fundamental assumption for axisymmetric calculations is that the 3-D flow structure during induction is short-lived. Gosman reports [11], "for axisymmetric chambers in the absence of complicating features such as port arrangements which produce pre-swirl, that: (i) The induction-generated mean flow pattern decays very rapidly during and after intake valve closure and the flow during compression is predominantly driven by piston motion. (ii) The induction generated turbulence also decays rapidly." However, in his experiments with a shrouded inlet valve a single strong tumbling vortex was found to persist long enough into compression to be sustained and enhanced by the compression. Our KIVA runs assume only solid body swirl (swirl ratios of 2.46 and 4.0) for the initial flow at -90° ATDC, 30 degrees after IVC. Considering the use of a shrouded valve to generate swirl in the test engine and in light of Gosman's results, our assumed initial conditions may not be accurate, but they are necessary to achieve the computational savings of an axisymmetric solution.

Figure 2-8 shows the location of fuel spray particles at three crank angles during injection. The fuel is injected from a point at the upper left hand corner of the axisymmetric plot. The left hand side of the plot is the centerline. The bottom curved surface is the piston bowl and the bottom flat surface is the top of the piston in the squish region. The right hand vertical surface is the cylinder wall and the flat top surface is the cylinder head. Injection starts at -15° ATDC and continues until +5°. By -5° reasonable penetration has been achieved, but combustion has started and evaporation is very rapid. By TDC evaporation has greatly reduced the penetration and only a few particles remain although injection is still going on.

Figures 2-9 thru 2-11 are plots of the swirl velocity. Note that since the swirl is in the negative direction the "L" in the plots represents the largest swirl velocities and the "H" represents the smallest. The swirl profile at -90° ATDC is strictly solid body with boundary layers. By -15.95°, just prior to the start of injection, the drag in the squish region is evident, but the profile is still basically solid body. There is a strongly swirling region at the radius just inside the squish region. This is due to the conservation of angular momentum of the squish flow. By -9.99° the momentum exchange between the flow and the fuel spray is evident. Its effect is to slow the swirl velocity down, conserving momentum. This is particularly true along the cylinder head where the spray's ability to entrain the swirling gas is limited. Conservation of angular momentum causes the swirl to increase as the piston passes TDC with the maximum swirl velocity increasing from 12.8 m/s at -90° to 14.7 m/s at +5° and then decaying to 9.4 m/s by +80° ATDC.

Figures 2-12 thru 2-14 are plots of velocities in the axisymmetric plane. At -90° ATDC these velocities are zero at the cylinder head and equal to the piston speed at the piston with a nearly linear profile from piston to head. By -30° flow out of the squish region has already started to alter the initial flow condition. By -16° the squish flow has developed into a well-defined clockwise vortex in the piston bowl, but does not penetrate into the boundary layer cells.

Injection starts at -15° ATDC. Injection is at a 24 degree angle with respect to the cylinder head. The velocities induced by the injection are an order of magnitude larger than the existing flow velocities. Since the plots are scaled to the highest velocities, plots from -10° to +10° ATDC are dominated by the spray and velocities away from the spray appear to be zero. The spray is able to entrain gas from below, but unable to entrain gas along the cylinder head. This results in a clockwise circulation into the base of the spray and out along the head as seen in Figure 2-13. Combustion starts at -7.2° ATDC. By +5° combustion is also having an effect on the flow. Velocities away from the combustion zone are augmented by the expansion of hot gases. By 10° the flow back into the squish region is well-defined. The excess from the flow along the cylinder head is bent down into the bowl generating another clockwise vortex. This vortex flow meets the combustion and spray generated flow in the middle of the bowl, creating a stagnation point. This stagnation point is also evident in the Total Fuel Mass Fraction (TFMF), oxygen and temperature plots. The flow is again dominated by the piston motion as the piston continues to move down.

Figures 2-15 thru 2-20 are contour plots of total fuel mass fraction (TFMF), oxygen mass fraction and temperature. They are best discussed together at each crank angle. At -9.99° ignition has not occurred and evaporation is slow. Fuel vapor is confined to a small region around the center of the spray. The evaporative cooling effect is very evident in thee same region on the temperature plot. By -5° ATDC combustion has started. Note that the temperature plot indicates a maximum cell temperature of 3498 K. This is extremely high, well above the adiabatic flame temperature of 2940 K. The relatively large timestep, when applied to the stiff set of chemical-reaction equations, causes pressure and temperature overshoots in large rapidly-burning cells. The major impact of these temperature overshoots is to drive the NO_x production rate calculated by KIVA way up. At TDC combustion is well underway. The premixed region extends out to the Low TFMF contour. Temperature profiles inside this region are very irregular with no distinct flame front. The oxygen inside this region is nearly depleted and the premixed burning phase is almost over. By 10° ATDC the temperature contours show a distinct diffusion flame front just behind the Low TFMF contour moving towards the curved portion of the bowl. During expansion the steep gradients are smoothed out by turbulent and numerical diffusion resulting in a large diffusive front. The expanding grid results in increasing and excessive numerical diffusion which quickly damps out all large scale convection. This limits the mixing between the large untouched air mass along the bottom of the bowl and the fuel-rich combustion region. The development of this large diffusive front coincides with the abrupt change in the burning rate seen in the burned fuel mass plot. The oxygen plots also show a very large region of unmixed air along the curved portion of the bowl. The mixing of fuel and air during the expansion process is severely limited. Since the numerical diffusivity could not be reduced without a substantial decrease in grid spacing and a corresponding increase in run time it was decided to increase the diffusivity even further. In order to compensate for the loss of large scale convection and reduce the unburned fuel at the end of the cycle, diffusivity was artificially increased after TDC.

In summary, these plots provide a self-consistent picture of the mixing and combustion process although this picture differs somewhat from our understanding of what really happens in a DI diesel. We would expect greater penetration of the fuel spray, significant convective and large-scale turbulent flow lasting well into the expansion process and more complete mixing of fuel and air with most of the fuel being burned by +80° ATDC. Deficiencies can be explained by the simplicity of the initial conditions, the coarse computational grid, and the universal problem of modeling turbulence and turbulent boundary flows. These deficiencies become most significant during the expansion process. For now, KIVA provides the best multi-dimensional picture of diesel combustion available. It is not our purpose to validate or improve KIVA, but to evaluate a two-step approach for predicting emissions. Results are at least reasonable and internally consistent, particularly near TDC where most of the critical NO chemistry takes place. KIVA should provide an adequate input for evaluating the SMM approach.

2.6 Processing KIVA Output

Program PRCMDM, listed in Appendix F.1, processes the KIVA output for input to the SMM. Its relationship to KIVA and the SMM are illustrated in Figure 1-4. Table 2-1 defines the input variables to PRCMDM. In order to keep the quantity of data generated by KIVA within reasonable limits the KIVA output is presorted into ten zones. This limits the number of mixing zones in the SMM to ten, but allows any combination of these ten zones to be used. Table 2-2 lists the ten zones and the various combinations used in our analysis. Table 2-3 defines the output variables from PRCMDM to the SMM. PRCMDM has four functions:

1. Inputs data from KIVA.
2. Combines the ten zone KIVA data to achieve the desired zone description.
3. Calculates the total mass flow, fuel vapor flow and burned fuel flow between zones using conservation of mass/species.
4. Outputs data for input to the SMM.

Ten zone KIVA output data for Test Case 17 is shown in Figures 2-21 thru 2-46. The zone mass plots, Figures 2-21 and 2-22 illustrate the growth and disappearance of zones. At the start of injection, -15° ATDC, only the air zone, zone 10, exists. As fuel is evaporated cells become richer and they are rezoned into progressively richer zones. In this way richer zones grow out of leaner ones. The coarse grid has again caused significant noise in this data. Initially we were concerned about the effect of this noise on the SMM results. To determine the extent of this effect, one set of data was smoothed before input to the SMM. The difference between the results using the raw data and the results using the smoothed data was negligible and all subsequent runs were made using raw data.

The data was also checked for consistency. The total zone mass plus the total zone liquid mass equaled the original charge mass plus the mass of fuel injected. The total zone liquid mass plus the total zone fuel vapor mass plus the total zone burned fuel mass equaled the mass of fuel injected. Mean zone temperature was highest in the stoichiometric zone. Zone mixing intensity is maximum around TDC and in zones where the fuel spray is most prominent. Mixing intensity decays during expansion. Zone mean TFMF is progressively higher in richer zones and within zone limits. Total zone volume is equal to the cylinder volume. NO_x mass fraction is highest in zones with the highest mean temperatures. Cumulative mass of fuel evaporated is equal to total zone fuel vapor mass plus total zone burned fuel mass less the original burned fuel mass. Total heat release agrees with total fuel burned and total wall heat transfer is about 15 percent of the total heat release.

CHAPTER 3

THE STOCHASTIC MIXING MODEL

3.1 Assumptions

The basic assumption underlying our two-step approach is that an inhomogeneous reactive flow, such as in a D.I. 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. Total fuel mass fraction (burned plus unburned) is used to define the zones. These zones are not fixed in space, but constantly change as the total fuel mass fraction distribution within the cylinder changes. There is no spatial resolution within the zones and each zone is considered to be perfectly macromixed. Figure 3-1 illustrates a typical zone arrangement. Output from a multi-dimensional model solution is used to define the zones, to specify the flow between zones and to constrain certain processes within the zones. It is also assumed that the slower emissions chemistry does not produce or use significant energy and is therefor only a perturbation of the major combustion and flow dynamics which are correctly modeled by the MDM.

3.2 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 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 element consists of two primary components, unburned fuel vapor and burned gas. The burned gas fraction (BGFR) includes air and burned products. The BGFR 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 (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 chemical properties, evaporation, heat transfer and volume.

Figures 3-2 and 3-3 illustrate the SMM's basic structure. Figure 1-4 illustrates the relationship between the SMM and the MDM. There are three primary inputs to the SMM:

1. Equilibrium data. Tables with standard enthalpy, specific heat, molecular weight, and equilibrium products are stored as a function of temperature, pressure and total equivalence ratio. These properties are calculated using the NASA equilibrium code as described in Appendix D.

2. MDM data. The processed MDM output as described in

Section 2.6 includes mass flow, zone fuel evaporated, zone volume, zone heat transfer, and zone mixing intensity.

3. NAMELIST data. Contains the SMM simulation control parameters, combustion and soot parameters, and fuel characteristics.

The equilibrium data and NAMELIST data are input at the start of the simulation by Program SMM. Program SMM updates the simulation time and initiates the mixing events. When it is time for the next MDM update, Program SMM calls Subroutine SMZ. Subroutine SMZ first completes the previous MDM timestep for each zone by updating the heat transfer, updating the chemical properties, and conserving volume. Subroutine SMZ 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 by Program SMM as the basic simulation time increment. Once these updates have been made, control returns to Program SMM and mixing continues until the next update.

3.3 Submodels

The following sections describe the various submodels included in the SMM. The fundamental structure of these submodels relies heavily on work done by Mansouri [2] and Sztenderowicz [21] although the overall structure and application is quite different.

3.3.1 Mixing

Program SMM calls Subroutine MIXING whenever it is time for a mixing event in a particular zone i. This subroutine performs zone mixing.

Our basic approach requires that the individual zones be modeled as stochastic mixing zones. Appendix C describes the details of this method. Each mixing zone is perfectly macromixed with the degree of micromixing determined by the mixing intensity, β_i. The method used for mixing is coalescence/dispersion.

Each zone consists of N_i equal mass elements. Turbulent mixing within zone i is characterized by the mixing intensity:

$$\beta_i = \frac{1}{\tau_{m_i}} \qquad (3.1)$$

where τ_{mi} is the characteristic time for all elements in the zone i ensemble to undergo one mix. For N_i elements, the time between element mixing events, t_{mi} is:

$$t_{m_i} = \frac{1}{N \beta_i} \qquad (3.2)$$

A single mixing event in zone i consists of the following:

1. Two elements within zone i are chosen at random. This is accomplished using a random number generator which produces values of a single random variable that is evenly distributed between zero and one. This value is multiplied by the number of elements in the zone and rounded up to the nearest integer. This integer identifies the element number, i. The probability that any one element will be chosen is $1/N_i$.
2. The properties of each element are updated.
3. The elements are combined and then separated again into two elements with equal properties, conserving species mass and enthalpy.
4. If the new elements satisfy the combustion criteria after mixing, they are burned.

The characteristic mixing time, τ_{mi}, is the same order of magnitude as the kinetic update time, consequently t_{mi} becomes very small for large values of N_i. The value of t_{mi} is updated for each zone at the start of each MDM timestep and the smallest of the zone mixing times is used by Program SMM for the basic simulation timestep.

3.3.2 Flow

Subroutine SMZ calls Subroutine FLOW at the start of each MDM timestep. As discussed in Section 2.5, Program PROCMDM uses conservation of mass to calculate net mass flow, fuel vapor mass flow, and burned fuel mass flow between zones. These flows represent convection, turbulent diffusion, and the rezoning of cells to richer or leaner zones due to changes in their total fuel mass fraction. These are net flows. They do not consider all exchanges back and forth across zone boundaries.

The flow between zones in the model must be accomplished within the model structure. This means exchanging elements between two ensembles of elements. In order to develop an effective algorithm for modeling the flow, the following objectives and constraints were considered:

1. Zone elements must be kept intact.
2. The selection of elements should adhere to the basic "random selection" criteria to the greatest extent possible.
3. The exchange of elements must transfer the correct net mass flow (FM).
4. The exchange of elements must transfer the correct amounts of fuel vapor (FMV) and burned fuel (FMBF). To accomplish this, combustion in each zone must approximate the MDM and the flow algorithm must include one for one exchange of elements across the boundary in addition to the net flow.
5. The resulting overall distribution of elements according to total fuel mass fraction should be continuous at zone boundaries and should converge to a single distribution as the number of zones increases.

A number of alternative algorithms were tried. The following algorithm best satisfied our objectives and constraints (Refer to Figure 3-1):

1. Calculate the number of elements required to flow between zones to satisfy the net total mass flow (FM). The net mass flow between any two zones will be from a donor zone to a receiving zone. Arrows in Figure 3-1 indicate the positive direction, but FM, FMV and FMBF may be independently positive or negative.

2. The flows are considered is sequence, starting with flow number one. (FM(1),FMV(1),FMBF(1))

3. Elements in the donor zone are sorted into three groups: (1) Elements containing fuel vapor (total fuel mass fraction greater than the upper limit for combustion), (2) Elements rich in burned fuel (burned fuel fraction greater than the lower limit for combustion) and (3) Lean elements (other).

4. When selecting the flow elements, if the required fuel vapor flow (FMV) is in the same direction as the total flow (FM) and exceeds the required burned fuel flow (FMBF), random elements are selected from Group 1 in the donor zone and added to the receiving zone. If the required burned fuel flow (FMBF) is in the same direction as the total flow (FM) and exceeds the required fuel vapor flow (FMV), random elements are selected from Group 2 in the donor zone and added to the receiving zone. Otherwise random elements are selected from Group 3 in the donor zone and added to the receiving zone. If the elements in a particular group run out and an element is required, a random element is selected from all the remaining elements in the donor zone and added to the receiving zone. This net flow process is continued until the total mass flow requirement (FM) is satisfied.

5. Once the net total mass flow has been achieved there may still be significant discrepancies in fuel vapor (FMV) and burned fuel (FMBF) flows. These discrepancies are cor-

rected by exchanging elements one for one between the two zones. Elements in both zones are sorted into the groups as described in item 3 above. One element is selected from each zone according to the same criteria as item 4 above. These elements are exchanged between the two zones. This process is repeated until the fuel vapor and burned fuel flows are within tolerance or one of the groups runs out of elements.

Subroutine FLOW accomplishes the net flows and calls Subroutines MIXINGA or MIXINGB if one for one exchange is required to accomplish the correct fuel vapor and burned fuel flows. Subroutine MIXINGA is used for flow to and from the air zone. Subroutine MIXINGB is used for all other flows.

3.3.3 Evaporation Model

The amount of fuel evaporated in each zone during the next MDM timestep is input with the MDM data by Subroutine SMZ at the start of each MDM timestep. If this amount exceeds the mass of one element and if there are already elements in the zone with which the fuel vapor can mix, Subroutine SMZ calls Subroutine EVAP.

Subroutine EVAP selects a random element already in the zone, updates its properties and mixes it with a pure fuel vapor element. The sensible and latent heat required to bring a liquid fuel element to saturation temperature and evaporate it is subtracted from the enthalpy of the mixed elements. Otherwise species mass and enthalpy are conserved as in a normal mixing event. The elements are separated into two elements with equal properties. This process is repeated until the mass of fuel vapor added is equal to the required evaporated fuel mass for the timestep. Required evaporation in excess of the mass of an integer number of elements is carried over to the next MDM timestep.

3.3.4 Ignition Delay and Combustion Model

Elements are tested to determine if they satisfy the combustion criteria whenever chemical properties are updated and before and after each mixing event. Subroutine PROP is called by Subroutine SMZ when the time since the last kinetic update exceeds the specified kinetic update time and prior to the mixing of two elements. If an element contains unburned fuel Subroutine PROP will call Subroutine CMBUST. Subroutine CMBUST is also called after mixing if the mixed elements contain unburned fuel. If an element satisfies the combustion criteria, Subroutine CMBUST instantaneously burns the element at constant pressure to equilibrium products. A new temperature is calculated for the products by Subroutine BTEMP and the element's burned gas fraction (BGFR) is set to one.

The combustion criteria are:

1. The element must contain unburned fuel. (BGFR < 1)
2. The element's ignition preparation factor must exceed one. ($PREP_i > 1$).
3. The element's total fuel equivalence ratio must be within combustible limits. ($\phi_L < \phi < \phi_R$)

The ignition delay preparation factor in element i is calculated as follows:

$$PREP_i = \int \frac{dt}{\tau_{id_i}(t)} \approx \sum_j \frac{\Delta t_j}{\tau_{id_i}(t_j)} \tag{3.3}$$

where the ignition delay time is expressed as [22]:

$$\tau_{id_i}(t_j) = 3.45E\text{-}3\ p^{-1.02} \exp(2100/T_i) \quad (s) \qquad (3.4)$$

Combustible equivalence ratio limits of 0.3 to 1.5 were found to best reproduce zone combustion as predicted by KIVA.

The SMM combustion model is not constrained by the combustion predicted in the KIVA solution. Two significant problems with the KIVA solution (Section 2.5) made this necessary: (1) KIVA's initial burning was too fast, (2) Excessive numerical diffusion damped out large scale convection and mixing, resulting in significant unburned fuel. The SMM was able to correct these deficiencies to some extent, but in the process the quantity of burned versus unburned fuel in the SMM solution was very different from the KIVA solution. This caused problems with the SMM flow algorithm which is constrained to match the flow of burned and unburned fuel in the KIVA solution. Ideally, if the KIVA solution were correct, the SMM combustion should be constrained to agree.

3.3.5 Heat Transfer Model

Wall heat transfer is updated at the end of each MDM timestep by Subroutine QWALL. QWALL is called by Subroutine SMZ. The wall heat transfer calculated by KIVA includes only convection/conduction. Radiation heat transfer is not calculated by KIVA. The purpose of Subroutine QWALL is to distribute the zone heat transfer specified by KIVA among the zone elements. The heat transfer to a particular element is assumed to be proportional to its surface area and to the temperature difference between the element and the wall:

$$Q_i = h A (T_i - T_w) = (mv_i)^{2/3} (T_i - T_w) \tag{3.5}$$

where:

Q_i = Wall heat transfer for element i.

T_w = Wall temperature.

T_i = Temperature of element i.

v_i = Specific volume of element i.

Given that this relationship is true for all elements:

$$Q_i = \frac{Q_w v_i^{2/3} (T_i - T_w)}{\sum_i v_i^{2/3} (T_i - T_w)} \tag{3.6}$$

Q_i is added to the element enthalpy for each element.

3.3.6 Volume Constraint

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 effects conservation of energy through the PV term in the First Law. Considering conservation of energy for one element:

$$\Delta E_i = Q_i - W_i = Q_i - \int_1^2 p dV_i \tag{3.7}$$

or:

$$\Delta H_i = Q_i + \int_1^2 V_i dp = Q_i + .5[V_i(t_1) + V_i(t_2)]\Delta p \tag{3.8}$$

where:

$\Delta H_i = H_i(t_2) - H_i(t_1)$ = change in enthalpy of element i

Q_i = heat transfer into element i

V_i = volume of element i

p = pressure

The volume constraint is updated at time $t_{2'}$. At this time all other MDM timestep processes have been completed (mixing, combustion, heat transfer). These processes are accomplished at constant pressure with no volume constraint. The additional enthalpy change which results from adiabatically updating the element volume may be expressed as:

$$[\Delta H_i]_{volume} = mc_p(t_{2'})[T_i(t_2) - T_i(t_{2'})] = .5\left[V_i(t_1) + \frac{mR_i(t_{2'})T_i(t_2)}{p(t_2)}\right]\Delta p$$

where: (3.9)

t_1 = start of the MDM timestep

$t_{2'}$ = end of the MDM timestep before the volume update

t_2 = end of the MDM timestep after the volume update

$c_p(t) = c_p(t_{2'})$ = specific heat at constant pressure

$R(t) = R(t_{2'})$ = gas constant

Subroutine VOLUME uses an iterative technique to calculate new element temperatures and a new SMM pressure while satisfying the volume constraint. Solving for $T_i(t_2)$, Equation (3.9) becomes:

$$T_i(t_2) = \frac{T_i(t_{2'}) + .5v_i(t_1)\Delta p/c_p(t_{2'})}{1 - \dfrac{.5R(t_{2'})\Delta p}{c_p(t_{2'})p(t_2)}} \tag{3.10}$$

The iterative procedure is as follows:

1. A value for $p(t_2)$ is assumed. For the first iteration $p(t_2)=p(t_1)$. Afterwards $p(t_2)$ is calculated on the previous iteration.

2. $\Delta p=p(t_2)-p(t_1)$.

3. New element temperatures and volumes are calculated using Equation (3.10) and the ideal gas law.

4. Total element volume is calculated and compared to the required value. If the total element volume is within tolerance the iteration stops and element properties are updated. If not, a new value for $p(t_2)$ is calculated using:

$$[p(t_2)]_{new} = \left[\frac{V_{SMM}}{V_{MDM}} \right] [p(t_2)]_{old} \tag{3.11}$$

where:

$V_{SMM} = \sum_i (mv_i)$ = sum of the element volumes

V_{MDM} = Required total cylinder volume

This value is used to start another iteration.

Subroutine VOLUME is called by Subroutine SMZ at the end of every MDM timestep.

3.3.7 NO Model

Nitric oxide (NO) is the predominant oxide of nitrogen produced in an engine. The principal source of NO is the oxidation of atmospheric oxygen. In lean and near-stoichiometric mixtures the principal reactions governing the formation of NO are those proposed by Zeldovich: [23]

1. $O + N_2 = NO + N$ (3.12)

2. $N + O_2 = NO + O$ (3.13)

Lavoie, Heywood and Keck [24] suggest an extension to this mechanism especially for rich mixtures:

3. $N + OH = NO + H$ (3.14)

Assuming a steady-state approximation for the nitrogen atom concentration, [N], and using this extended Zeldovich mechanism, rate expressions recommended by Bowman [25] reduce to the following simplified expression:

$$\frac{d[NO]}{dt} = 2k_1^+[O][N_2]\left[\frac{1 - [NO]^2/\ K[O_2][N_2]}{1 + k_1^+[NO]/(k_2^+[O_2] + k_3^+[OH])}\right] \text{ (gmole/cc}\cdot\text{s)}, \quad (3.15)$$

where:

[ ] = species concentration (gmole/cc)

k_r^+, k_r^- = forward and backward reaction coefficients

K = $(k_1^+/k_1^-)(k_2^+/k_2^-)$

Since NO production in the post-flame gases dominates flame-front produced NO, combustion and NO formation processes are assumed to be decoupled. Concentrations of O, O2, OH, H and N2 may then be approximated by their equilibrium values:

$$\frac{d[NO]}{dt} = \frac{2k_1^+U_2(1 - \alpha^2)}{\rho_i(1 + \alpha U_3)} \quad \text{(gmole/cc}\cdot\text{s)} \quad (3.16)$$

where:

T_i = temperature of element i (K)

ρ_i = gas density of element i (g/cc)

$[\ ]_e$ = equilibrium species concentration (gmole/cc)

α = $[NO]/U_1$

U_1 = $[NO]_e$

U_2 = $[N_2]_e[O]_e$

$$U_3 = \frac{k_1^+[N_2]_e[O]_e}{k_2^+[N]_e[O_2]_e + k_3^+[N]_e[OH]_e}$$

k_1^+ = $7.6E13 \exp(-38000/T_i)$ (cc/gmole·s) [26]

k_2^+ = $1.5E9 \exp(-19500/T_i)$ (cc/gmole·s) [26]

k_3^+ = $4.1E13$ (cc/gmole·s) [26]

Subroutine PROP updates NO concentration in an element using Equation (3.16). Equilibrium values for U1, U2, and U3 are provided in the NASA equilibrium data for a range of temperatures, pressures and equivalence ratios of the burned gas. Subroutine SPECNO interpolates between the tabular values to calculate U1, U2, and U3 at the specified temperature, pressure and equivalence ratio.

3.3.8 Soot Model

Diesel particulates consist primarily of soot on which some unburned hydrocarbons have been absorbed. The individual particles are found to be clusters of many small spheres or spherules of carbon. [27] A typical composition of dry soot might be $CH_{.27}O_{.22}N_{.01}$, but this varies widely. Spherules have a concentric lamellate structure much like the layers of an onion. Spherules vary in diameter between 10 and 80 nm, but most are in the 15-30 nm range. Spherule density is approximately 1.8 g/cc.

Most of the information available on the fundamentals of soot formation comes from studies in simple premixed and diffusion flames, stirred reactors, shock tubes, and constant volume combustion bombs. [28] Soot measurements in DI diesel engines and in similar fuel rich diffusion flames show high concentrations of soot in and around the fuel-rich cores. This indicates that pyrolysis is an important source of soot. Amann and Siegla [27] conclude that the production of diesel particulates involves a complex series of chemical and physical processes. These are represented in Figure 3-4.

The precise details of the chemistry leading to the formation of soot are not well understood. Figure 3-5 represents a simple mechanistic model for the nucleation of soot. [28] At low temperatures an aromatic hydrocarbon can produce soot via a relatively fast, direct route that involves condensation of the aromatic rings into a graphitelike structure. This production increases with temperature up to around 1800K. Experiments by Prado and Lahaye [29] support such a condensation mechanism. Above 1800K, a slower indirect route is favored that requires break-up into smaller fragments which polymerize to ultimately form soot nuclei. An ionic mechanism proposed by Howard [30] may also contribute to soot formation, but it does not appear to be a major contributor.

Given the very limited knowledge about these mechanisms and the total lack of quantitative prediction methods, we ultimately selected an empirical correlation for predicting soot formation. Wang, Matula and Farmer [31] studied soot formation for toluene behind reflected shock waves over the temperature range 1400 K to 2500 K and the pressure range 2.5 to 10 atmospheres using a laser beam attenuation technique. Their results were consistent with the nucleation mechanism discussed above and they included two correlations, one with oxygen in the mixture and one without. This provides a low oxygen limit on the formation rate rather than having a rate which gets very large as the oxygen goes to zero. The large temperature and pressure range of their data approaches that found in diesel combustion.

The correlation equation of the apparent soot formation rate for toluene/argon/oxygen mixtures is given by:

$$R_{soot} = \frac{5.55E16\ [C_7H_8]^{2.59}[Ar]^{.13}\exp[-41.8/RT - 48.1\sigma(1/RT - 1/RT_m)]}{[O_2]^{.71}} \quad (g/cc\cdot s) \qquad (3.17)$$

where:

[ ] = species concentration (gmole/cc)

R = Universal gas constant

T_m = 1800 K

$$\sigma \begin{cases} 0 \text{ for } T \leq T_m \\ 1 \text{ for } T > T_m \end{cases}$$

For toluene/argon mixtures (low O_2 limit):

$$R_{soot} = 1.04E13\,[C_7H_8]^{1.48}[Ar]^{.24}\exp[-29.7/RT + 39.7\sigma(1/RT - 1/RT_m)] \quad (g/cc \cdot s) \qquad (3.18)$$

These rate equations were multiplied by a calibrating constant (SOOTC) and applied directly in the model with:

$$[C_7H_8] = [C_{10.8}H_{18.7}] \qquad (3.19)$$

$$[Ar] = \rho_i /\ MW - [C_{10.8}H_{18.7}] - [O_2] \qquad (3.20)$$

$$\dot{m}_{soot_i} = \begin{matrix}\text{soot mass formation rate}\\ \text{for element i}\end{matrix} = m_e v_i R_{soot_i} \quad (g/s) \qquad (3.21)$$

where:

m_e = element mass (g)

v_i = specific volume of element i (cc/g)

The purpose of the calibrating constant is to relate the rate of sooting for diesel fuel in a turbulent flow to that of toluene in a shock tube experiment. All the soot mass formed during a timestep is assumed to take the form of new spherules of density ρ_{soot} and radius r_o. The soot surface area contributed by these new spherules is:

$$\Delta A_{form_i} = \frac{3\dot{m}_{soot_i}\Delta t}{\rho_{soot} r_o} \quad (cm^2) \qquad (3.22)$$

Occurring simultaneously with soot formation is soot oxidation. Park and Appleton [32] have shown that the surface reaction rate for the oxidation of soot in a flame is nearly the same as that for pyrolytic graphite. In lean and near-stoichiometric mixtures where 02 is the primary oxidant the semi-empirical formula proposed by Nagle and Strickland-Constable [33] has proven very satisfactory for predicting this reaction rate. Measurements taken by Neoh and Howard [34] indicate that in fuel rich flames the OH radical becomes the principal oxidant and that the rate predicted by Nagle and Strickland-Constable under-predicts soot oxidation. This effect could be significant in the richer region of the diesel fuel spray where most of the soot is formed, although the overall diesel equivalence ratio is very lean. Since the quantitative effect of the OH radical has not been thoroughly evaluated for the full range of equivalence ratios encountered in diesel combustion, only the Nagle and Strickland-Constable formula will be used here:

$$\omega_{ox_i} = 12 \left[\frac{k_A p_{O2} \chi}{1 + k_Z p_{O2}} + k_B p_{O2} (1 - \chi) \right] \quad (g/cm^2 \cdot s) \qquad (3.23)$$

where:

$$\chi = \frac{1}{1 + k_T / k_B p_{O2}}$$

$$k_A = 20.\ \exp(-15000/T_i)$$

$$k_B = 4.46E\text{-}3\ \exp(7640/T_i)$$

$$k_T = 1.51E5\ \exp(-48000/T_i)$$

$$k_Z = 21.3\ \exp(2060/T_i)$$

p_{O2} = partial pressure of O_2 in element i (atm)

After formation and oxidation during kinetic timestep, Δt, the final soot mass becomes:

$$m_{soot_{i,2}} = m_{soot_{i,1}} + \dot{m}_{soot_i} \Delta t - \omega_{ox} (A_{soot_{i,1}} + .5\ \Delta A_{form_i})\ (g) \qquad (3.24)$$

and the final soot area becomes:

$$A_{soot_{i,2}} = A_{soot_{i,1}} \left(\frac{m_{soot_{i,2}}}{m_{soot_{i,1}}} \right)^{2/3} \ (cm^2) \qquad (3.25)$$

where:

ω_{ox} = soot oxidation surface recession rate ($g^2/cm \cdot s$)

$m_{soot_{i,j}}$ = mass of soot in element i at time j (g)

$A_{soot_{i,j}}$ = surface area of soot in element i at time j (cm^2)

Subroutine PROP calls Subroutine SOOT which calculates soot formation. Subroutine PROP calculates soot oxidation and updates the quantity of soot in each element.

CHAPTER FOUR

EXPERIMENTAL DATA

4.1 Data Requirement

In order to evaluate the Stochastic Mixing Model it was necessary to obtain or generate test data. The calculation of Nitric Oxide (NO) by the SMM is dependent on only one calibrating constant. This is the scaling factor for mixing intensity. This constant is adjusted to match the mass of fuel burned in each zone and the overall pressure trace to the MDM results. This adjustment does not consider NO and does not consider experimental results. Consequently, NO 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. Most diesel NO data is derived from either probe sampling, spectroscopic analysis or exhaust measurements. Probe studies provide local NO measurements at various crank angles, but do not provide cylinder-averaged values. Spectroscopic analysis is severely limited in direct injection diesels because of the opaque diesel spray and overwhelming soot radiation. Exhaust measurements do not resolve crank angle dependence. One technique that does provide this data is to dump and quench the cylinder contents for chemical analysis at various crank angles. Fortunately, the University of Wisconsin-Madison has had an ongoing study using this technique and their results will be used in our analysis. [19,35,36,37,38] The specific test cases we have used are those discussed in Reference [35].

4.2 Description of the Test Engine and Apparatus

The test engine used at the University of Wisconsin is a single-cylinder direct-injection diesel engine. The specifications for this engine are listed in Table 4-1. Dumping of the cylinder contents is achieved by cutting a one-inch diameter steel diaphragm mounted in the cylinder head, allowing the cylinder gas to expand into a quench chamber. This process is repeated at various crank angles for a fixed engine operating condition, providing a history of cylinder-averaged NO over the combustion cycle.

Figure 4-1 is a diagram of the cylinder head and combustion chamber. This head was specifically designed and manufactured for their experiments. It contains a one inch diameter dumping port, injector hole, exhaust port, and intake port with a shrouded intake valve. The shrouded intake valve allows experiments at various swirl ratios. Shroud adjustment was calibrated at steady flow conditions for a reasonable range of swirl values using a paddle-wheel transducer.

Figure 4-2 is a diagram of the dumping system. Its major components are the quench chamber, the ball valve which isolates the quench chamber from the engine immediately after dumping, the connecting tube which holds the diaphragm and cutting mechanism, the cutter actuating mechanism, and the pressure safety valve. The diaphragm is held at one end of the connecting tube by clamping between outer and inner concentric tubes. The cutter is a third concentric tube which slides inside the inner clamping tube. When the cutter tube is forced down by the actuating mechanism the diaphragm is sheared around its circumference.

The rapidly expanding cylinder gases cause it to fold upward around a diagonal cross-member. This process takes about 0.1 ms. 80% of the cylinder gases are collected. The quench tank is isolated from the connecting tube and engine by a ball valve. The tank is designed to provide an adequate volume of helium quenching gas and to dissipate the shock produced by the inflow.

Figure 4-3 is a schematic of the dumping and control system. The dumping event is triggered by a signal from a magnetic pickup placed on the camshaft. This signal is received by a timing circuit which actuates the cutter mechanism solenoid and synchronizes engine shutdown and isolation. This includes closing the ball valve, the engine intake and exhaust valves, and the fuel cut-off valve.

The engine is equipped with an electric dynamometer and a digital counter to measure speed. Fuel consumption is measured using a fuel weighing balance and electronic timer. Air supply is measured using a critical flow orifice. Cylinder pressure is measured using a piezoelectric transducer.

A complete test run proceeds as follows:

1. The engine is started and warmed up.
2. With the diaphragm in place and the ball valve open, the quench tank is pumped out using a vacuum pump and refilled with helium. This is repeated several times to ensure that all air has been removed from the system. The final helium pressure is set slightly above atmospheric. Quench tank temperature and pressure are recorded.
3. The triggering signal is set to occur at the desired crank angle. This value will only approximate the dump angle. The actual value is obtained by analyzing the cylinder pressure trace.
4. The timing circuit is activated and the cylinder is

dumped on the next complete cycle after receipt of the triggering signal.

5. The cylinder pressure recorder is also activated for the dumping cycle.

6. A portion of the collected gas in the quench tank is passed through a drier and filter and stored in a Tedler bag for gas analysis. A Barber Colman gas chromatograph (GC) is used to measure O_2,N_2,CH_4,CO and CO_2. Non-dispersive infrared (NDIR) analysis is also used to measure CO_2. The remainder of the gas is passed through a chemiluminescent analyzer (CLA) for NO and NO_x analysis.

4.3 The Test Cases

Table 4-2 describes the five test cases. Safety considerations limited the engine speed to 1000 RPM and the engine load to an overall equivalence ratio of 0.5. Runs using an eight-hole injector were made at two swirl ratios, zero and ten percent EGR, and two injection timings.

Each NO versus crank angle history represents a series of cylinder dumps at constant engine conditions. The effect of cycle-to-cycle variations was analyzed by multiple dumps at a single crank angle. For NO levels below 1000 ppm the variation was less than 10 percent. For NO levels above 1000 ppm it was less than 2 percent.

Complete test data and pressure traces are listed in Appendix G. Note that NO mass fractions must be multiplied by a correction factor to account for helium dilution.

CHAPTER FIVE

MODEL EVALUATION AND SENSITIVITY

5.1 Sensitivity to Simulation Parameters

The first step in evaluating the Stochastic Mixing Model approach is to consider its internal consistency: its sensitivity to 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, the mixing intensity scaling factor, and the number and definition of the zones on the results and on element distributions.

5.1.1 Number of Elements

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 (ELMM), specified as a model input parameter, and the total mass of injected fuel and intake air per cycle, specified by the engine operating conditions. A random number generator is used in many of the SMM submodels to select elements for mixing and exchange with other zones. Included in the model input parameters is a random number seed which determines the series of random numbers selected 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. Figures 5-1 and 5-2 show mean maximum pressure, mean maximum NO and mean maximum soot 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. Each run uses 10 zones, a mixing intensity factor of 1.1 and MDM data for Test Run 17. Four different element sizes were used for element totals of 1437, 2875, 5750 and 11500 (ELMM=0.0012, 0.0006, 0.0003, and 0.00015 g). The curves connect the four mean data points. The vertical lines indicate the standard deviation and the tick marks indicate the 95 per cent confidence interval for the mean value. [51] Two important observations may be made about this data. First, the standard deviation decreases with more elements and second the mean value changes with the number of elements, approaching an asymptotic limit with more elements. Both of these observations are as expected and may be attributed to the stabilization of the distribution of element properties 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 elements chosen. Figure 5-3 shows the distribution of elements for these cases as a function of total fuel mass fraction and the number of elements. These distributions converge as the number of elements is increased. Typical of all the distributions examined is that they start off with a large group of elements that are very rich and a large group that are very lean. These two groups should gradually mix and converge with increased crank angle to a distribution centered on the overall fuel mass fraction. This occurs in our results although our distributions always have a significant number of very lean elements left at the end. This is due to the incomplete mixing predicted by KIVA.

Computer run time for the SMM varies directly with the number of elements, so for computational efficiency of a single run it is desirable to have fewer elements. However, standard deviation decreases with the number of elements and fewer runs are required with more elements for the same computational accuracy. A compromise number of 5750 elements (ELMM=0.0003 g) was selected for the remainder of our runs. Mean results for this number of elements are within 5 per cent of their asymptotic values and the 95 per cent confidence factor range for ten runs is less than plus or minus 5 per cent. Run time from the start of injection to 40° ATDC for one run on a VAX 750 is approximately 90 minutes.

5.1.2 Mixing Intensity Scaling Factor

Most important among the physical parameters is the mixing intensity scaling factor (CBETA). As shown in Equation C.16 mixing intensity may be derived from basic principles to within a linear scaling factor. This scaling factor must be specified in the model input. Figure 5-4 shows cylinder pressure, mass of fuel burned, NO, and soot versus crank angle and CBETA. Included are plots of the experimental test results, the KIVA results and the SMM results. Each SMM curve represents the mean of 10 stochastic runs with 5750 elements and 10 zones, using MDM data for Test Case 17.

Initial burning and pressure rise in the SMM are slower than the KIVA results. This may be attributed to the ignition delay submodel included in the SMM which slows down this initial burning phase. KIVA does not consider pre-ignition chemistry and its initial burning is too rapid. For the range of mixing intensity factors considered, the maximum pressure predicted by the SMM is reasonably close to the KIVA results. Increasing CBETA results in increased burning and higher pressures. This is consistent with increased mixing. With CBETA fixed, trends in maximum pressure predictions at other engine operating conditions are also consistent with the KIVA and experimental data. The SMM pressure trace eventually converges with the KIVA and experimental results. The discrepancy in the pressure traces from peak pressure to convergence is attributed to possible diaphragm leakage in the experimental results and to incomplete combustion predicted by KIVA, which may be seen in the mass-burned plot. The value of CBETA selected for comparison to the experimental data (CBETA=0.9) was chosen to give the best matchup between SMM and KIVA pressure traces. Experimental results were not considered in determining CBETA.

The shape and the magnitude of the NO curves agree well with the experimental results for this test case. NO concentration increases with CBETA, pressure and mass-burned. This is consistent with increased mixing and earlier combustion.

Unlike NO, soot formation predictions are dependent on a calibrating constant (SOOTC). The value used (SOOTC=0.001) was chosen to give agreement between exhaust soot predicted by the SMM (Test Run 17, CBETA equal to 0.9) and the experimental results. Since toluene combustion generates far more soot than diesel fuel, this constant is substantially different from unity. The application of the toluene shock-tube correlations to the diesel environment is, however, highly speculative. This value was held constant for all subsequent runs. In order to use the experimental results to calibrate the soot submodel it was necessary to convert an exhaust Bosch Number to percent Carbon. [52] Soot calculations made by the SMM are considered qualitatively and are not used for quantitative evaluation of the model. The soot curves show a maximum near the end of injection followed by rapid oxidation. Increased mixing reduces the amount of soot produced and increases the amount of soot oxidized. This is consistent with our general knowledge about diesel soot emissions.

Figure 5-5 shows the distribution of elements as a function of total fuel mass fraction and mixing intensity at different crank angles. As CBETA increases, the rich and lean peaks converge more rapidly resulting in narrower and taller distributions. This is consistent with more mixing.

5.2 Sensitivity to Zones

The number and definition of stochastic mixing zones used in the SMM is fundamental to the basic hypothesis of our approach and a critical parameter in determining the results. We assume that an inhomogeneous flow may be broken down into a discrete number of zones which individually may be modeled as well-mixed on a microscopic scale. 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. Increasing the number of zones and consequently decreasing their size should improve the validity of our hypothesis. We would expect that as the number of zones is increased and our hypothesis becomes valid, the results should converge to a solution. Increasing the number of zones would eventually become computationally unmanageable and other model hypothesis, such as having simply-connected zones, would begin to break down. Our concern was that this might occur before converging to a solution.

As discussed in Section 2.6, the KIVA output is sorted into 10 zones. Any combination of these ten zones may be used in the SMM. Table 2-2 lists the zone definitions used in our analysis. Runs were made using 5,7,8,9 and 10 zones. Two different 8 zone definitions were used: one with more division around stoichiometric and one with more division richer than stoichiometric. All runs were made using 5750 total elements, with CBETA equal to 0.3, and using MDM data for Test Case 17.

Figure 5-6 shows cylinder pressure, fuel-mass burned, NO concentration and soot versus crank angle and zone definition. Included are the SMM, KIVA and experimental results. The results for 5 zones are very different from the others. The fuel-mass burned versus crank angle plot is much slower and has a different shape. Cylinder pressure for 5 zones is less and does not ultimately converge with the other cases. The shape of the soot profile is again dramatically different for the 5 zone case. With 8 zones the curves begin to converge. Pressure and burned fuel plots are very similar for 8, 9 and 10 zones. The NO and soot curves are more sensitive to small changes in temperature and converge more slowly, but the difference for 9 and 10 zones is very small. Of the two cases with 8 zones, more subdivision around stoichiometric results in a distribution most similar to the 9 zone case. This may be attributed to there being more elements and greater temperature sensitivity to fuel mass fraction in the near-stoichiometric interval.

The most critical mechanism by which the zone definition effects these results appears to be through the fuel mass fraction distribution. Figure 5-7 shows these distributions for the various zone definitions. Increasing the number of zones results in more boundaries across which the flow is specified and increasingly constrains the overall distribution. The larger zones in the 5 and 7 zone models tend to develop large peaks in their fuel mass fraction distribution around zone means. This effect is much less evident with more zones where the fuel is forced to be in the appropriate zone and fuel mass fraction interval. 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 converge rapidly with more than 8 zones. This is consistent with our mixing hypothesis. Ten zones are used in the runs for comparison to the experimental results.

5.3 Comparison to the MDM Results

Sections 5.1 and 5.2 compare SMM results to global MDM results such as average cylinder pressure, fuel-mass burned, NO and soot. The ability of the SMM to reproduce individual zone processes as specified by the MDM solution is also important. Figures 5-8 thru 5-11 compare zone fuel mass fraction and zone fuel-mass burned in the SMM and MDM.

As described in Section 3.3.4, SMM combustion is not constrained by KIVA. The ignition delay predicted by the SMM compares very well with the KIVA ignition delay, which is specified by the experimental results and provided as input to KIVA. (See Figs. 5-8 and 5-9) However, once combustion is allowed to occur in the KIVA solution it takes off much too rapidly. The SMM combustion is constrained by the pre-ignition chemistry criteria and proceeds more slowly. This is particularly apparent in the richer zones where lower temperatures and the rich combustion constraint result in much slower SMM combustion rates. Except for Zone 1, the two plots ultimately converge, but quickly start to diverge again as the stable concentration gradients predicted by the KIVA solution prematurely slow KIVA combustion after +20° ATDC.

The decision not to constrain SMM combustion was made because of the apparent deficiencies in the KIVA combustion solution, but the cost of this decision is seen in the Total Fuel Mass Fraction plots (Figs. 5-10 and 5-11). The quantity of burned versus unburned fuel in the SMM solution was very different from the KIVA solution. This caused problems with the SMM flow algorithm which attempts to match the flow of burned and unburned fuel to the KIVA solution. Burned and unburned-fuel flow errors are less than two percent of the total fuel before +20°, but increase to as much as 20 percent of the total fuel after +20°. As a result, the zone fuel-mass fractions do not precisely match KIVA, particularly after +20° ATDC. Ideally, if the KIVA solution were correct, the SMM combustion should be constrained to agree. Because of the apparent deficiencies in the KIVA combustion solution we chose to have the best agreement occur early in the cycle and around top dead center. Most of the critical NO chemistry is complete by 20° ATDC so that evaluation of our two-step approach is still valid using NO as a criteria. We should, however, be cautious with any conclusions dependent on results after 20° ATDC.

CHAPTER SIX

COMPARISON TO EXPERIMENTAL RESULTS AND ANALYSIS

6.1 Comparison to Experimental Results

The next step in evaluating the Stochastic Mixing Model approach is the comparison of model results to experimental results and trends. This section compares model predictions to the experimental test case results described in Section 4.3. The experimental results include data for two injection timings, two swirl ratios and two levels of exhaust gas recirculation (EGR). KIVA and SMM runs were made for each of these test cases. SMM results represent the mean of 10 stochastic runs with identical engine operating conditions, but different random number seeds. All the SMM runs use a mixing intensity factor (CBETA) of 0.9 and approximately 5750 elements (ELMM=0.0003 g). Table 6-1 summarizes the important features of the model and experimental results. Figures 6-1 through 6-6 are plots of these results.

The pressure traces and fuel-mass burned plots provide important global comparisons. Unfortunately, the comparison of pressure traces was a problem for two reasons: (1) Initial KIVA combustion was too rapid and combustion during the expansion stroke was incomplete. These effects were partially corrected in the SMM by not constraining the SMM combustion to agree with KIVA, but as a result their pressure traces represent different heat release profiles. (2) The experimental pressure traces start out looking normal, but for Test Cases 17, 18, 20 and 21 they seem to "fizzle out". This discrepancy was discussed in Section 2.5.1 and is attributed to possible leakage around the dumping diaphragm in the test engine. The mixing intensity scaling factor used for subsequent comparison runs (CBETA=0.9) was selected to best match the maximum SMM pressure to the maximum KIVA pressure for Test Case 17. Once this was done, the maximum SMM pressure compared well to the maximum KIVA pressure for each run. This is an important indication of model consistency. Ignition delay and initial pressure rise predicted by the SMM compare well with the experimental results. Towards the end of the cycle the incomplete mixing of fuel and air predicted by KIVA leaves some very rich zones with significant unburned fuel. The fuel-mass burned results for both KIVA and the SMM show only 80-90 percent burned fuel at +80° ATDC. In zones where the mean fuel mass fraction is within combustible limits the SMM ultimately mixes and burns more fuel than KIVA, but in richer zones many elements never satisfy combustible limits and do not burn. The SMM fuel-mass burned results are consistent with the experimental results in that the two high swirl cases (18 and 21) and the early injection case (19) result in more complete combustion, but the SMM is not able to burn all the fuel because of the KIVA constraints.

NO results will be discussed one test case at a time, comparing the results of advanced injection timing, increased swirl and increased EGR to the basic test case, Test Case 17. The curves from all five test cases are plotted together in Figure 6-6. The ability of the SMM to predict NO is an excellent quantitative indication of its ability to predict slow chemistry. There are no calibrating factors in the NO calculation and the bulk of the NO chemistry occurs prior to +20° ATDC where the SMM results are most valid.

NO results for Test Case 17 are plotted in Figure 6-1. The NO plot shows excellent agreement with the experimental data although the experimental results show a slight increase towards the end of the cycle while the SMM results are nearly constant. NO results for Test Case 18 are plotted in Figure 6-2. The increased swirl in this case results in less fuel spray penetration and increased mixing intensity. Ultimately more of the fuel is mixed and burned than in Test Case 17, but due to less penetration, premixed combustion is less and combustion occurs in a richer mixture. This results in lower burned-gas temperatures, less NO and more soot. The NO reduction from Test Case 17 to Test Case 18 is approximately 40 percent in the SMM versus 26 percent in the experimental results. NO results for Test Case 19 are plotted in Figure 6-3. Agreement between the SMM and the experimental NO results is not as good as in the other cases. The SMM predicts only a 31 percent increase in NO between Case 17 and Case 19 (10° injection advance) versus a 90 percent increase in the experimental results. This 90 percent increase is in agreement with that predicted in other experiments with similar operating conditions. [52] The SMM NO trace does not start up as quickly and falls off at +20° ATDC. Possible causes of this disagreement include: (1) Breakdown of the model after +20° ATDC (results are more consistent before +20°). (2) Inaccuracy of the KIVA initial flow conditions which would have a greater impact in the advanced injection case. (3) Inaccuracy of KIVA initial burning due to the lack of pre-ignition chemistry in our application. NO results for Test Case 20 are plotted in Figure 6-4. Ten percent EGR results in higher gas heat capacities and lower temperatures. This results in less NO and more soot. Again the SMM results agree reasonably well with the experimental results. The SMM predicts a 55 percent reduction in NO between Test Case 17 and Test Case 20 versus a 58 percent decrease in the experimental results. NO results for Test Case 21 are plotted in Figure 6-5, showing the combined effect of increasing swirl and EGR. The SMM predicts a 58 percent reduction in NO between Test Case 17 and Test Case 21 versus a 66 percent decrease in the experimental results.

Two limitations must be considered when analyzing the soot results: (1) The expression for soot production, Equation 3.17, includes a calibrating constant. The soot constant (SOOTC=0.001) used for all the comparison runs was selected to match the soot loading at +80° ATDC in the SMM to the experimental results for Test Case 17. The application of the toluene shock-tube correlations to the diesel environment is, as stated before, highly speculative. (2) Important soot chemistry occurs after +20° ATDC where the SMM assumptions begin to break down. Because of these limitations the quantitative validity of the soot results is unclear and they are only discussed qualitatively.

In all cases (Figs. 6-1 thru 6-5), the soot plot reaches a maximum around the end of injection and then rapidly oxidizes. Maximum soot is approximately two orders of magnitude larger than the soot at exhaust. The hump at +20° ATDC is attributed to the soot production rate (Equation 3.17) increasing as element temperatures approach 1800 K. Cylinder gas temperatures are well above 1800 K at TDC and drop below 1800 K during expansion, passing through this maximum around +20° ATDC. The trade-off between this effect, decreasing unburned fuel and rapid soot oxidation is a possible explanation for this hump occurring to a varying degree in each of the test cases. Trends in the final soot loading for all test cases are correct, but only Test Case 19 shows good agreement in magnitude with the experimental results. Both the experimental and SMM results indicate a 25 percent reduction in soot from Test Case 17 to Test Case 19 at +80° ATDC. Better agreement for Test Case 19 than for the other test cases is attributed to the soot chemistry being more nearly complete for Cases 17 and 19 by +20° ATDC where the SMM results are most valid. Significant soot oxidation is still in progress after +20° for the other test cases.

6.2 Learning from the SMM Results

In addition to predicting global properties such as pressure, soot, and NO the SMM can provide detailed information about the reactive flow not obtainable from laboratory measurements. Examples of this are the turbulent distribution of fuel mass fraction and NO in the combustion chamber.

Figures 6-7 through 6-10 are fuel mass fraction and mass weighted NO distributions as a function of total fuel mass fraction broken down by zones. The mass-weighted NO distributions are calculated as follows:

$$\text{mass-weighted NO} = \frac{\sum_{i=j} [NO]_i}{N} \qquad \text{(ppm)} \qquad (6.1)$$

where:

$[NO]_i$ = mass fraction of NO in element i

N = total number of elements in all zones

j = all elements in the ΔTFMF increment

The total fuel mass fraction increment used is 0.01. Refer to the zone definitions in Table 2-3.

In Test Case 17 at -5° ATDC (Fig. 6-7) the individual zone distributions are not yet fully developed. The fuel is dispersed over all the zones and many of the elements are very lean (4856 of 5644 elements are air zone elements). NO (Fig. 6-8) is most significant around stoichiometric and in the leaner elements and zones. In the early injection case, Test Case 19, injection is complete and, although there are still many lean elements, all of the zones have a broad and significant TFMF distribution with a fairly flat zone total. The NO, produced primarily in the stoichiometric elements, has mixed very rapidly into other elements and zones. The quantity and broad distribution of NO in even the richest zones (1 and 2) is surprising.

By 5° ATDC (Fig. 6-9) the typical "two-hump" TFMF distribution has developed in both test cases. This shape is due to the fuel vapor, which is introduced as pure vapor elements, gradually mixing in with air elements. These two groups of elements, starting from the right and left of the TFMF distribution, gradually converge. Case 19 has proceeded further in converging than Case 17 because of its earlier injection. Zone 1 has nearly disappeared by +5° in Case 19 while it is the dominant rich zone in Case 17. The NO (Fig. 6-10) has dispersed even more completely by this time and the mass-weighted NO distribution begins to correspond closely with the TFMF distribution although there is still a definite peak around stoichiometric. The concentration of NO is significant even in Zone 1.

By 25° ATDC the double humps in the TFMF plots (Fig. 6-13) have nearly merged. The distributions in Test Case 19 continue to be more peaked and narrow. The NO distribution in both cases (Fig. 6-14) conforms closely to the TFMF distribution except for the air zone elements where there is no NO. This indicates nearly homogeneous mixing of NO among the combustion zone elements and little mixing with the air zone elements segregated by the KIVA solution.

CHAPTER SEVEN

SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

This thesis proposes and evaluates a Two-Step Approach for calculating slow and complex chemistry in inhomogeneous turbulent reactive flows, specifically in a direct-injection diesel engine. The first step is to complete a Multi-Dimensional Model (MDM) solution of the reactive flow. This is accomplished for a direct-injection diesel using the KIVA computer code. The output of this solution is 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 MDM information. The SMM generates distributions of turbulent properties within each zone which are necessary to calculate the slow emissions chemistry. This approach is evaluated for consistency by analyzing zone property distributions, the effect of changing zone boundaries, the effect of increasing the number of zones, the sensitivity to various physical and model parameters, the ability of the SMM to reproduce MDM results and the variance of SMM results over multiple stochastic runs. It is evaluated for accuracy by comparison to experimental data and trends.

Weaknesses and deficiencies noted in the direct-injection diesel application of this approach were:

1. The coarse grid spacing used in the KIVA runs for computational economy caused excess numerical diffusion especially during expansion. This damped-out large scale turbulence and

convection very early in the expansion stroke, limiting mixing and combustion in both the KIVA and SMM results.

2. The global combustion chemistry used in the KIVA runs does not consider pre-ignition chemistry. Initial combustion in all the KIVA runs was too fast.

3. Because of these known deficiencies in KIVA, the SMM was not constrained to follow the KIVA heat release. Instead an ignition delay model was included in the SMM and elements were burned as they mixed when they satisfied the combustion criteria. Consequently the balance of burned and unburned fuel in the zones as specified by KIVA and as calculated in the SMM were not the same. This made it difficult for the SMM flow algorithm to satisfy burned and unburned fuel flow constraints, particularly after +20° ATDC.

4. The SMM mixing algorithm broke down after +20° ATDC when the KIVA large-scale flow was damped-out and gradients became stable.

5. The axisymetric grid used in KIVA for computational economy probably reduced the effect of increased swirl. Initial conditions were also somewhat simplistic and may have effected results, particularly in the early injection case.

6. The soot model used in the SMM was developed for toluene and requires calibration for application to diesel fuel. The accuracy of a diesel fuel application is questionable.

Consistent and encouraging results noted in the direct-injection diesel application of the stochastic mixing model approach were:

1. The standard deviation of pressure, soot and NO decreases with more elements and the mean value approaches an asymptotic limit with more elements. Total fuel mass fraction distributions also converge with more elements.

2. Pressure, soot and NO histories converge as the number of mixing zones is increased. Total fuel mass fraction distributions also converge. Nine or ten zones were required for convergence in our application.

3. SMM and KIVA pressure traces were consistent with different engine operating conditions for a fixed mixing intensity scaling factor.

4. SMM and experimental NO histories showed good agreement, both in magnitude and in trend, as the engine operating conditions were changed. The one exception was for the early injection case where the SMM predicted only half the increase in NO specified by the experimental data.

This Two-Step Approach is an excellent example of the unique potential for the application of multi-dimensional models. The KIVA code provided detailed information about the diesel reactive flow that could not be obtained by any other means. As MDM codes are exercised and reworked their limitations and deficiencies will be resolved.

Recommendations for future effort using KIVA and the Stochastic Mixing Model approach are:

1. Individual KIVA submodels should be validated using experimental data.

3. A 3-D KIVA computation with more realistic initial conditions should be made for comparison to simpler 2-D computations.

3. Pre-ignition chemistry needs to be included in the KIVA solution. Once the MDM combustion calculation is improved, combustion in the SMM should be constrained to agree.

4. A more sophisticated understanding is needed relating the number of mixing zones and efficiency of the mixing model to turbulent parameters in the KIVA solution. Use of a $k-\varepsilon$ turbulence model vice the subgrid scale model in the KIVA code would facilitate calculation of a realistic turbulent length scale for this purpose.

The Two-Step Approach shows great promise for calculating slow and complex chemistry in turbulent reactive flows. Our direct-injection diesel application of this approach was remarkably successful in predicting NO histories. Limitations in our application were due primarily to KIVA model limitations and inadequacies and to externally-imposed economies on KIVA computer time. The Stochastic Mixing Model appears to be internally consistent and reasonably economical in terms of run time. It should be stressed that the submodels included in the SMM are not intended to be unique, but only to represent one example of how this approach might be applied.

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TABLE 2-1

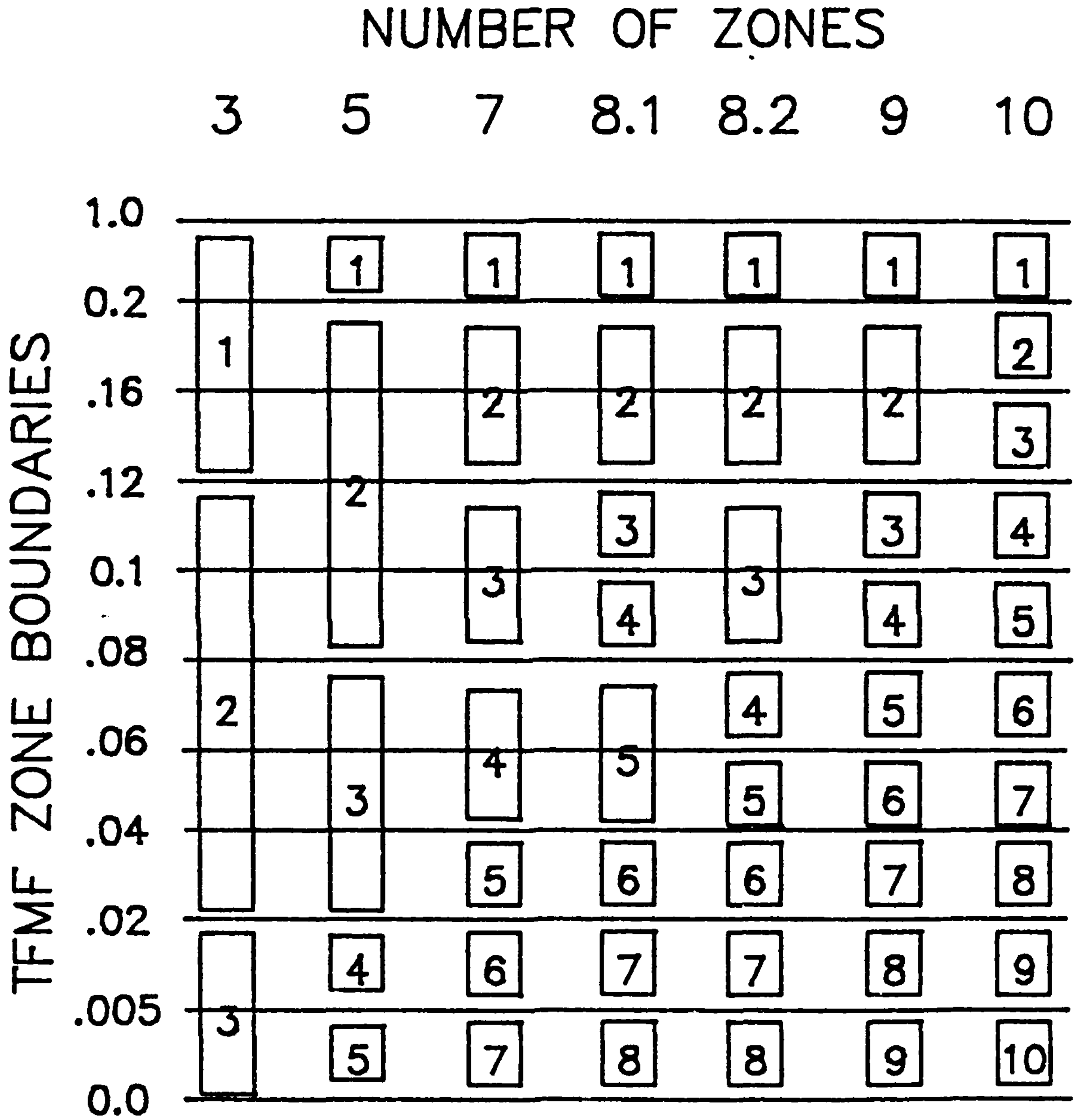
INPUT VARIABLES TO PROGRAM PRCMDM FROM KIVA

ZM(NZ)	Total mass of gas in zone NZ. (g)
ZML(NZ)	Total liquid fuel mass in zone NZ. (g)
ZMV(NZ)	Total fuel vapor mass in zone NZ. (g)
ZMBF(NZ)	Total mass of burned fuel in zone NZ. (g)
ZTEMP(NZ)	Mass average temperature in zone NZ. (K)
ZQCOMB(NZ)	Zone NZ chemical heat release during timestep. (cal)
ZMEVAP(NZ)	Zone NZ fuel mass evaporated during timestep. (g)
ZQWALL(NZ)	Zone NZ heat transfer from wall during timestep. (cal)
ZMFBRN(NZ)	Zone NZ fuel mass burned turing timestep. (g)
ZNO(NZ)	Zone NZ NO_x total mass. (g)
ZVOL(NZ)	Zone NZ volume. (cc)
ZFMF(NZ)	Zone NZ average total fuel mass fraction.
ZBETA(NZ)	Zone NZ mixing intensity. (1/s)

TABLE 2-2

INPUT VARIABLES TO STOCHASTIC MIXING MODEL FROM PROGRAM PRCMDM

FM(NF)	Total gaseous mass flow from zone NF to zone NF+1 during timestep. May be positive or negative. (g)
FMV(NZ)	Fuel vapor mass flow from zone NF to zone NF+1. (g)
ZML(NZ)	Total liquid fuel mass in zone NZ. (g)
FMBF(NZ)	Burned fuel mass flow from zone NF to zone NF+1. (g)
ZTEMP(NZ)	Mass average temperature in zone NZ. (K)
ZMEVAP(NZ)	Zone NZ fuel mass evaporated during timestep. (g)
ZQWALL(NZ)	Zone NZ heat transfer from wall during timestep. (cal)
ZMFBRN(NZ)	Zone NZ fuel mass burned turing timestep. (g)
ZVOL(NZ)	Zone NZ volume. (cc)
ZFMF(NZ)	Zone NZ average total fuel mass fraction.
ZBETA(NZ)	Zone NZ mixing intensity. (1/s)
ZMA	Air zone total mass (g)
ZMVA	Air zone fuel vapor mass (g)
ZMBFA	Air zone burned fuel mass (g)



TFMF ZONE BOUNDARIES	3	5	7	8.1	8.2	9	10
1.0 – 0.2	1	1	1	1	1	1	1
0.2 – .16		2	2	2	2	2	2
.16 – .12							3
.12 – 0.1	2		3	3	3	3	4
0.1 – .08				4		4	5
.08 – .06		3	4	5	4	5	6
.06 – .04					5	6	7
.04 – .02			5	6	6	7	8
.02 – .005	3	4	6	7	7	8	9
.005 – 0.0		5	7	8	8	9	10

Table 2-3 Mixing Zone Definitions

TABLE 4-1

ENGINE SPECIFICATIONS

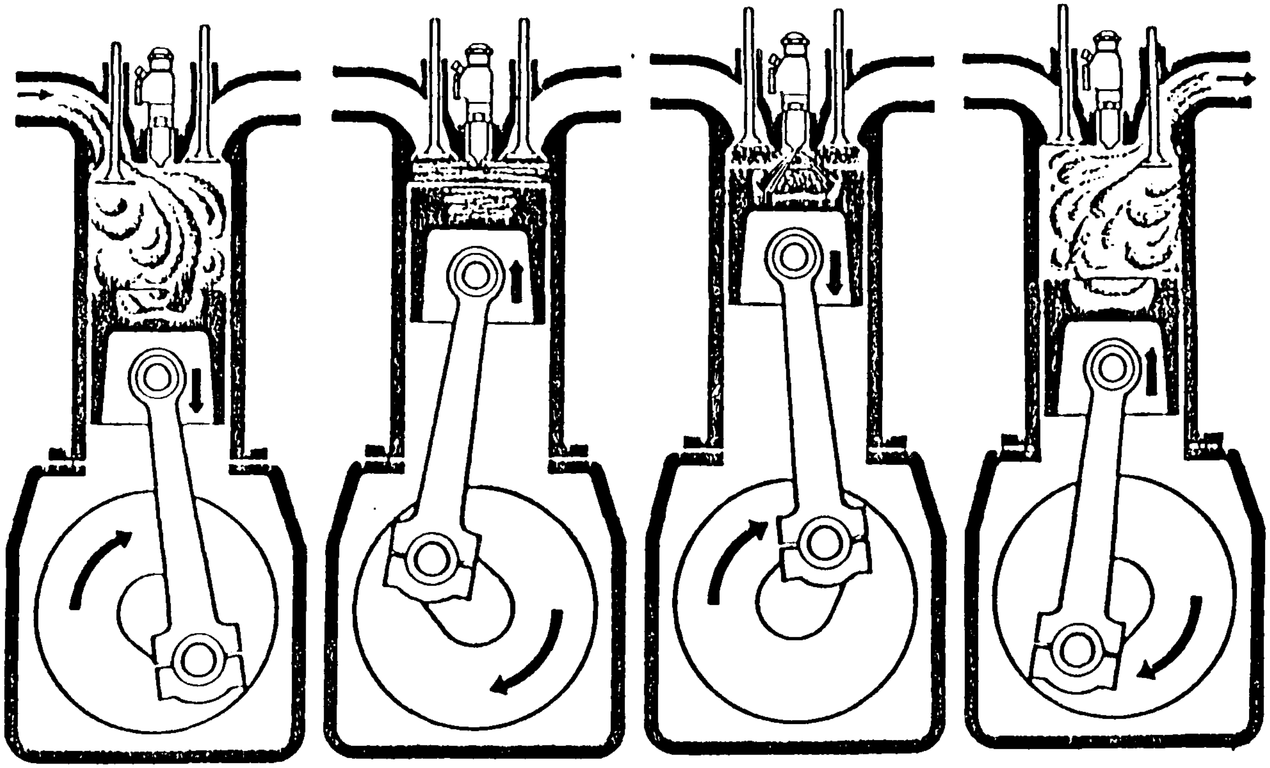
Engine Type	LABECO TACOM single cylinder experimental engine
Bore	11.43 cm
Stroke	11.43 cm
Displacement	1172.8 cc
Compression Ratio	16.79:1
Conrod Length	22.86 cm
Squish Clearance	.092 cm
IVC	-120°ATDC
EVO	+120°ATDC
Injector Nozzle	8 holes X .025 cm diam X 157° injection angle
Opening Pressure	21.02 MPa
Piston Bowl	8.89 cm diam X 1.27 cm max depth X 74.29 cc volume

Table 4-2 TACOM Engine Test Cases

RUN	17	18	19	20	21
Equivalence Ratio	0.50	0.50	0.50	0.50	0.50
Swirl Ratio	2.46	2.46	2.46	2.46	2.46
Nozzle Type	8-hole	8-hole	8-hole	8-hole	8-hole
EGR (%)	0.00	0.00	0.00	10.0	10.0
Engine Speed (RPM)	1001	1001	998	999	1002
Intake Temp (°K)	339.	339.	339.	339.	339.
Start of Injection (° ATDC)	-15	-15	-15	-15	-15
Injection Duration (CA °)	18.	18.	18.	18.	18.
Start of Combustion (° ATDC)	-7.8	-8.4	-15.0	-7.8	-7.2
Peak Pressure (atm)	1049	1053	1343	1006	1017
Dry Exhaust NO (ppm)	842	625	1600	356	290
Exhaust Temp (°K)	658	646	642	667	645
Smoke (Bosch No.)	4.2	4.3	3.3	5.7	6.9

Table 6-1 Comparison of Experimental and SMM Results - Summary of Major Features

RUN	INJECT (° ATDC)	SWIRL	EGR (%)	P_{max} (atm)	$[NO]_{80°}$ (ppm)	$Soot_{max}$ (%C)	$Soot_{80°}$ (%C)	$(m_{bf})_{80°}$ (g)	Comments
17(SMM)	-15.	2.46	0.0	76.3	841.	11.3	0.016	0.0488	Slight hump at +20° in soot plot.
17(exp)				70.9	842.		0.016		
18(SMM)	-15.	4.00	0.0	76.1	508.	11.2	0.269	0.0502	Hump at +20° in soot plot.
18(exp)				71.7	625.		0.017		
19(SMM)	-25.	2.46	0.0	86.7	1100.	7.36	0.013	0.0489	NO drops off substantially around +20°.
19(exp)				91.4	1600.		0.011		Burning much slower than KIVA at the start.
20(SMM)	-15.	2.46	10.0	69.8	378.	9.97	0.425	0.0486	Slight soot hump at +20°.
20(exp)				68.4	356.		0.030		
21(SMM)	-15.	4.00	10.0	72.6	353.	9.83	0.566	0.0502	Soot hump at +20°.
21(exp)				69.2	290.		0.049		



Intake Compression Combustion Exhaust

The Four-Stroke Diesel Engine [3]

Figure 1-1

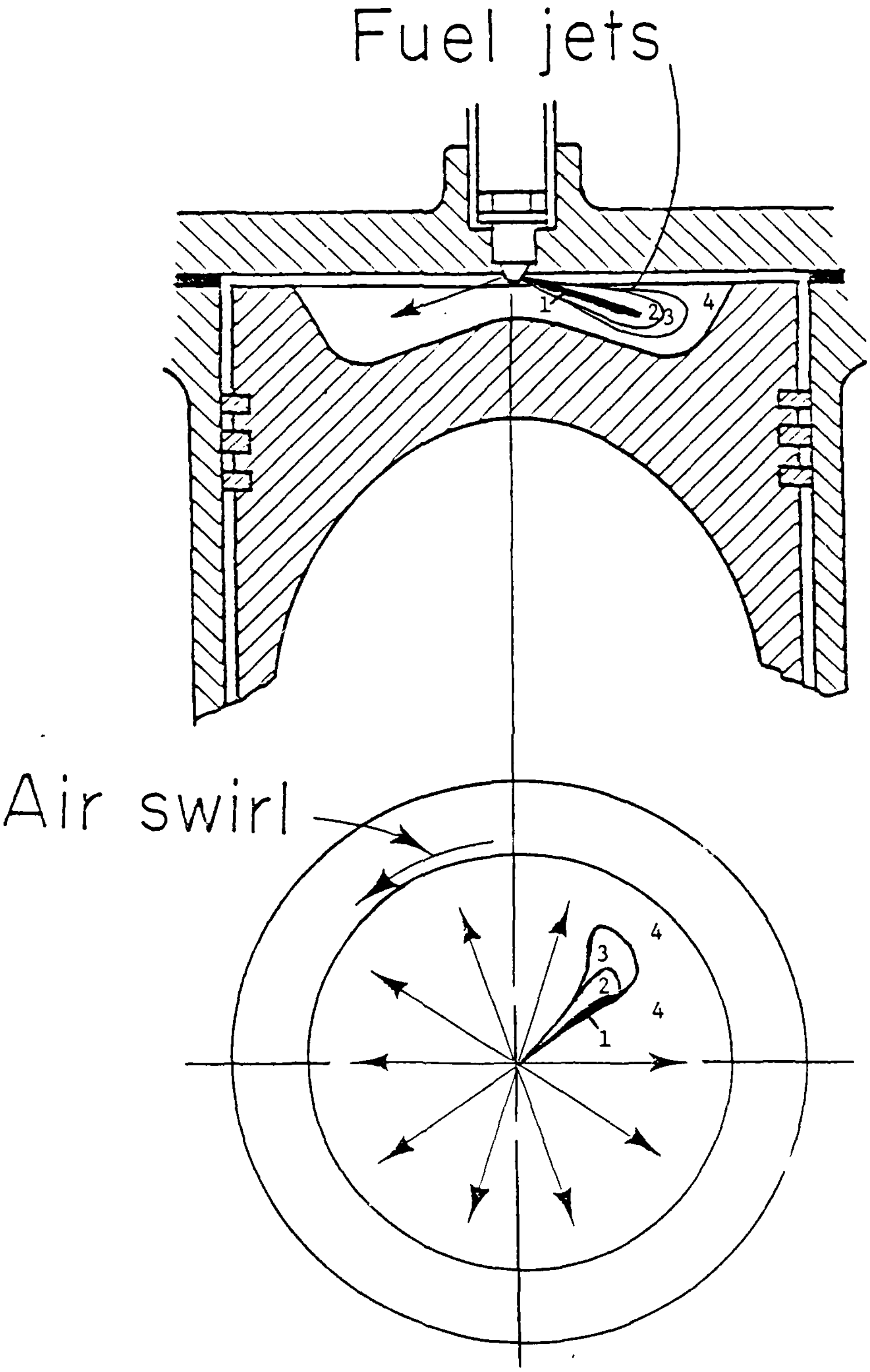


Figure 1-2 Schematic of Direct-Injection Diesel Cylinder and and Fuel Spray Showing Four Typical Mixing Zones

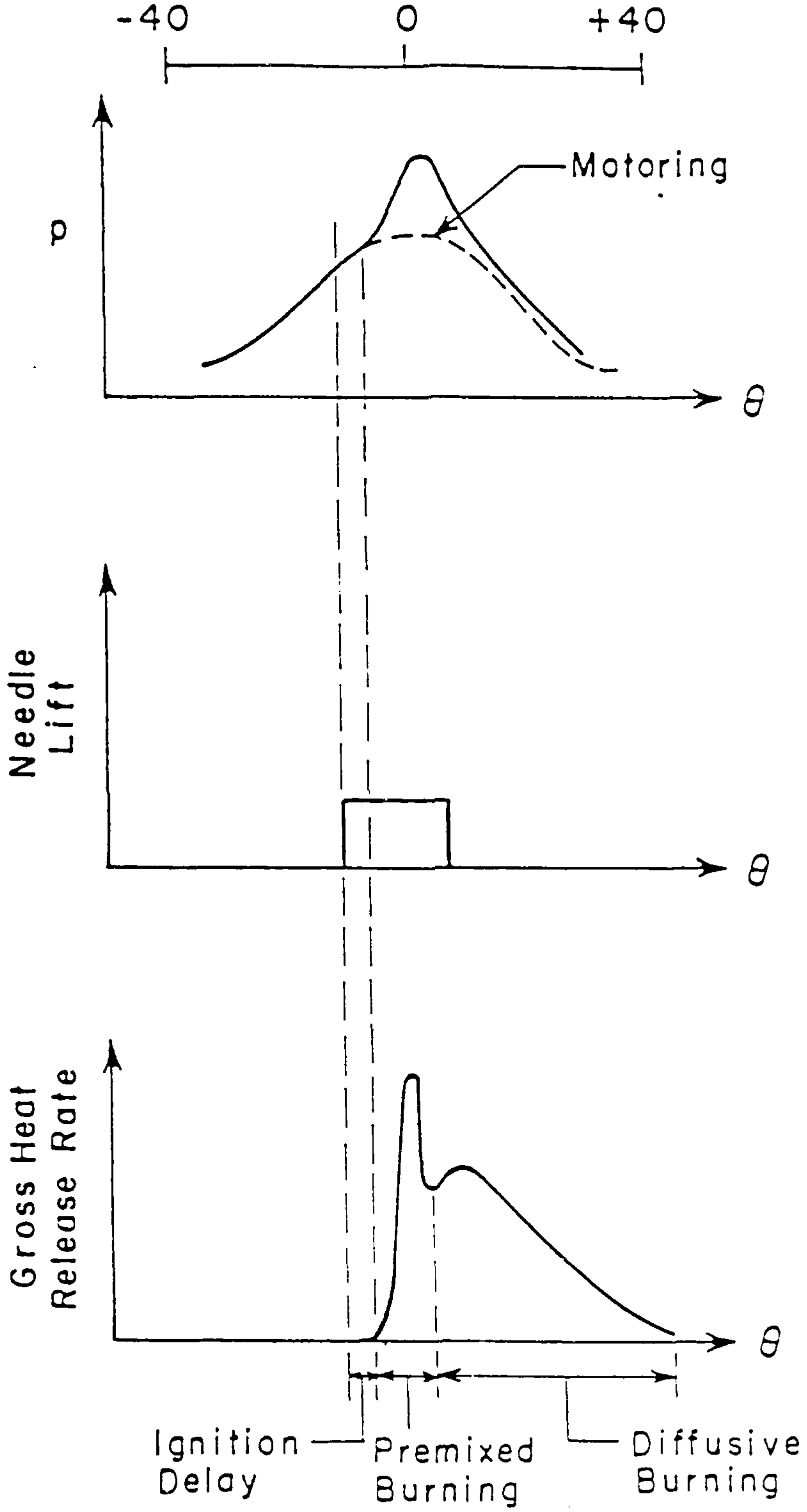
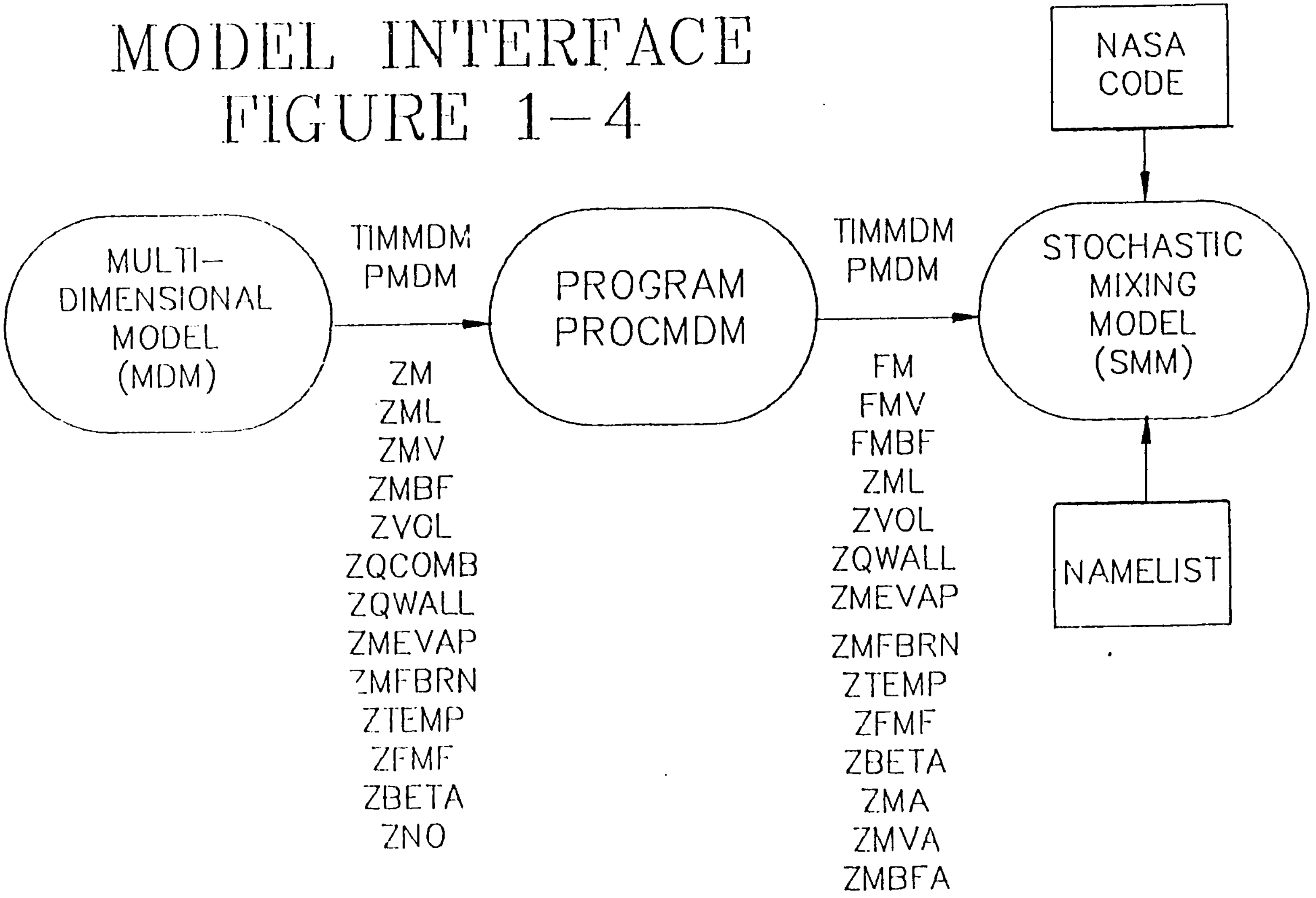


Figure 1-3 Pressure, Needle Lift, and Heat Release Profiles of a Direct Injection Diesel Engine [3]

MODEL INTERFACE
FIGURE 1–4



AD-A175 155 A STOCHASTIC MIXING MODEL FOR PREDICTING EMISSIONS IN A 2/4
DIRECT INJECTION (U) MASSACHUSETTS INST OF TECH
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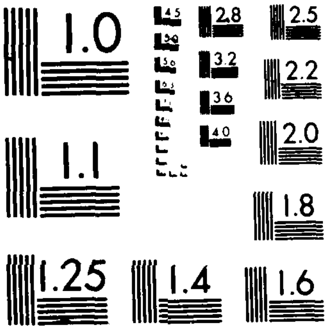


CROCOPY RESOLUTION TEST CHART

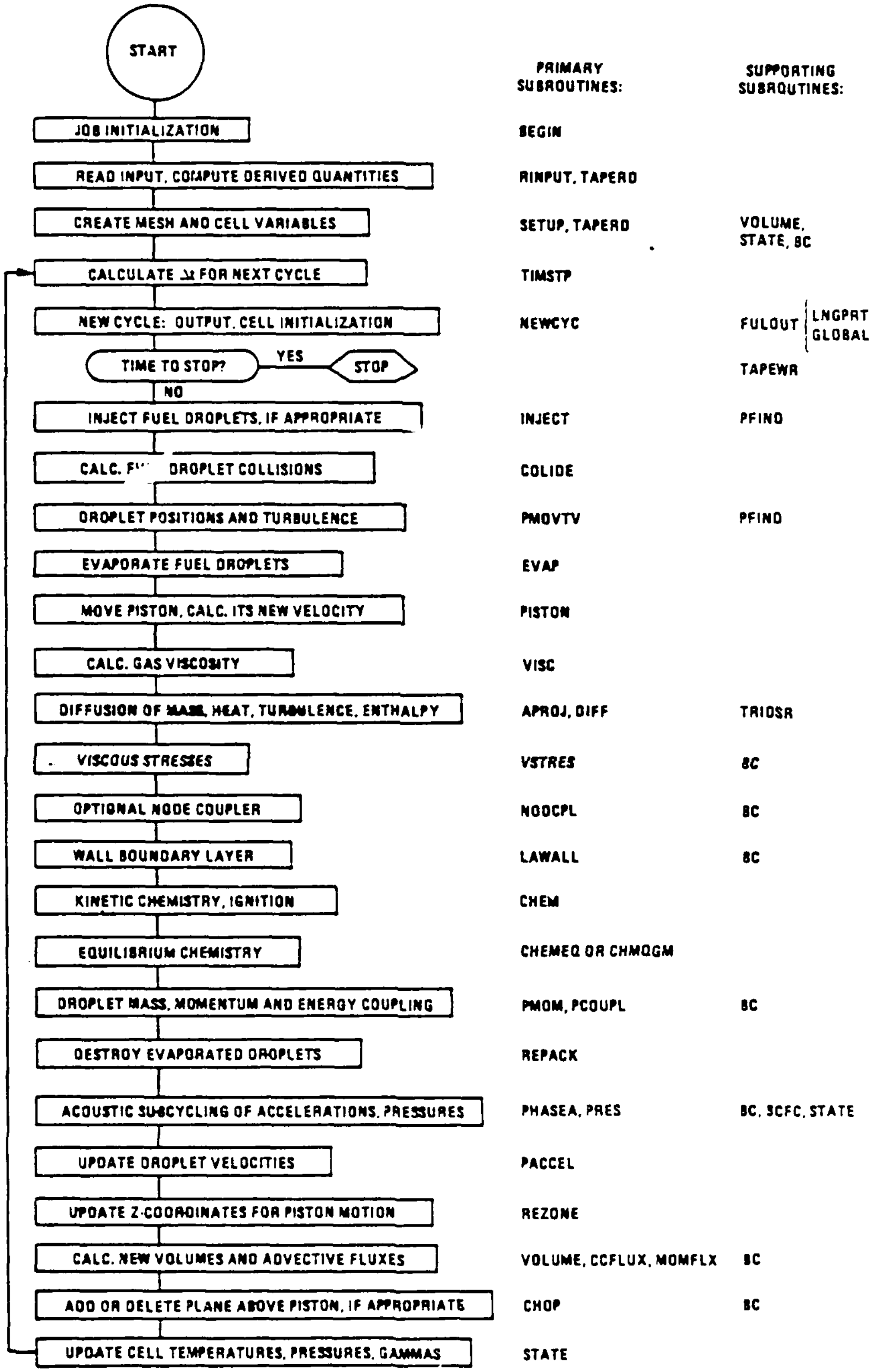


Figure 2-1 General flow diagram for the revised KIVA program. [15]

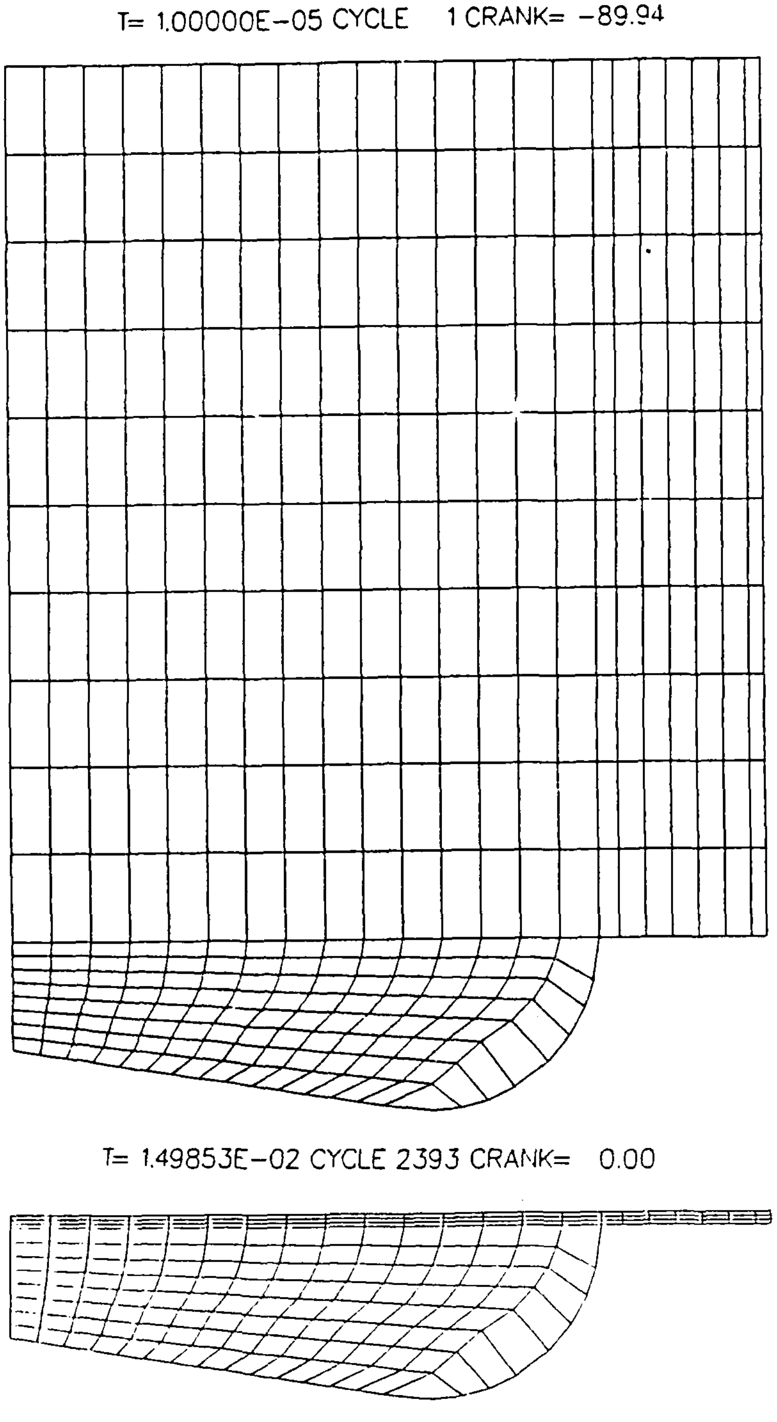


Figure 2-2 KIVA Computational Grid

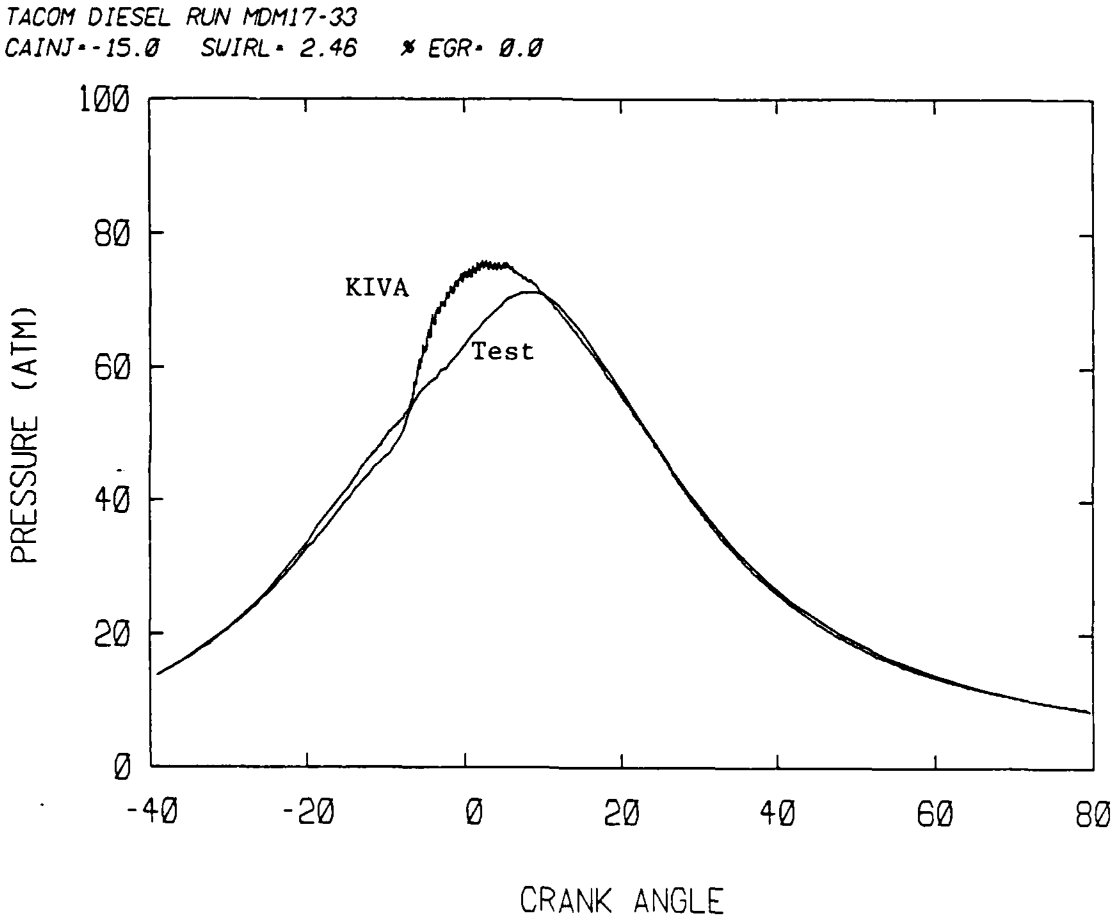


Figure 2-3 KIVA Pressure Trace VS. Test Results (Run 17)

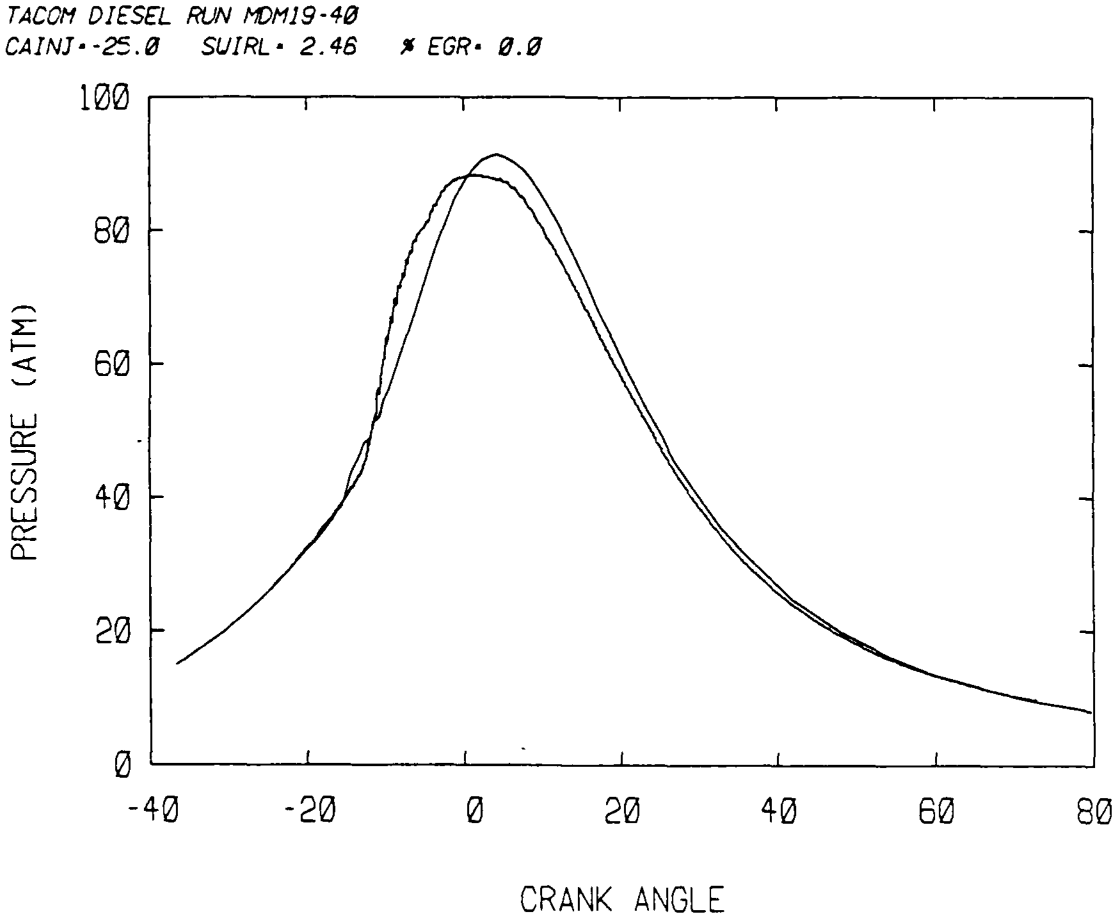


Figure 2-4 KIVA Pressure Trace VS. Test Results
(Run 19)

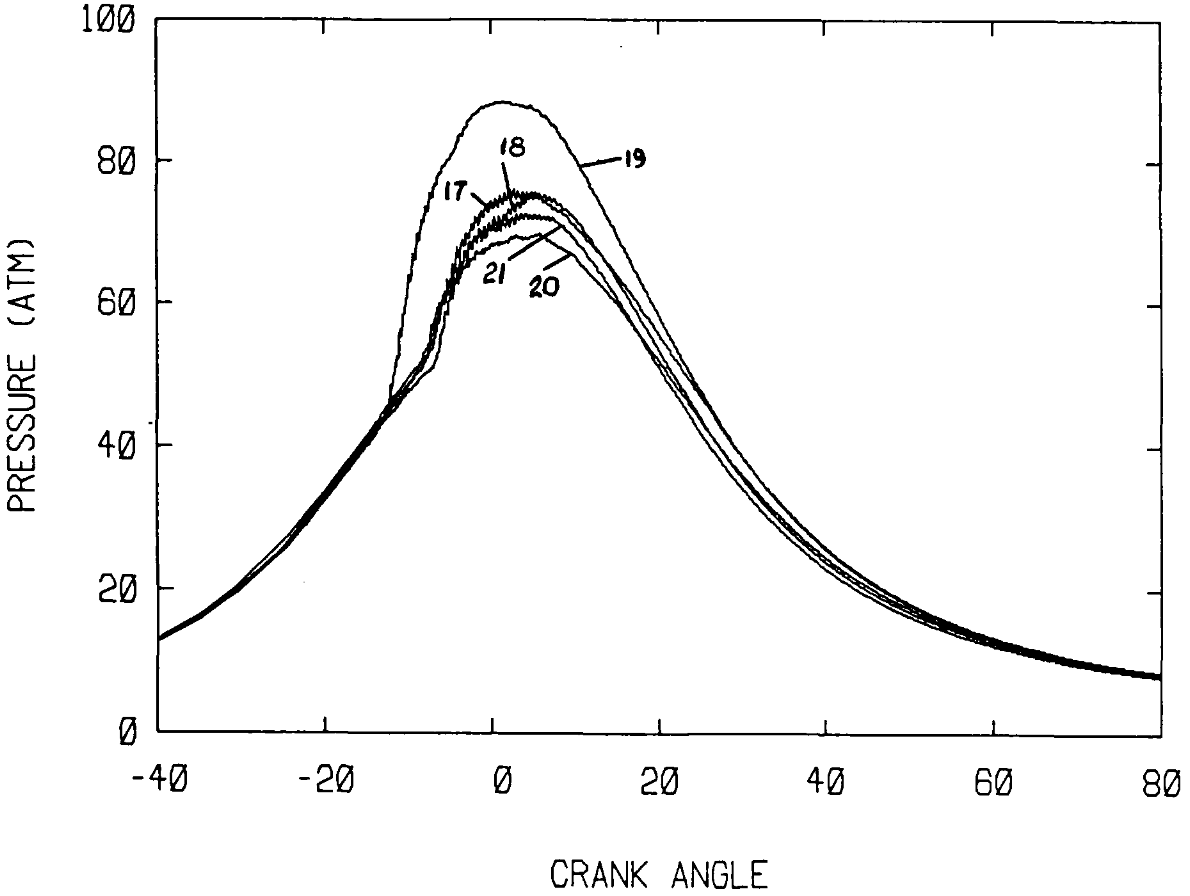


Figure 2-5 KIVA Pressure Traces (All Runs)

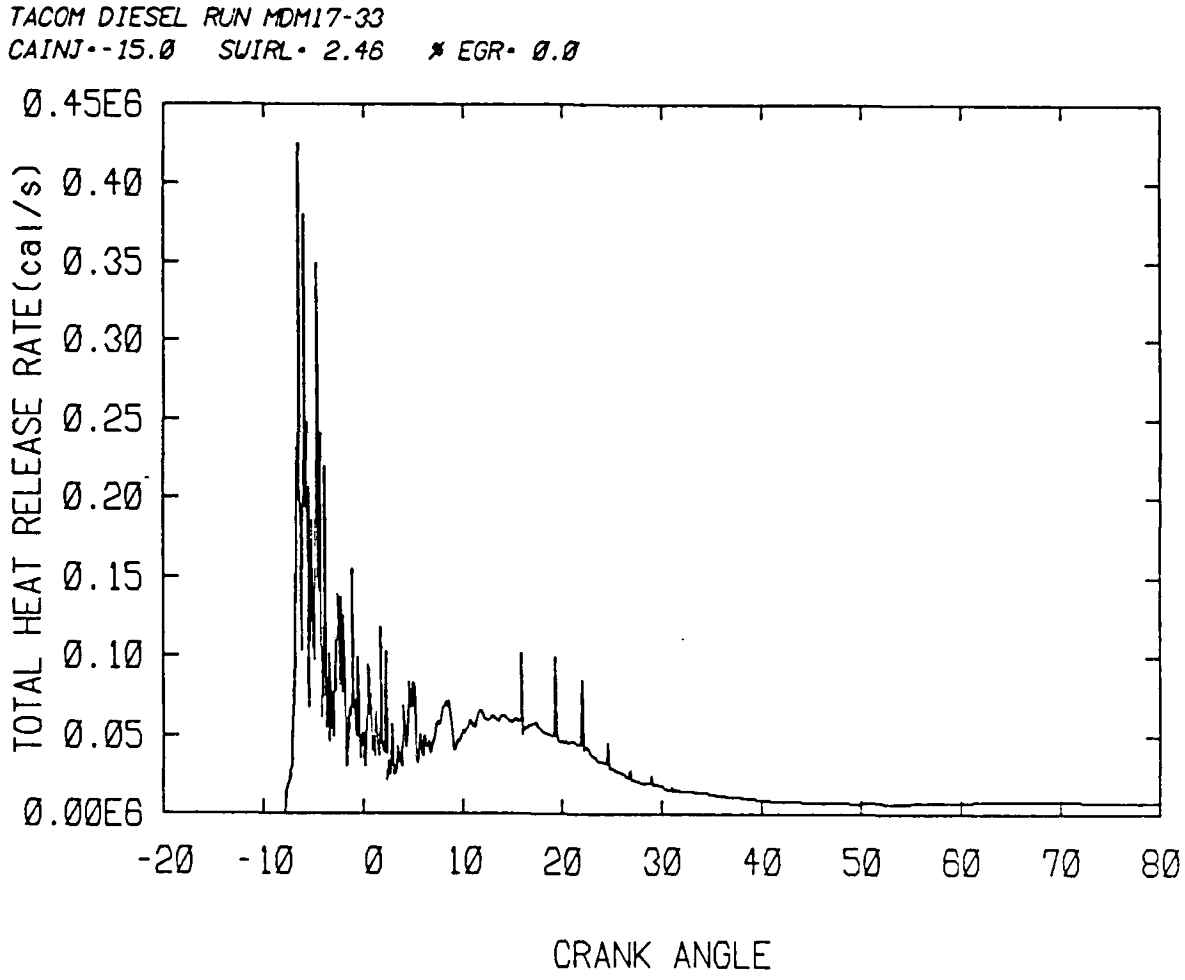


Figure 2-6 KIVA Heat Release Rate (Run 17)

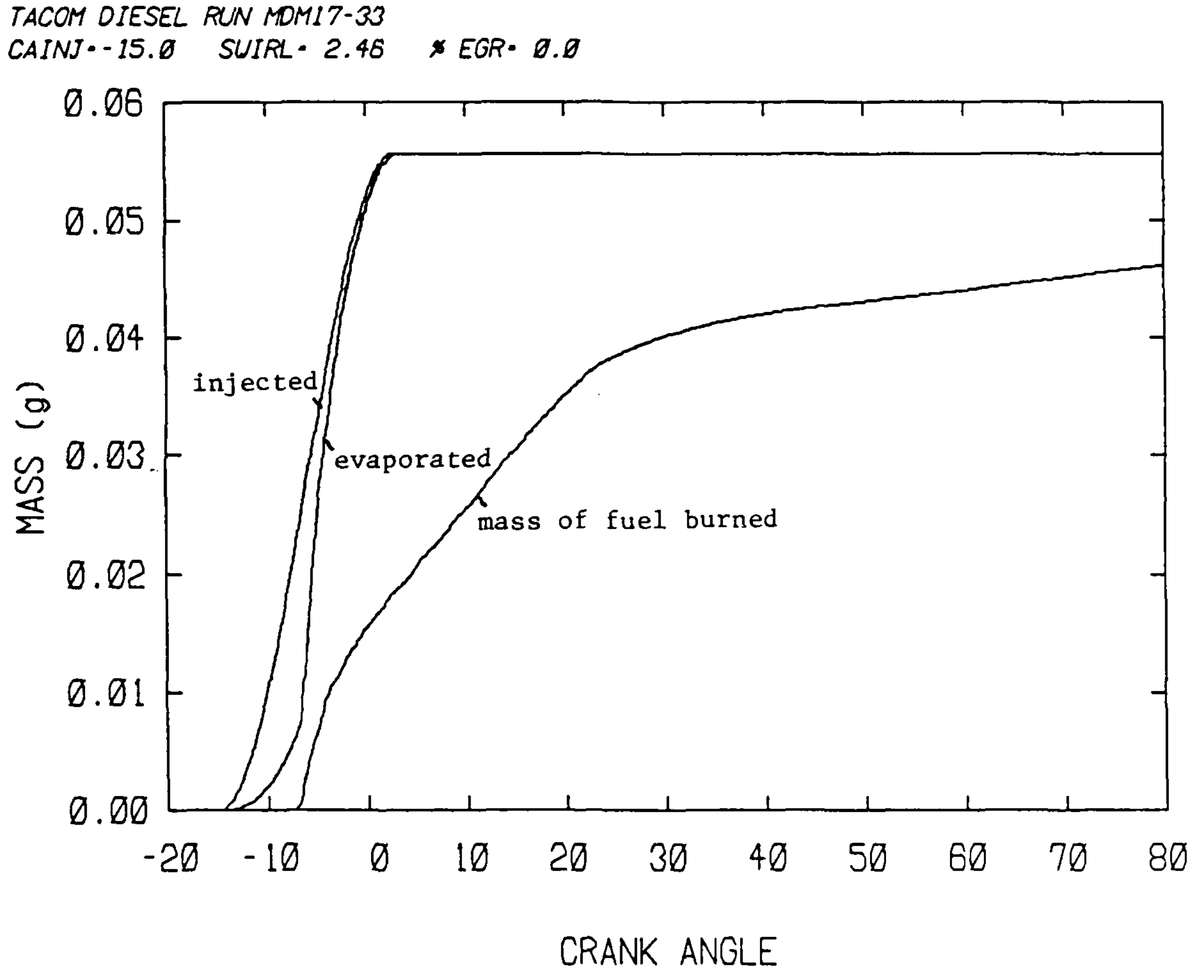


Figure 2-7 KIVA Fuel Mass History (Run 17)

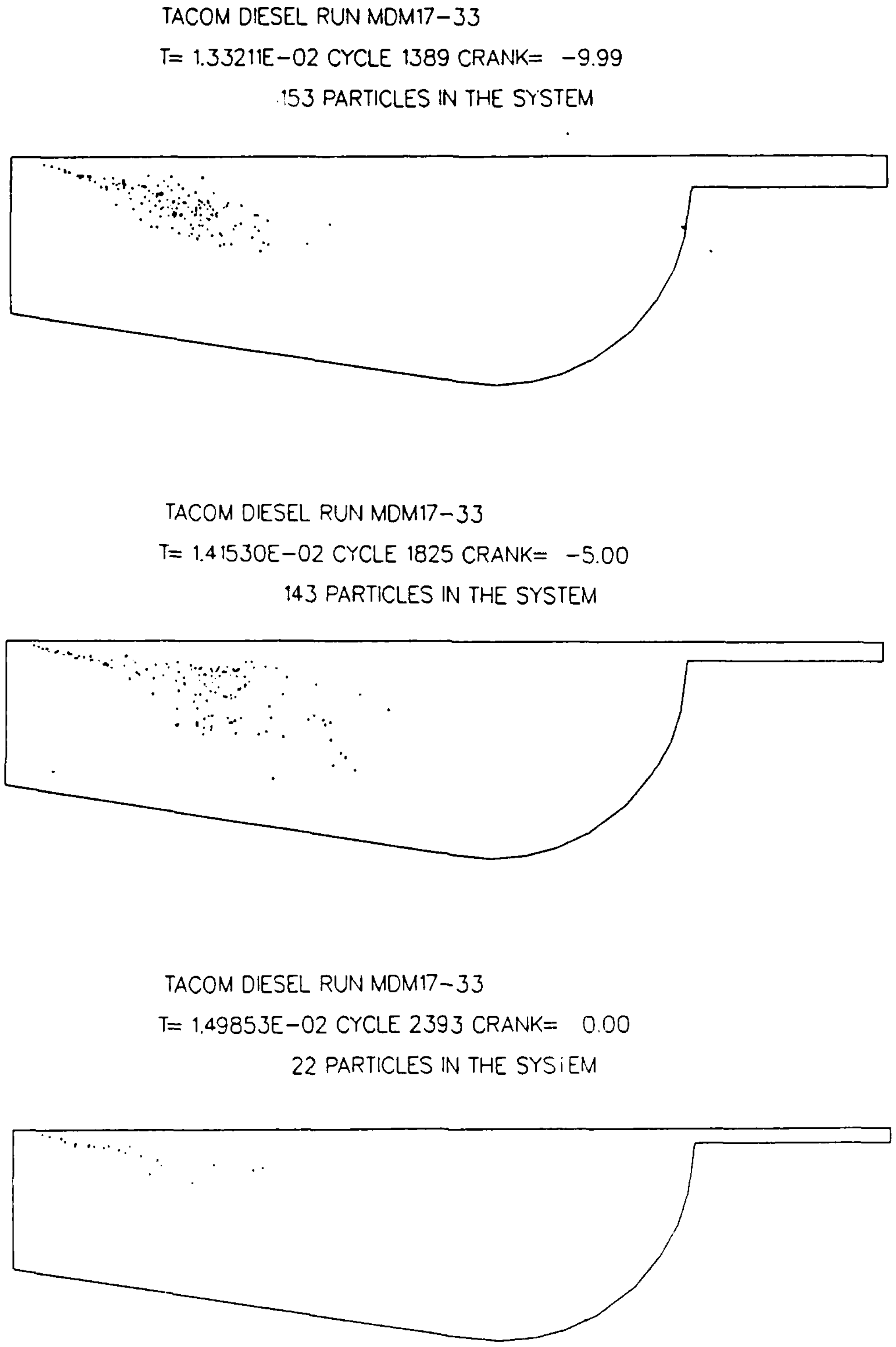


Figure 2-8 KIVA Injection Particle Plot
(Run 17)

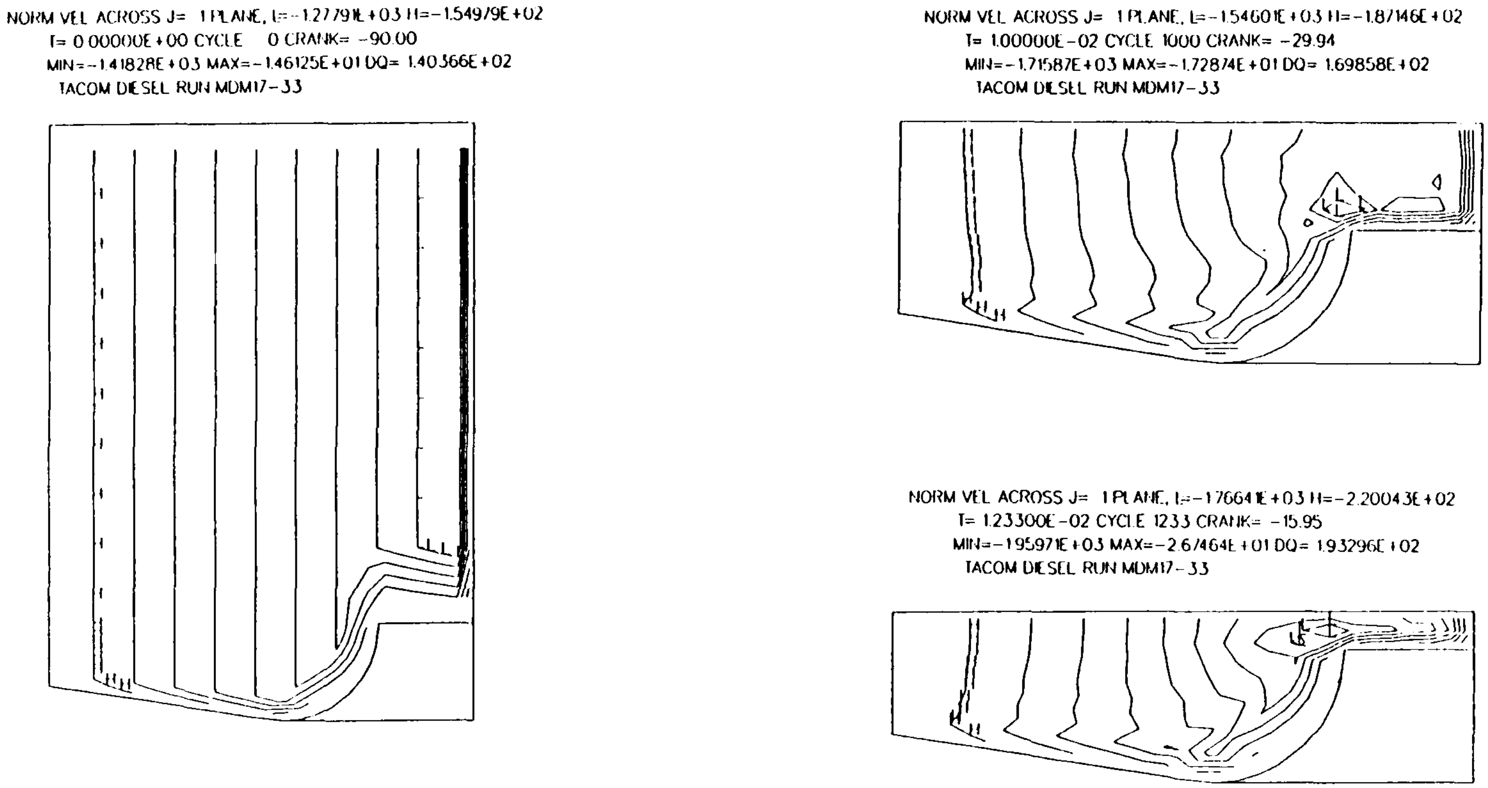
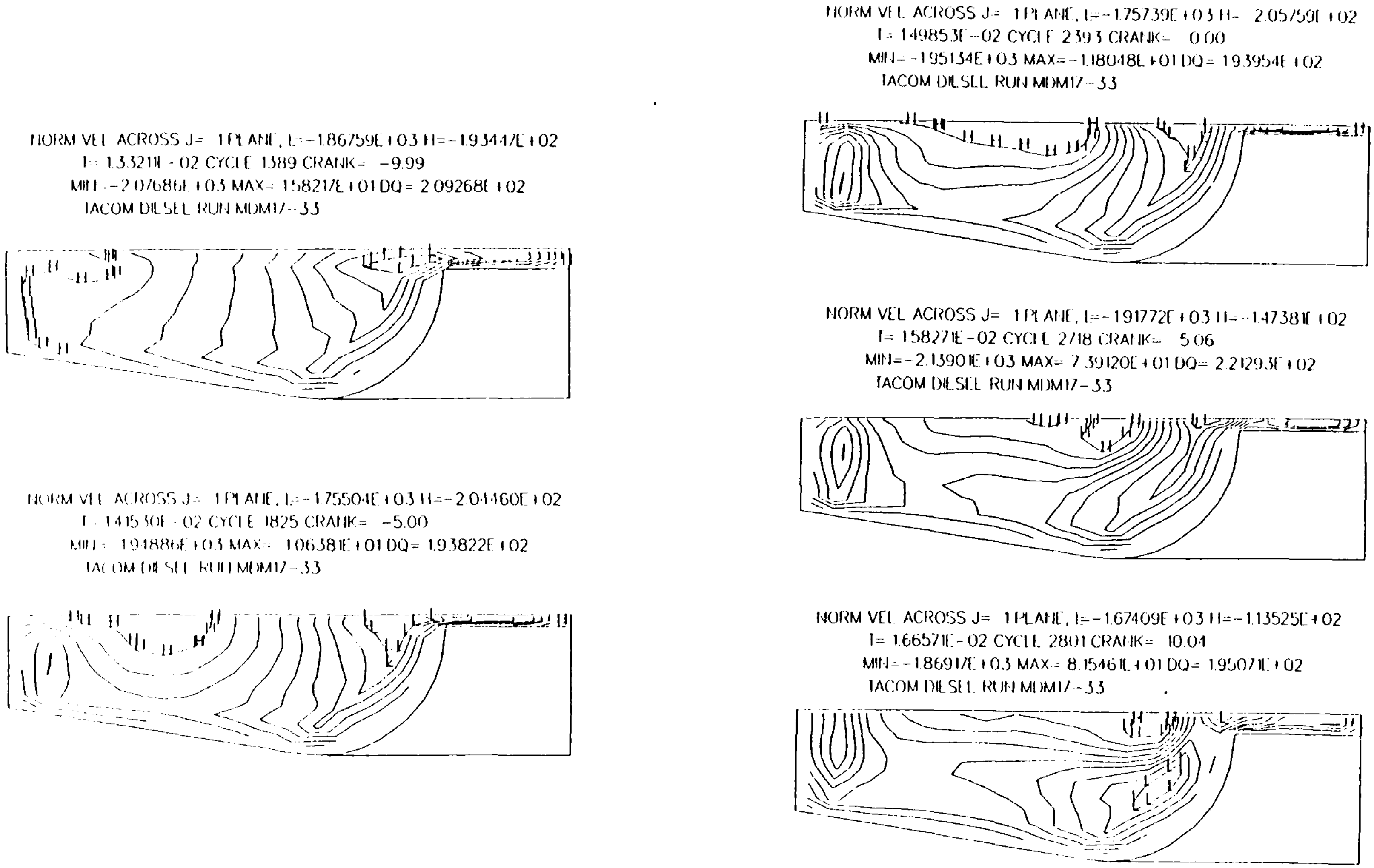


Figure 2-9 KIVA Swirl Velocity
(Run 17)



NORM VEL ACROSS J= 1 PLANE, L=-1.86759E+03 H=-1.93447E+02
T= 1.33211E-02 CYCLE 1389 CRANK= -9.99
MIN=-2.07686E+03 MAX= 1.58217E+01 DQ= 2.09268E+02
TACOM DIESEL RUN MDM17-33

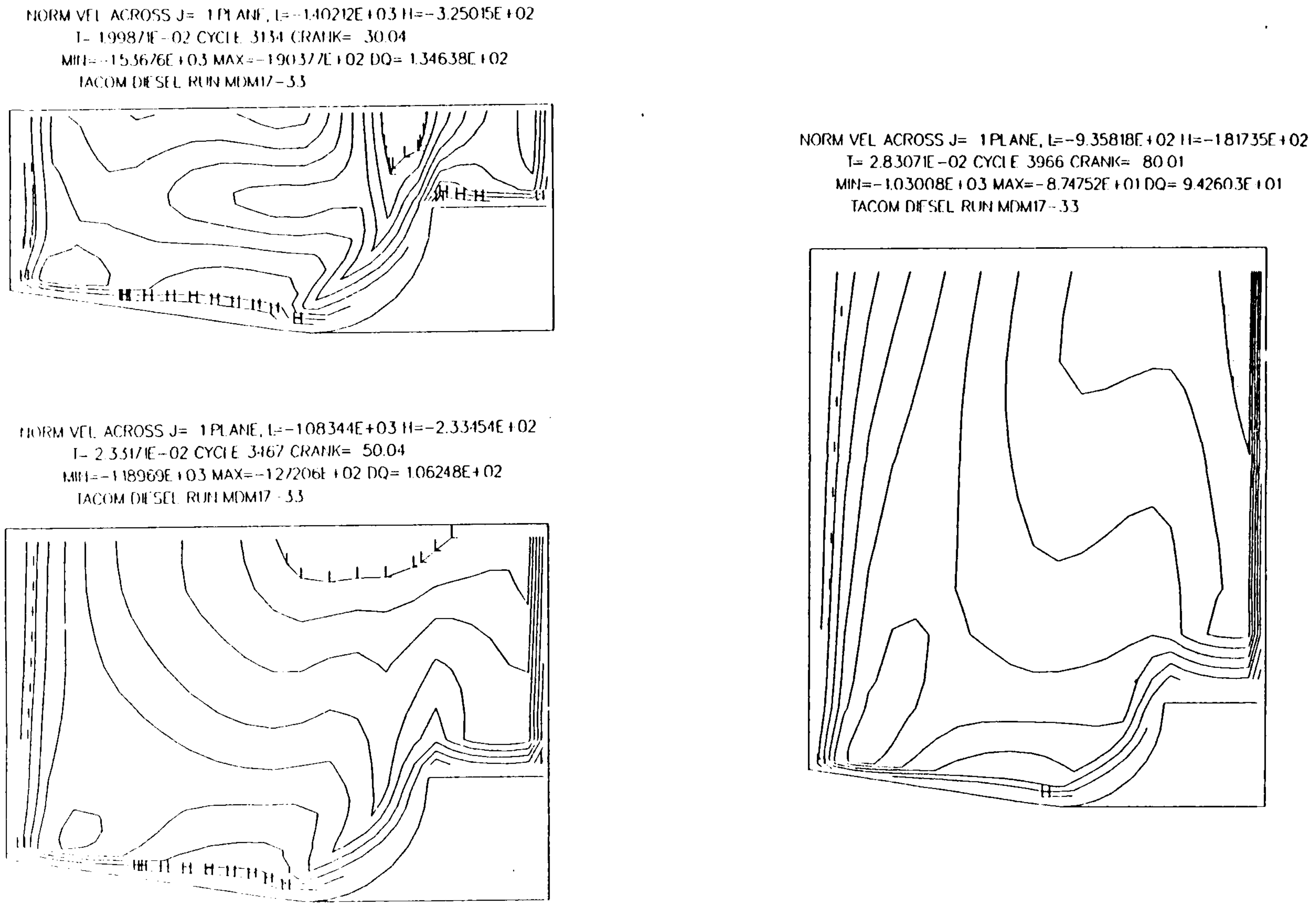
NORM VEL ACROSS J= 1 PLANE, L=-1.75504E+03 H=-2.04460E+02
T= 1.41530E-02 CYCLE 1825 CRANK= -5.00
MIN= 1.94886E+03 MAX= 1.06381E+01 DQ= 1.93822E+02
TACOM DIESEL RUN MDM17-33

NORM VEL ACROSS J= 1 PLANE, L=-1.75739E+03 H= 2.05759E+02
T= 1.49853E-02 CYCLE 2393 CRANK= 0.00
MIN=-1.95134E+03 MAX=-1.18048E+01 DQ= 1.93954E+02
TACOM DIESEL RUN MDM17-33

NORM VEL ACROSS J= 1 PLANE, L=-1.91772E+03 H=-1.47381E+02
T= 1.58271E-02 CYCLE 2718 CRANK= 5.06
MIN=-2.13901E+03 MAX= 7.39120E+01 DQ= 2.21293E+02
TACOM DIESEL RUN MDM17-33

NORM VEL ACROSS J= 1 PLANE, L=-1.67409E+03 H=-1.13525E+02
T= 1.66571E-02 CYCLE 2801 CRANK= 10.04
MIN=-1.86917E+03 MAX= 8.15461E+01 DQ= 1.95071E+02
TACOM DIESEL RUN MDM17-33

Figure 2-10 KIVA Swirl Velocity (cont)
(Run 17)

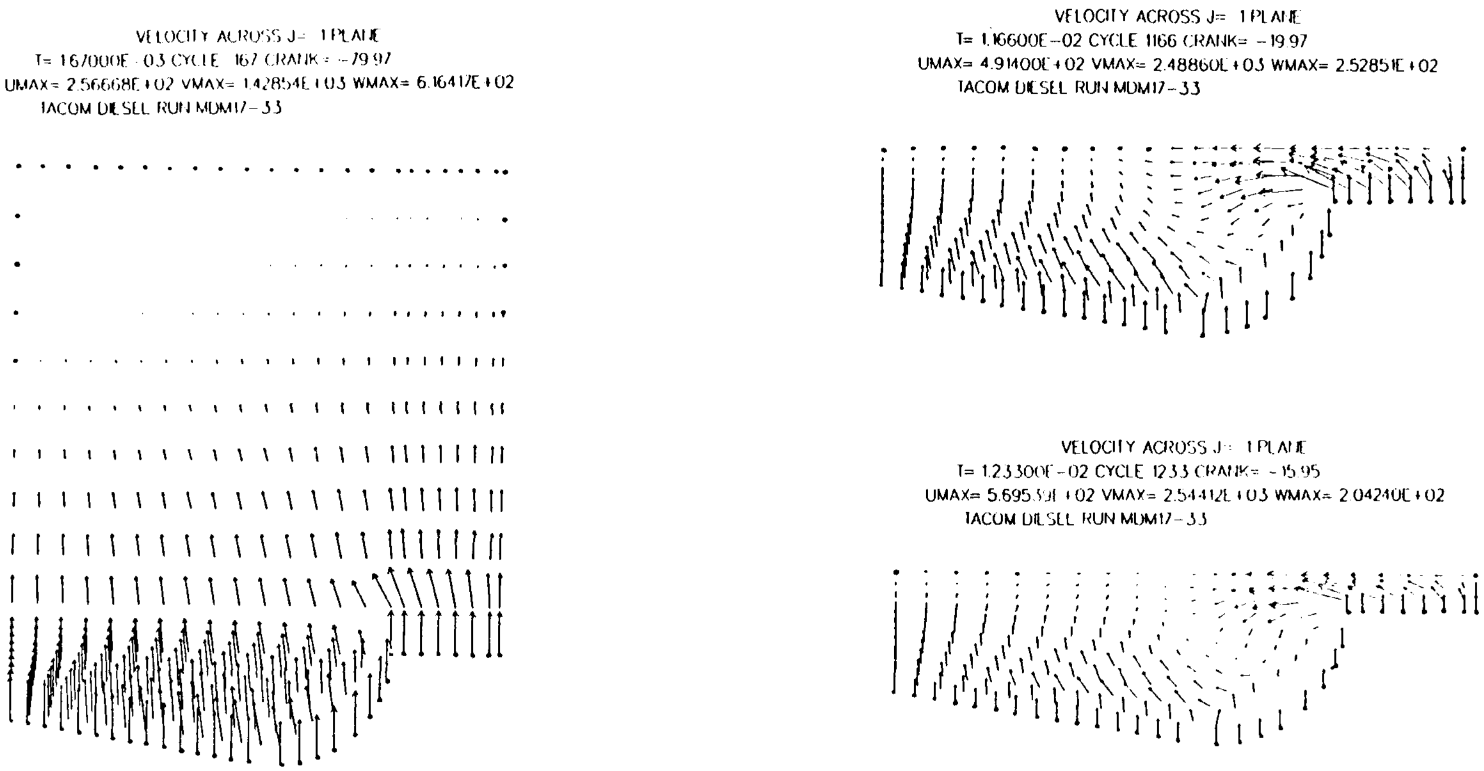


NORM VEL ACROSS J= 1 PLANE, L=-1.40212E+03 H=-3.25015E+02
T= 1.99871E-02 CYCLE 3134 CRANK= 30.04
MIN=-1.53676E+03 MAX=-1.90377E+02 DQ= 1.34638E+02
TACOM DIESEL RUN MDM17-33

NORM VEL ACROSS J= 1 PLANE, L=-1.08344E+03 H=-2.33454E+02
T= 2.33171E-02 CYCLE 3467 CRANK= 50.04
MIN=-1.18969E+03 MAX=-1.27206E+02 DQ= 1.06248E+02
TACOM DIESEL RUN MDM17-33

NORM VEL ACROSS J= 1 PLANE, L=-9.35818E+02 H=-1.81735E+02
T= 2.83071E-02 CYCLE 3966 CRANK= 80.01
MIN=-1.03008E+03 MAX=-8.74752E+01 DQ= 9.42603E+01
TACOM DIESEL RUN MDM17-33

Figure 2-11 KIVA Swirl Velocity (cont)

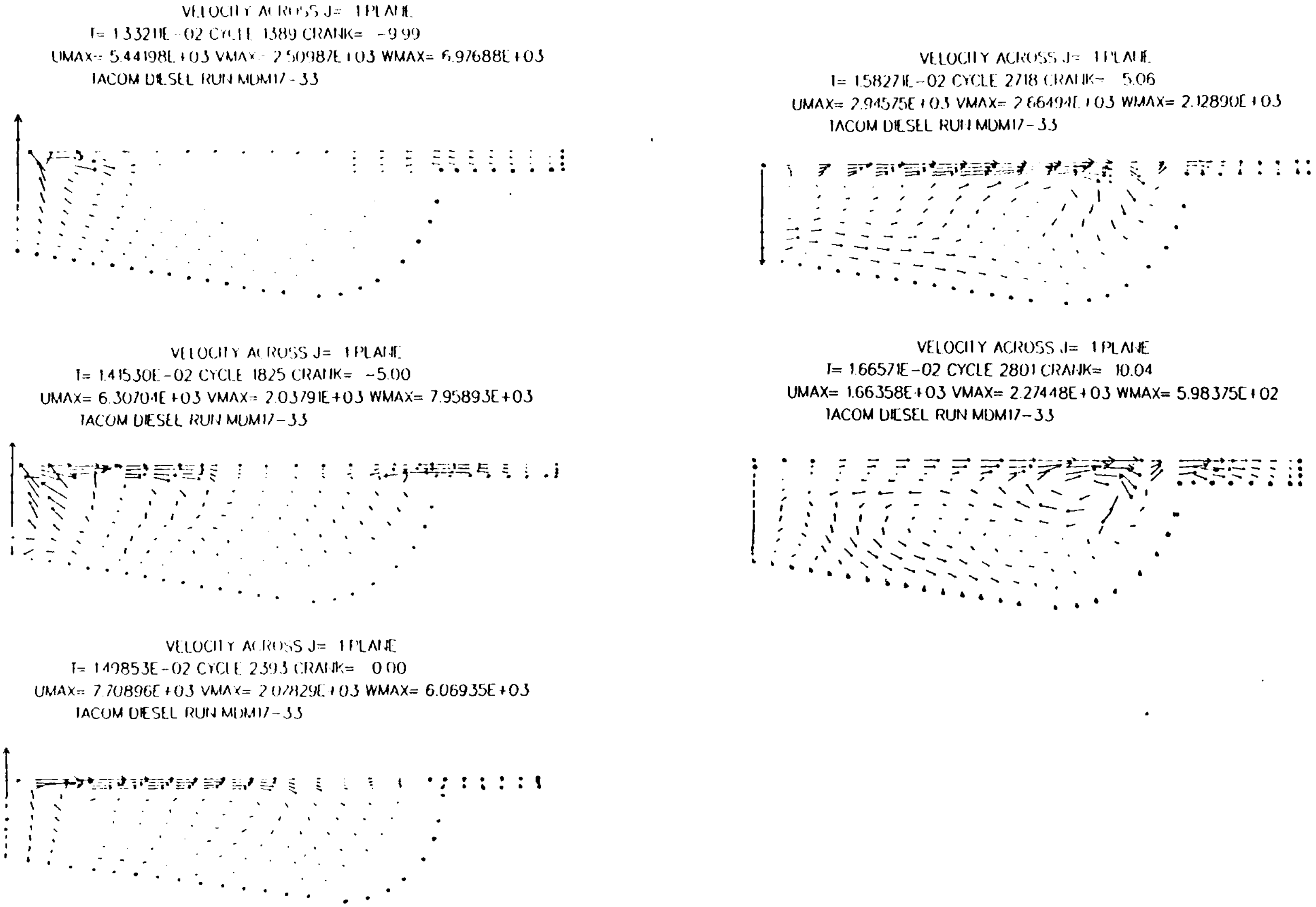


VELOCITY ACROSS J= 1 PLANE
T= 1.67000E-03 CYCLE 167 CRANK= -79.97
UMAX= 2.56668E+02 VMAX= 1.42854E+03 WMAX= 6.16417E+02
TACOM DIESEL RUN MDM17-33

VELOCITY ACROSS J= 1 PLANE
T= 1.16600E-02 CYCLE 1166 CRANK= -19.97
UMAX= 4.91400E+02 VMAX= 2.48860E+03 WMAX= 2.52851E+02
TACOM DIESEL RUN MDM17-33

VELOCITY ACROSS J= 1 PLANE
T= 1.23300E-02 CYCLE 1233 CRANK= -15.95
UMAX= 5.69559E+02 VMAX= 2.54412E+03 WMAX= 2.04240E+02
TACOM DIESEL RUN MDM17-33

Figure 2-12 KIVA In-Plane Velocities (Run 17)



VELOCITY ACROSS J= 1 PLANE
T= 1.33211E-02 CYCLE 1389 CRANK= -9.99
UMAX= 5.44198E+03 VMAX= 2.50987E+03 WMAX= 6.97688E+03
TACOM DIESEL RUN MDM17-33

VELOCITY ACROSS J= 1 PLANE
T= 1.41530E-02 CYCLE 1825 CRANK= -5.00
UMAX= 6.30704E+03 VMAX= 2.03791E+03 WMAX= 7.95893E+03
TACOM DIESEL RUN MDM17-33

VELOCITY ACROSS J= 1 PLANE
T= 1.49853E-02 CYCLE 2393 CRANK= 0.00
UMAX= 7.70896E+03 VMAX= 2.07829E+03 WMAX= 6.06935E+03
TACOM DIESEL RUN MDM17-33

VELOCITY ACROSS J= 1 PLANE
T= 1.58271E-02 CYCLE 2718 CRANK= 5.06
UMAX= 2.94575E+03 VMAX= 2.66494E+03 WMAX= 2.12890E+03
TACOM DIESEL RUN MDM17-33

VELOCITY ACROSS J= 1 PLANE
T= 1.66571E-02 CYCLE 2801 CRANK= 10.04
UMAX= 1.66358E+03 VMAX= 2.27448E+03 WMAX= 5.98375E+02
TACOM DIESEL RUN MDM17-33

Figure 2-13 KIVA In-Plane Velocities (cont)
(Run 17)

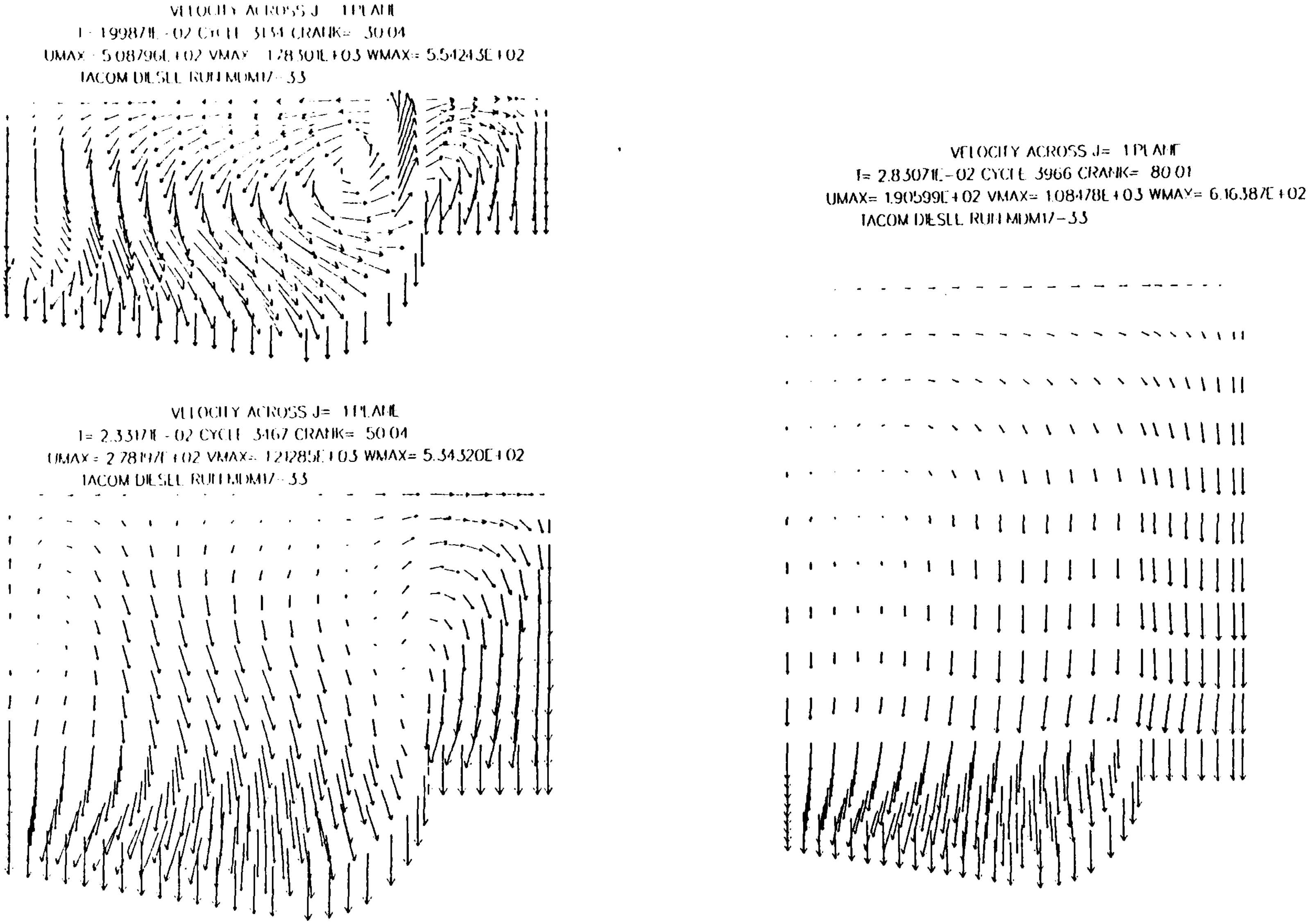
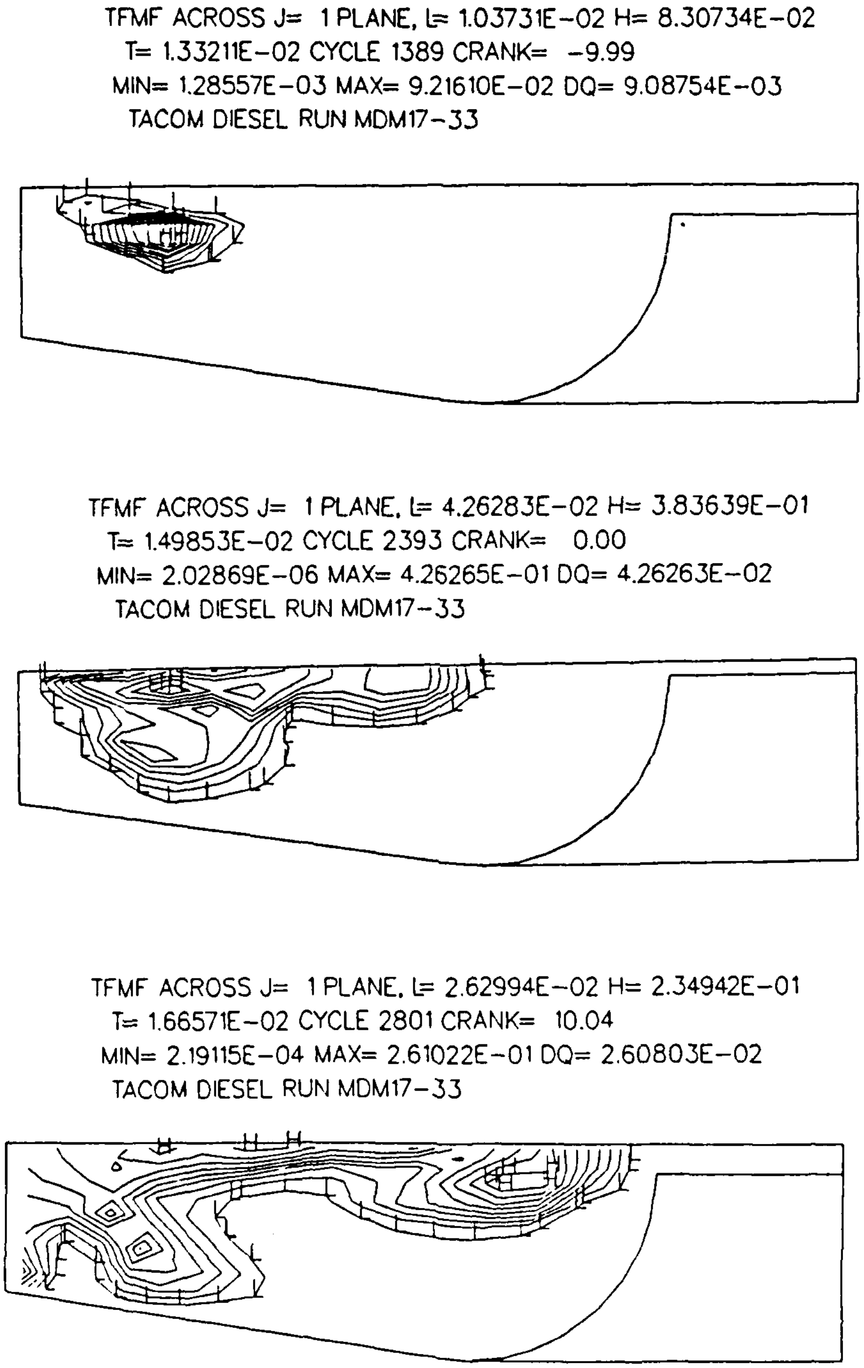


Figure 2-14 KIVA In-Plane Velocities (cont)
(Run 17)



TFMF ACROSS J= 1 PLANE, L= 1.03731E-02 H= 8.30734E-02
T= 1.33211E-02 CYCLE 1389 CRANK= -9.99
MIN= 1.28557E-03 MAX= 9.21610E-02 DQ= 9.08754E-03
TACOM DIESEL RUN MDM17-33

TFMF ACROSS J= 1 PLANE, L= 4.26283E-02 H= 3.83639E-01
T= 1.49853E-02 CYCLE 2393 CRANK= 0.00
MIN= 2.02869E-06 MAX= 4.26265E-01 DQ= 4.26263E-02
TACOM DIESEL RUN MDM17-33

TFMF ACROSS J= 1 PLANE, L= 2.62994E-02 H= 2.34942E-01
T= 1.66571E-02 CYCLE 2801 CRANK= 10.04
MIN= 2.19115E-04 MAX= 2.61022E-01 DQ= 2.60803E-02
TACOM DIESEL RUN MDM17-33

Figure 2-15 KIVA Total Fuel Mass Fraction Contours (Run 17)

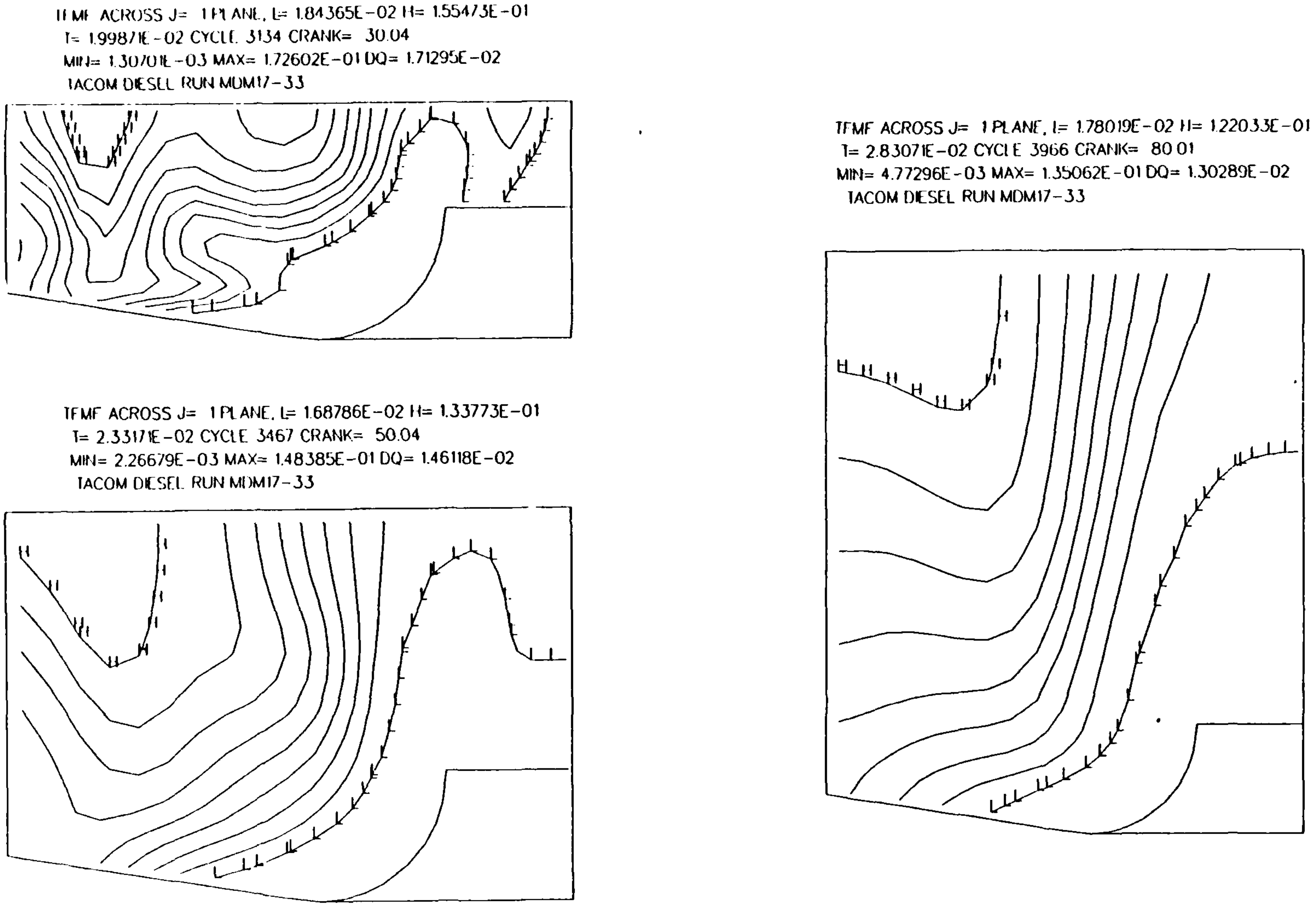


Figure 2-16 KIVA Total Fuel Mass Fraction Contours (cont)
(Run 17)

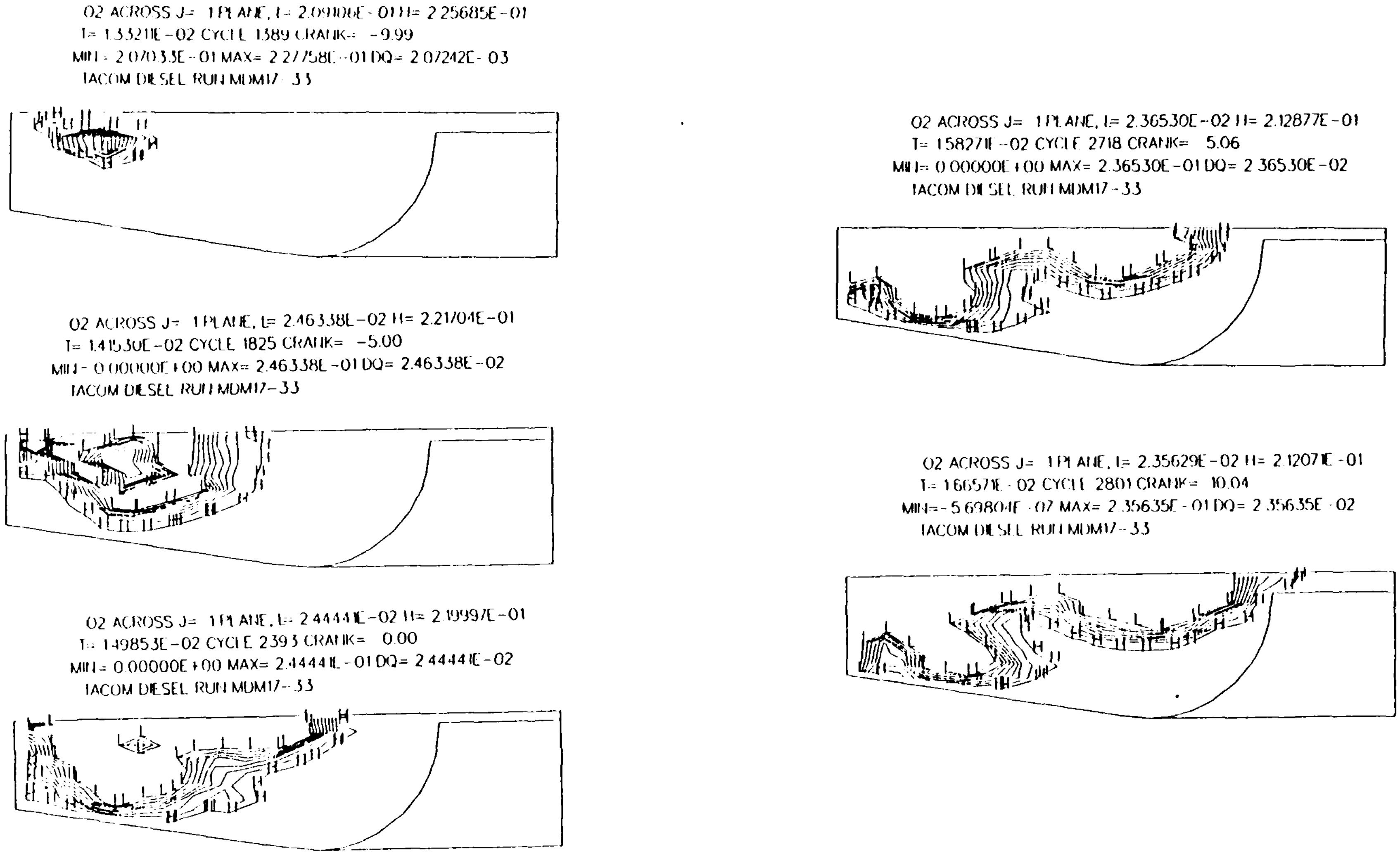


Figure 2-17 KIVA Oxygen Mass Fraction Contours
(Run 17)

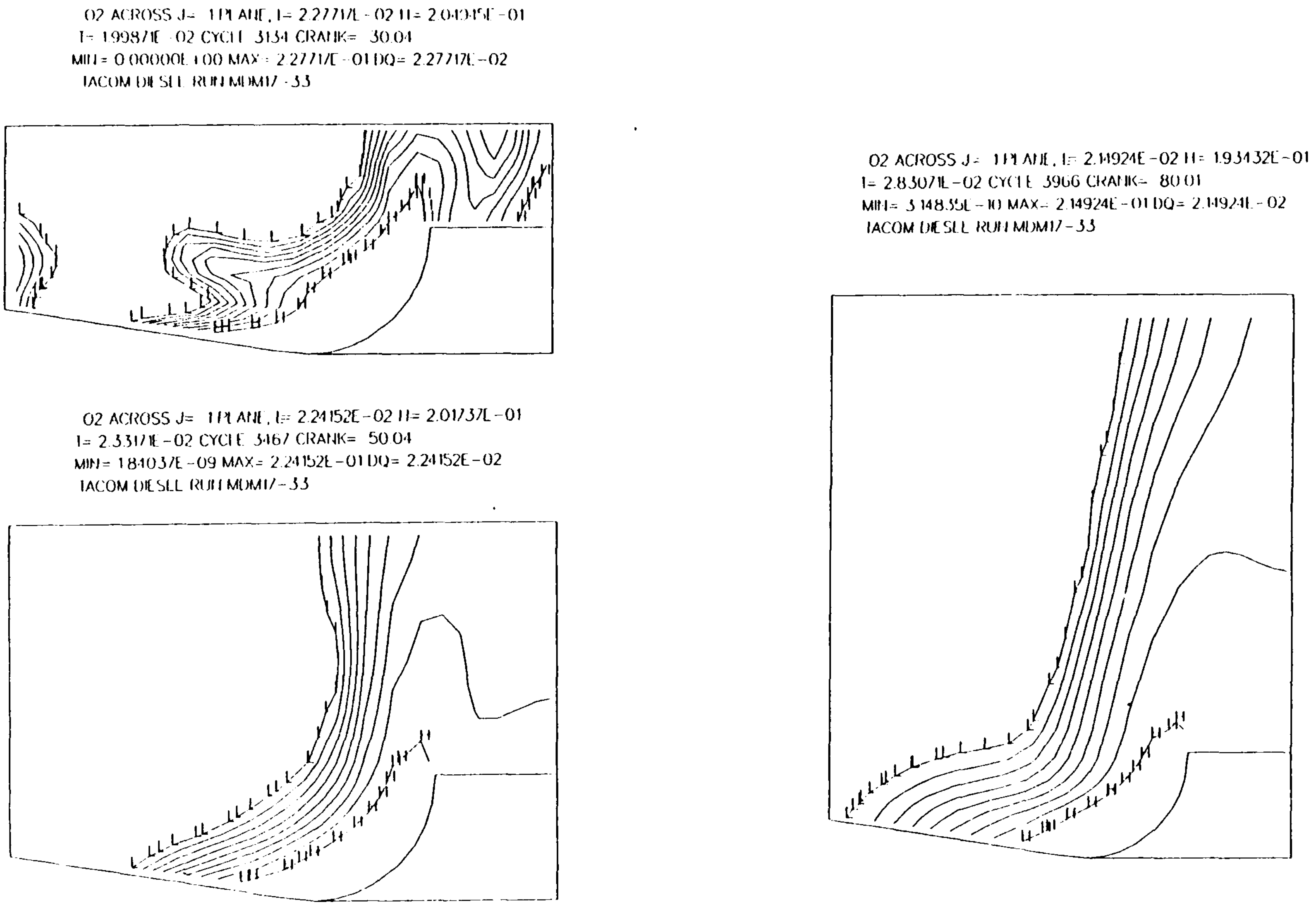
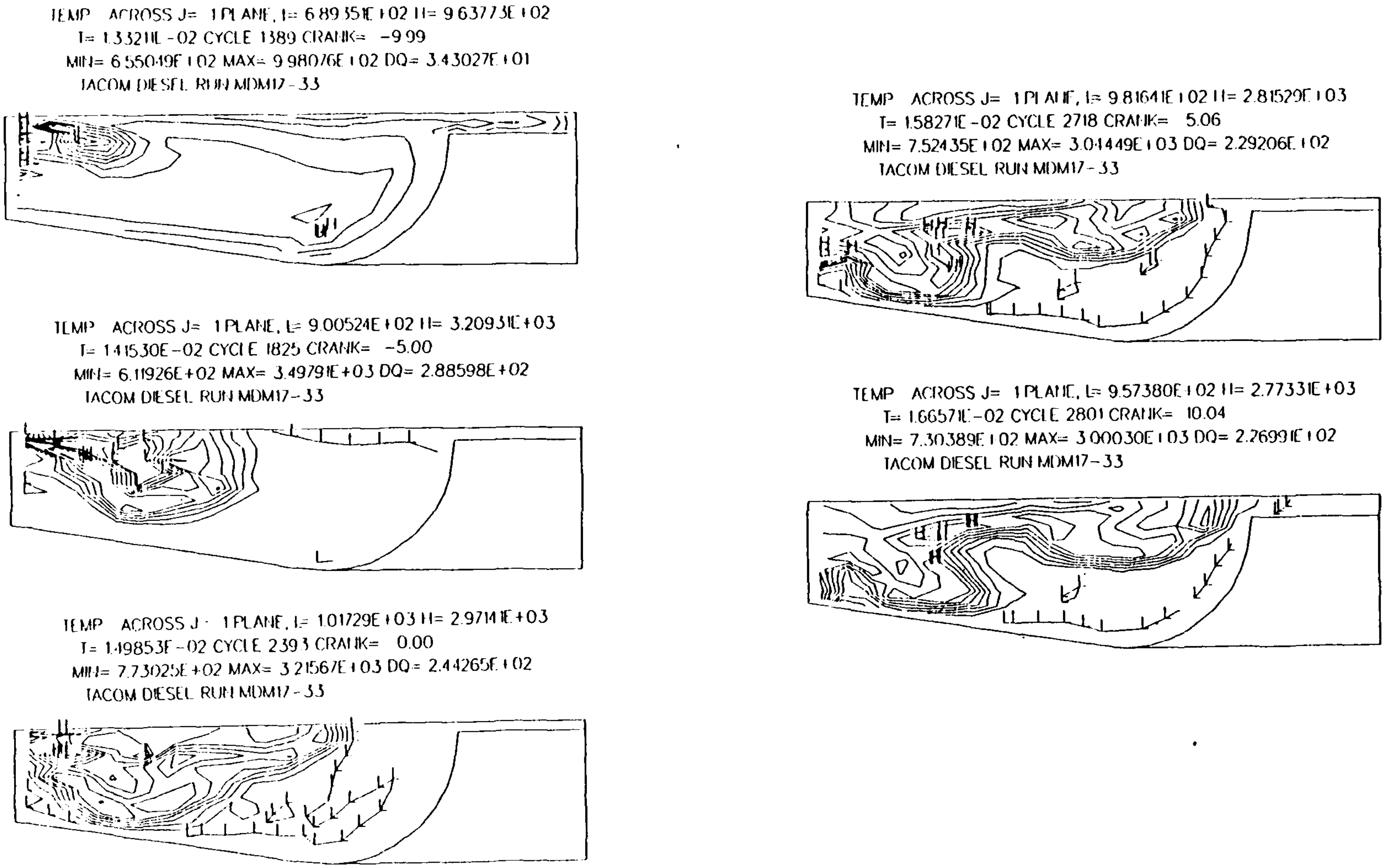


Figure 2-18 KIVA Oxygen Mass Fraction Contours (cont)
(Run 17)



TEMP ACROSS J= 1 PLANE, L= 6.89351E+02 H= 9.63773E+02
T= 1.33211E-02 CYCLE 1389 CRANK= -9.99
MIN= 6.55049E+02 MAX= 9.98076E+02 DQ= 3.43027E+01
TACOM DIESEL RUN MDM17-33

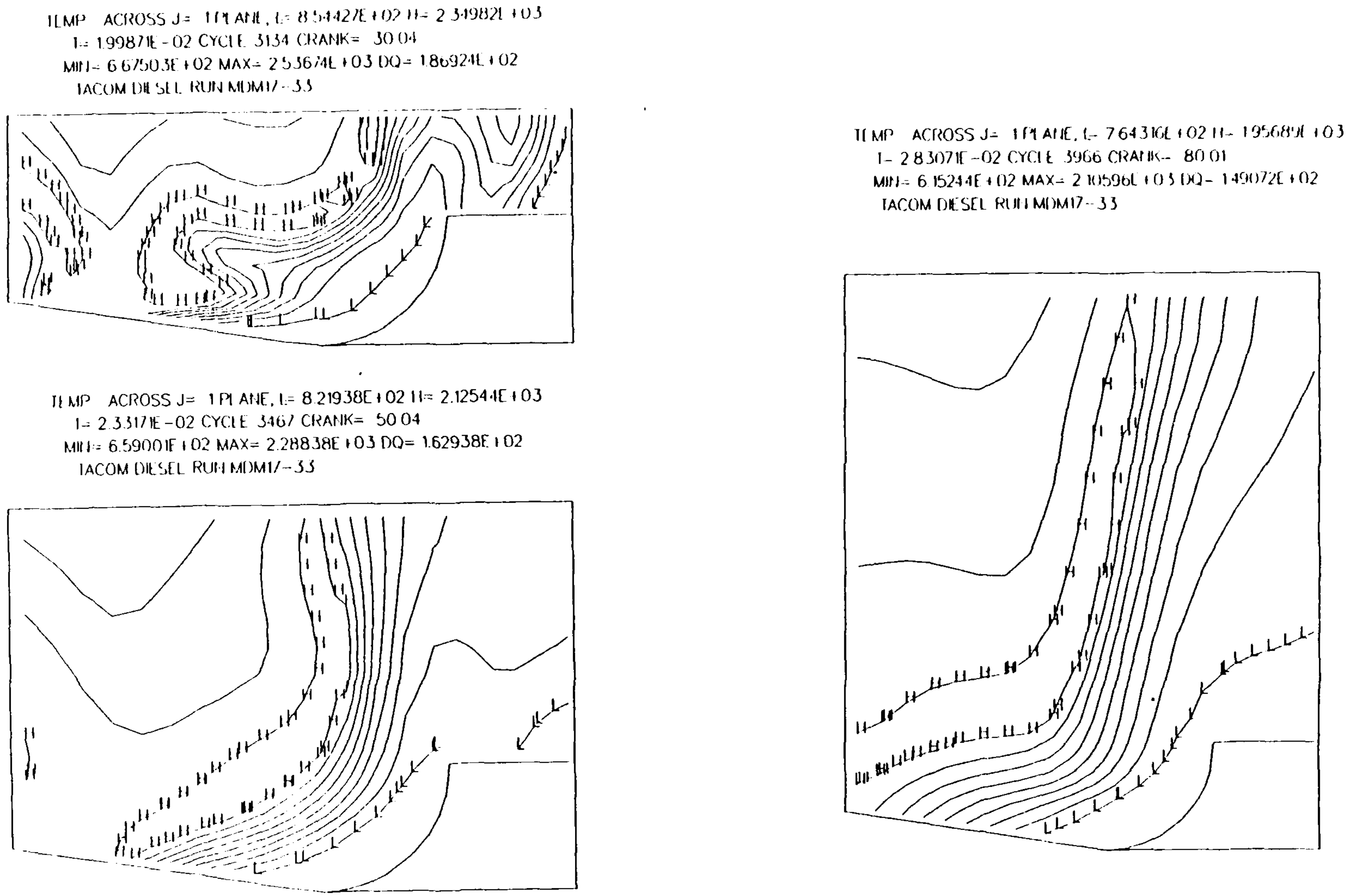
TEMP ACROSS J= 1 PLANE, L= 9.00524E+02 H= 3.20931E+03
T= 1.41530E-02 CYCLE 1825 CRANK= -5.00
MIN= 6.11926E+02 MAX= 3.49791E+03 DQ= 2.88598E+02
TACOM DIESEL RUN MDM17-33

TEMP ACROSS J= 1 PLANE, L= 1.01729E+03 H= 2.97141E+03
T= 1.49853E-02 CYCLE 2393 CRANK= 0.00
MIN= 7.73025E+02 MAX= 3.21567E+03 DQ= 2.44265E+02
TACOM DIESEL RUN MDM17-33

TEMP ACROSS J= 1 PLANE, L= 9.81641E+02 H= 2.81529E+03
T= 1.58271E-02 CYCLE 2718 CRANK= 5.06
MIN= 7.52435E+02 MAX= 3.04449E+03 DQ= 2.29206E+02
TACOM DIESEL RUN MDM17-33

TEMP ACROSS J= 1 PLANE, L= 9.57380E+02 H= 2.77331E+03
T= 1.66571E-02 CYCLE 2801 CRANK= 10.04
MIN= 7.30389E+02 MAX= 3.00030E+03 DQ= 2.26991E+02
TACOM DIESEL RUN MDM17-33

Figure 2-19 KIVA Temperature Contours
(Run 17)



TEMP ACROSS J= 1 PLANE, L= 8.54427E+02 H= 2.34982E+03
T= 1.99871E-02 CYCLE 3134 CRANK= 30.04
MIN= 6.67503E+02 MAX= 2.53674E+03 DQ= 1.86924E+02
TACOM DIESEL RUN MDM17-33

TEMP ACROSS J= 1 PLANE, L= 8.21938E+02 H= 2.12544E+03
T= 2.33171E-02 CYCLE 3467 CRANK= 50.04
MIN= 6.59001E+02 MAX= 2.28838E+03 DQ= 1.62938E+02
TACOM DIESEL RUN MDM17-33

TEMP ACROSS J= 1 PLANE, L= 7.64316E+02 H= 1.95689E+03
T= 2.83071E-02 CYCLE 3966 CRANK= 80.01
MIN= 6.15244E+02 MAX= 2.10596E+03 DQ= 1.49072E+02
TACOM DIESEL RUN MDM17-33

Figure 2-20 KIVA Temperature Contours (cont)
(Run 17)

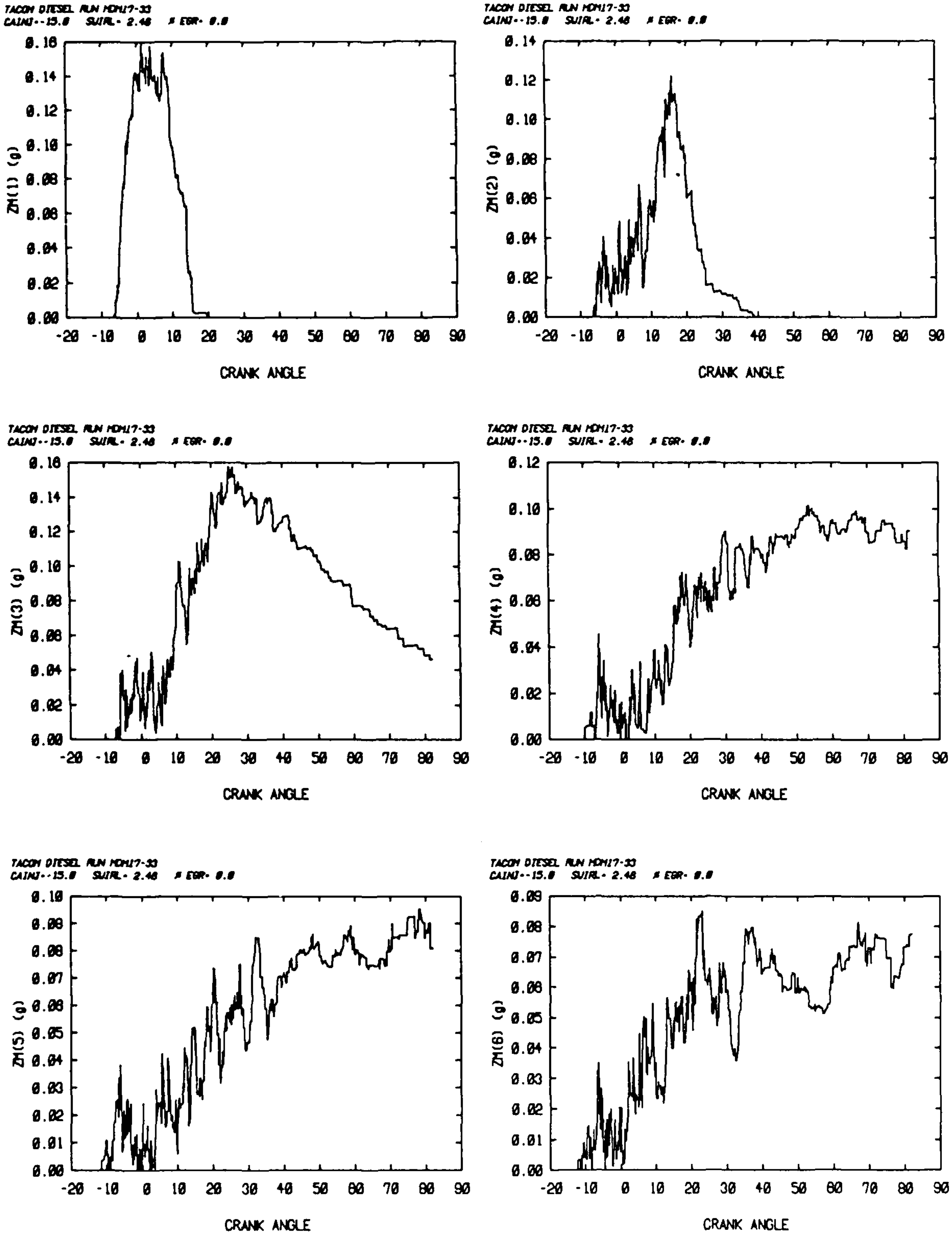


Figure 2-21 KIVA Zone Mass

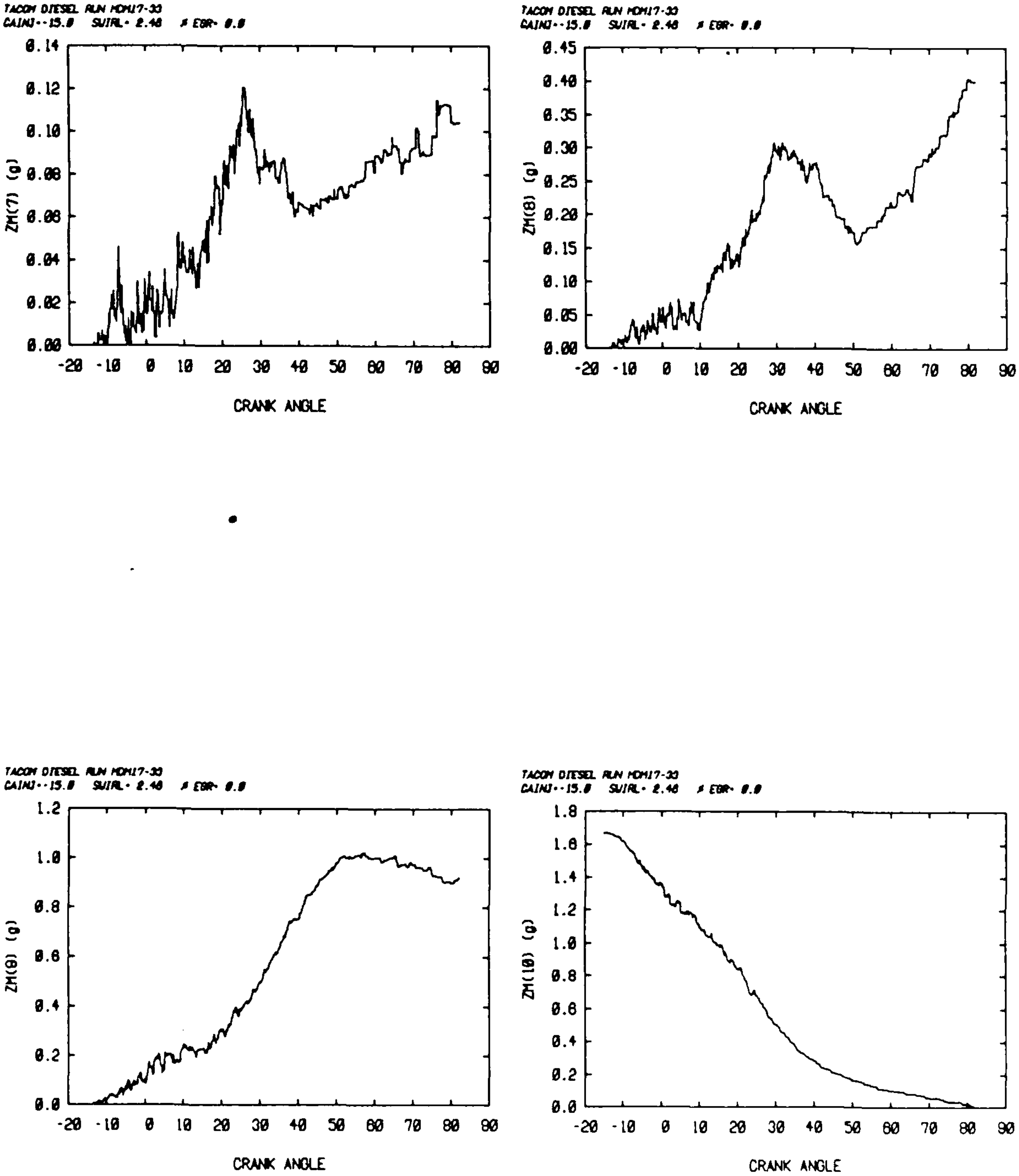


Figure 2-22 KIVA Zone Mass (cont)

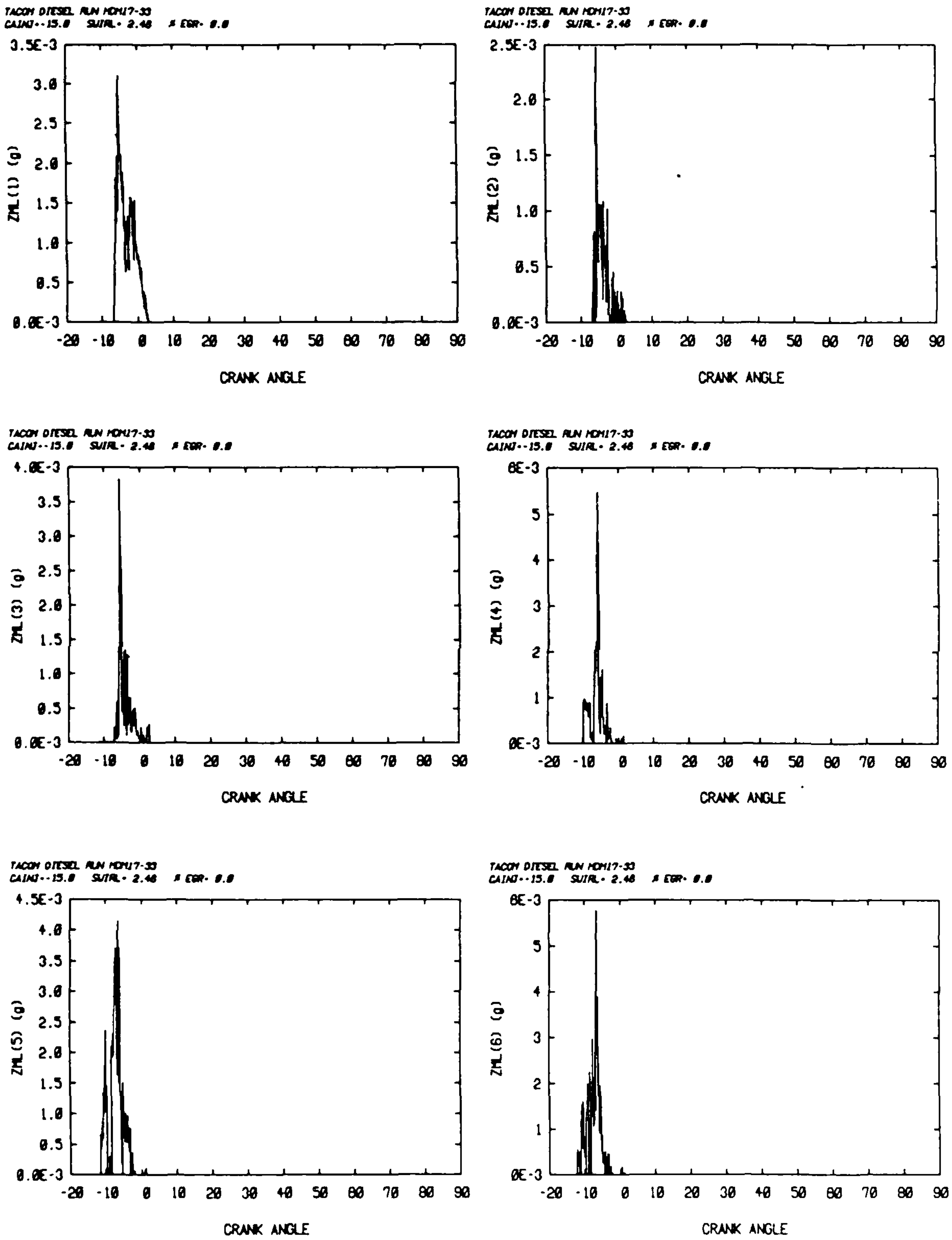


Figure 2-23 KIVA Zone Liquid Fuel Mass

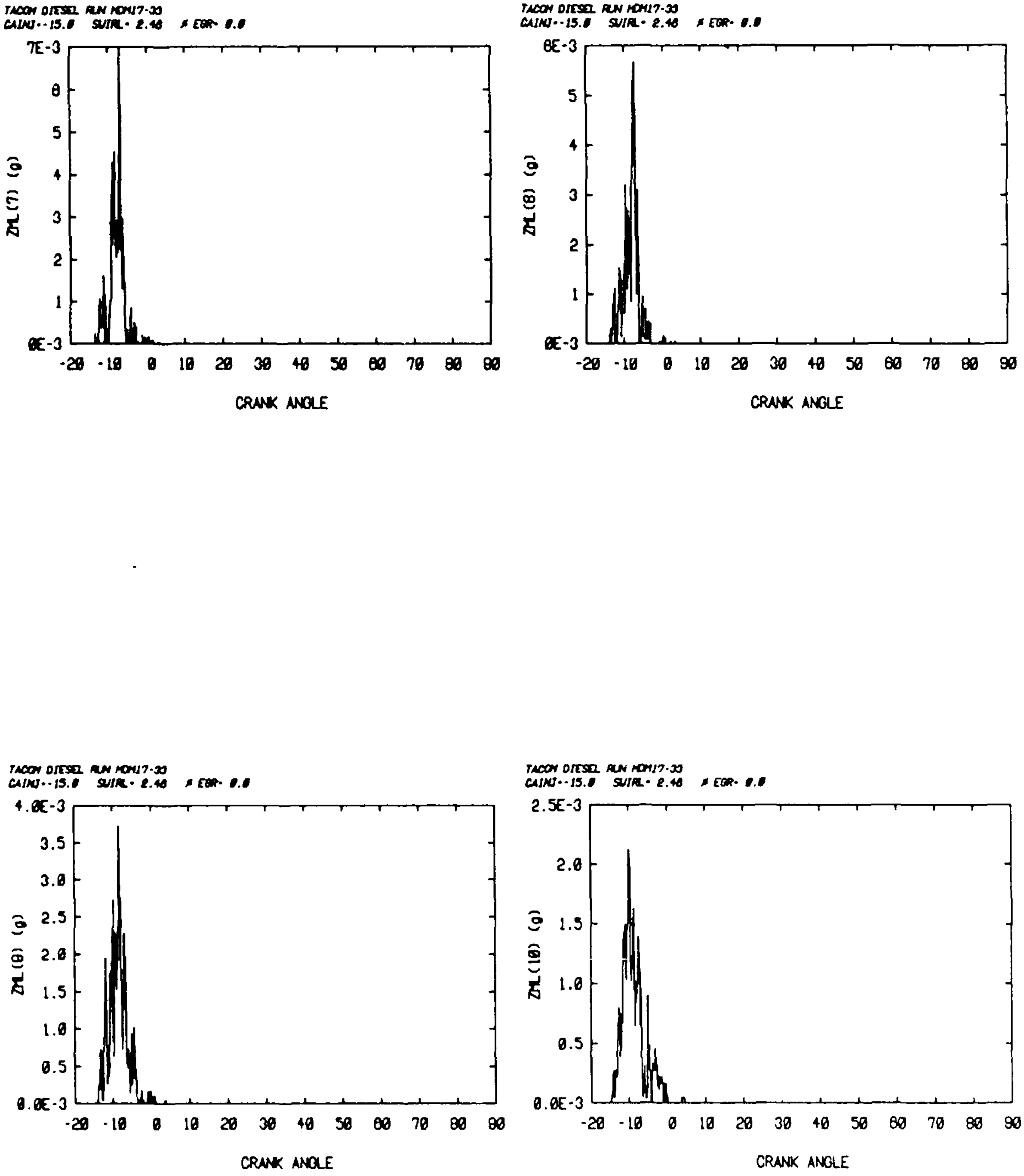


Figure 2-24 KIVA Zone Liquid Fuel Mass (cont)

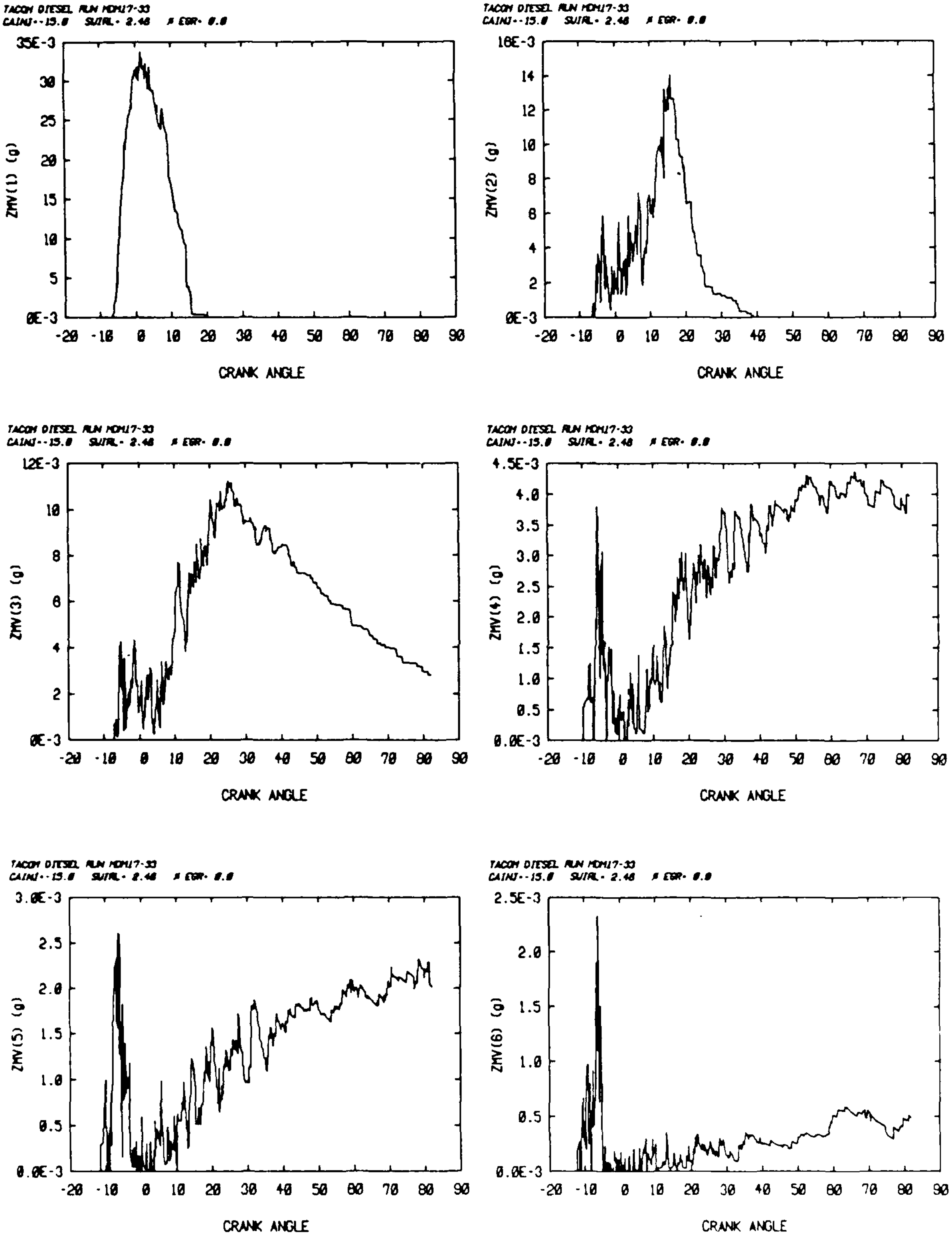


Figure 2-25 KIVA Zone Fuel Vapor Mass

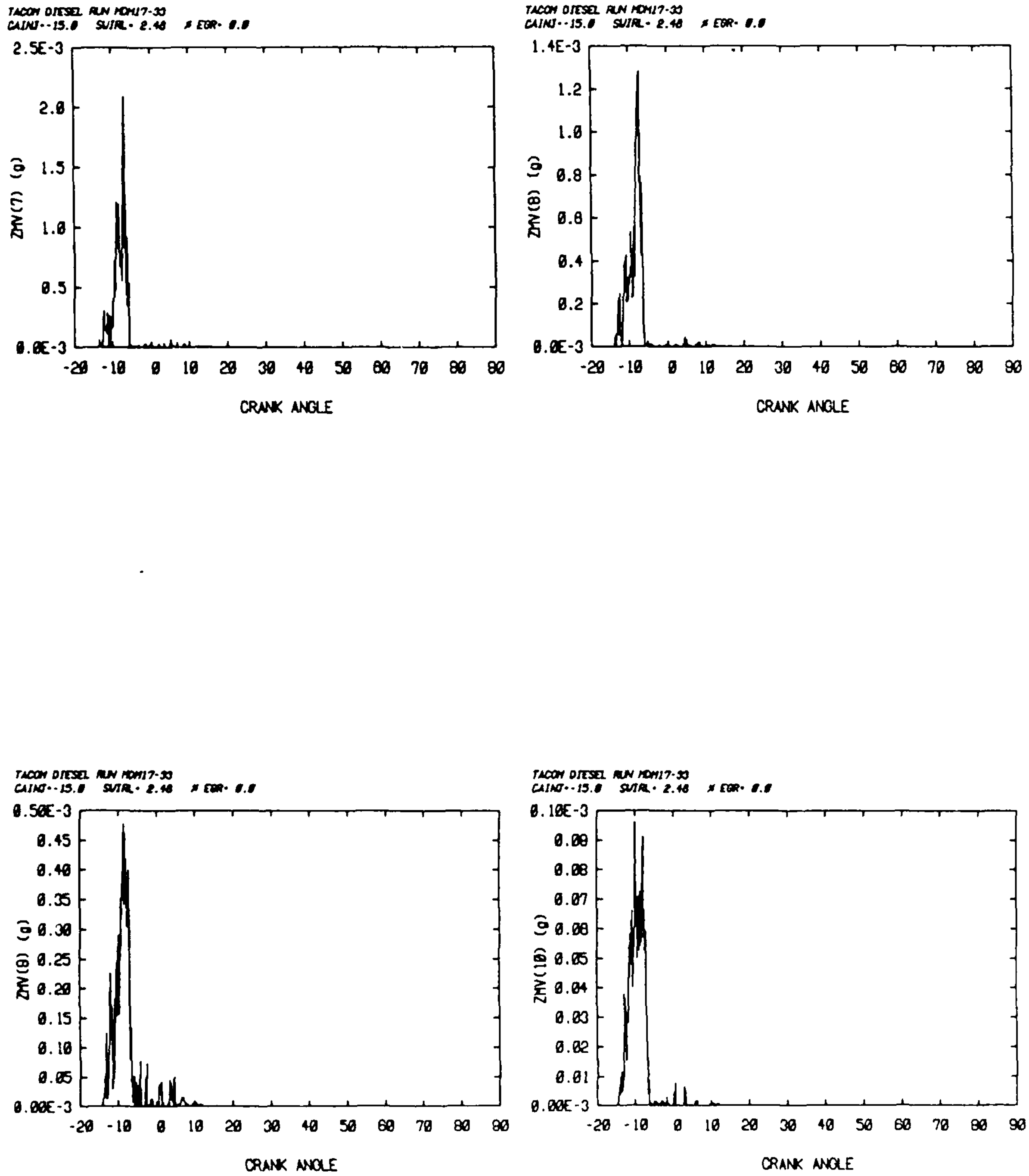


Figure 2-26 KIVA Zone Fuel Vapor Mass (cont)

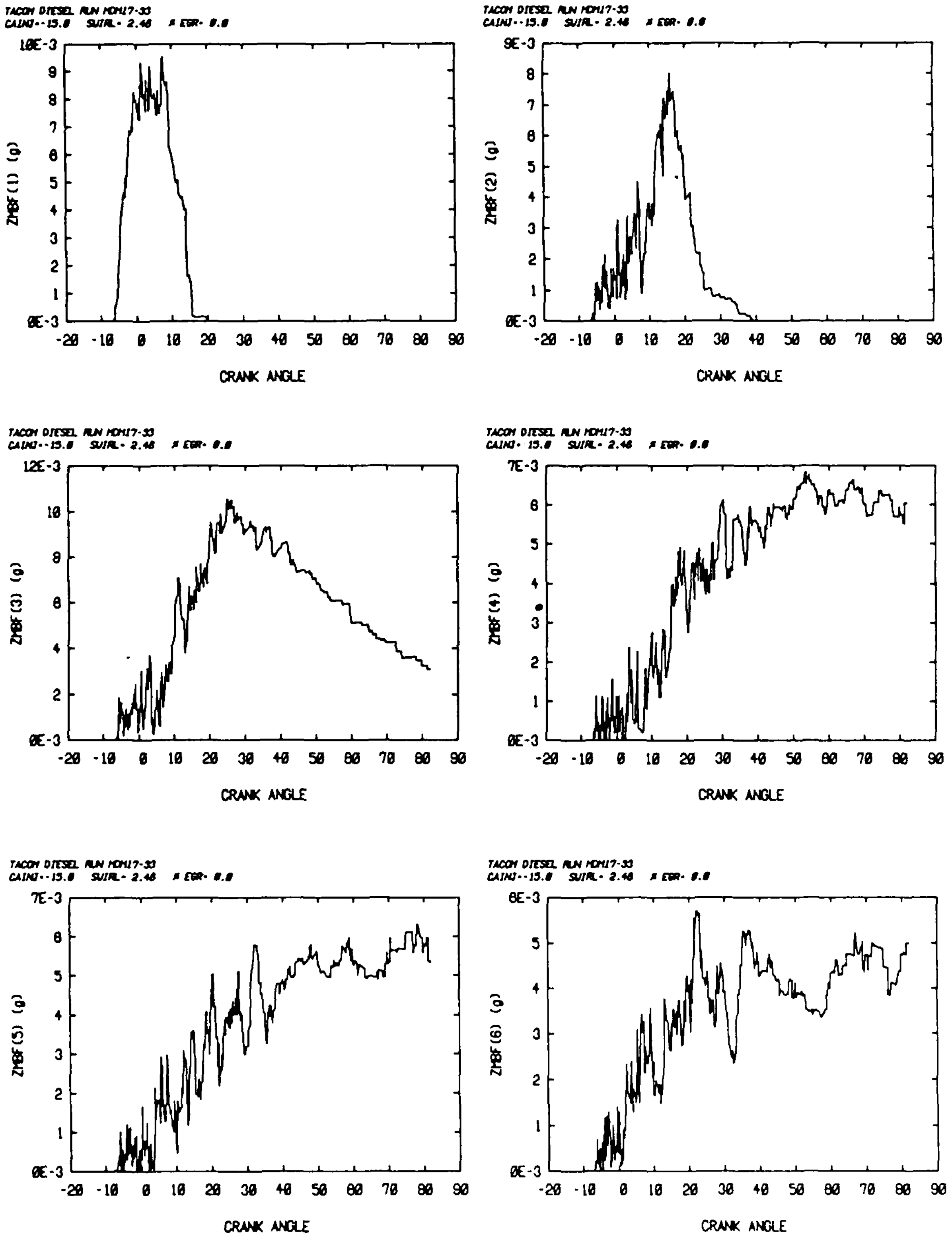


Figure 2-27 KIVA Zone Burned Fuel Mass

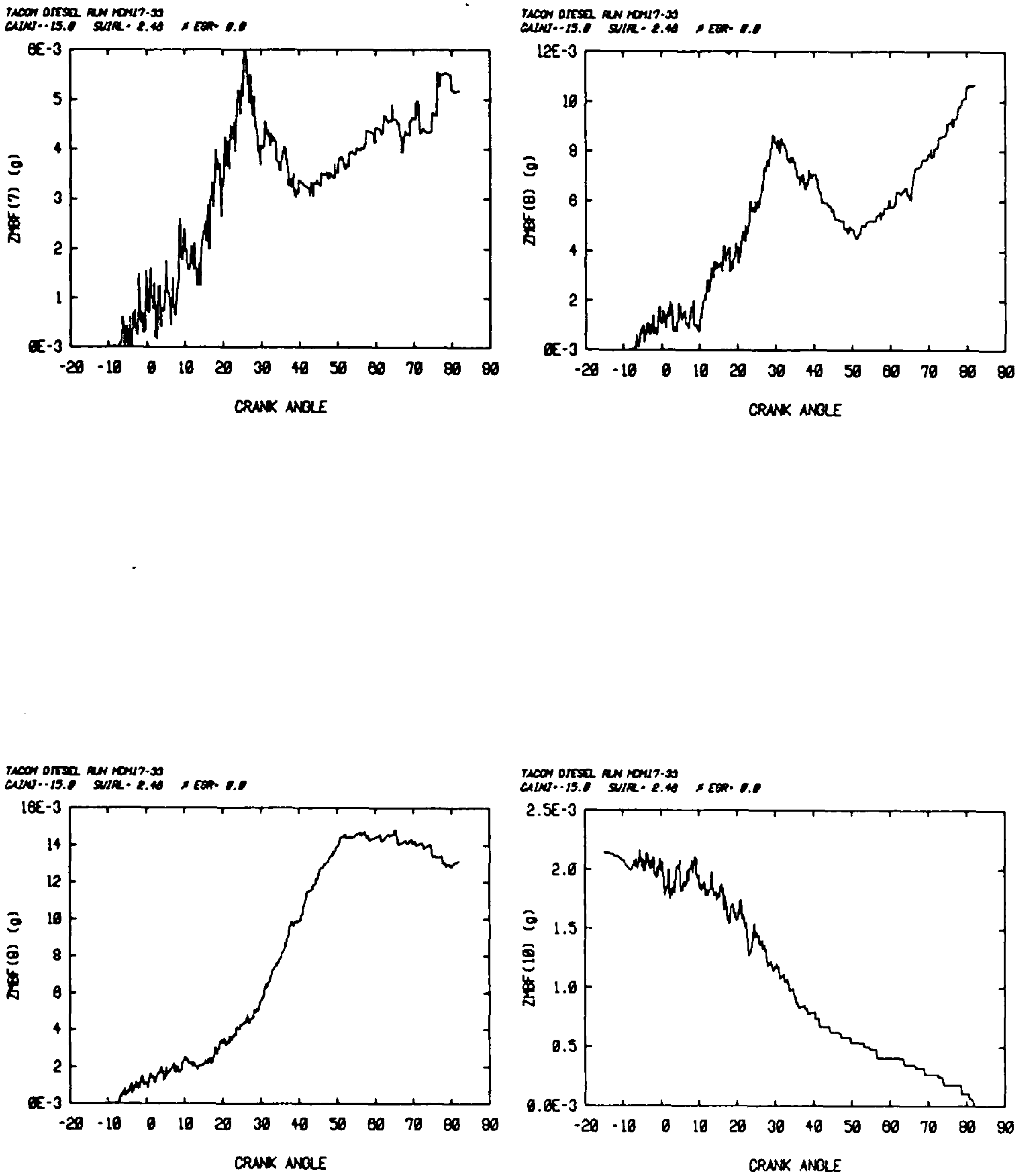


Figure 2-28 KIVA Zone Burned Fuel Mass (cont)

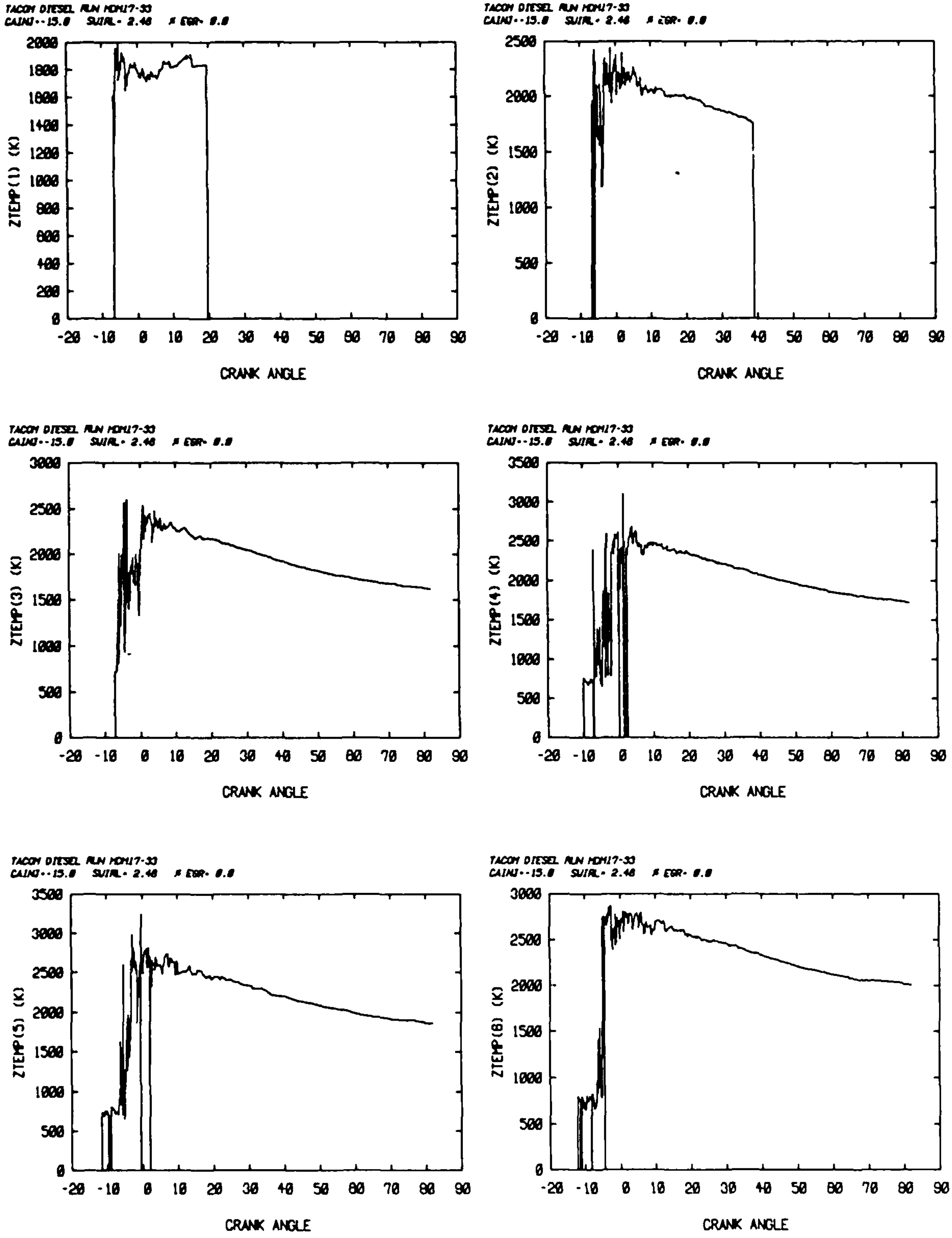


Figure 2-29 KIVA Zone Temperature

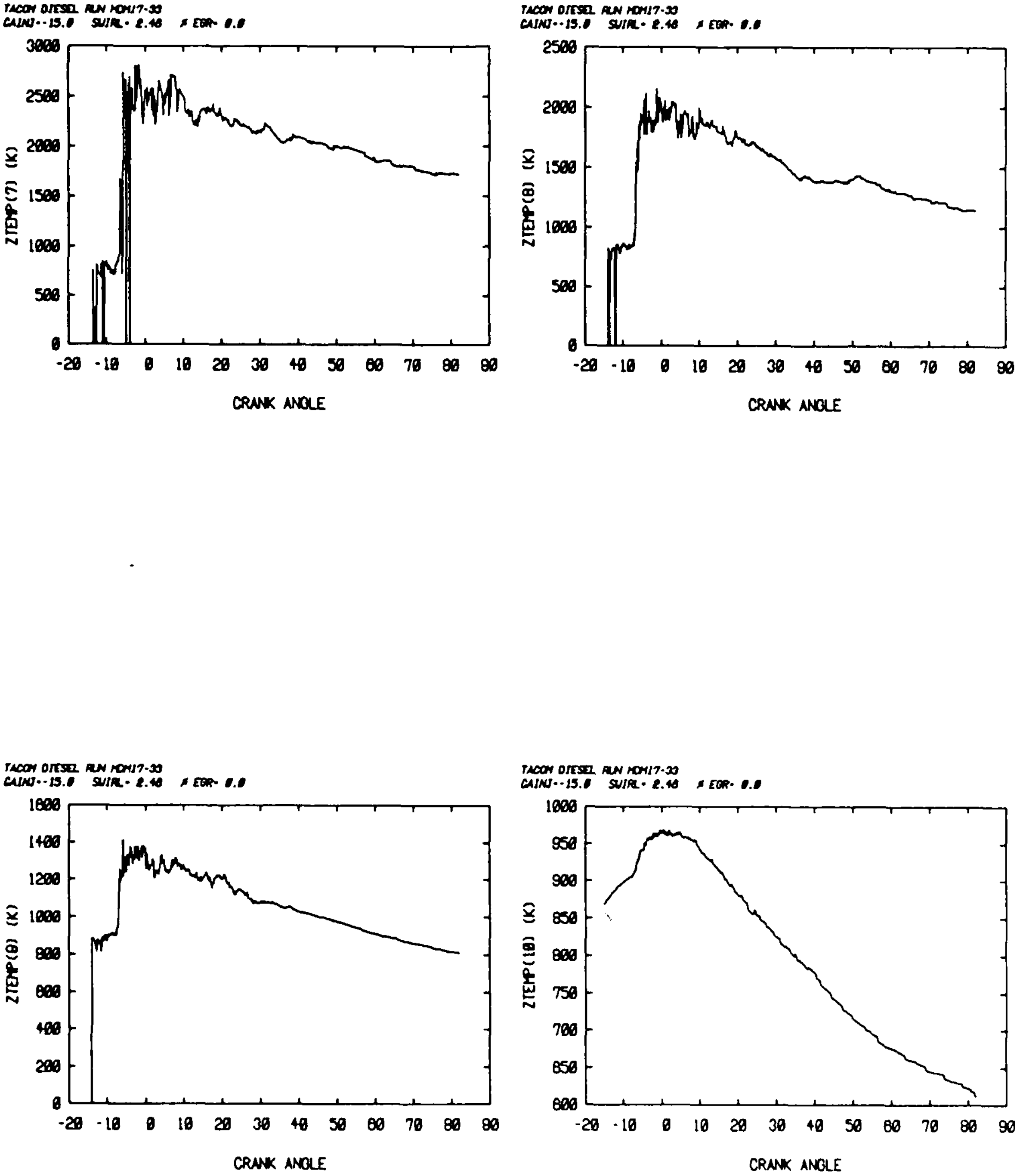


Figure 2-30 KIVA Zone Temperature (cont)

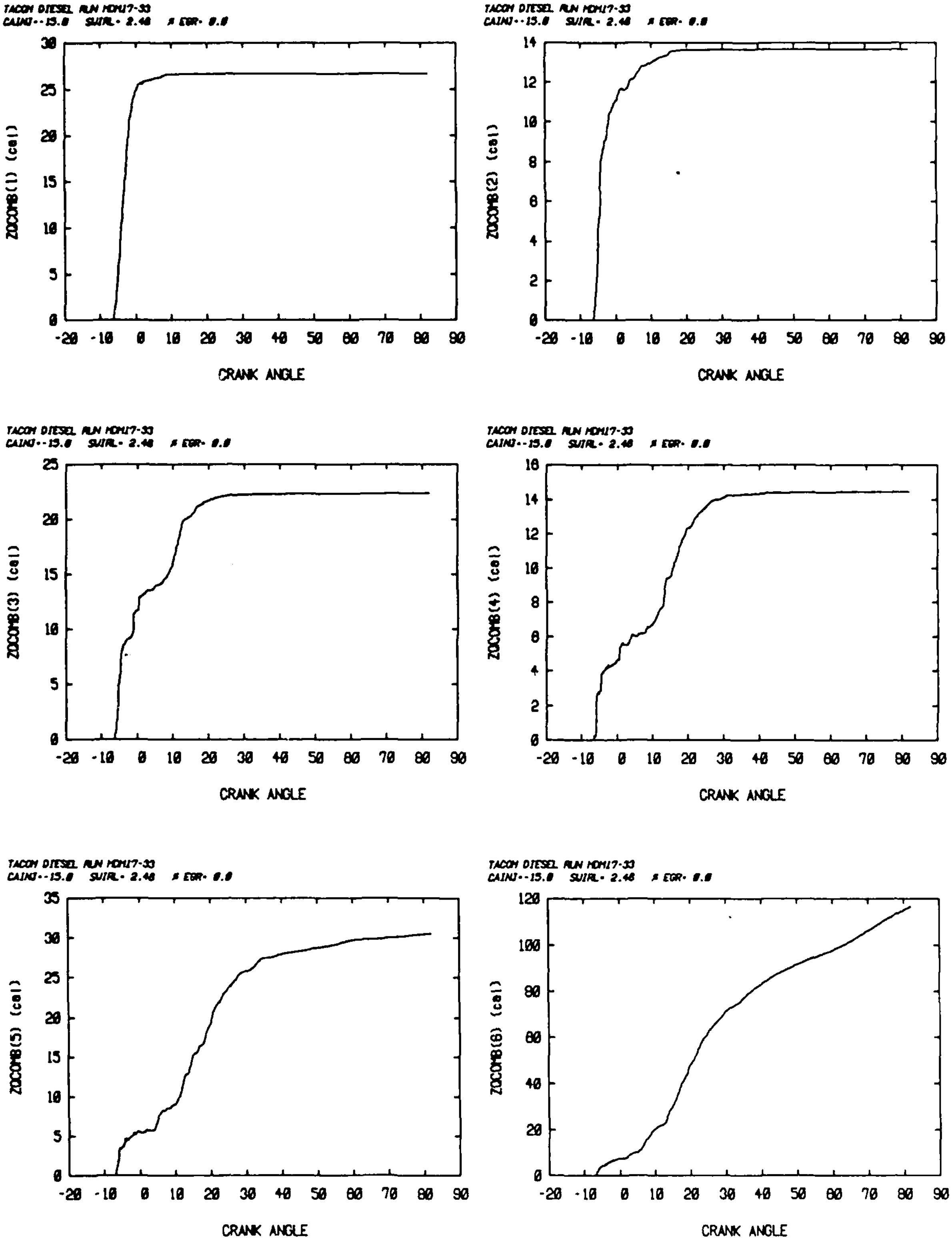


Figure 2-31 KIVA Zone Heat Release

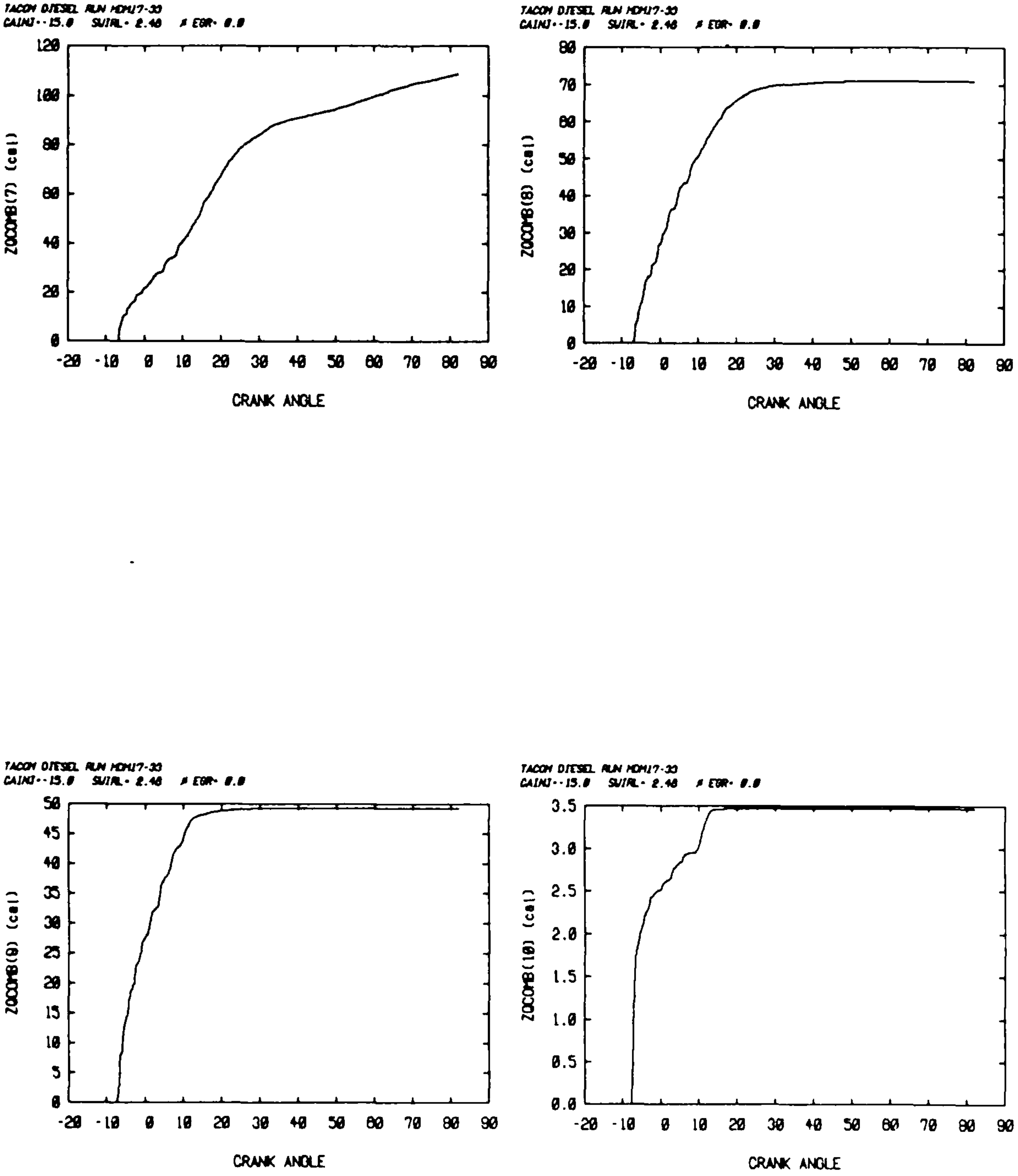


Figure 2-32 KIVA Zone Heat Release (cont)

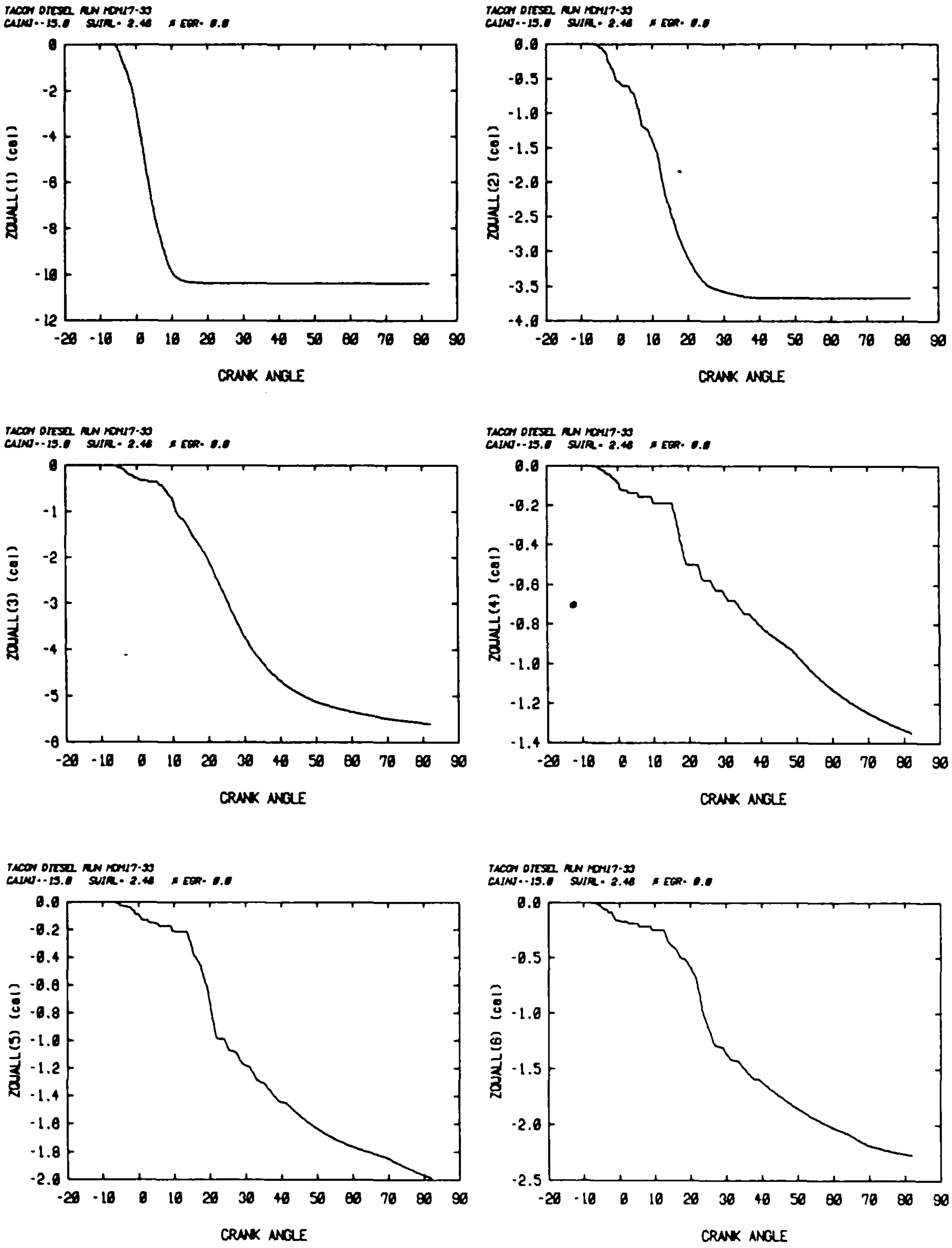


Figure 2-33 KIVA Zone Wall Heat Transfer

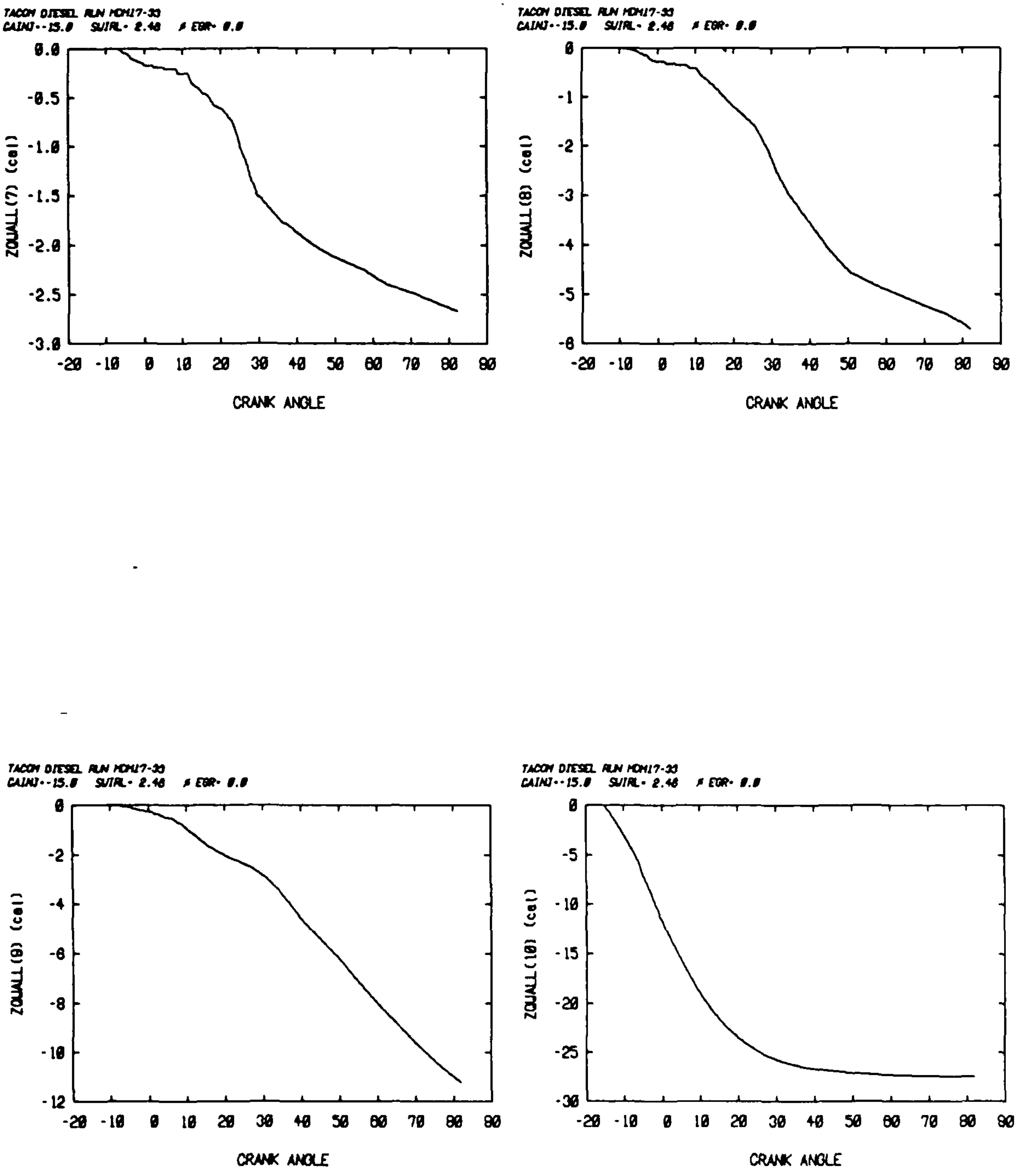


Figure 2-34 KIVA Zone Wall Heat Transfer (cont)

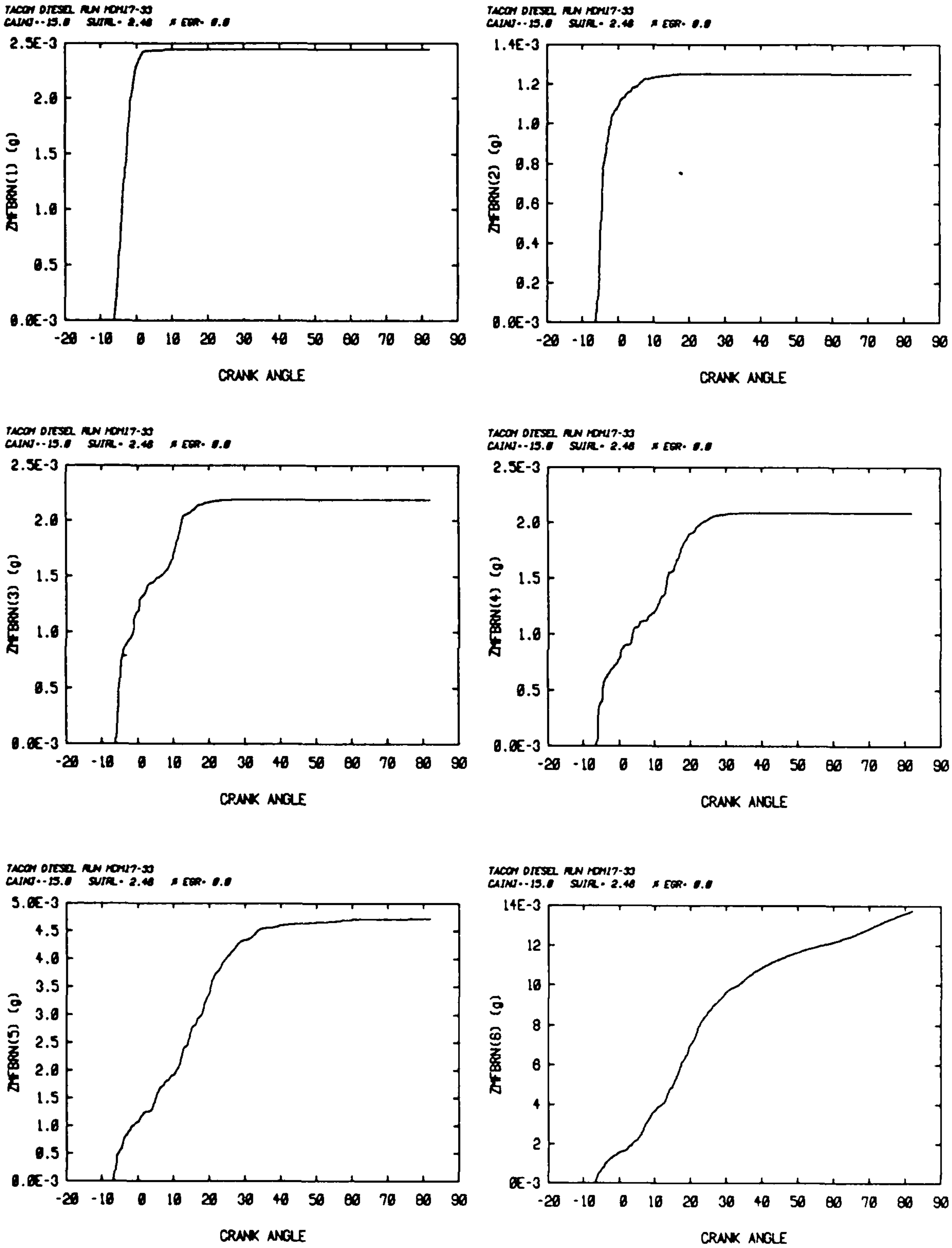


Figure 2-35 KIVA Zone Mass of Fuel Burned

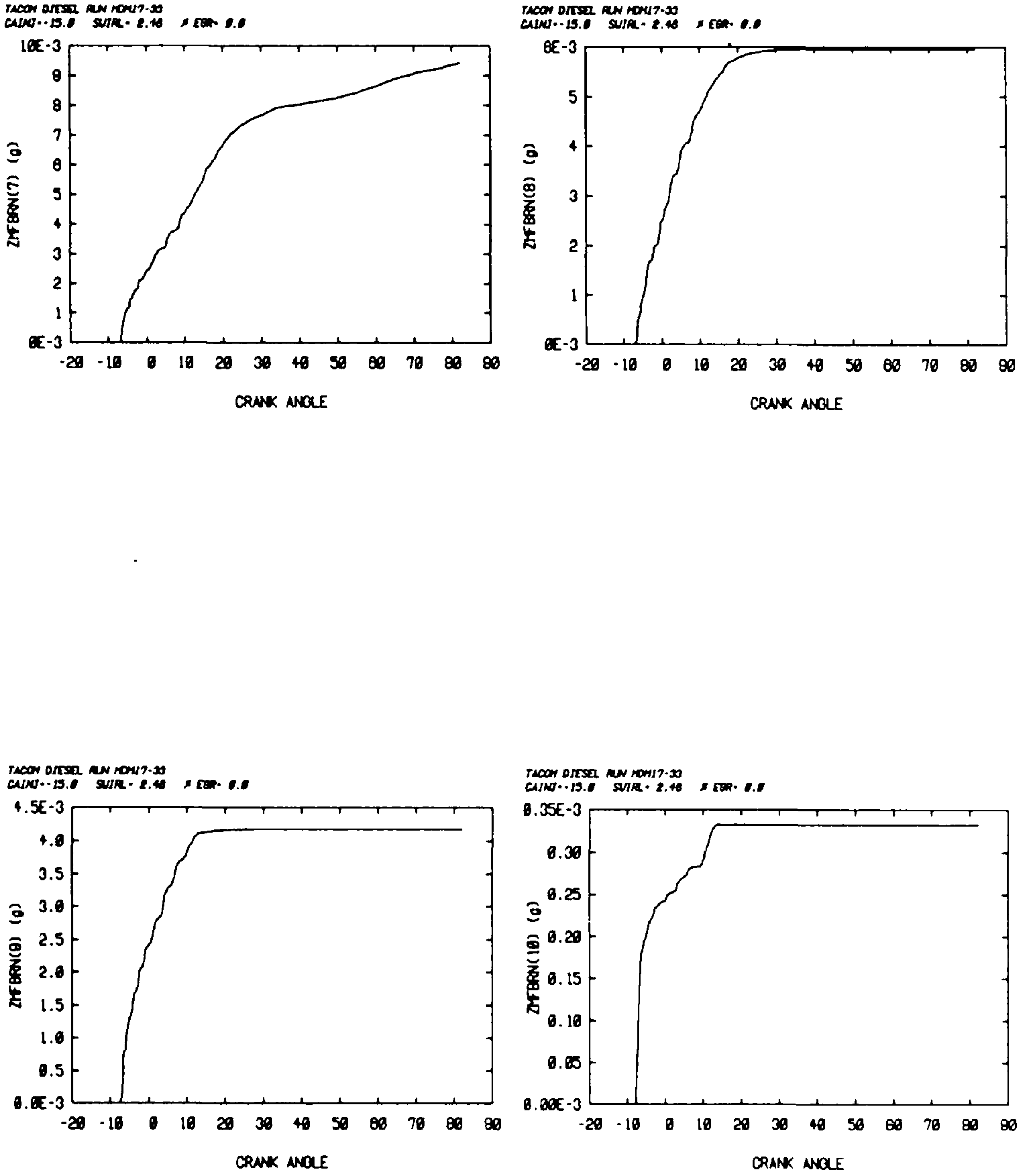


Figure 2-36 KIVA Zone Mass of Fuel Burned (cont)

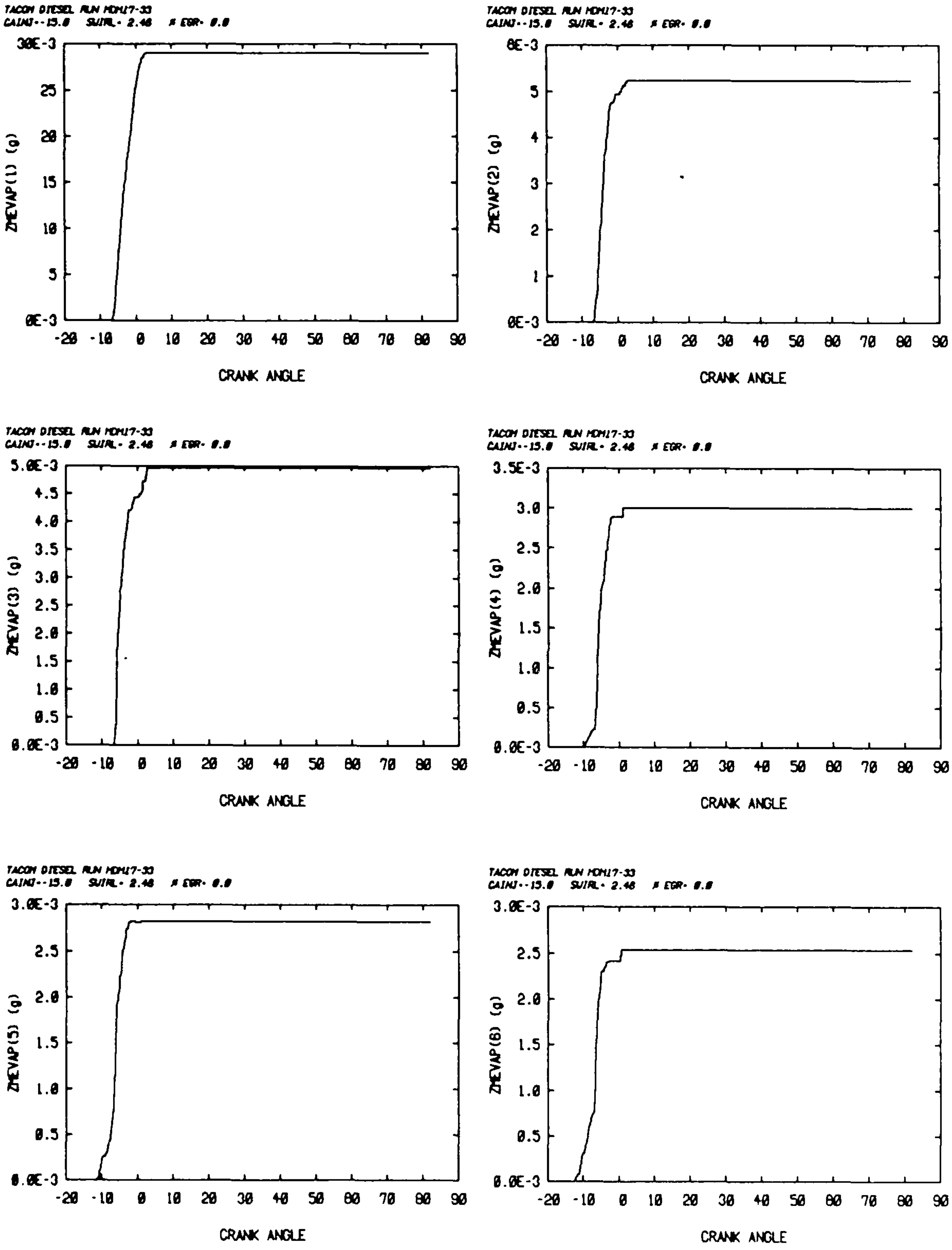


Figure 2-37 KIVA Zone Mass of Fuel Evaporated

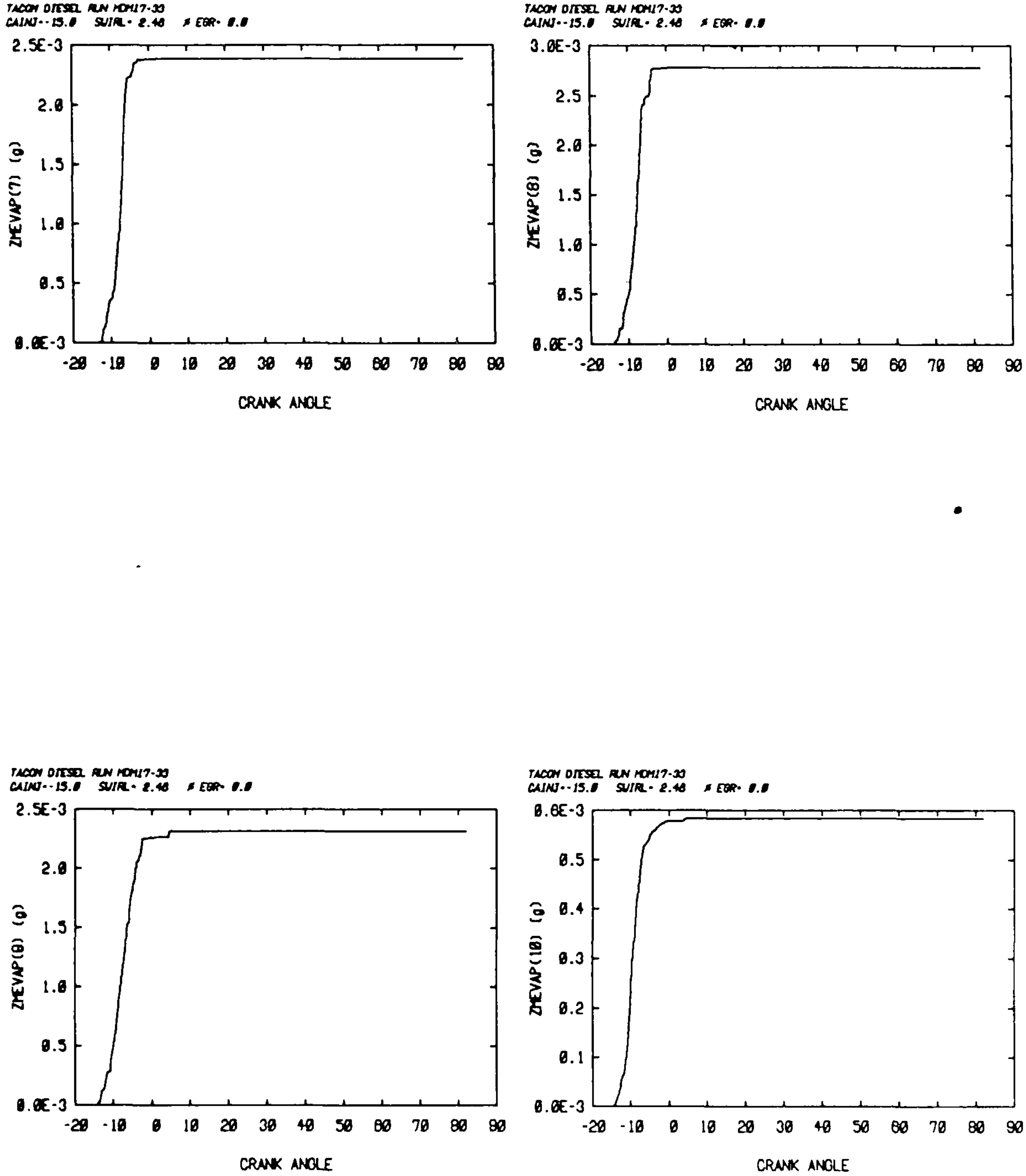


Figure 2-38 KIVA Zone Mass of Fuel Evaporated (cont)

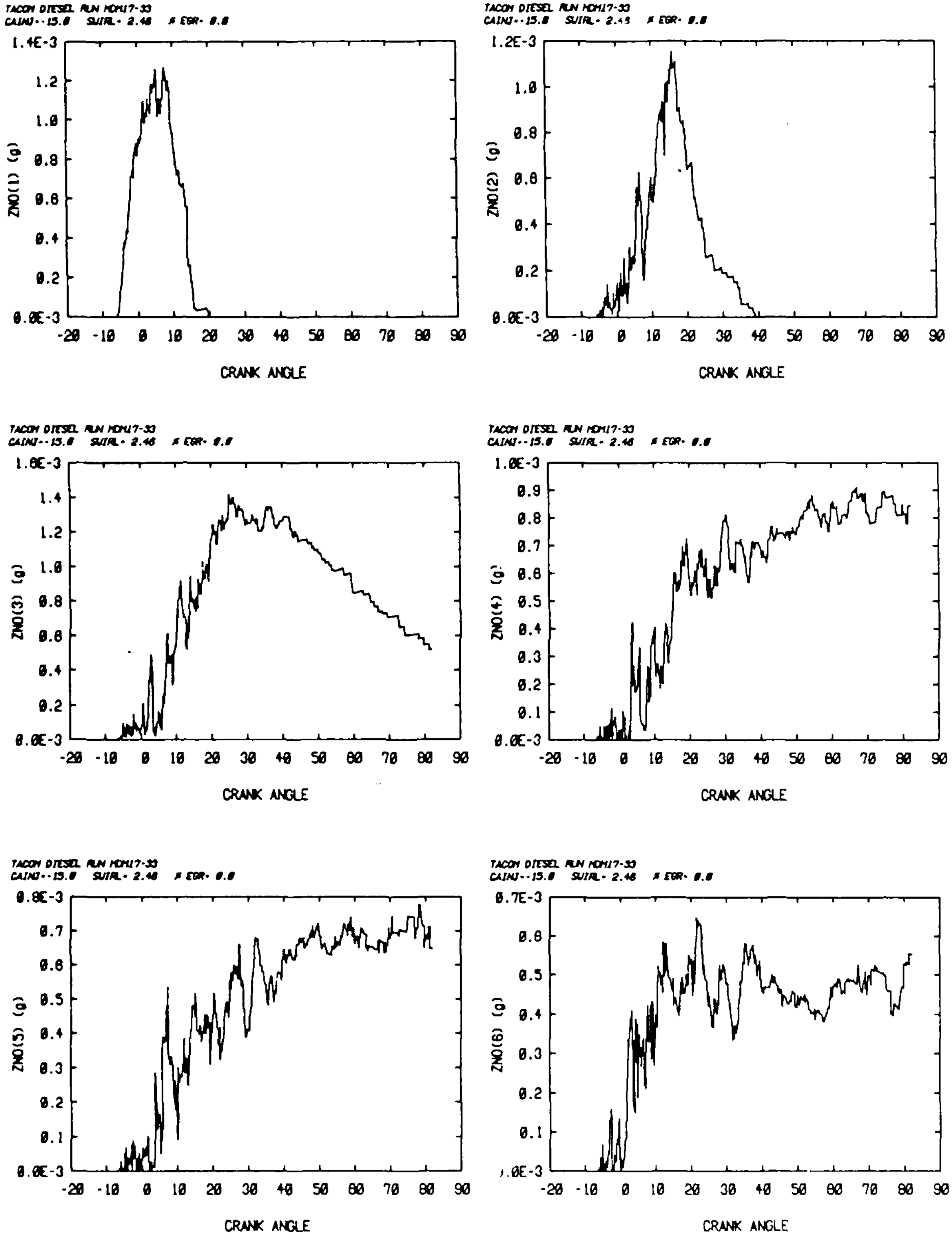


Figure 2-39 KIVA Zone Mass of Nitric Oxide

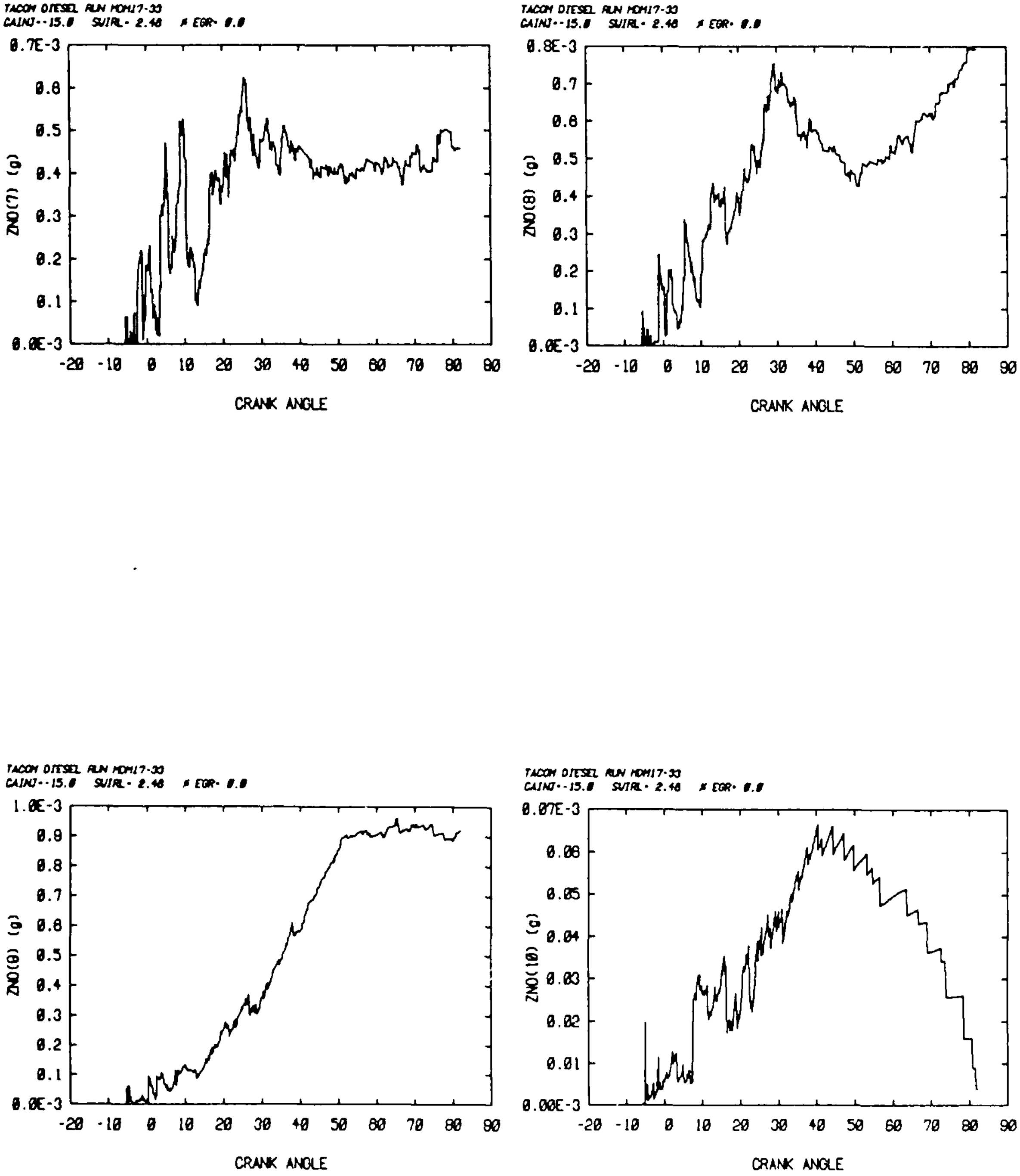


Figure 2-40 KIVA Zone Mass of Nitric Oxide (cont)

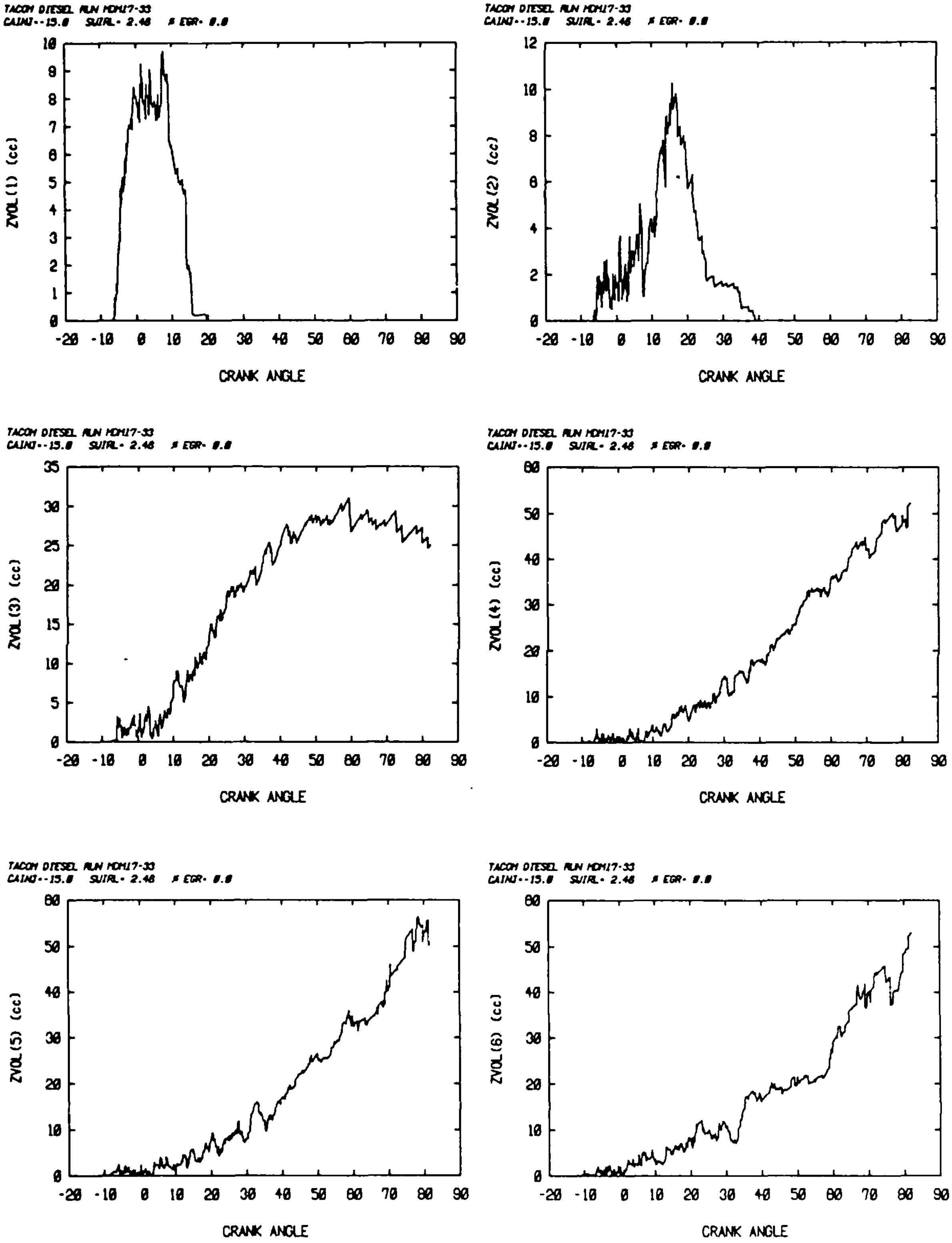


Figure 2-41 KIVA Zone Volume

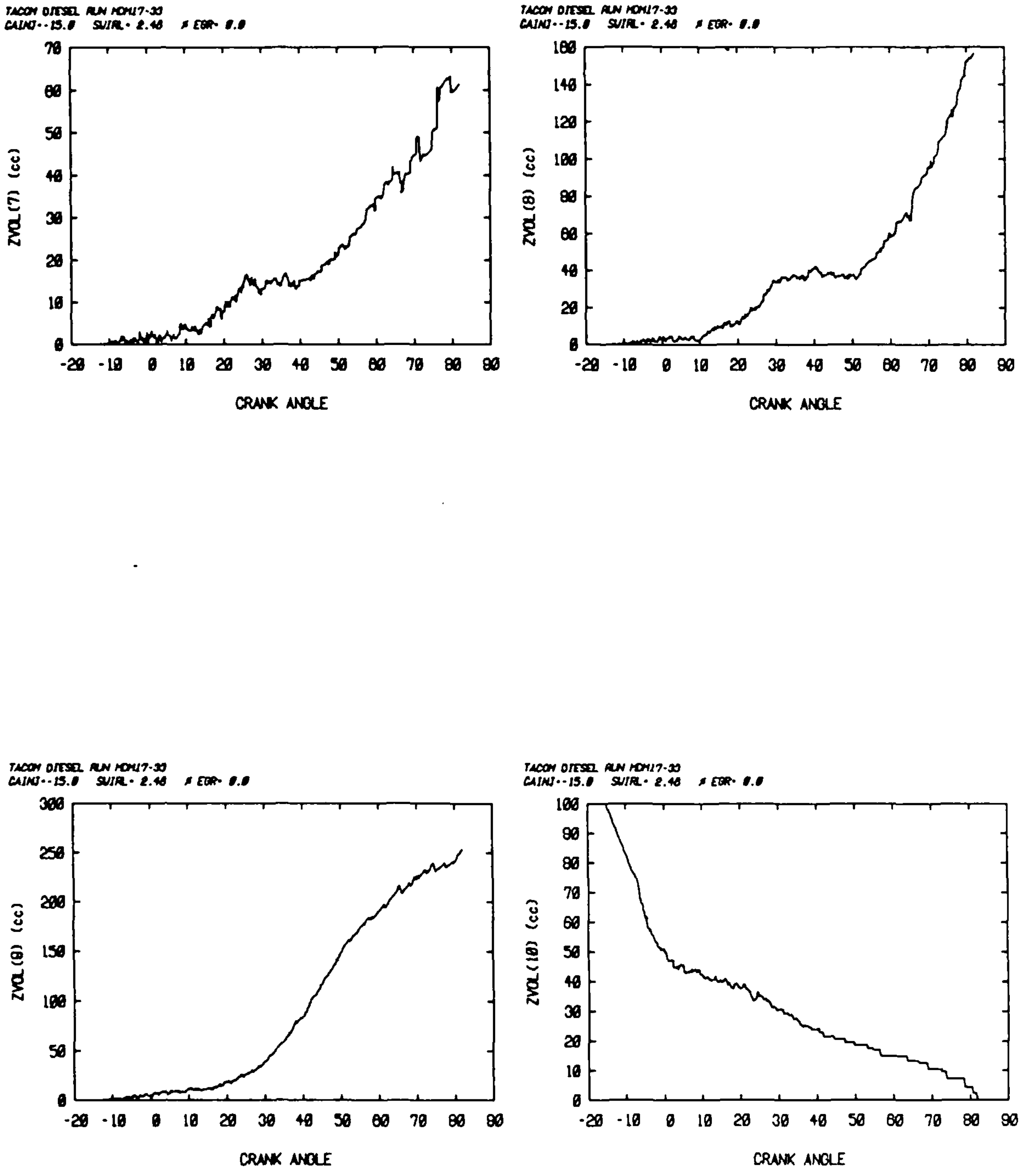


Figure 2-42 KIVA Zone Volume (cont)

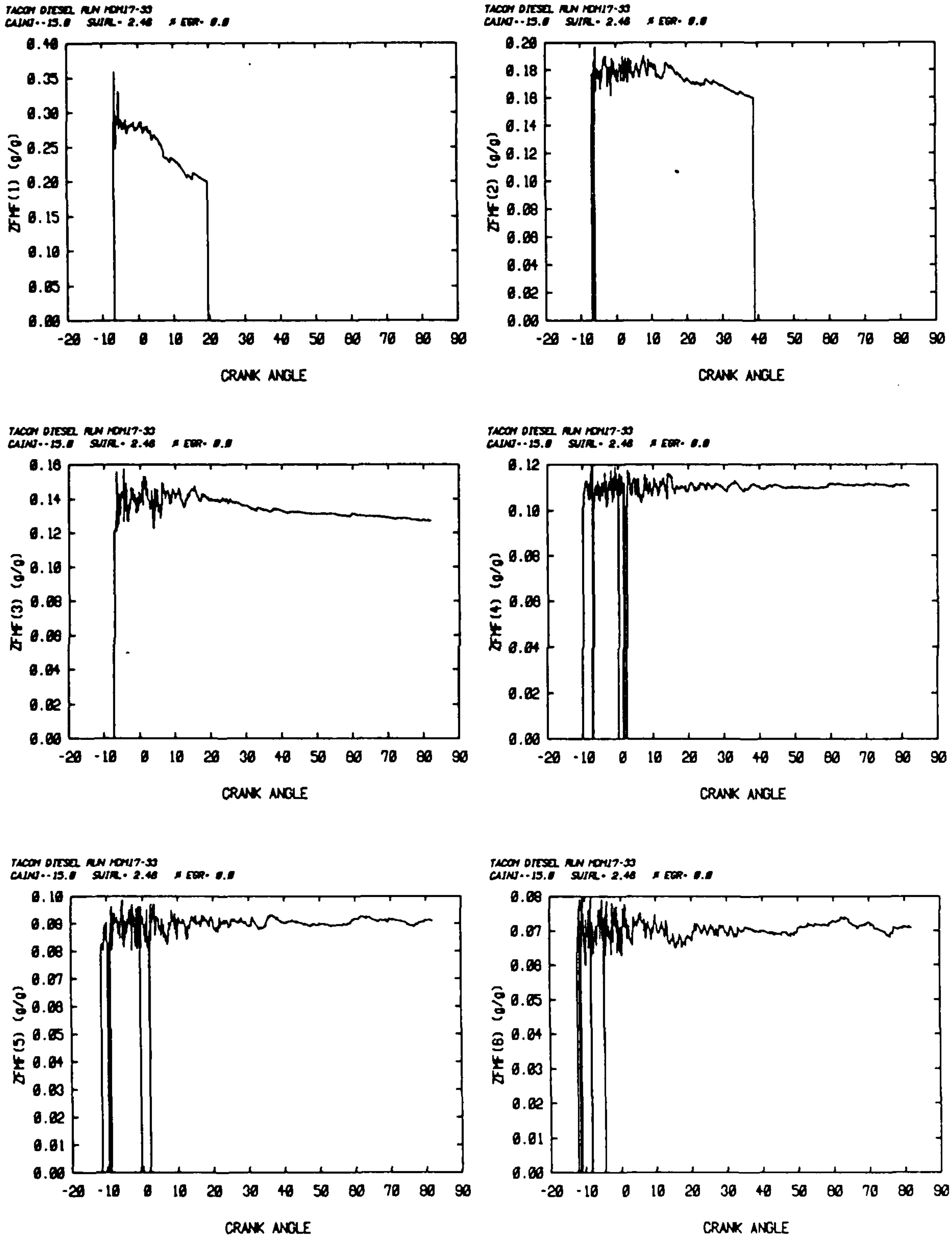


Figure 2-43 KIVA Zone Fuel Mass Fraction

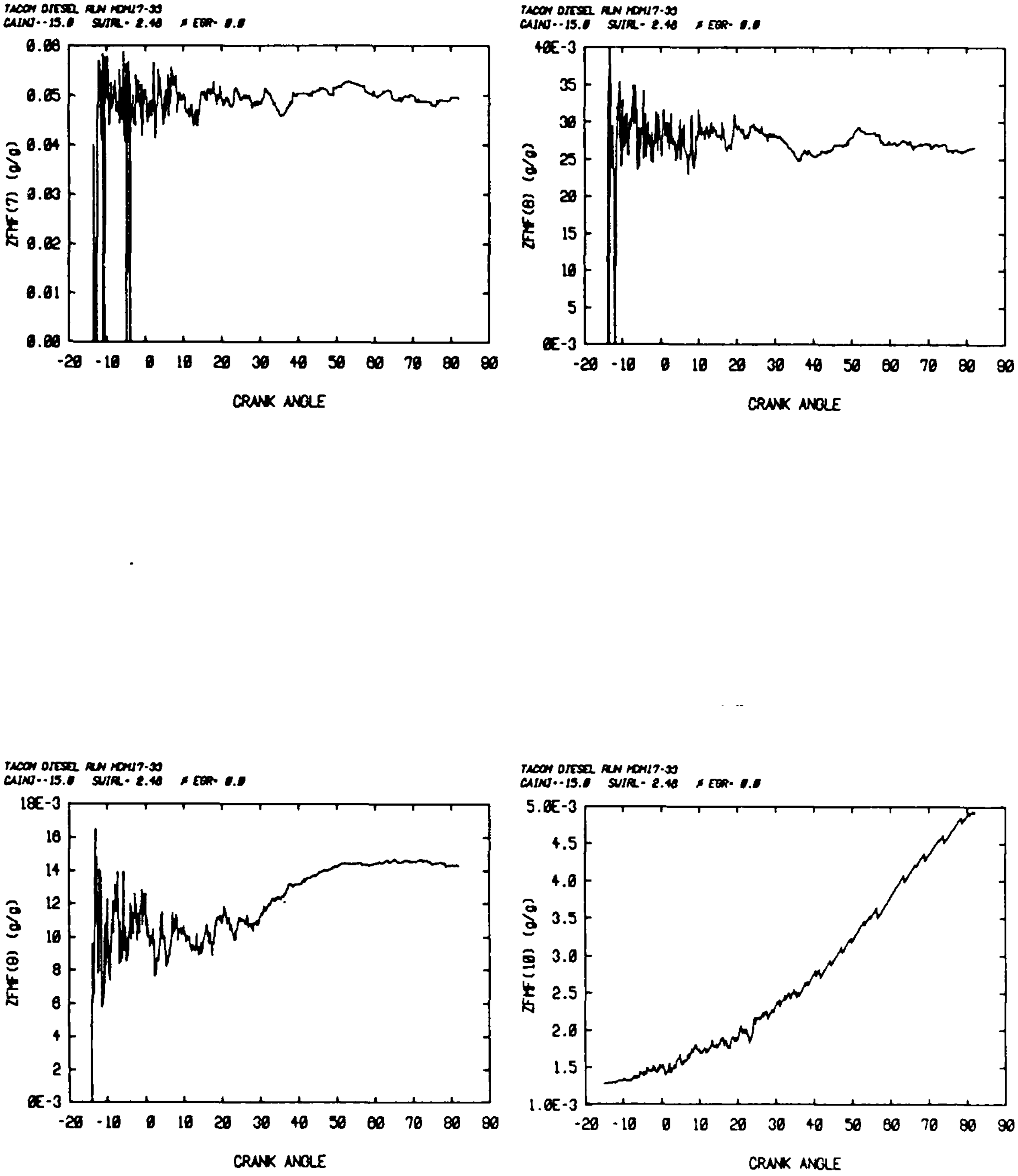


Figure 2-44 KIVA Zone Total Fuel Mass Fraction (cont)

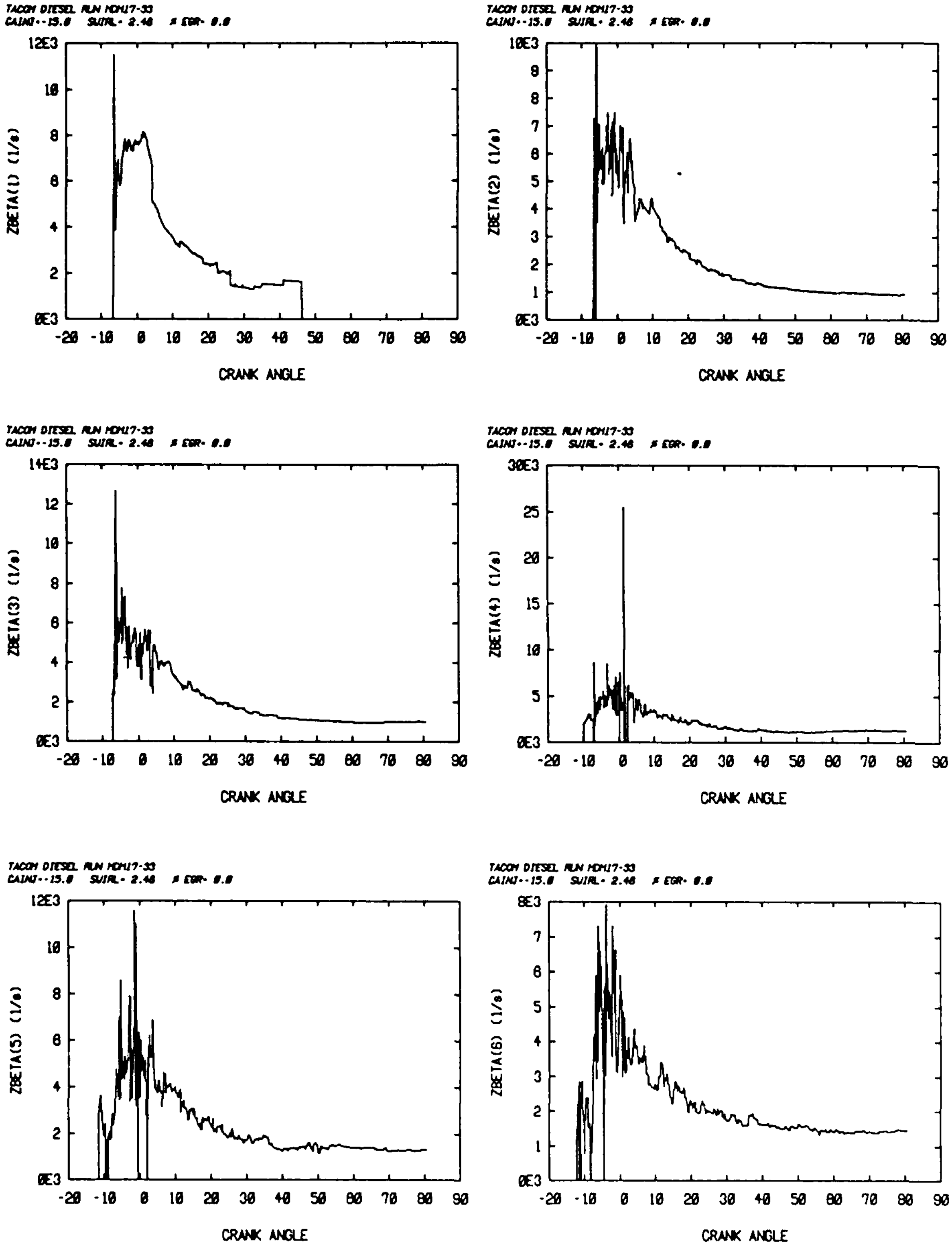


Figure 2-45 KIVA Zone Mixing Intensity

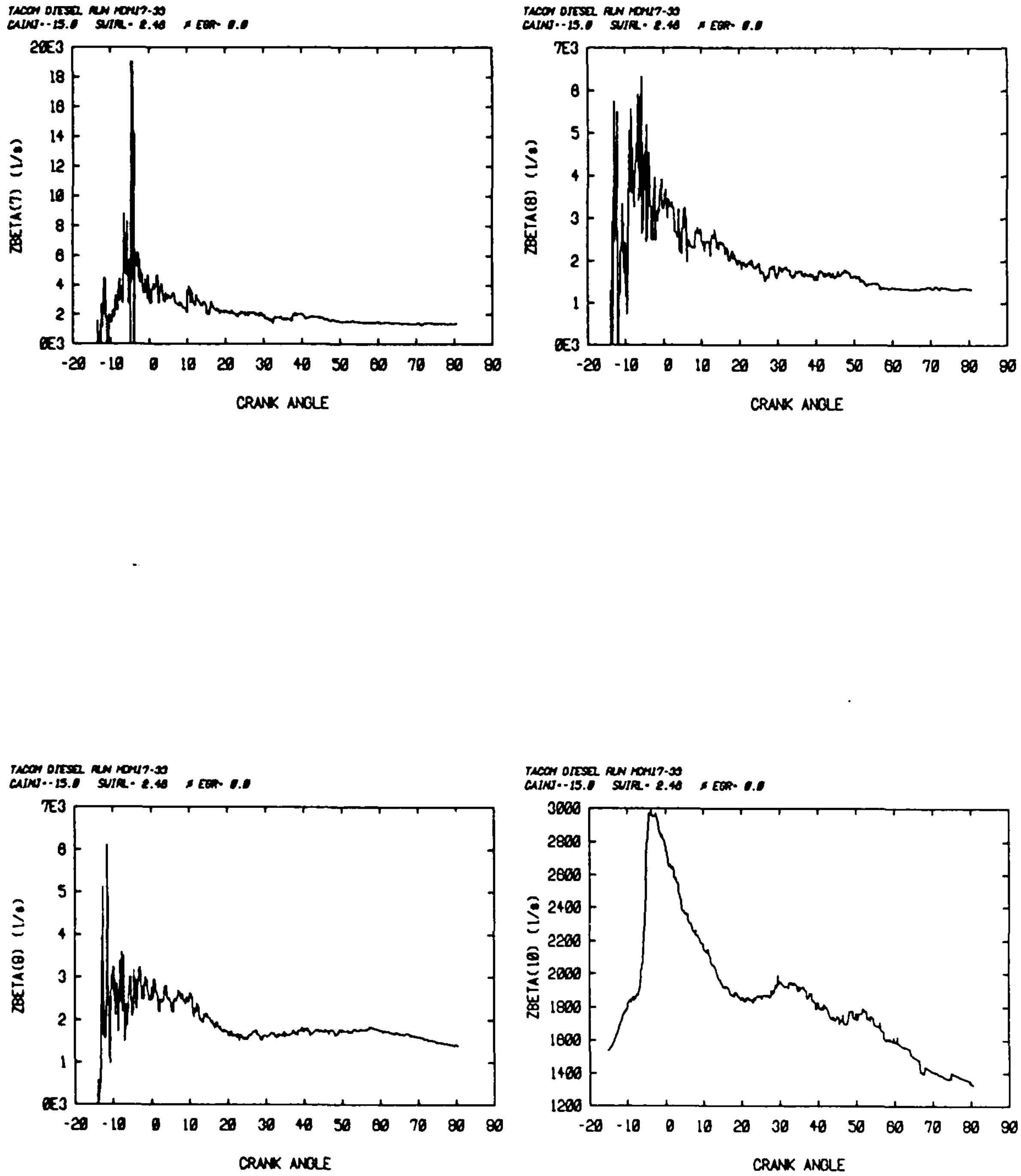
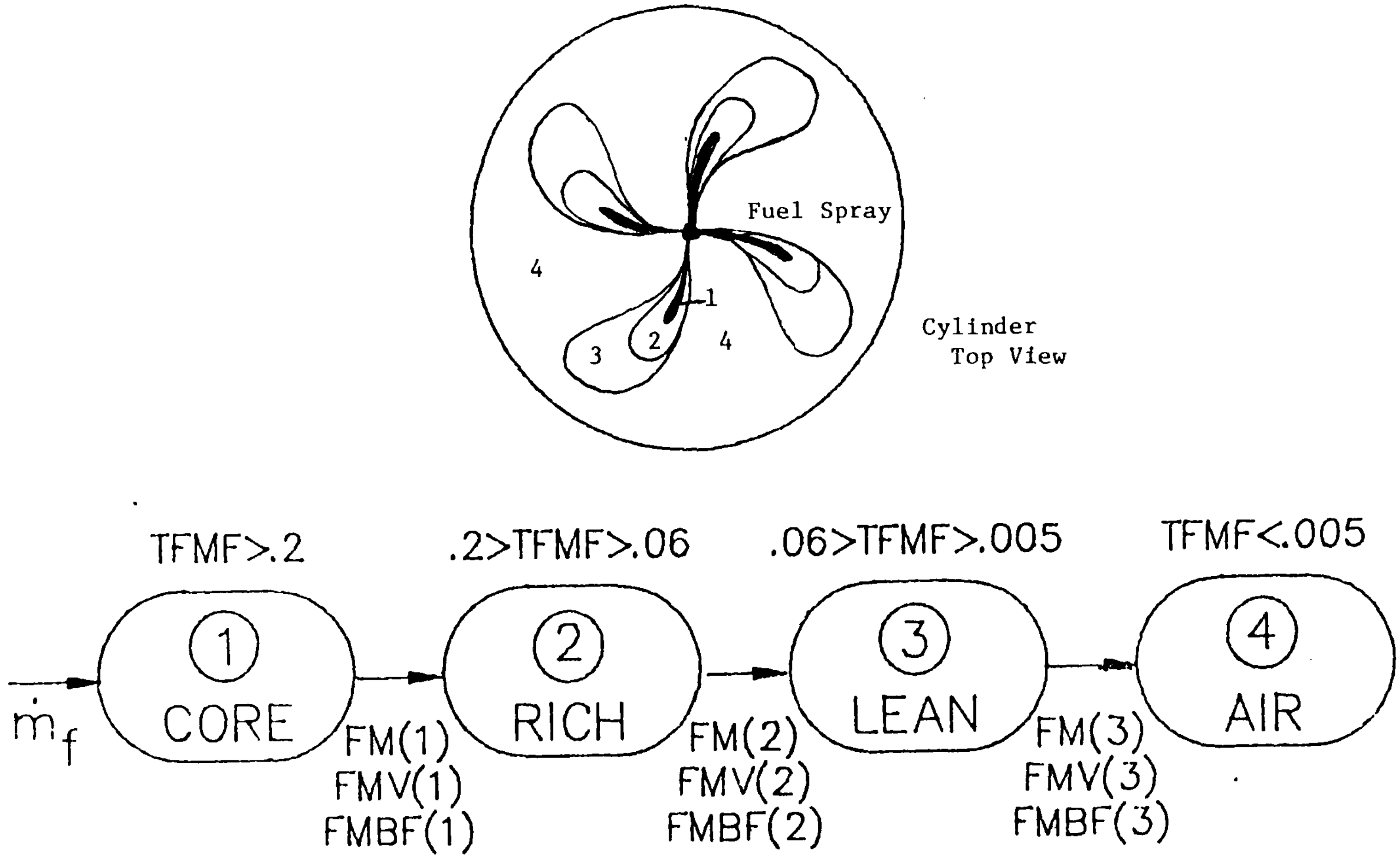
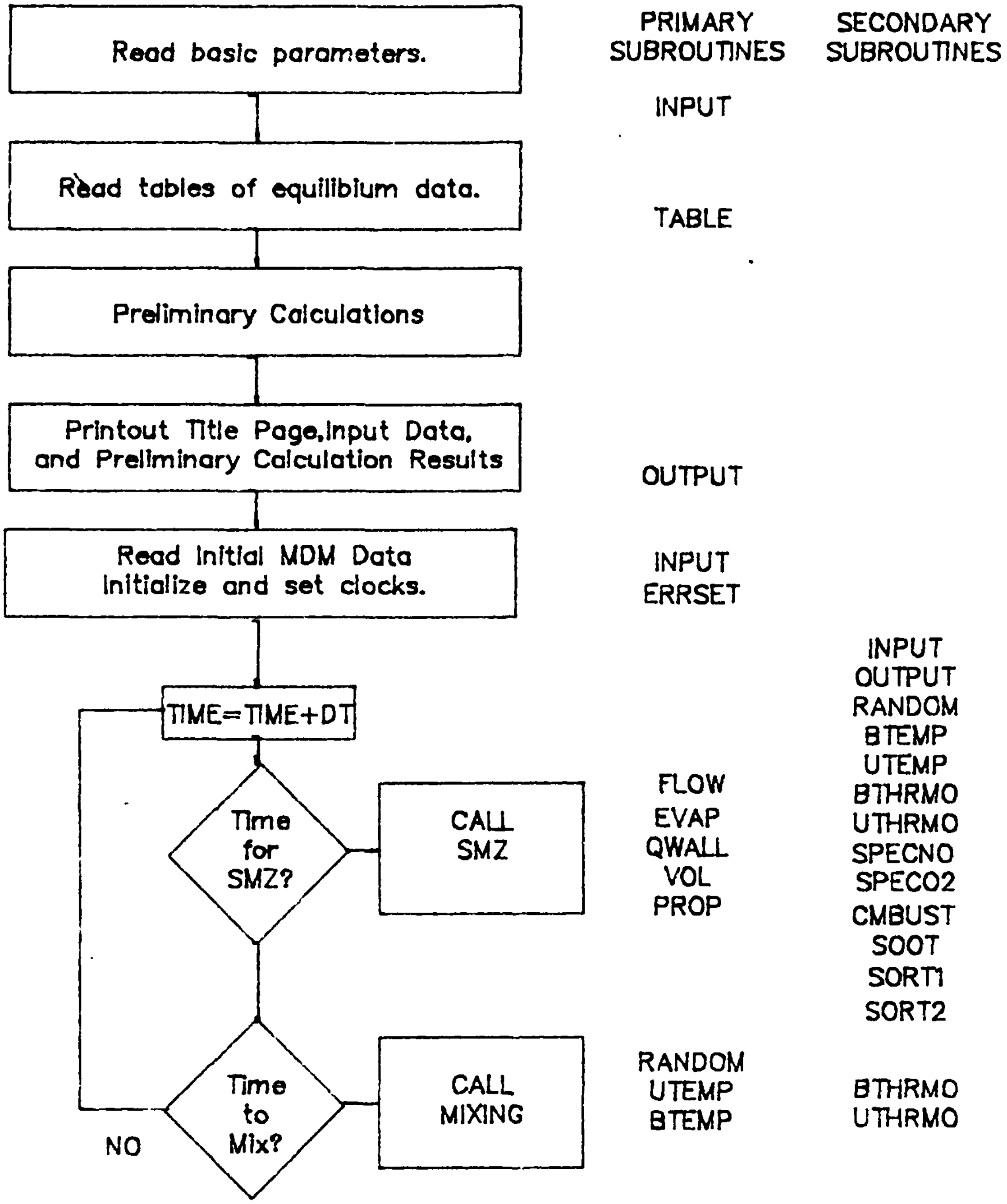


Figure 2-46 KIVA Zone Mixing Intensity (cont)



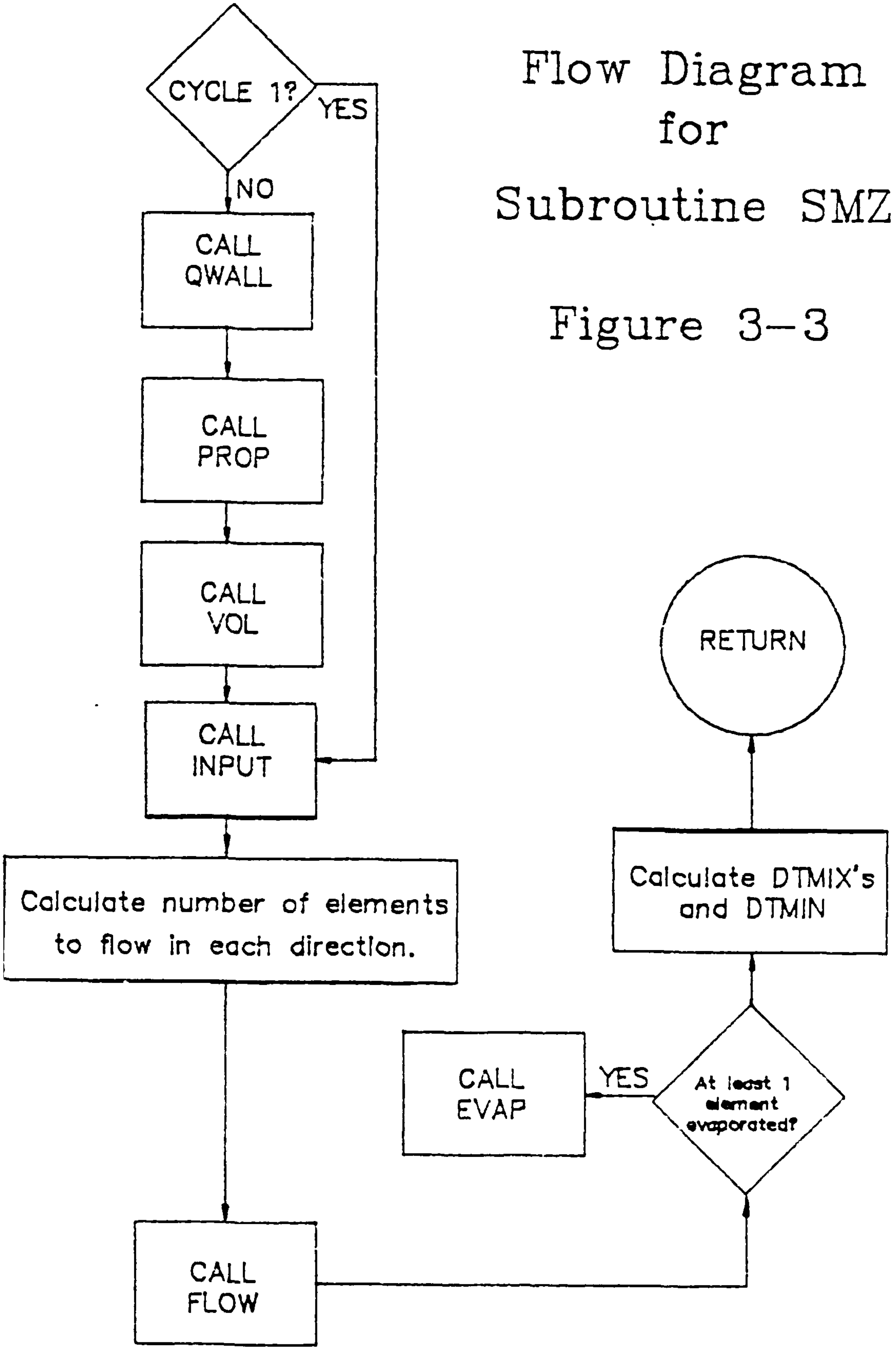
TYPICAL 4-ZONE MODEL

FIGURE 3-1



Flow Chart for PROGRAM SMM

Figure 3-2



Flow Diagram
for
Subroutine SMZ

Figure 3-3

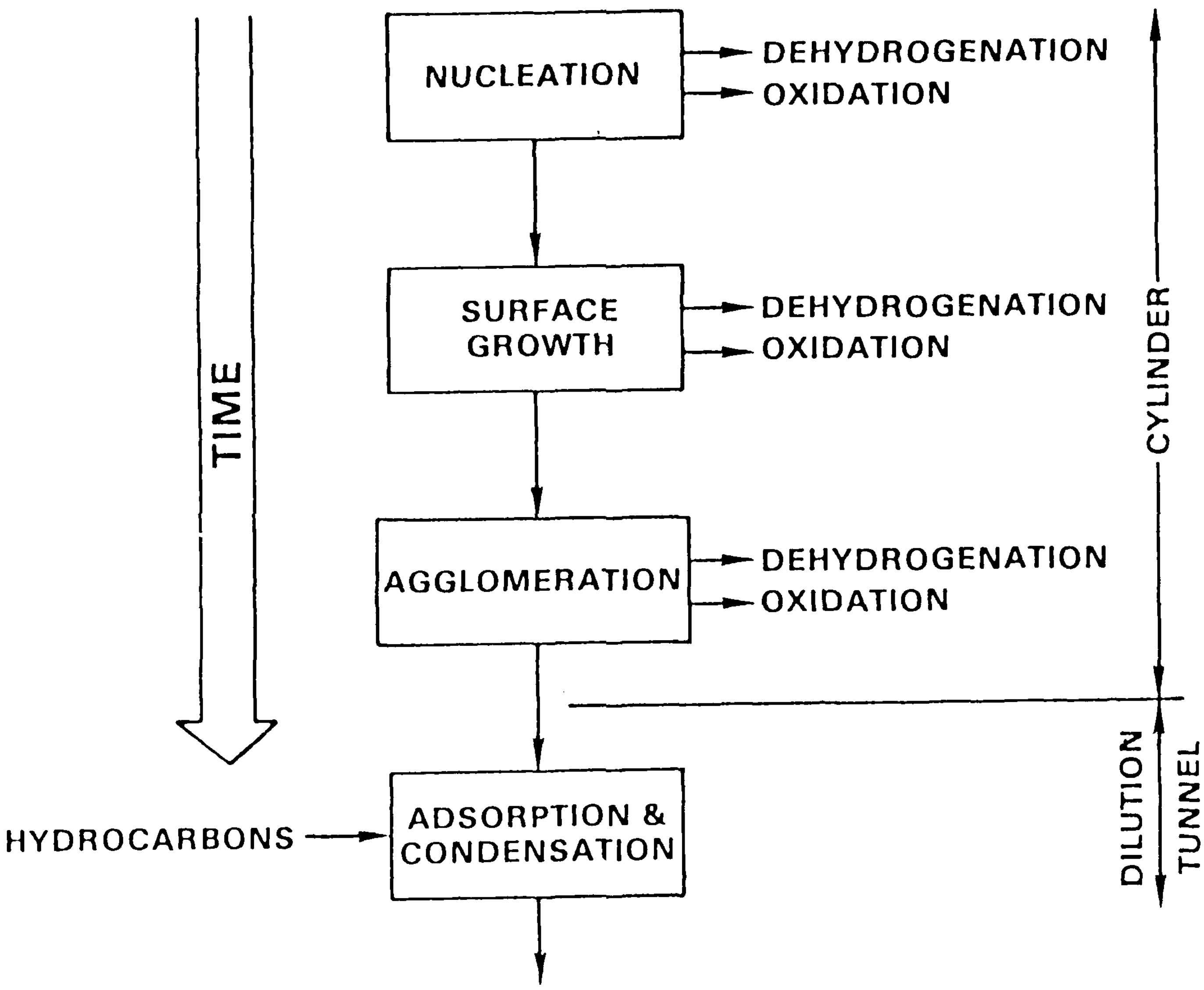


Figure 3-4 Production of Diesel Particulates [41]

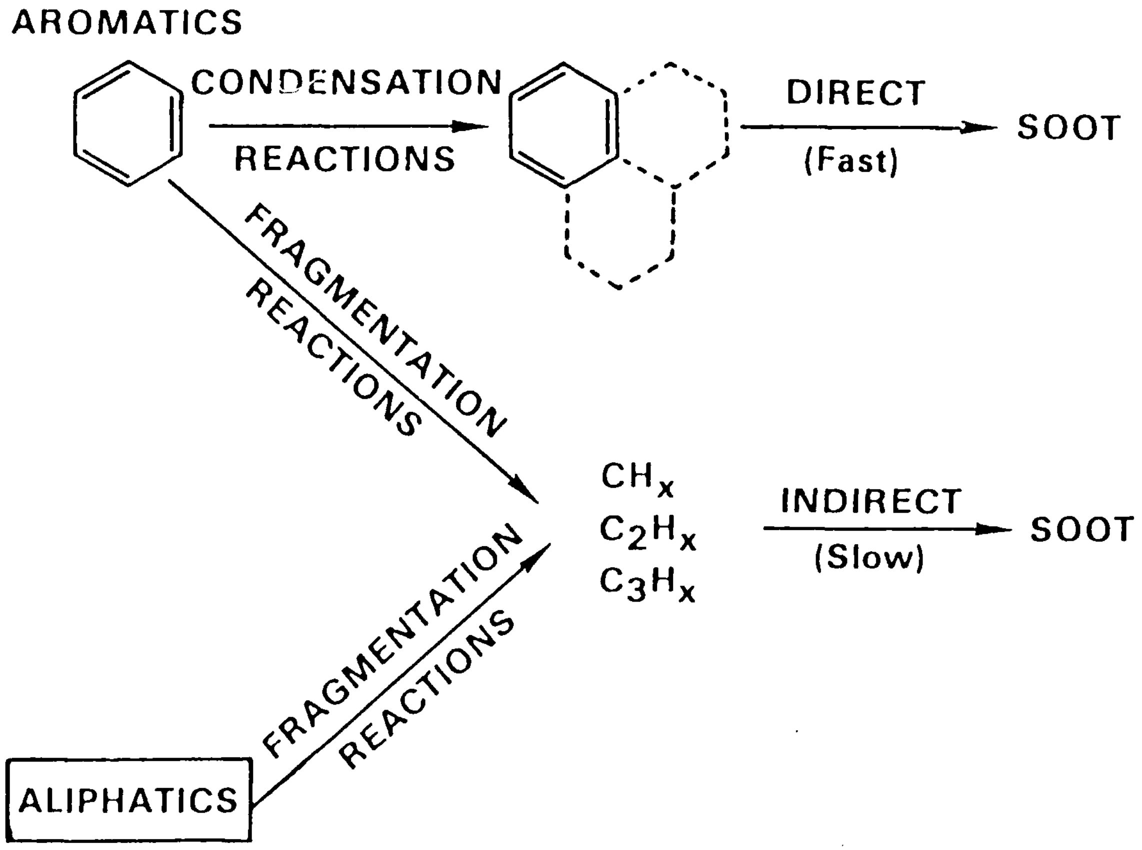
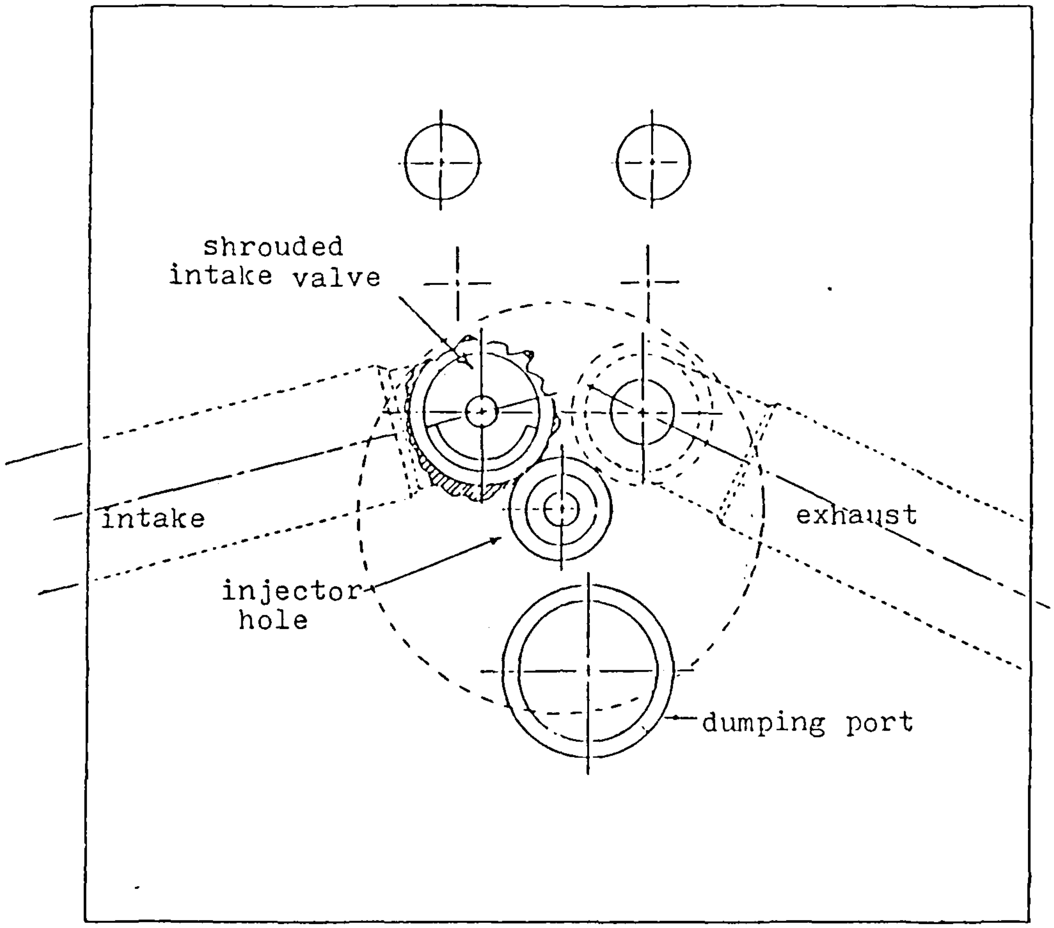
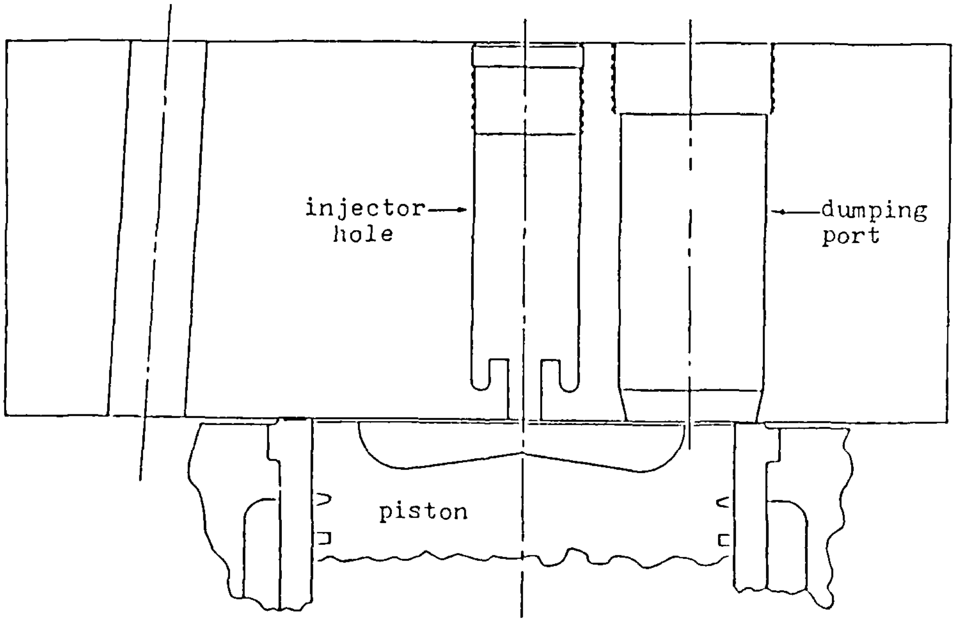


Figure 3-5 Mechanistic Model for the Nucleation of Soot [42]

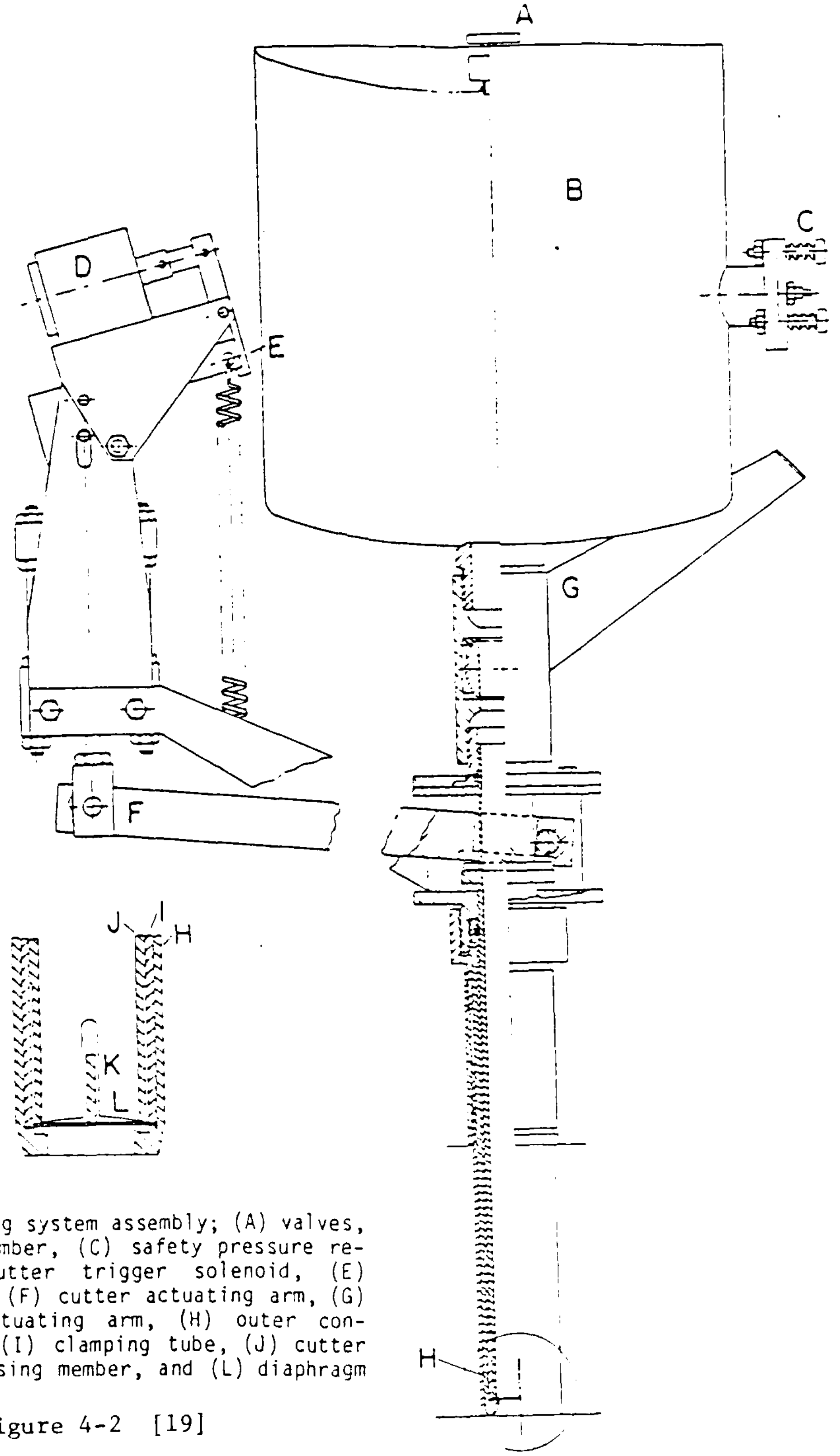


Simplified top view of the engine head



Simplified side view of the engine head and the piston [19]

Figure 4-1



Dumping system assembly; (A) valves, (B) quench chamber, (C) safety pressure release, (D) cutter trigger solenoid, (E) trigger latch, (F) cutter actuating arm, (G) ball valve actuating arm, (H) outer connecting tube, (I) clamping tube, (J) cutter tube, (K) crossing member, and (L) diaphragm

Figure 4-2 [19]

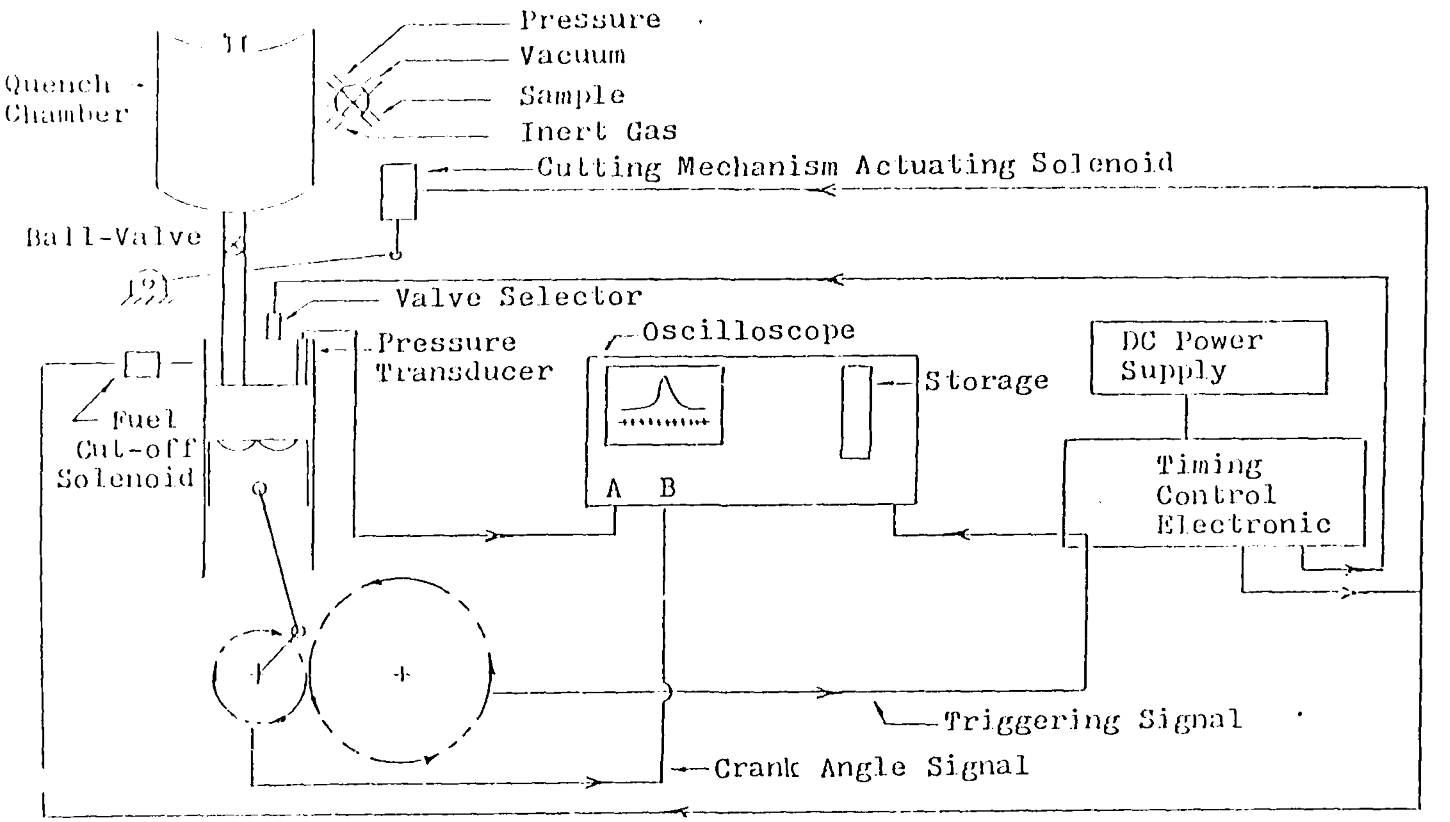
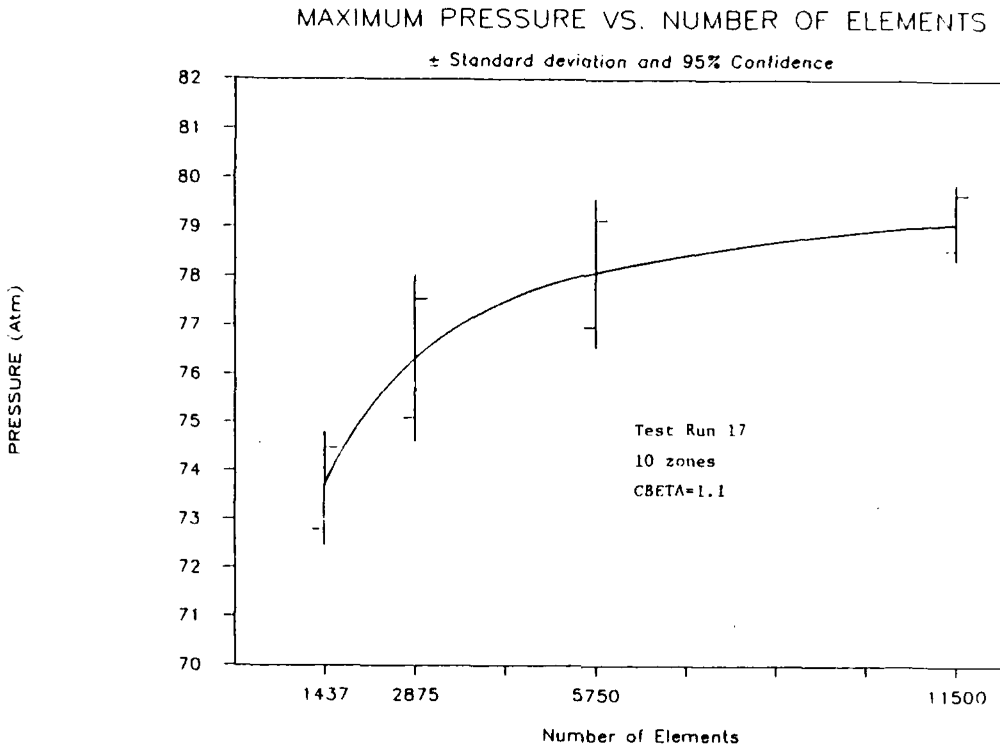


Figure 4-3   Schematic of the dumping and the control system [19]



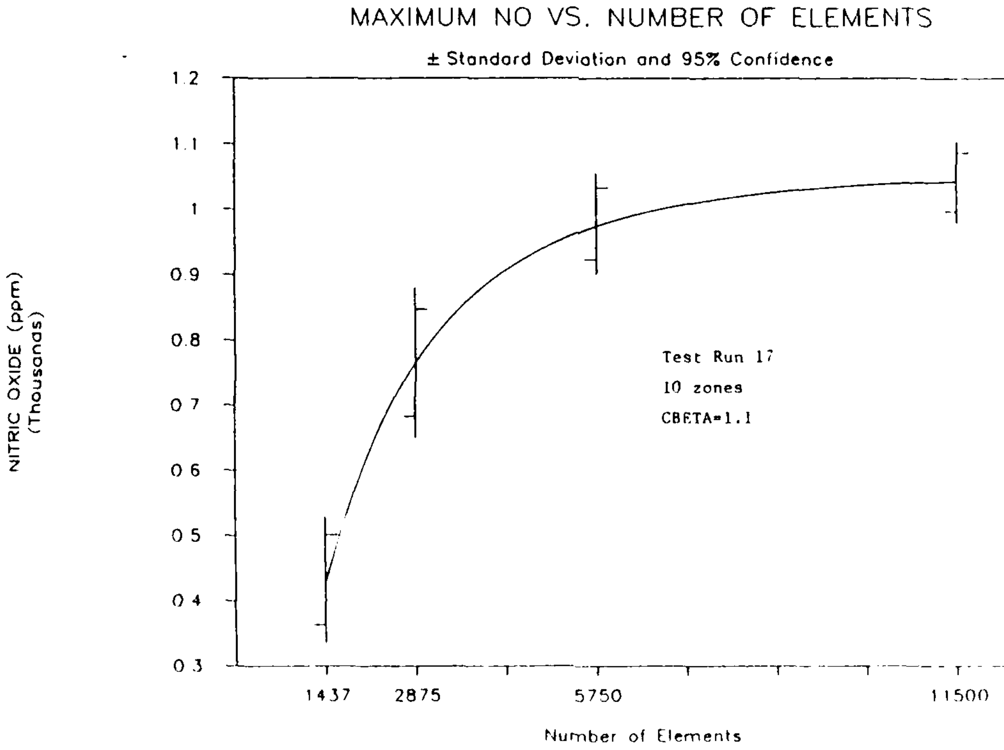


Figure 5-1 Effect of Number of Elements on Pressure and NO

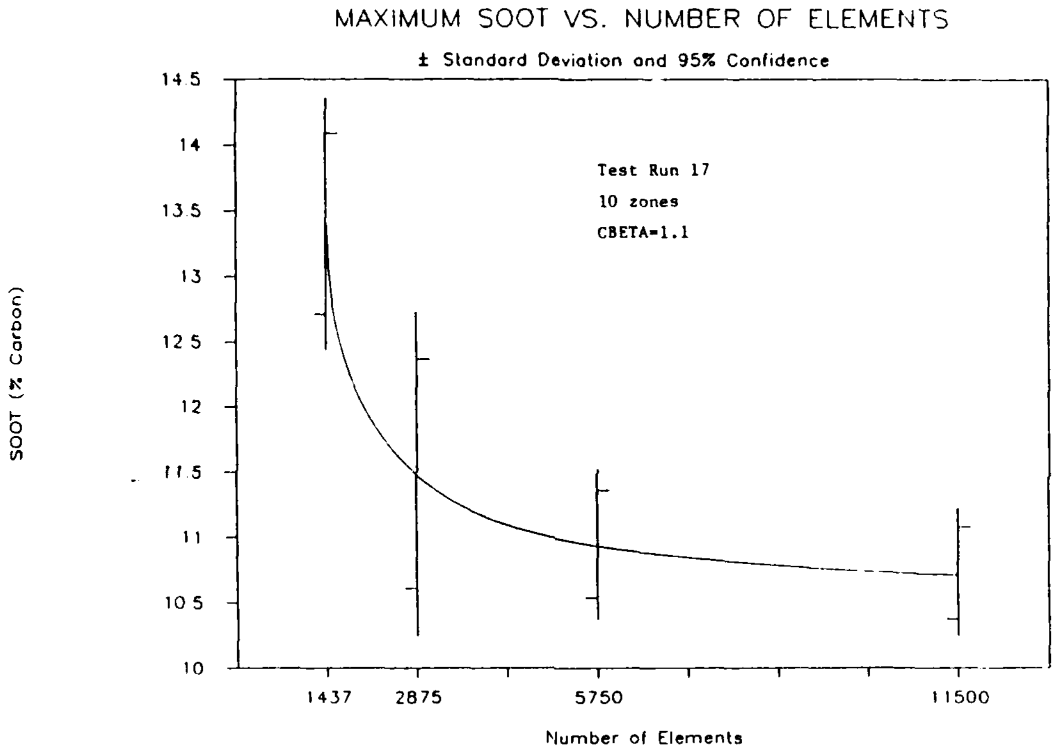


Figure 5-2 Effect of Number of Elements on Maximum Soot

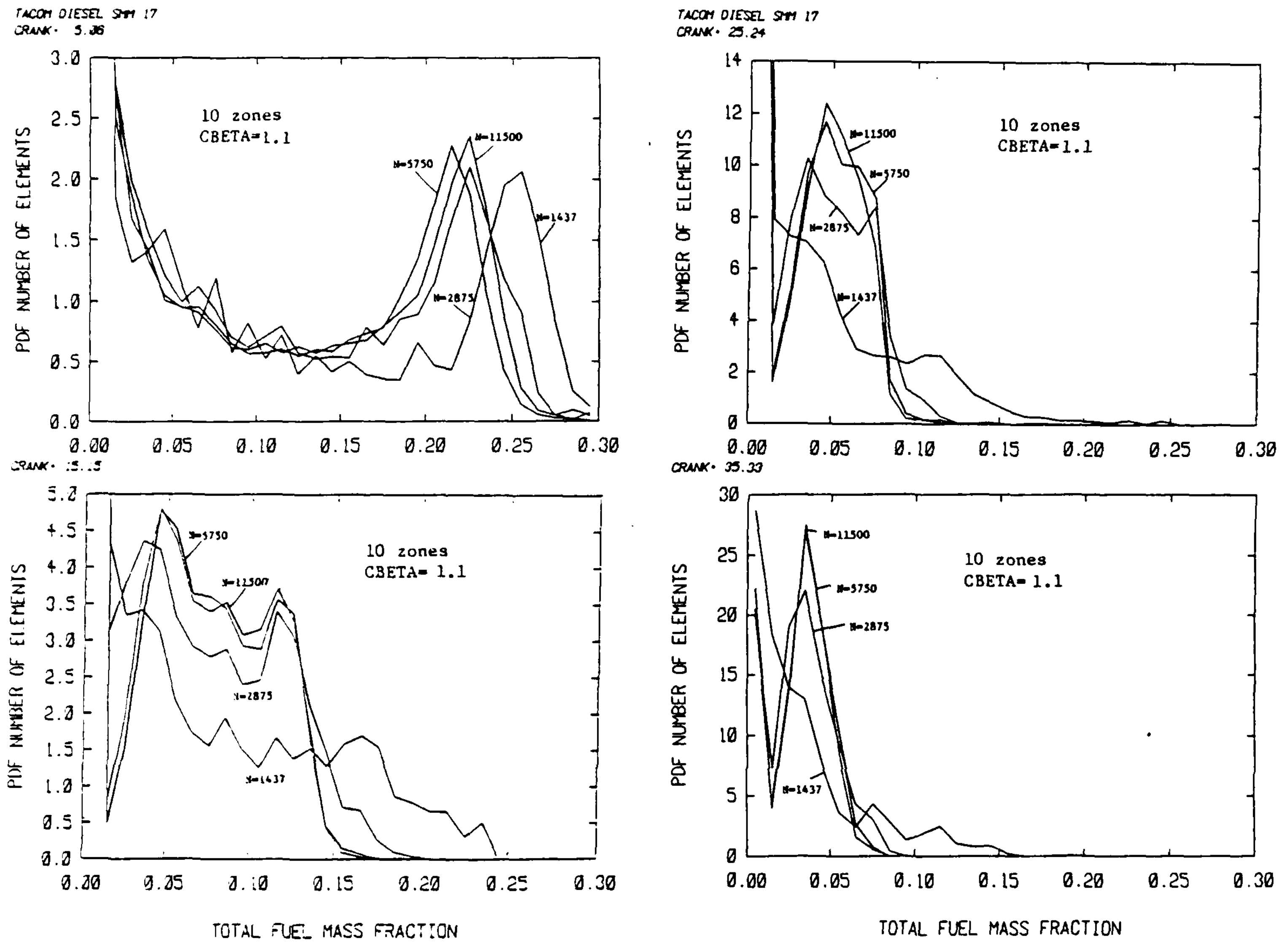


Figure 5-3 Effect of Number of Elements on Fuel Mass Fraction Distribution

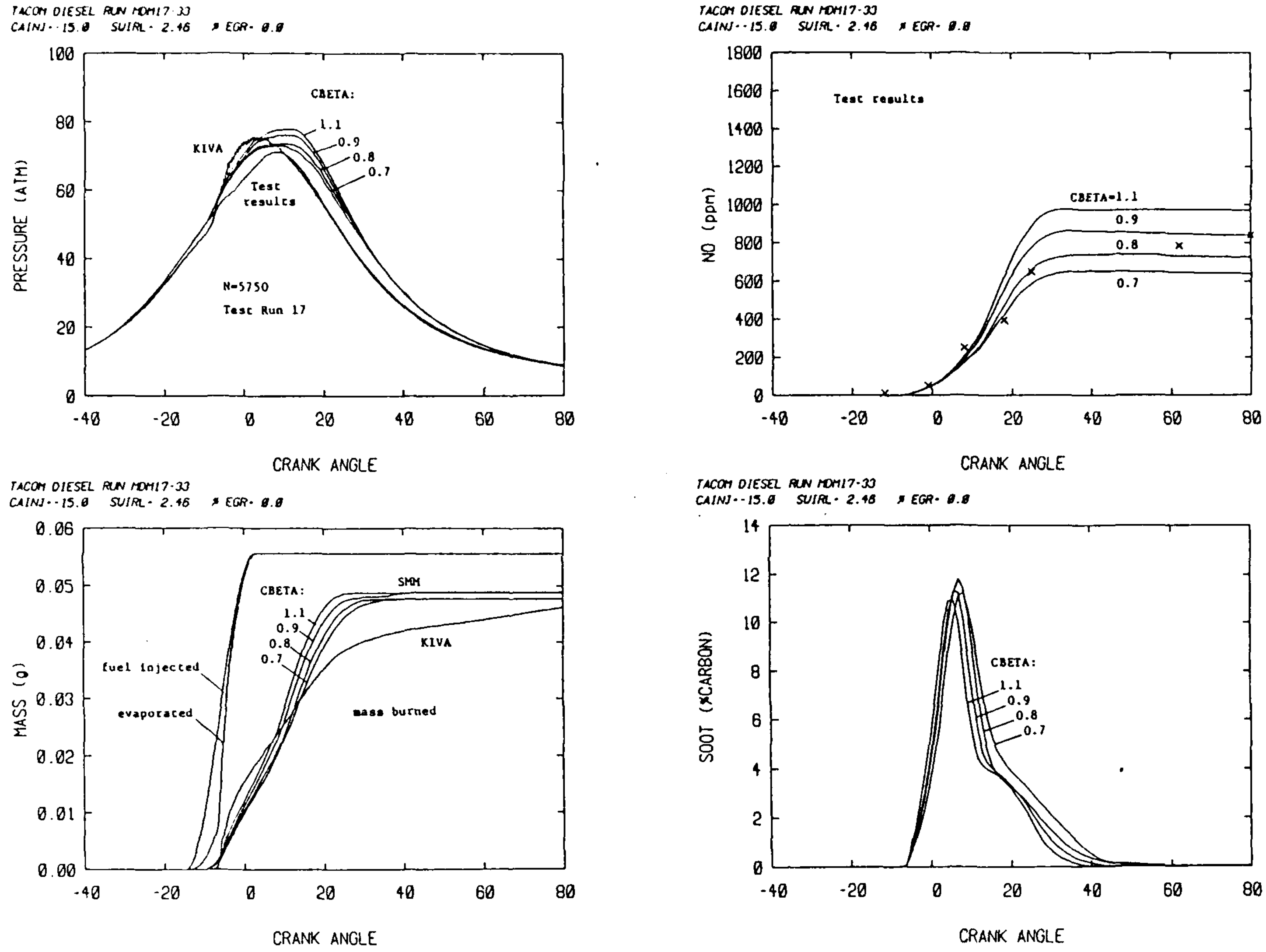


Figure 5-4 Effect of Mixing Intensity Scaling Factor (CBETA) on Mixing Model Results

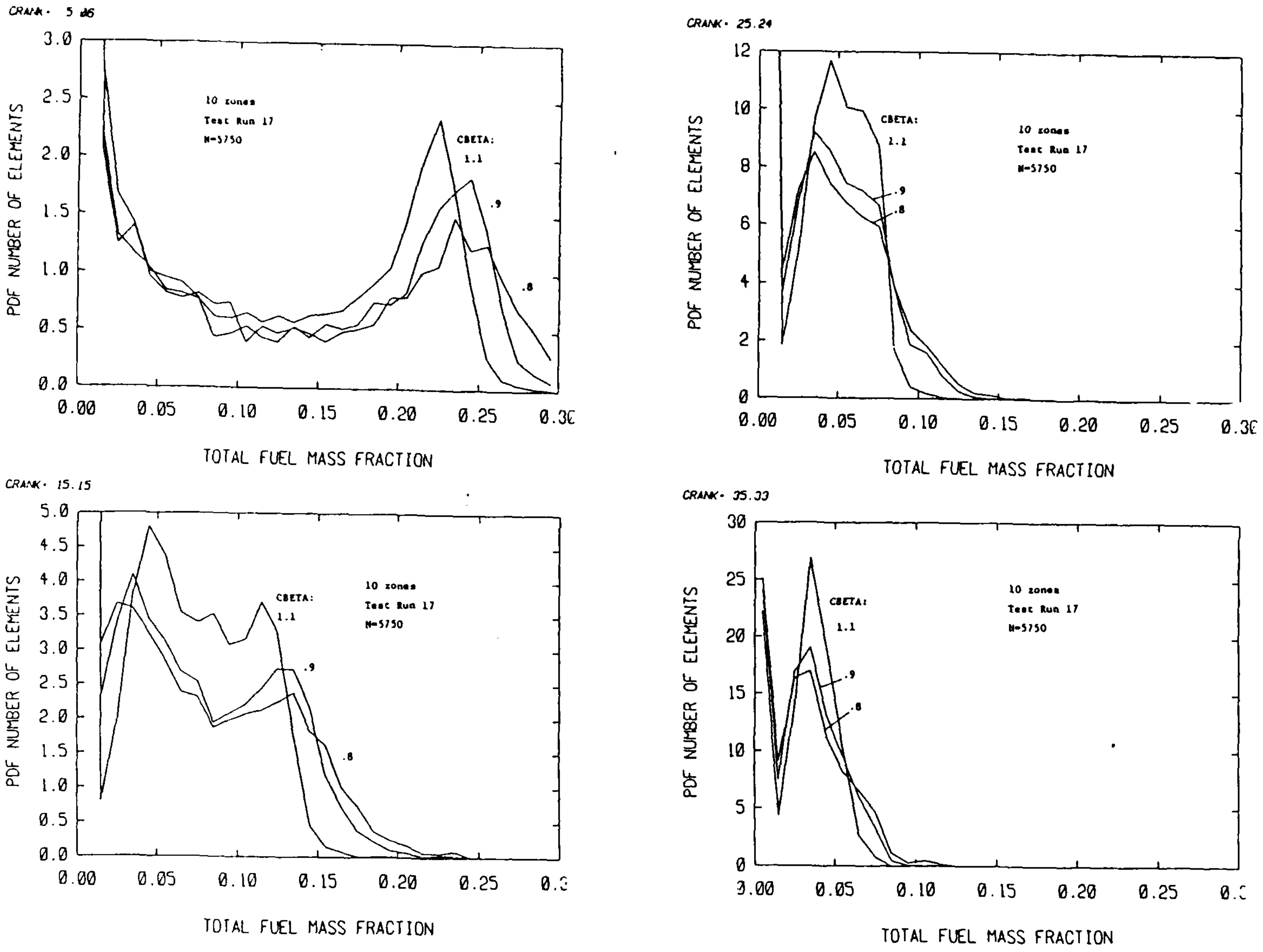


Figure 5-5 Effect of Mixing Intensity Scaling Factor (CBETA) on Fuel Mass Fraction Distribution

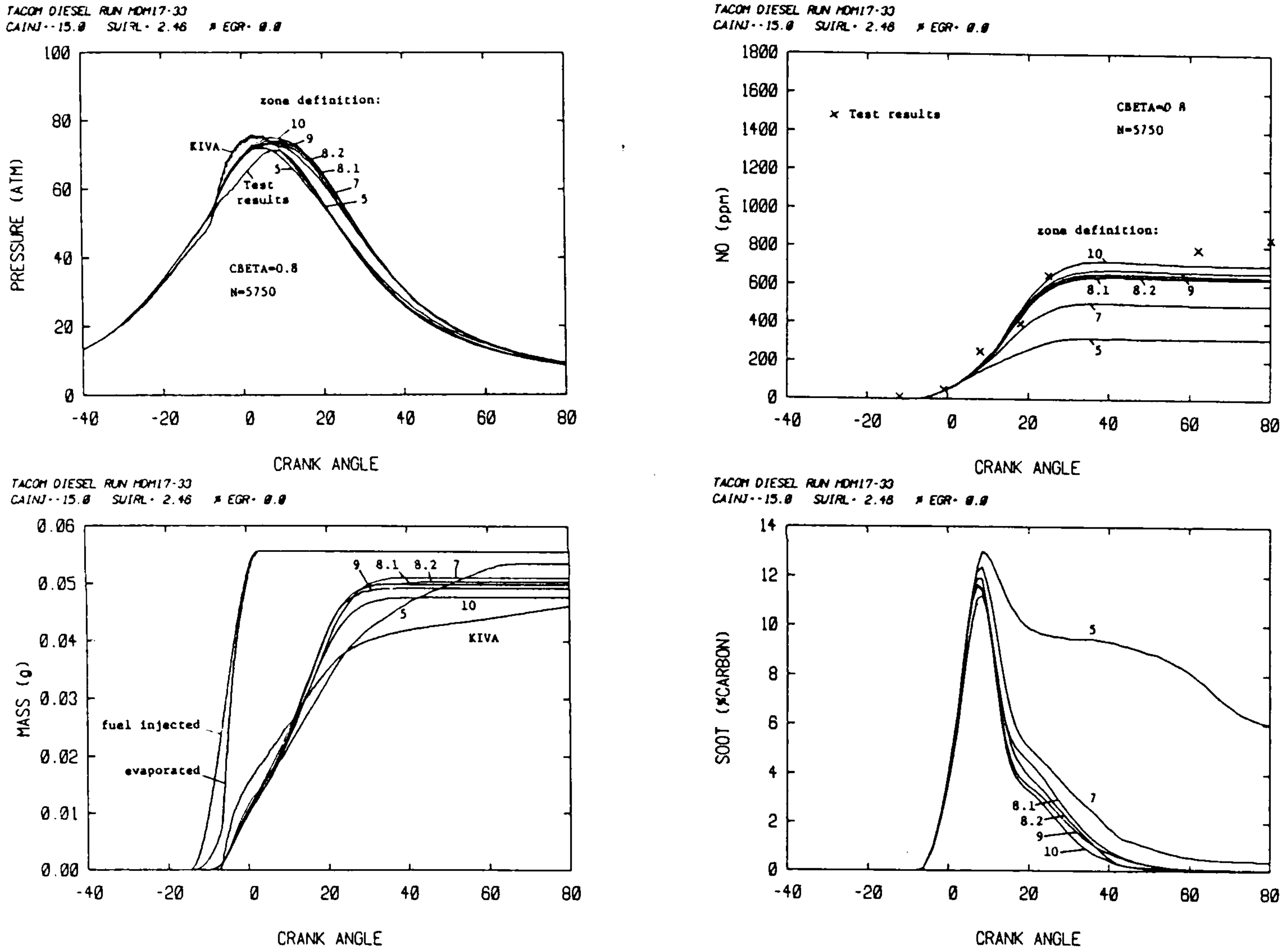


Figure 5-6 Effect of Mixing Zone Definition on Stochastic Mixing Model Results

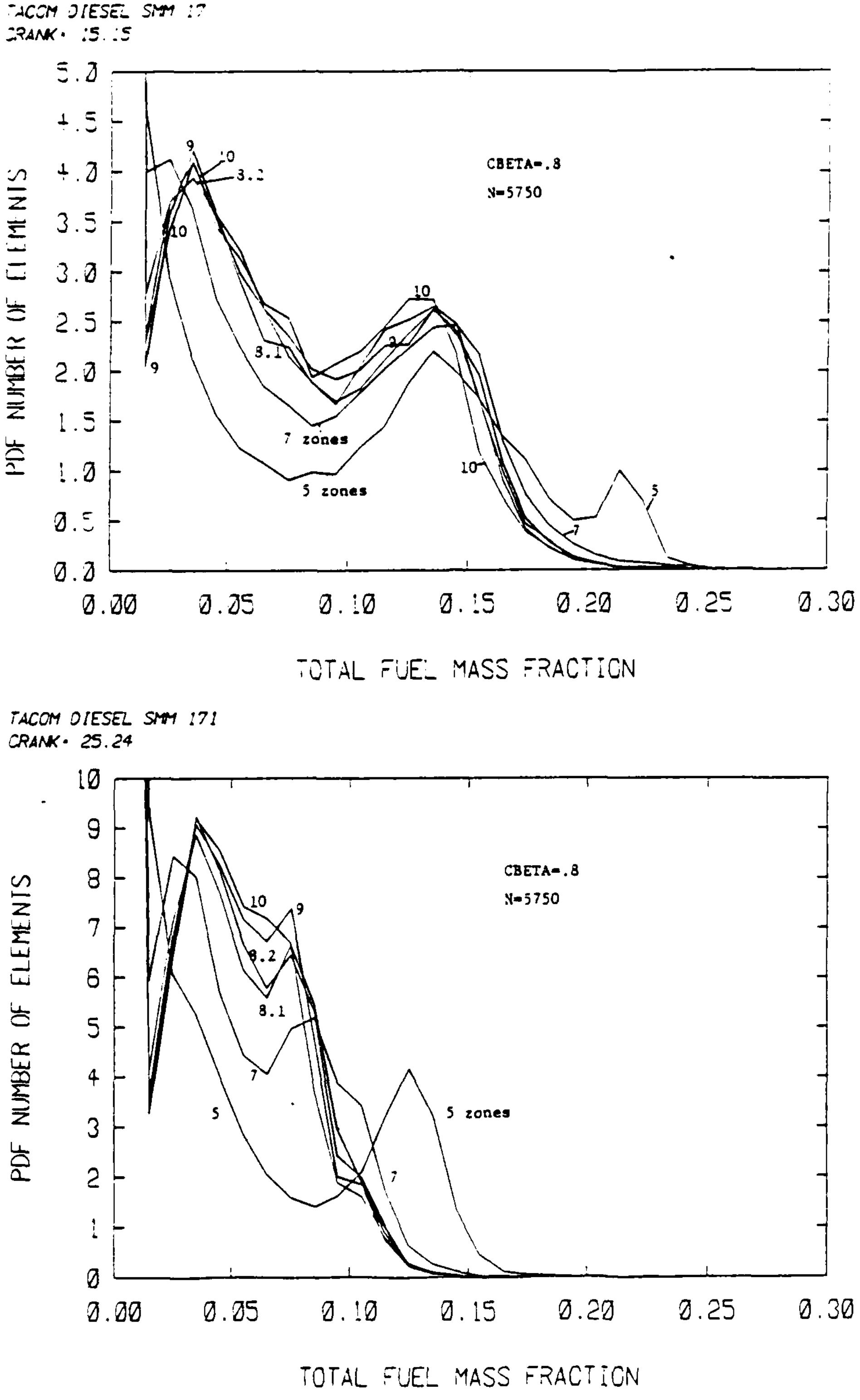


Figure 5-7 Effect of Number and Limits of Zones on Fuel Mass Fraction Distribution

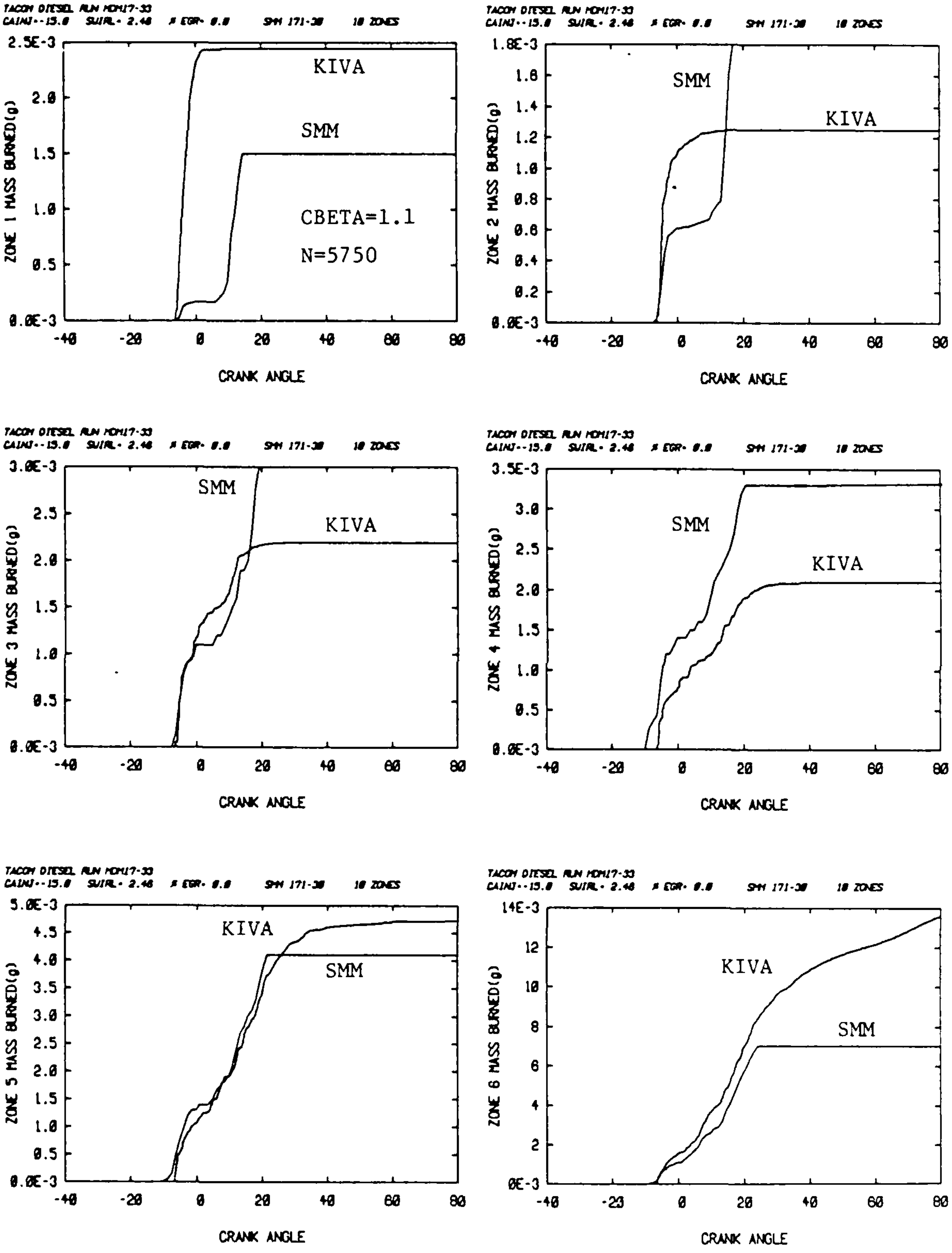


Figure 5-8 Comparison of SMM versus KIVA Zone Fuel-Mass Burned

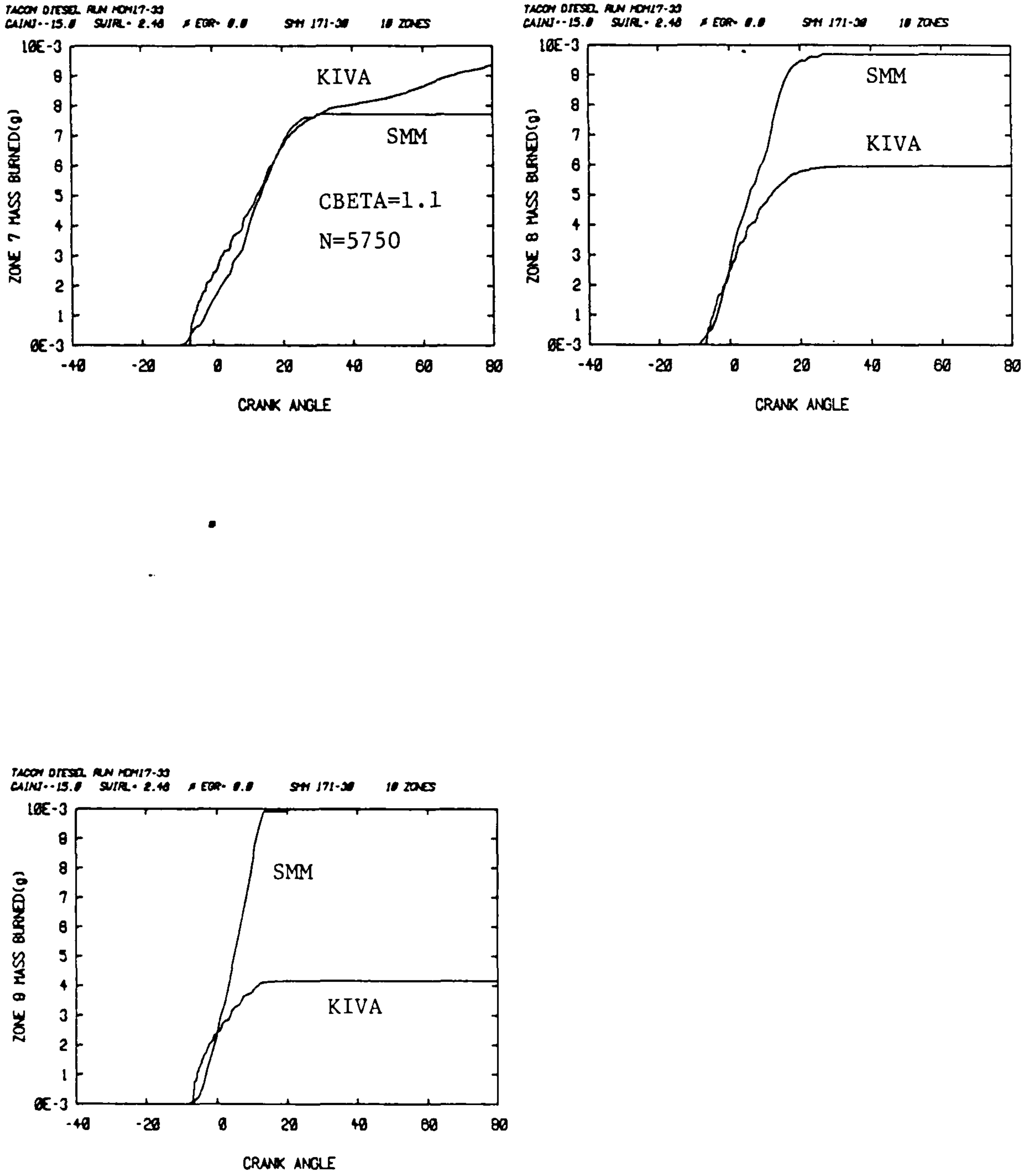


Figure 5-9 Comparison of SMM versus KIVA Zone Fuel-Mass Burned

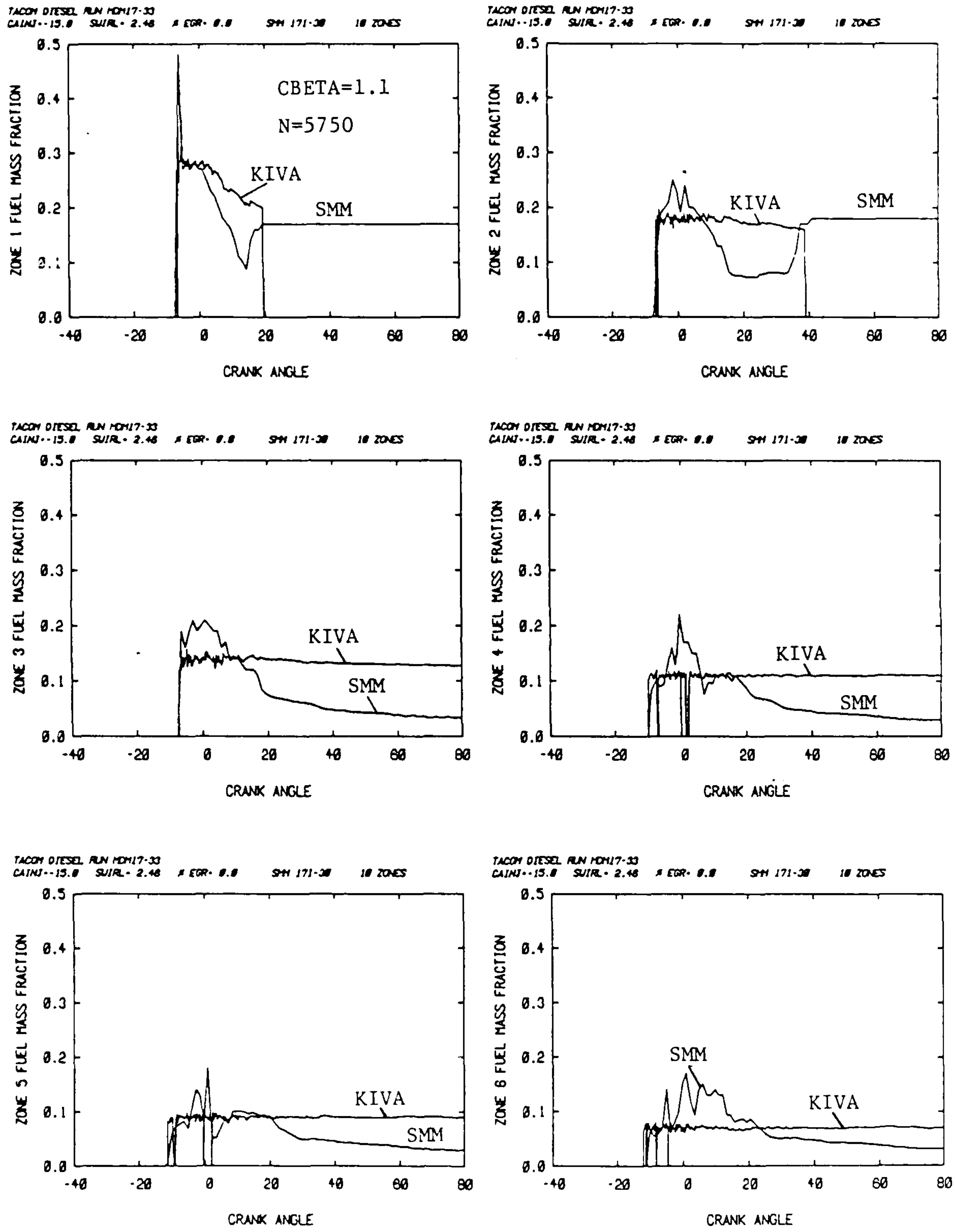


Figure 5-10 Comparison of SMM versus KIVA Total Fuel Mass Fraction

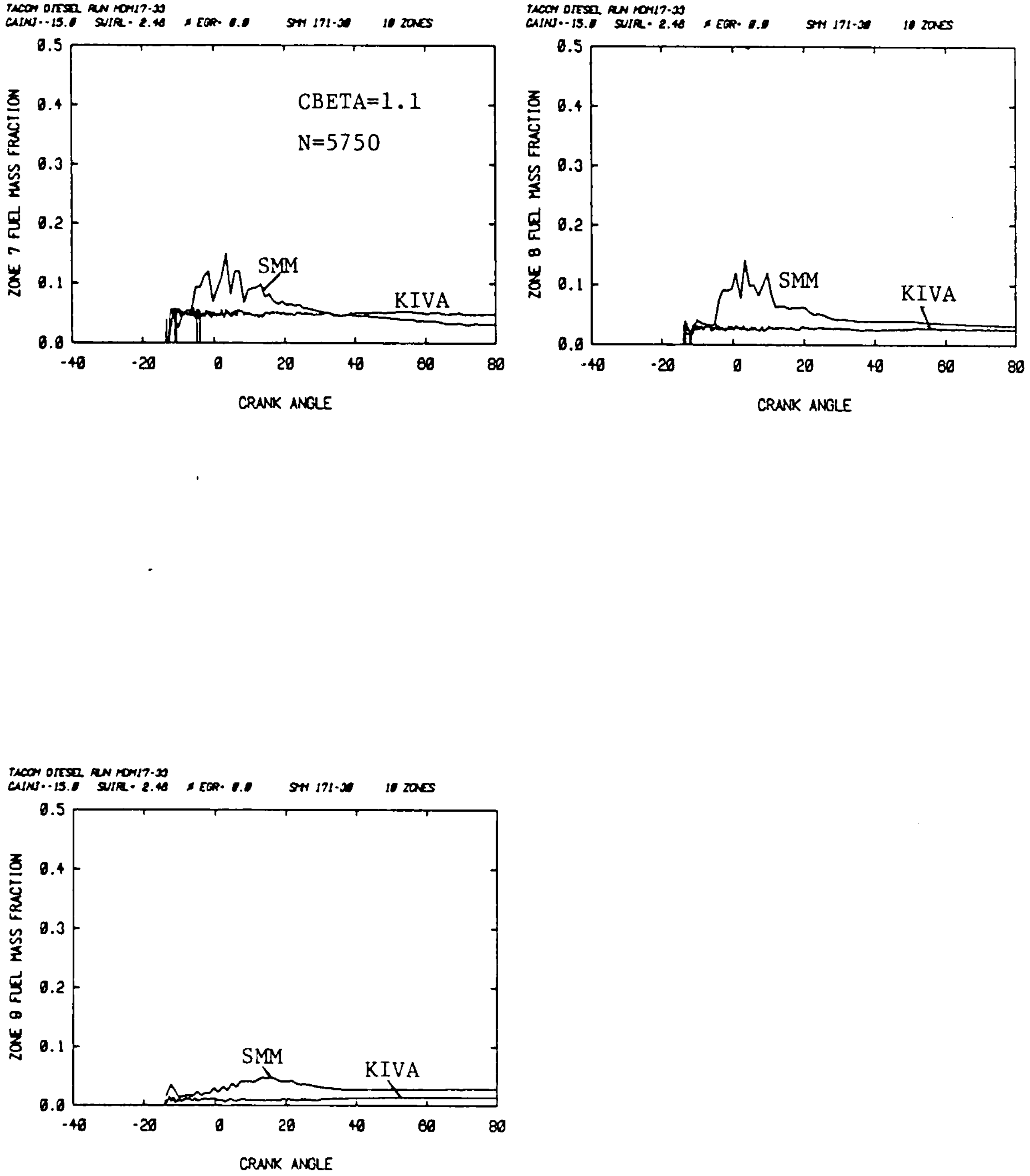


Figure 5-11 Comparison of SMM versus KIVA Total Fuel Mass Fraction (cont)

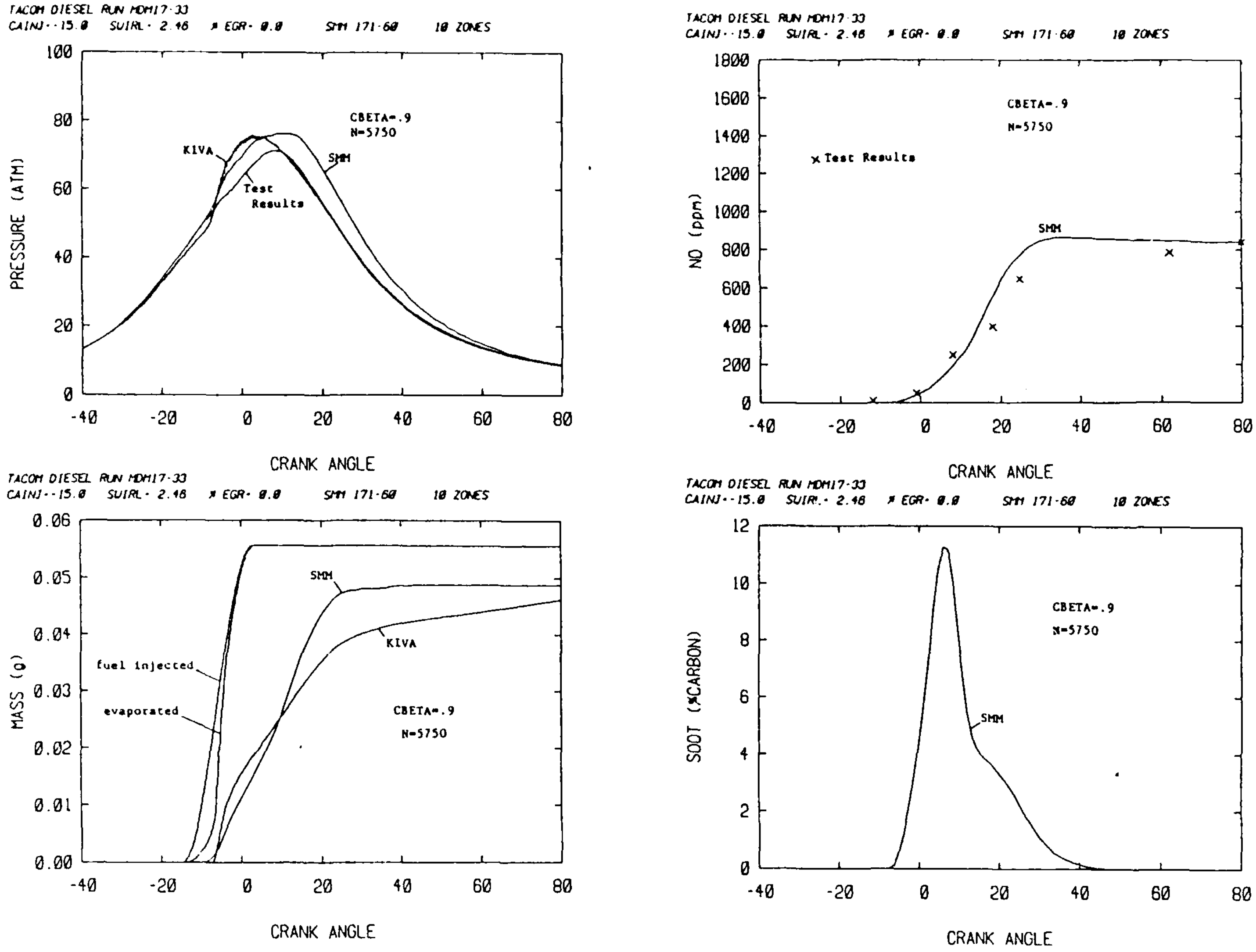


Figure 6-1 Stochastic Mixing Model Results for Test Run 17

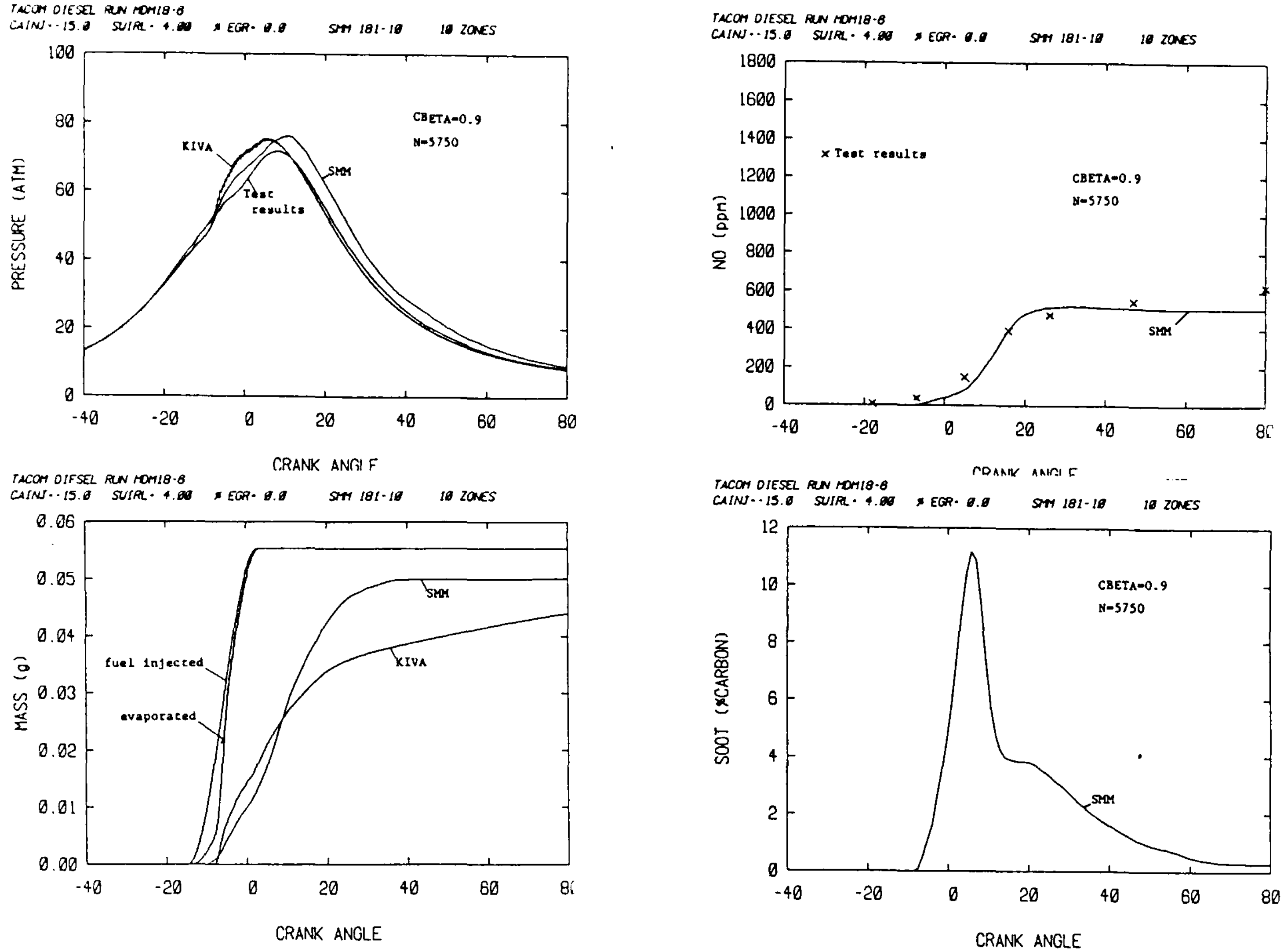


Figure 6-2 Stochastic Mixing Model Results for Test Run 18

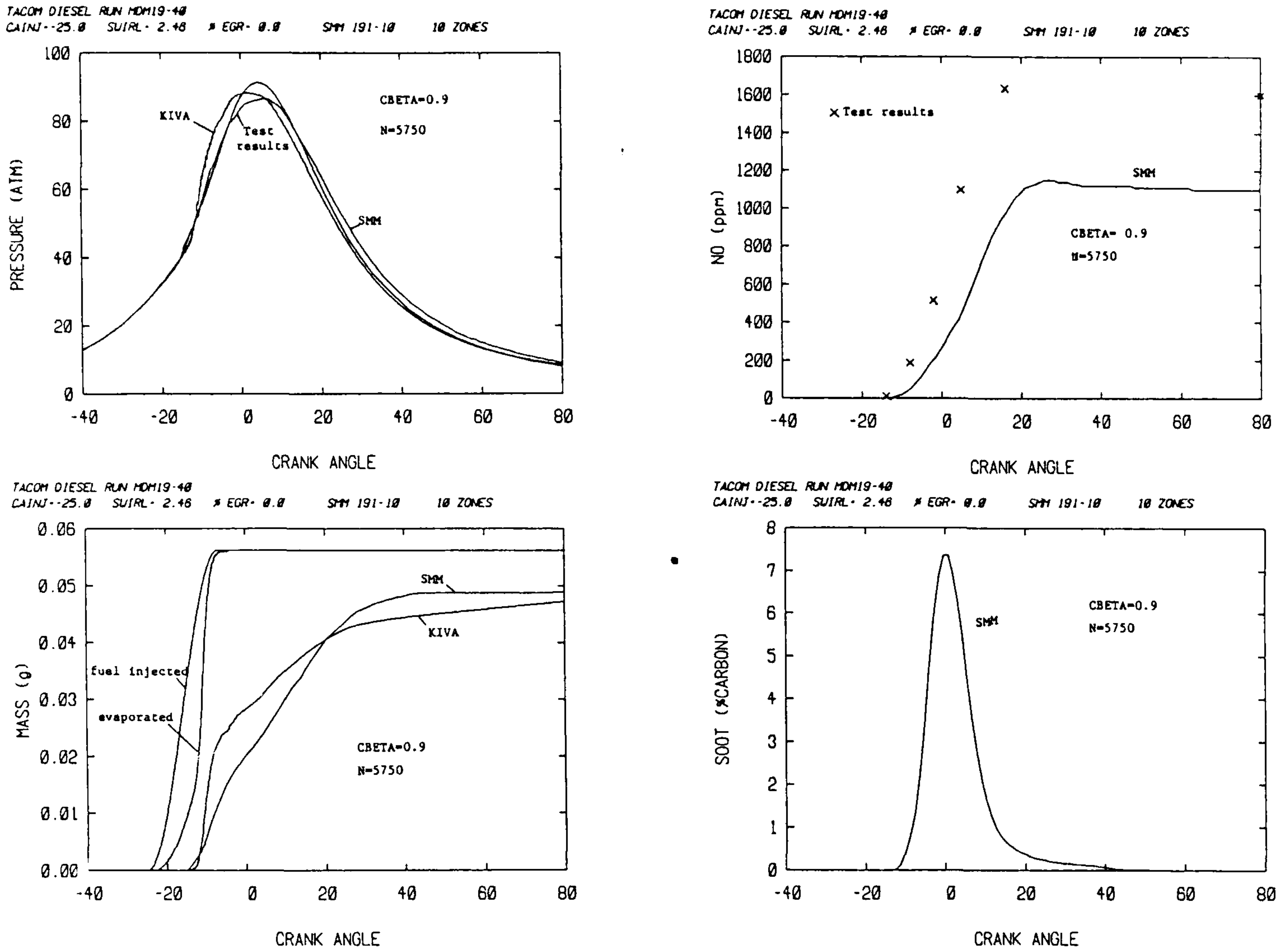


Figure 6-3 Stochastic Mixing Model Results for Test Run 19

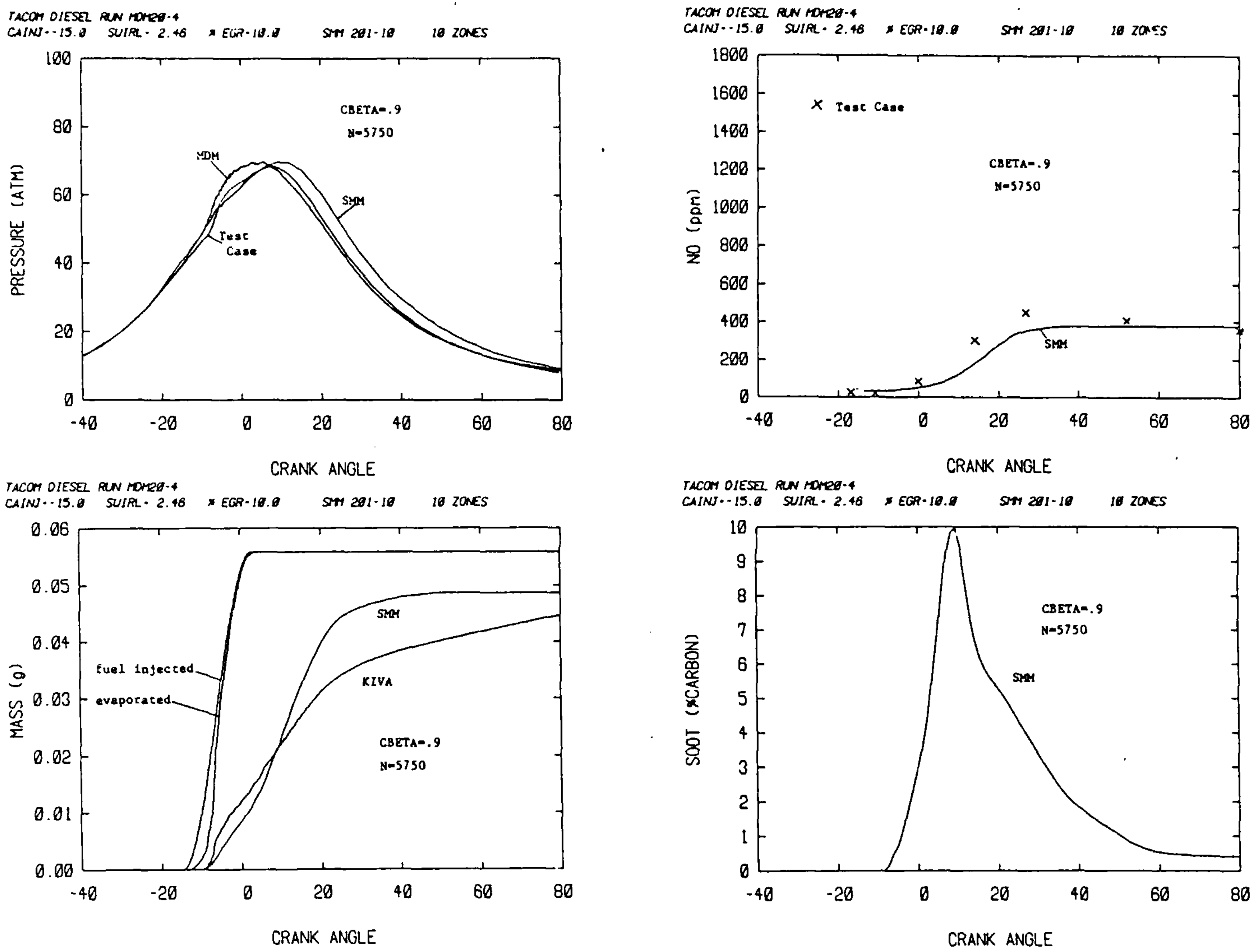


Figure 6-4 Stochastic Mixing Model Results for Test Run 20

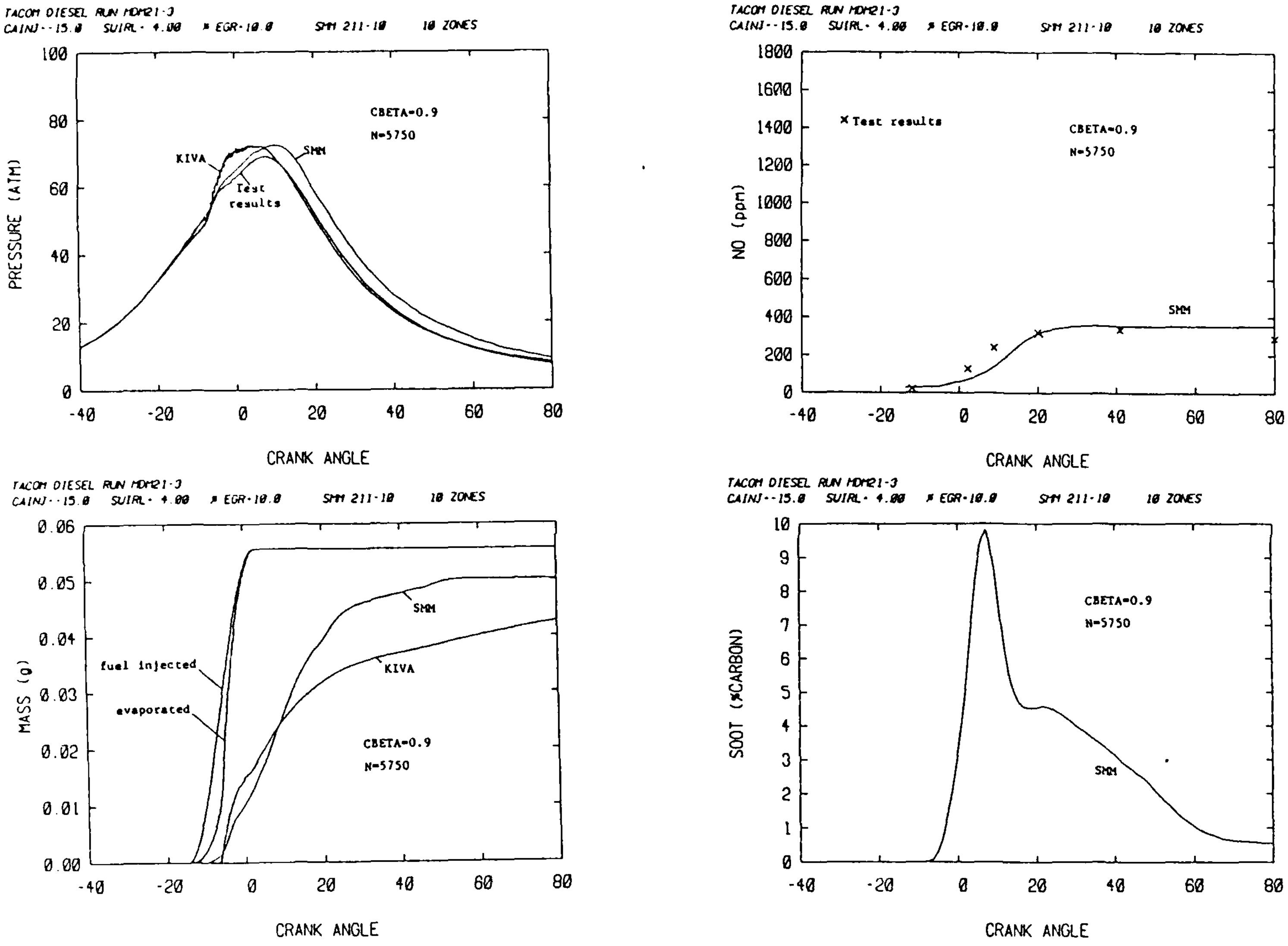


Figure 6-5 Stochastic Mixing Model Results for Test Run 21

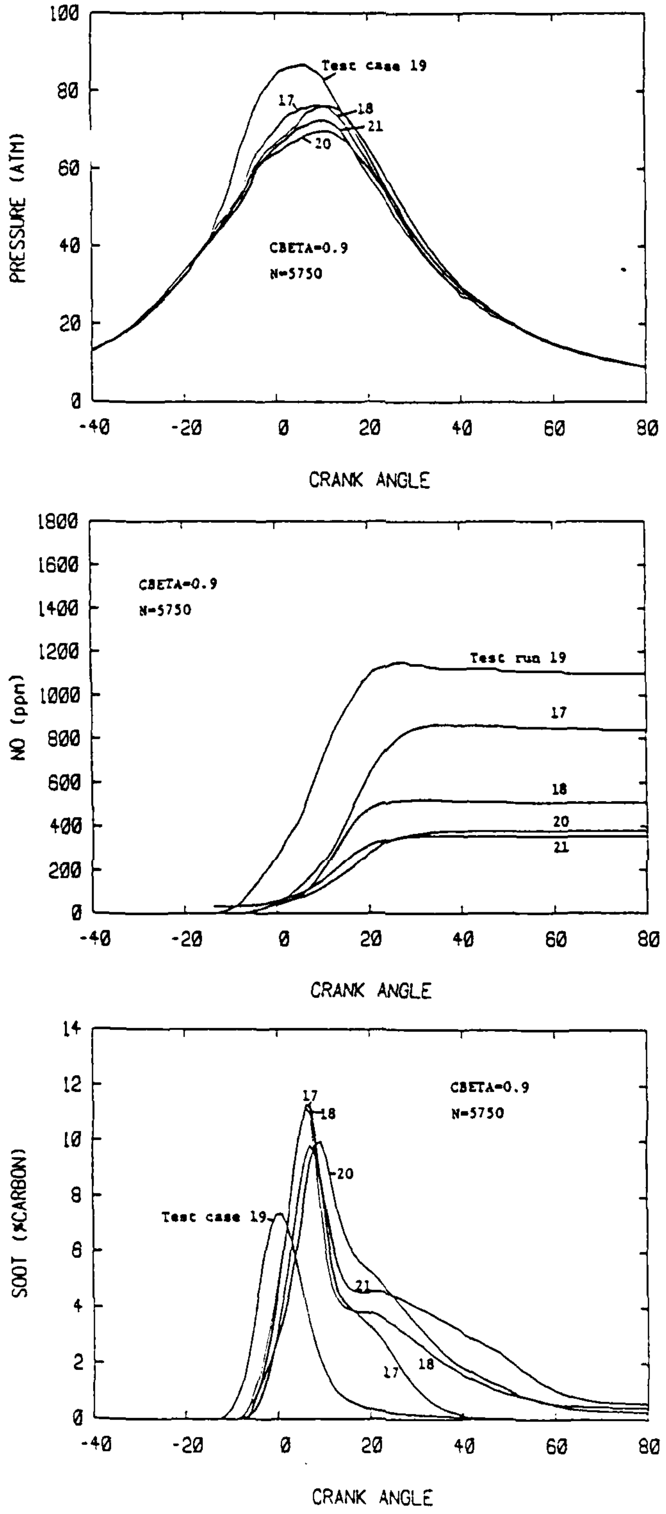


Figure 6-6 Comparison of Stochastic Mixing Model Results for Different Operating Conditions

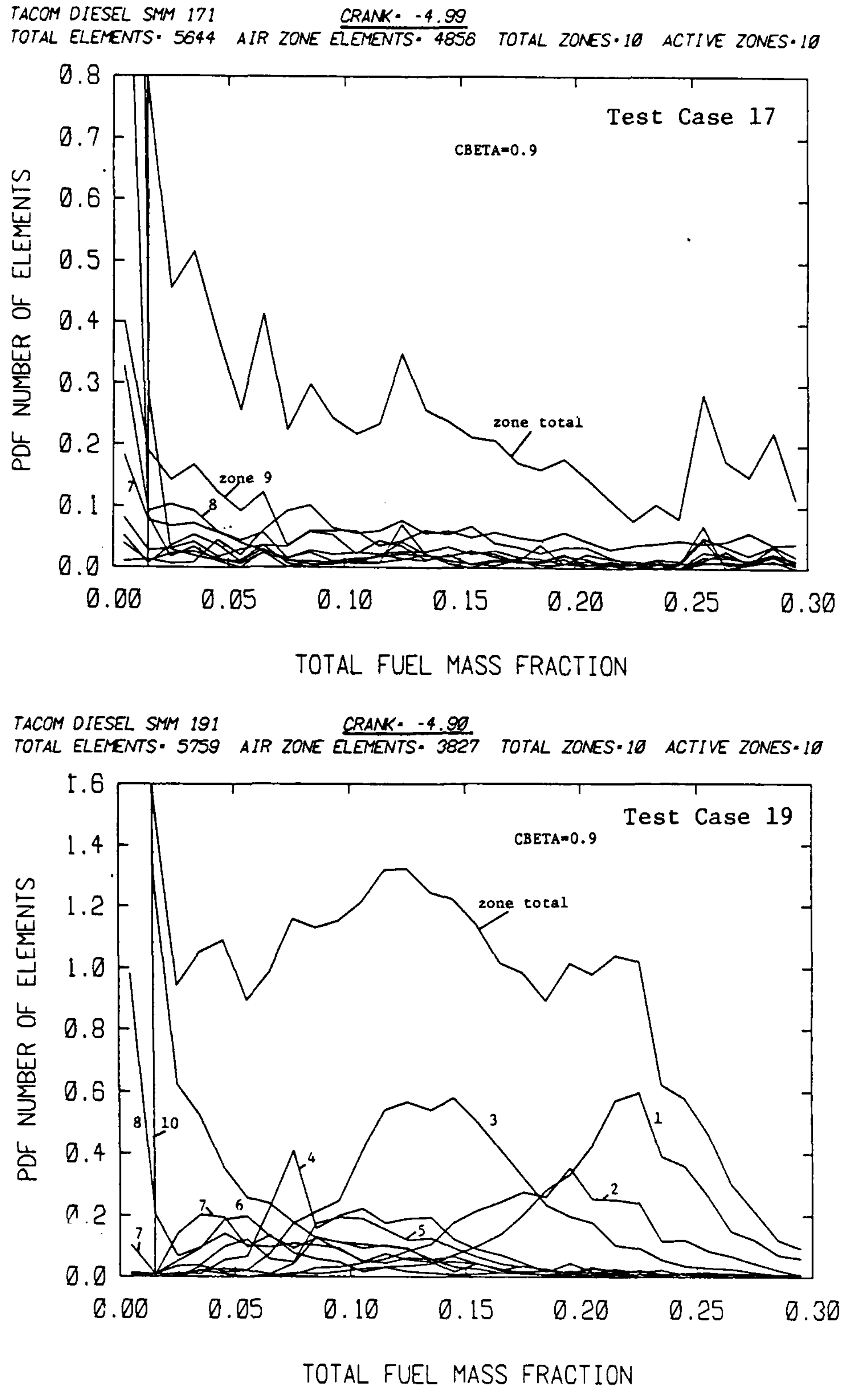


Figure 6-7 Fuel Mass Fraction Distribution by Mixing Zone
(Test Case 17 and 19)

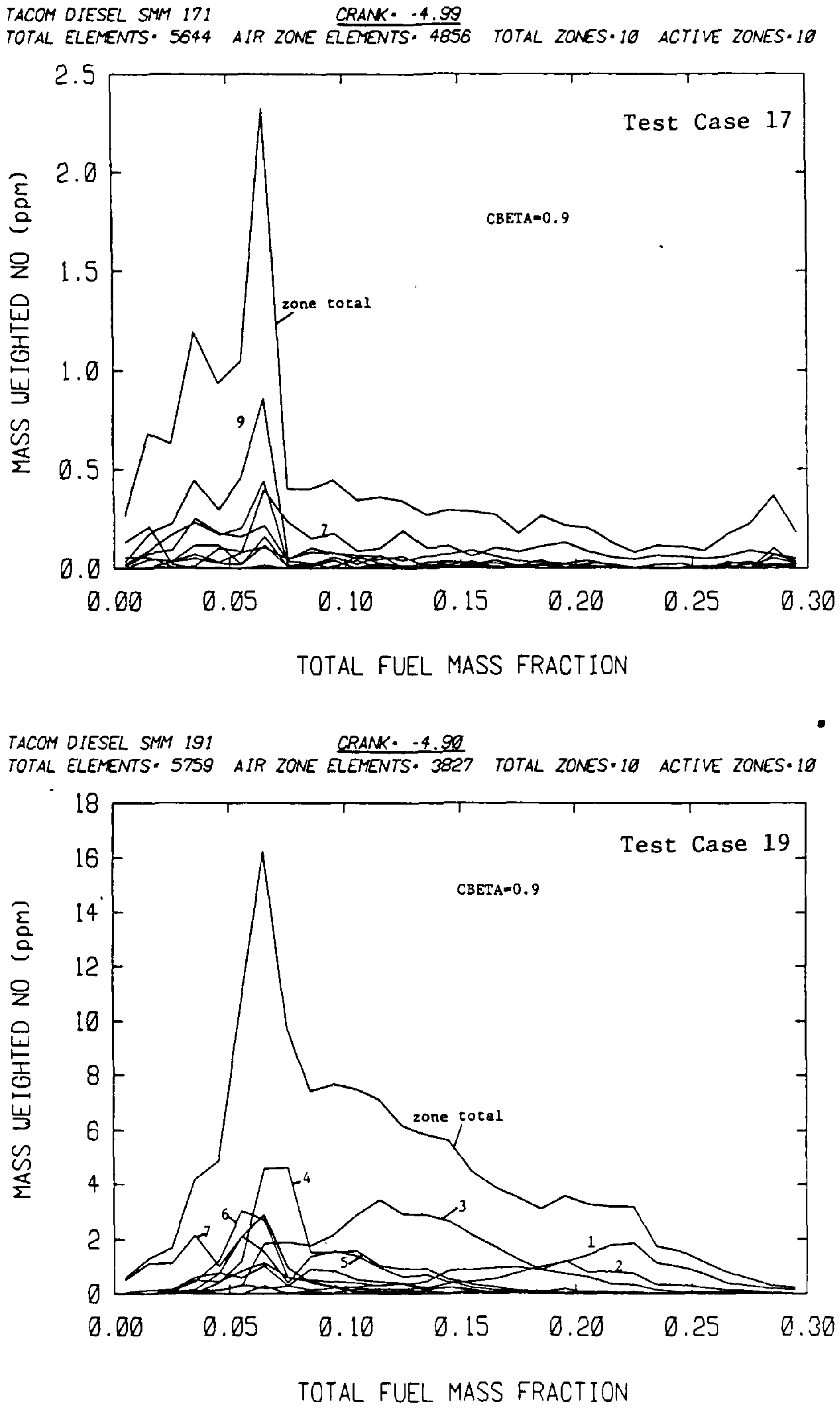


Figure 6-8 Mass-Weighted NO Distribution by Mixing Zone (Test Case 17 and 19)

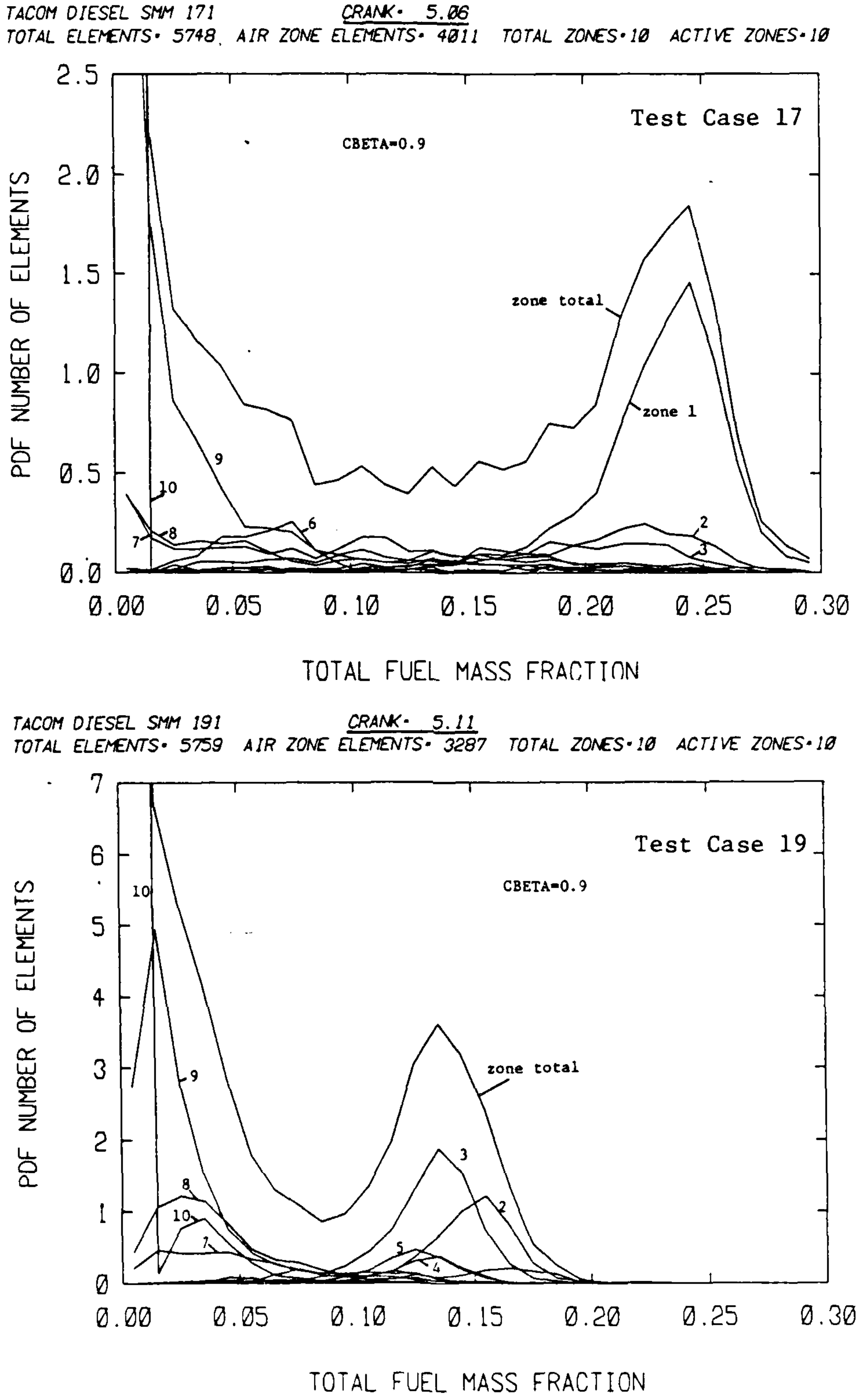


Figure 6-9 Fuel Mass Fraction Distribution by Mixing Zone (Test Case 17 and 19)

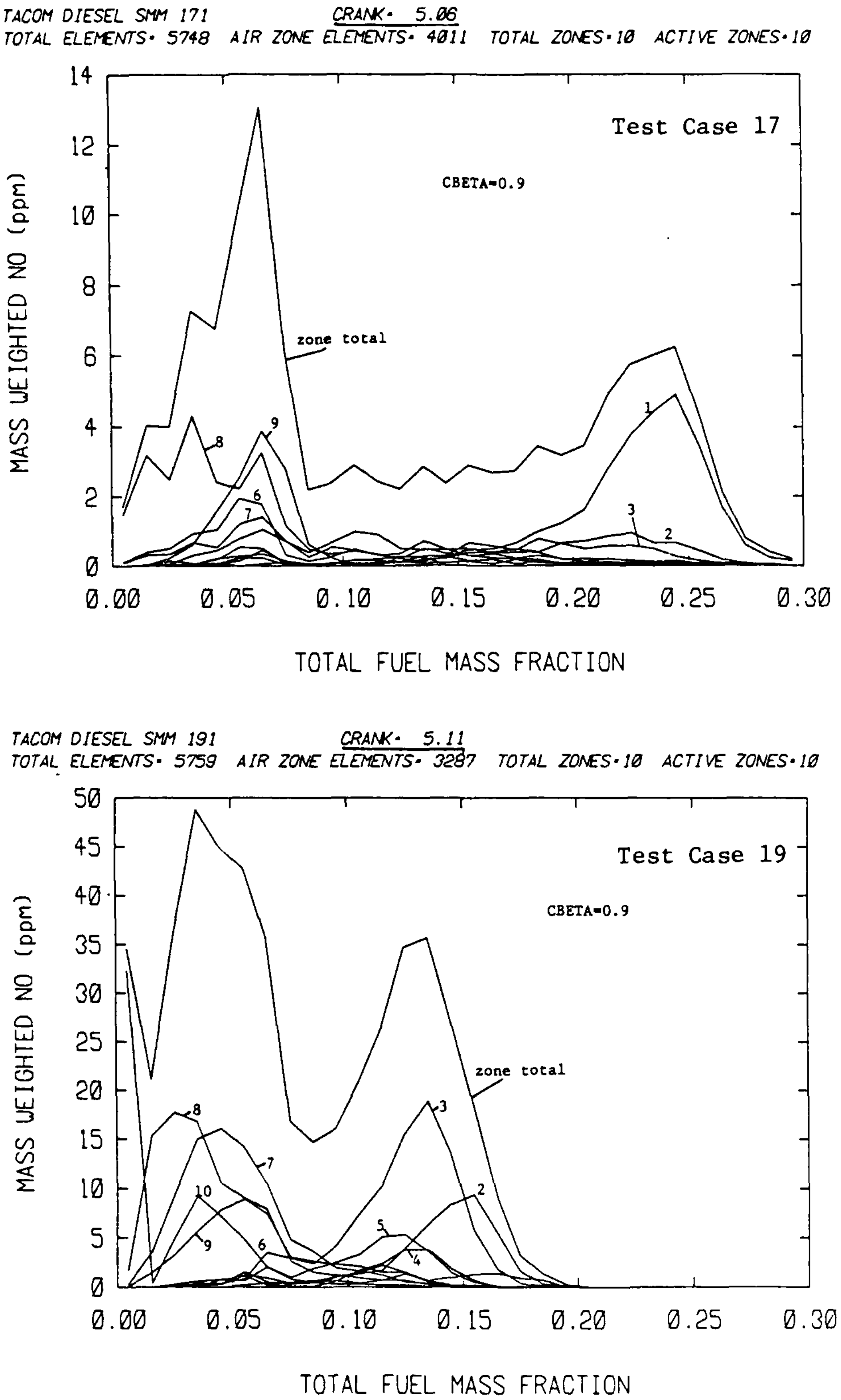
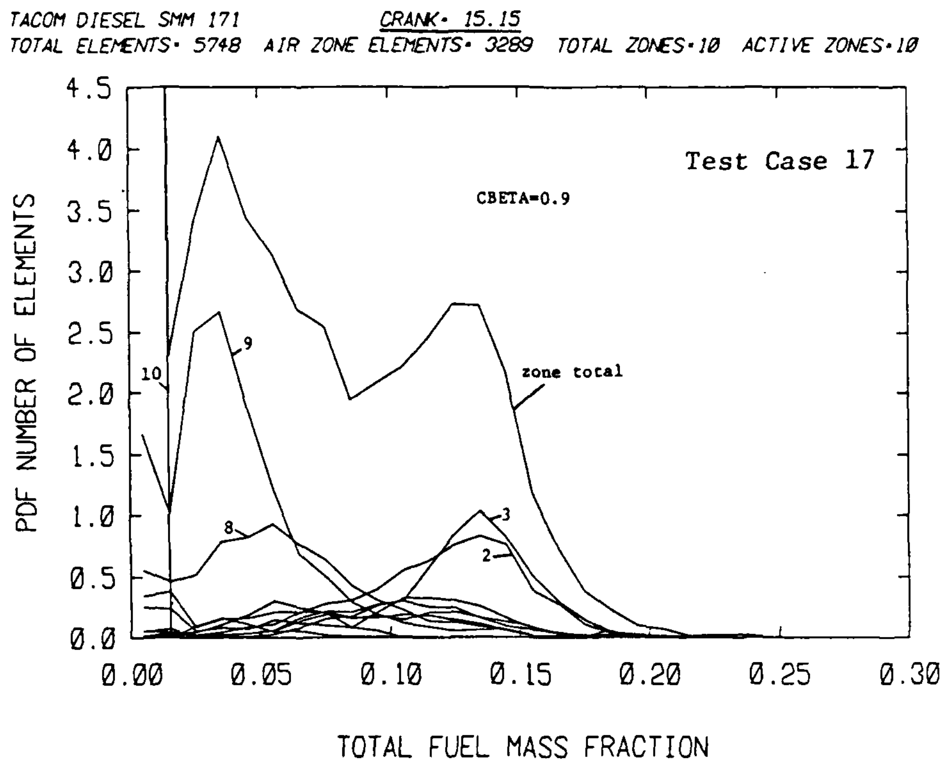


Figure 6-10 Mass-Weighted NO Distribution by Mixing Zone (Test Case 17 and 19)



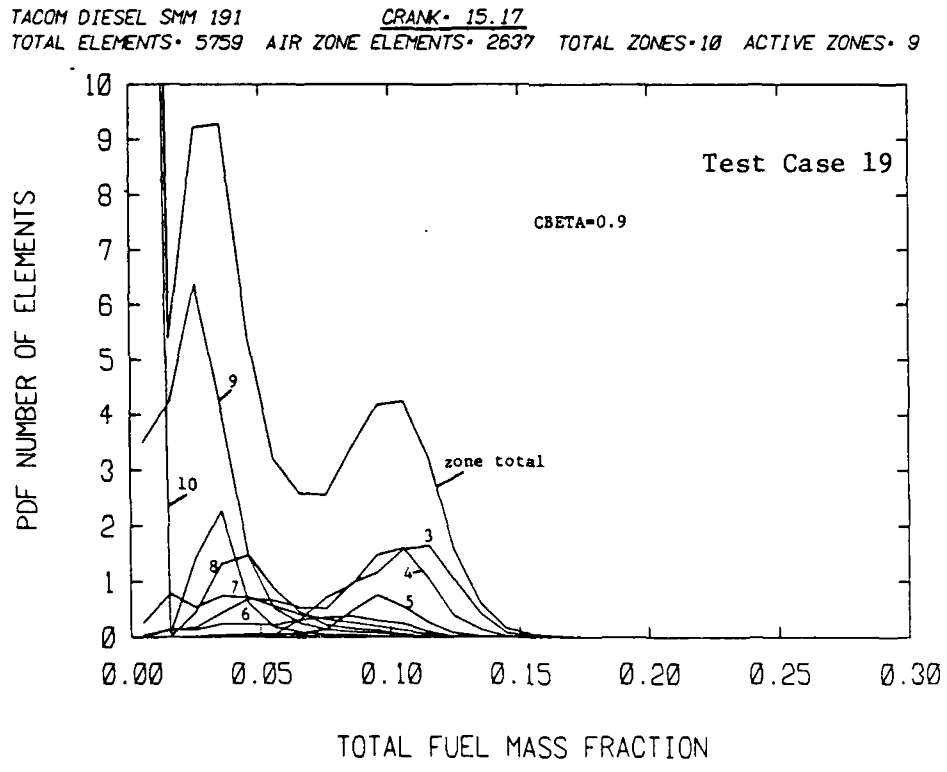


Figure 6-11 Fuel Mass Fraction Distribution by Mixing Zone (Test Case 17 and 19)

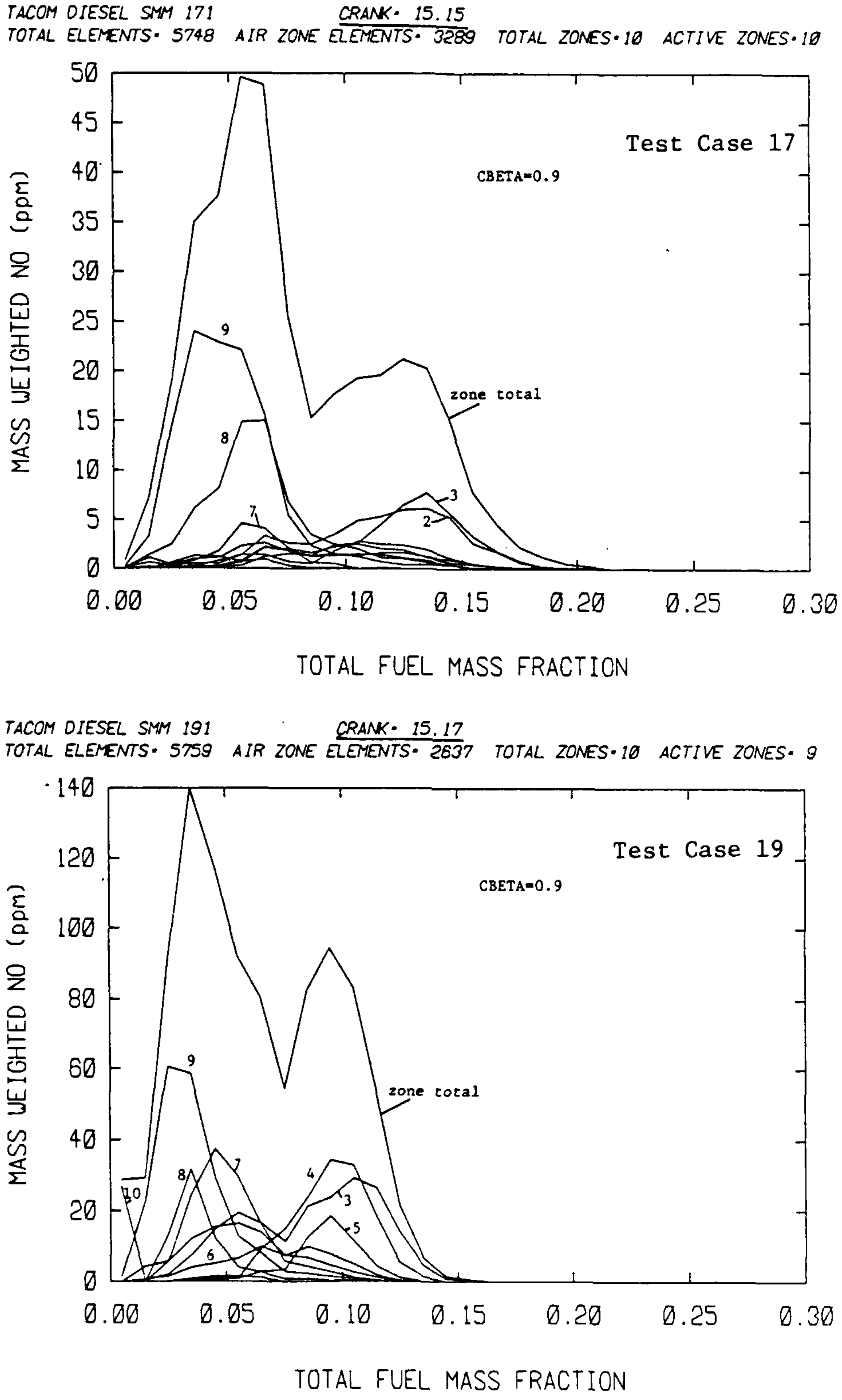


Figure 6-12 Mass-Weighted NO Distribution by Mixing Zone (Test Case 17 and 19)

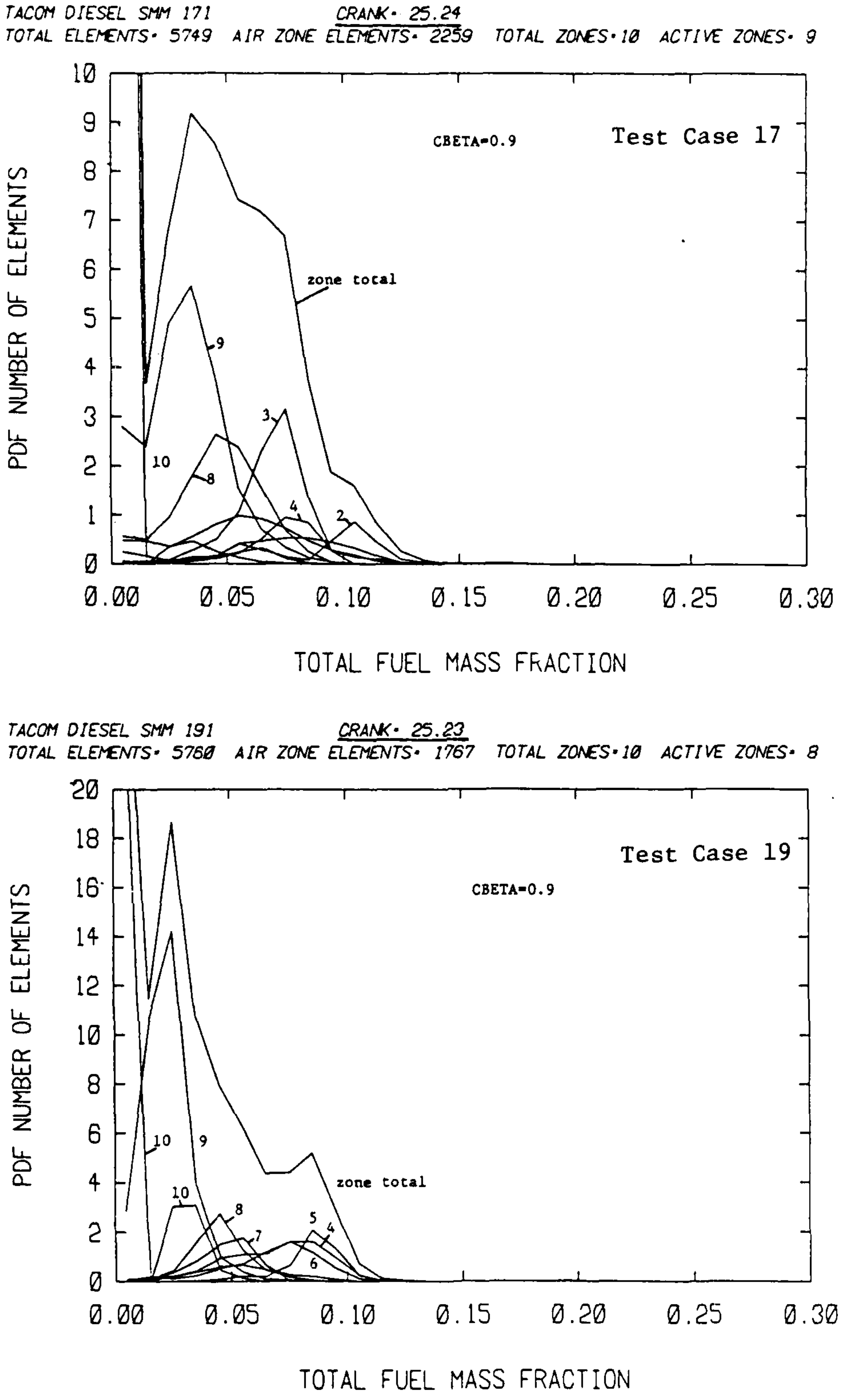


Figure 6-13 Fuel Mass Fraction Distribution by Mixing Zone (Test Case 17 and 19)

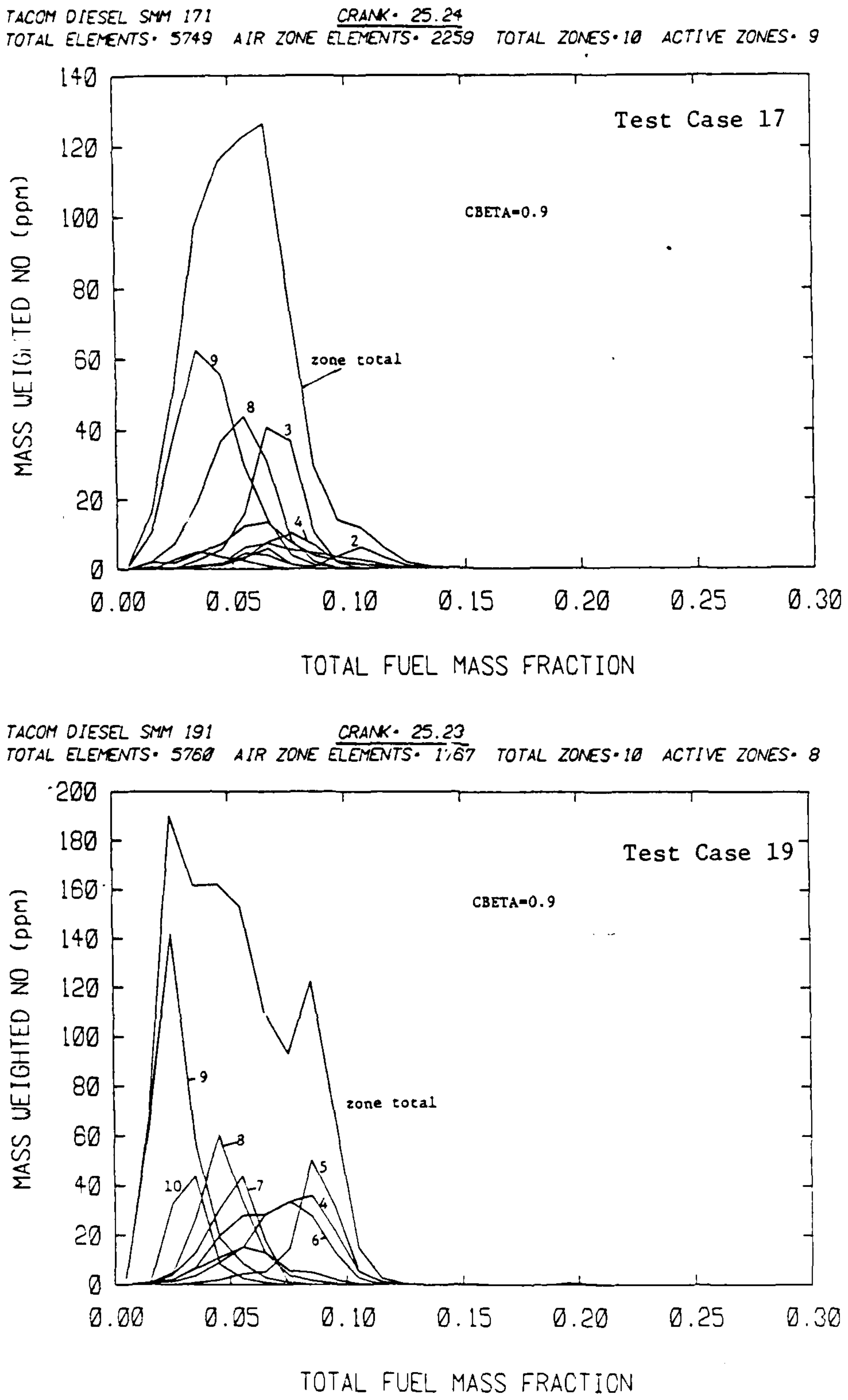


Figure 6-14 Mass-Weighted NO Distribution by Mixing Zone
(Test Case 17 and 19)

APPENDIX A

KIVA INPUT

A.1 Test Case Number 17

```
TACOM DIESEL RUN MDM17-33
 NX        22
 NY         1
 NZ        18
 LWALL      1
 NCHOP      3
 LPR        3
 JSECTR     1
 NCFILM 9999
 NCTAP8 9999
 NCLAST 9999
 CAFILM     5.0
 CAFIN     80.0
 ANGMOM     1.0
 CYL        1.0
 DY         0.0
 PGSSW      1.0
 SAMPL      0.0
 DTI        1.0E-5
 DTMAX      1.0E-5
 TLIMD      1.0
 TWFIN     9.99E+9
 FCHEM      0.25
 STROKE    11.43
 SQUISH     0.092
 RPM     1.001E+3
 ATDC    -90.0
 CONROD    22.86
 OFFSET     0.0
 SWIRL      2.46
 THSECT     0.5
 THNOZL    12.5
 SSSF       2.5
 TEMPI    455.0
 A0         0.0
 B0         1.0
 ANC4       0.05
 ARTVIS     1.0
 UVFREE     1.0
```

```
ADIA      0.0
CHARLF    2.0
ANUO      0.0
VISRAT-.66666667
RGAS   8.3143E+7
TCUT    800.0
TCUTE  1200.0
EPSCHM    0.02
OMGCHM    1.0
TKEI     0.02
ATKE     .05
DTKE     1.0
AIRMU1  1.457E-5
AIRMU2  110.0
AIRLA1  252.0
AIRLA2  200.0
AIRDIF  2.341E-6
EXPDIF    0.6
TWALL   400.0
RPR       1.1
RSC       1.1
XIGNIT    0.0
T1IGN   1.37E-02
T2IGN   1.57E-02
CA1IGN   -7.8
CA2IGN   -1.0
IIGNL1    0
IIGNR1    0
JIGNF1    0
JIGND1    0
KIGNB1    0
KIGNT1    0
IIGNL2    0
IIGNR2    0
JIGNF2    0
JIGND2    0
KIGNB2    0
KIGNT2    0
KWIKEQ    1
KOLIDE    1
EVAPP     1.0
T1INJ    -1.0
T2INJ    -1.0
CA1INJ  -15.0
CA2INJ    3.0
TSPMAS  0.05573
TNPARC 1000.0
RHOP    0.7452
TPI     350.0
VELINJ  1.66E+4
CONE    157.0
DCONE    12.5
TILT      0.0
```

```
  SMR        9.5E-4
  SURTEN    25.04
  TCRIT    659.0
  TURB        1.0
  NPO        31
  NUNIF       0
   1   1 0.0          0.4700
   2   1 0.2          0.4393
   3   1 0.4          0.4087
   4   1 0.6          0.3780
   5   1 0.8          0.3473
   6   1 1.0          0.3167
   7   1 1.2          0.2860
   8   1 1.4          0.2553
   9   1 1.6          0.2247
  10   1 1.8          0.1940
  11   1 2.0          0.1633
  12   1 2.2          0.1327
  13   1 2.4          0.1020
  14   1 2.6          0.0713
  15   1 2.8          0.0407
  16   1 3.175        0.0
  16   2 3.4          0.0210
  16   3 3.6          0.0740
  16   4 3.8          0.1660
  16   5 4.05         0.3500
  16   6 4.22         0.5500
  16   7 4.334        0.7500
  16   8 4.401        0.9500
  16   9 4.445        1.2700
  17   9 4.6          1.27
  18   9 4.8          1.27
  19   9 5.0          1.27
  20   9 5.2          1.27
  21   9 5.4          1.27
  22   9 5.6          1.27
  23   9 5.715        1.27
  NSP        12
RHO1      0.0      MW1     148.6     HTF1    -26.614
RHO2  5.1739E-4    MW2      32.0     HTF2      0.0
RHO3  1.7380E-3    MW3      28.0     HTF3      0.0
RHO4  6.8139E-6    MW4      44.0     HTF4    -93.965
RHO5  9.4661E-6    MW5      18.0     HTF5    -57.103
RHO6      0.0      MW6       1.0     HTF6     51.631
RHO7      0.0      MW7       2.0     HTF7      0.0
RHO8      0.0      MW8      16.0     HTF8     58.989
RHO9      0.0      MW9      14.0     HTF9    112.520
RHO10     0.0      MW10     17.0     HTF10     9.289
RHO11     0.0      MW11     28.0     HTF11   -27.200
RHO12     0.0      MW12     30.0     HTF12    21.456
  NRK         4
CF1  2.0000E10     EF1   1.5780E+4   ZF1       0.0
CB1       0.0      EB1       0.0     ZB1       0.0
```

```
 AM1     40   619    0     0     0     0     0     0     0     0     0     0
 BM1      0     0    0   432   374     0     0     0     0     0     0     0
 AE1     0.250    1.500    0.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE1     0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 CF2   1.5587E14 EF2    6.7627E+4 ZF2        0.0
 CB2   7.5000E12 EB2       0.0    ZB2        0.0
 AM2      0     1    2     0     0     0     0     0     0     0     0     0
 BM2      0     0    0     0     0     0     0     0     2     0     0     2
 AE2     0.000    0.500    1.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE2     0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
         1.000    0.000    0.000    1.000
 CF3   2.6484E10 EF3    5.9418E+4 ZF3        1.0
 CB3   1.6000E+9 EB3    1.9678E+4 ZB3        1.0
 AM3      0     2    1     0     0     0     0     0     0     0     0     0
 BM3      0     0    0     0     0     0     0     2     0     0     0     2
 AE3     0.000    1.000    0.500    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE3     0.000    0.000    0.000    0.000    0.000    0.000    0.000    1.000
         0.000    0.000    0.000    1.000
 CF4   2.1230E14 EF4    5.7020E+4 ZF4        0.0
 CB4      0.0    EB4       0.0    ZB4        0.0
 AM4      0     0    1     0     0     0     0     0     0     2     0     0
 BM4      0     0    0     0     0     2     0     0     0     0     0     2
 AE4     0.000    0.000    0.500    0.000    0.000    0.000    0.000    0.000
         0.000    1.000    0.000    0.000
 BE4     0.000    0.000    0.000    0.000    0.000    1.000    0.000    0.000
         0.000    0.000    0.000    1.000
  NRE       6
 AS1   0.990207  BS1    -51.7916  CS1    0.993074  DS1   -0.343428  ES1
0.0111668
 AN1      0     0    0     0     0     0     1     0     0     0     0     0
 BN1      0     0    0     0     0     2     0     0     0     0     0     0
 AS2   0.431310  BS2    -59.6554  CS2    3.503350  DS2   -0.340016  ES2
0.0158715
 AN2      0     1    0     0     0     0     0     0     0     0     0     0
 BN2      0     0    0     0     0     0     0     2     0     0     0     0
 AS3   0.794709  BS3  -113.2080  CS3    3.168370  DS3   -0.443814  ES3
0.0269699
 AN3      0     0    1     0     0     0     0     0     0     0     0     0
 BN3      0     0    0     0     0     0     0     0     2     0     0     0
 AS4  -0.652939  BS4     -9.8232  CS4    3.930330  DS4    0.163490
ES4  -0.0142865
 AN4      0     1    0     0     0     0     1     0     0     0     0     0
 BN4      0     0    0     0     0     0     0     0     0     2     0     0
 AS5   1.158882  BS5    -76.8472  CS5    8.532155  DS5   -0.868320  ES5
0.0463471
 AN5      0     1    0     0     2     0     0     0     0     0     0     0
 BN5      0     0    0     0     0     0     0     0     0     4     0     0
 AS6   0.980875  BS6     68.4453  CS6  -10.5938   DS6    0.574260
ES6  -0.0414570
```

```
AN6     0    1    0    0    0    0    0    0    0    0    2    0
BN6     0    0    0    2    0    0    0    0    0    0    0    0
```

A.2 Test Case Number 18

```
TACOM DIESEL RUN MDM18-6
 NX         22
 NY          1
 NZ         18
 LWALL       1
 NCHOP       3
 LPR         3
 JSECTR      1
 NCFILM 9999
 NCTAP8 9999
 NCLAST 9999
 CAFILM      5.0
 CAFIN      80.0
 ANGMOM      1.0
 CYL         1.0
 DY          0.0
 PGSSW       1.0
 SAMPL       0.0
 DTI         1.0E-5
 DTMAX       1.0E-5
 TLIMD       1.0
 TWFIN     9.99E+9
 FCHEM       0.25
 STROKE    11.43
 SQUISH      0.092
 RPM      1.001E+3
 ATDC      -90.0
 CONROD    22.86
 OFFSET      0.0
 SWIRL       4.0
 THSECT      0.5
 THNOZL     12.5
 SSSF        2.5
 TEMPI     465.0
 AO          0.0
 BO          1.0
 ANC4        0.05
 ARTVIS      1.0
 UVFREE      1.0
 ADIA        0.0
 CHARLF      2.0
 ANUO        0.0
 VISRAT-.66666667
 RGAS   8.3143E+7
 TCUT      800.0
 TCUTE    1200.0
```

```
EPSCHM    0.02
OMGCHM   1.0
TKEI     0.02
ATKE     0.05
DTKE     1.0
AIRMU1  1.457E-5
AIRMU2  110.0
AIRLA1  252.0
AIRLA2  200.0
AIRDIF  2.341E-6
EXPDIF    0.6
TWALL   400.0
RPR       1.1
RSC       1.1
XIGNIT    0.0
T1IGN   1.358E-2
T2IGN   1.51E-2
CA1IGN   -8.4
CA2IGN   -1.0
IIGNL1    0
IIGNR1    0
JIGNF1    0
JIGND1    0
KIGNB1    0
KIGNT1    0
IIGNL2    0
IIGNR2    0
JIGNF2    0
JIGND2    0
KIGNB2    0
KIGNT2    0
KWIKEQ    1
KOLIDE    1
EVAPP     1.0
T1INJ    -1.0
T2INJ    -1.0
CA1INJ  -15.0
CA2INJ    3.0
TSPMAS  0.05546
TNPARC 1000.0
RHOP    0.7452
TPI     350.0
VELINJ  1.66E+4
CONE    157.0
DCONE    12.5
TILT     0.0
SMR     9.5E-4
SURTEN   25.04
TCRIT   659.0
TURB      1.0
NPO      31
NUNIF     0
 1   1 0.0        0.4700
```

```
   2   1 0.2        0.4393
   3   1 0.4        0.4087
   4   1 0.6        0.3780
   5   1 0.8        0.3473
   6   1 1.0        0.3167
   7   1 1.2        0.2860
   8   1 1.4        0.2553
   9   1 1.6        0.2247
  10   1 1.8        0.1940
  11   1 2.0        0.1633
  12   1 2.2        0.1327
  13   1 2.4        0.1020
  14   1 2.6        0.0713
  15   1 2.8        0.0407
  16   1 3.175      0.0
  16   2 3.4        0.0210
  16   3 3.6        0.0740
  16   4 3.8        0.1660
  16   5 4.05       0.3500
  16   6 4.22       0.5500
  16   7 4.334      0.7500
  16   8 4.401      0.9500
  16   9 4.445      1.2700
  17   9 4.6        1.27
  18   9 4.8        1.27
  19   9 5.0        1.27
  20   9 5.2        1.27
  21   9 5.4        1.27
  22   9 5.6        1.27
  23   9 5.715      1.27
 NSP       12
RHO1      0.0     MW1     148.6    HTF1    -26.614
RHO2  5.1086E-4 MW2      32.0    HTF2      0.0
RHO3  1.7162E-3 MW3      28.0    HTF3      0.0
RHO4  6.7631E-6 MW4      44.0    HTF4    -93.965
RHO5  9.8146E-6 MW5      18.0    HTF5    -57.103
RHO6      0.0     MW6       1.0    HTF6     51.631
RHO7      0.0     MW7       2.0    HTF7      0.0
RHO8      0.0     MW8      16.0    HTF8     58.989
RHO9      0.0     MW9      14.0    HTF9    112.520
RHO10     0.0     MW10     17.0    HTF10     9.289
RHO11     0.0     MW11     28.0    HTF11   -27.200
RHO12     0.0     MW12     30.0    HTF12    21.456
 NRK        4
CF1   2.0000E10 EF1   1.5780E+4 ZF1        0.0
CB1       0.0     EB1      0.0     ZB1        0.0
AM1     40   619     0      0      0      0      0      0      0      0      0      0
BM1      0     0     0    432    374      0      0      0      0      0      0      0
AE1     0.250    1.500    0.000    0.000    0.000    0.000    0.000    0.000
        0.000    0.000    0.000    0.000
BE1     0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
        0.000    0.000    0.000    0.000
CF2   1.5587E14 EF2   6.7627E+4 ZF2        0.0
```

```
 CB2   7.5000E12 EB2       0.0    ZB2       0.0
 AM2     0     1     2     0     0     0     0     0     0     0     0     0
 BM2     0     0     0     0     0     0     0     0     2     0     0     2
 AE2     0.000    0.500    1.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE2     0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
         1.000    0.000    0.000    1.000
 CF3   2.6484E10 EF3   5.9418E+4 ZF3        1.0
 CB3   1.6000E+9 EB3   1.9678E+4 ZB3        1.0
 AM3     0     2     1     0     0     0     0     0     0     0     0     0
 BM3     0     0     0     0     0     0     0     2     0     0     0     2
 AE3     0.000    1.000    0.500    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE3     0.000    0.000    0.000    0.000    0.000    0.000    0.000    1.000
         0.000    0.000    0.000    1.000
 CF4   2.1230E14 EF4   5.7020E+4 ZF4        0.0
 CB4     0.0     EB4       0.0    ZB4       0.0
 AM4     0     0     1     0     0     0     0     0     0     2     0     0
 BM4     0     0     0     0     0     2     0     0     0     0     0     2
 AE4     0.000    0.000    0.500    0.000    0.000    0.000    0.000    0.000
         0.000    1.000    0.000    0.000
 BE4     0.000    0.000    0.000    0.000    0.000    1.000    0.000    0.000
         0.000    0.000    0.000    1.000
  NRE       6
 AS1   0.990207   BS1    -51.7916   CS1    0.993074   DS1   -0.343428   ES1
0.0111668
 AN1     0     0     0     0     0     0     1     0     0     0     0     0
 BN1     0     0     0     0     0     2     0     0     0     0     0     0
 AS2   0.431310   BS2    -59.6554   CS2    3.503350   DS2   -0.340016   ES2
0.0158715
 AN2     0     1     0     0     0     0     0     0     0     0     0     0
 BN2     0     0     0     0     0     0     0     2     0     0     0     0
 AS3   0.794709   BS3  -113.2080   CS3    3.168370   DS3   -0.443814   ES3
0.0269699
 AN3     0     0     1     0     0     0     0     0     0     0     0     0
 BN3     0     0     0     0     0     0     0     0     2     0     0     0
 AS4  -0.652939   BS4     -9.8232   CS4    3.930330   DS4    0.163490
ES4  -0.0142865
 AN4     0     1     0     0     0     0     1     0     0     0     0     0
 BN4     0     0     0     0     0     0     0     0     0     2     0     0
 AS5   1.158882   BS5    -76.8472   CS5    8.532155   DS5   -0.868320   ES5
0.0463471
 AN5     0     1     0     0     2     0     0     0     0     0     0     0
 BN5     0     0     0     0     0     0     0     0     0     4     0     0
 AS6   0.980875   BS6     68.4453   CS6  -10.5938    DS6    0.574260
ES6  -0.0414570
 AN6     0     1     0     0     0     0     0     0     0     0     2     0
 BN6     0     0     0     2     0     0     0     0     0     0     0     0
```

A.3 Test Case Number 19

```
TACOM DIESEL RUN MDM19-40
 NX        22
 NY         1
 NZ        18
 LWALL      1
 NCHOP      3
 LPR        3
 JSECTR     1
 NCFILM 9999
 NCTAP8 9999
 NCLAST 9999
 CAFILM     5.0
 CAFIN     80.0
 ANGMOM     1.0
 CYL        1.0
 DY         0.0
 PGSSW      1.0
 SAMPL      0.0
 DTI        1.0E-5
 DTMAX      1.0E-5
 TLIMD      1.0
 TWFIN     9.99E+9
 FCHEM      0.25
 STROKE    11.43
 SQUISH     0.092
 RPM      0.998E+3
 ATDC     -90.0
 CONROD    22.86
 OFFSET     0.0
 SWIRL      2.46
 THSECT     0.5
 THNOZL    12.5
 SSSF       2.5
 TEMPI    445.0
 AO         0.0
 BO         1.0
 ANC4       0.05
 ARTVIS     1.0
 UVFREE     1.0
 ADIA       0.0
 CHARLF     2.0
 ANUO       0.0
 VISRAT-.66666667
 RGAS   8.3143E+7
 TCUT     800.0
 TCUTE   1200.0
 EPSCHM     0.02
 OMGCHM     1.0
 TKEI      0.02
```

```
ATKE       0.05
DTKE       1.0
AIRMU1   1.457E-5
AIRMU2   110.0
AIRLA1   252.0
AIRLA2   200.0
AIRDIF   2.341E-6
EXPDIF     0.6
TWALL    400.0
RPR        1.1
RSC        1.1
XIGNIT     0.0
T1IGN    1.25E-02
T2IGN    1.53E-02
CA1IGN   -15.0
CA2IGN    -1.0
IIGNL1     0
IIGNR1     0
JIGNF1     0
JIGND1     0
KIGNB1     0
KIGNT1     0
IIGNL2     0
IIGNR2     0
JIGNF2     0
JIGND2     0
KIGNB2     0
KIGNT2     0
KWIKEQ     1
KOLIDE     1
EVAPP      1.0
T1INJ     -1.0
T2INJ     -1.0
CA1INJ   -25.0
CA2INJ    -7.0
TSPMAS   0.05628
TNPARC   1000.0
RHOP     0.7452
TPI      350.0
VELINJ   1.66E+4
CONE     157.0
DCONE     12.5
TILT       0.0
SMR      9.5E-4
SURTEN    25.04
TCRIT    659.0
TURB       1.0
NPO       31
NUNIF      0
  1    1 0.0        0.4700
  2    1 0.2        0.4393
  3    1 0.4        0.4087
  4    1 0.6        0.3780
```

```
  5    1 0.8        0.3473
  6    1 1.0        0.3167
  7    1 1.2        0.2860
  8    1 1.4        0.2553
  9    1 1.6        0.2247
 10    1 1.8        0.1940
 11    1 2.0        0.1633
 12    1 2.2        0.1327
 13    1 2.4        0.1020
 14    1 2.6        0.0713
 15    1 2.8        0.0407
 16    1 3.175      0.0
 16    2 3.4        0.0210
 16    3 3.6        0.0740
 16    4 3.8        0.1660
 16    5 4.05       0.3500
 16    6 4.22       0.5500
 16    7 4.334      0.7500
 16    8 4.401      0.9500
 16    9 4.445      1.2700
 17    9 4.6        1.27
 18    9 4.8        1.27
 19    9 5.0        1.27
 20    9 5.2        1.27
 21    9 5.4        1.27
 22    9 5.6        1.27
 23    9 5.715      1.27
 NSP        12
RHO1       0.0    MW1     148.6    HTF1    -26.614
RHO2  5.1753E-4   MW2      32.0    HTF2      0.0
RHO3  1.7390E-3   MW3      28.0    HTF3      0.0
RHO4  6.3055E-6   MW4      44.0    HTF4    -93.965
RHO5  1.2499E-5   MW5      18.0    HTF5    -57.103
RHO6       0.0    MW6       1.0    HTF6     51.631
RHO7       0.0    MW7       2.0    HTF7      0.0
RHO8       0.0    MW8      16.0    HTF8     58.989
RHO9       0.0    MW9      14.0    HTF9    112.520
RHO10      0.0    MW10     17.0    HTF10     9.289
RHO11      0.0    MW11     28.0    HTF11   -27.200
RHO12      0.0    MW12     30.0    HTF12    21.456
 NRK        4
CF1   2.0000E10   EF1   1.5780E+4  ZF1        0.0
CB1        0.0    EB1       0.0    ZB1        0.0
AM1     40   619     0     0     0     0     0     0     0     0     0     0
BM1      0     0     0   432   374     0     0     0     0     0     0     0
AE1     0.250   1.500   0.000   0.000   0.000   0.000   0.000   0.000
        0.000   0.000   0.000   0.000
BE1     0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
        0.000   0.000   0.000   0.000
CF2   1.5587E14   EF2   6.7627E+4  ZF2        0.0
CB2   7.5000E12   EB2       0.0    ZB2        0.0
AM2      0     1     2     0     0     0     0     0     0     0     0     0
BM2      0     0     0     0     0     0     0     0     2     0     0     2
```

```
AE2    0.000    0.500    1.000    0.000    0.000    0.000    0.000    0.000
       0.000    0.000    0.000    0.000
BE2    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
       1.000    0.000    0.000    1.000
CF3   2.6484E10 EF3    5.9418E+4 ZF3        1.0
CB3   1.6000E+9 EB3    1.9678E+4 ZB3        1.0
AM3     0     2     1     0     0     0     0     0     0     0     0     0
BM3     0     0     0     0     0     0     0     2     0     0     0     2
AE3    0.000    1.000    0.500    0.000    0.000    0.000    0.000    0.000
       0.000    0.000    0.000    0.000
BE3    0.000    0.000    0.000    0.000    0.000    0.000    0.000    1.000
       0.000    0.000    0.000    1.000
CF4   2.1230E14 EF4    5.7020E+4 ZF4        0.0
CB4      0.0     EB4       0.0     ZB4        0.0
AM4     0     0     1     0     0     0     0     0     0     2     0     0
BM4     0     0     0     0     0     2     0     0     0     0     0     2
AE4    0.000    0.000    0.500    0.000    0.000    0.000    0.000    0.000
       0.000    1.000    0.000    0.000
BE4    0.000    0.000    0.000    0.000    0.000    1.000    0.000    0.000
       0.000    0.000    0.000    1.000
 NRE       6
AS1   0.990207   BS1    -51.7916  CS1     0.993074  DS1   -0.343428  ES1
0.0111668
AN1     0     0     0     0     0     0     1     0     0     0     0     0
BN1     0     0     0     0     0     2     0     0     0     0     0     0
AS2   0.431310   BS2    -59.6554  CS2     3.503350  DS2   -0.340016  ES2
0.0158715
AN2     0     1     0     0     0     0     0     0     0     0     0     0
BN2     0     0     0     0     0     0     0     2     0     0     0     0
AS3   0.794709   BS3  -113.2080   CS3     3.168370  DS3   -0.443814  ES3
0.0269699
AN3     0     0     1     0     0     0     0     0     0     0     0     0
BN3     0     0     0     0     0     0     0     0     2     0     0     0
AS4  -0.652939   BS4     -9.8232  CS4     3.930330  DS4    0.163490
ES4  -0.0142865
AN4     0     1     0     0     0     0     1     0     0     0     0     0
BN4     0     0     0     0     0     0     0     0     0     2     0     0
AS5   1.158882   BS5    -76.8472  CS5     8.532155  DS5   -0.868320  ES5
0.0463471
AN5     0     1     0     0     2     0     0     0     0     0     0     0
BN5     0     0     0     0     0     0     0     0     0     4     0     0
AS6   0.980875   BS6     68.4453  CS6   -10.5938    DS6    0.574260
ES6  -0.0414570
AN6     0     1     0     0     0     0     0     0     0     0     2     0
BN6     0     0     0     2     0     0     0     0     0     0     0     0
```

A.4 Test Case Number 20

```
TACOM DIESEL RUN MDM20-4
 NX        22
```

```
NY         1
NZ        18
LWALL      1
NCHOP      3
LPR        2
JSECTR     1
NCFILM 9999
NCTAP8 9999
NCLAST 9999
CAFILM    10.0
CAFIN     80.0
ANGMOM     1.0
CYL        1.0
DY         0.0
PGSSW      1.0
SAMPL      0.0
DTI        1.0E-5
DTMAX      1.0E-5
TLIMD      1.0
TWFIN     9.99E+9
FCHEM      0.25
STROKE    11.43
SQUISH     0.092
RPM      0.999E+3
ATDC     -90.0
CONROD    22.86
OFFSET     0.0
SWIRL      2.46
THSECT     0.5
THNOZL    12.5
SSSF       2.5
TEMPI    459.0
AO         0.0
BO         1.0
ANC4       0.05
ARTVIS     1.0
UVFREE     1.0
ADIA       0.0
CHARLF     2.0
ANUO       0.0
VISRAT-.66666667
RGAS   8.3143E+7
TCUT     800.0
TCUTE   1200.0
EPSCHM     0.02
OMGCHM     1.0
TKEI      0.02
ATKE      0.05
DTKE      1.0
AIRMU1  1.457E-5
AIRMU2  110.0
AIRLA1  252.0
AIRLA2  200.0
```

```
AIRDIF  2.341E-6
EXPDIF    0.6
TWALL   400.0
RPR       1.1
RSC       1.1
XIGNIT    0.0
T1IGN   1.33E-2
T2IGN   1.55E-2
CA1IGN   -7.8
CA2IGN   -1.0
IIGNL1    0
IIGNR1    0
JIGNF1    0
JIGND1    0
KIGNB1    0
KIGNT1    0
IIGNL2    0
IIGNR2    0
JIGNF2    0
JIGND2    0
KIGNB2    0
KIGNT2    0
KWIKEQ    1
KOLIDE    1
EVAPP     1.0
T1INJ    -1.0
T2INJ    -1.0
CA1INJ  -15.0
CA2INJ    3.0
TSPMAS  0.05597
TNPARC 1000.0
RHOP    0.7452
TPI     350.0
VELINJ  1.66E+4
CONE    157.0
DCONE    12.5
TILT      0.0
SMR      9.5E-4
SURTEN   25.04
TCRIT   659.0
TURB      1.0
NPO      31
NUNIF     0
 1    1 0.0        0.4700
 2    1 0.2        0.4393
 3    1 0.4        0.4087
 4    1 0.6        0.3780
 5    1 0.8        0.3473
 6    1 1.0        0.3167
 7    1 1.2        0.2860
 8    1 1.4        0.2553
 9    1 1.6        0.2247
10    1 1.8        0.1940
```

```
  11    1 2.0       0.1633
  12    1 2.2       0.1327
  13    1 2.4       0.1020
  14    1 2.6       0.0713
  15    1 2.8       0.0407
  16    1 3.175     0.0
  16    2 3.4       0.0210
  16    3 3.6       0.0740
  16    4 3.8       0.1660
  16    5 4.05      0.3500
  16    6 4.22      0.5500
  16    7 4.334     0.7500
  16    8 4.401     0.9500
  16    9 4.445     1.2700
  17    9 4.6       1.27
  18    9 4.8       1.27
  19    9 5.0       1.27
  20    9 5.2       1.27
  21    9 5.4       1.27
  22    9 5.6       1.27
  23    9 5.715     1.27
  NSP       12
 RHO1      0.0    MW1     148.6    HTF1    -26.614
 RHO2  4.7866E-4  MW2      32.0    HTF2      0.0
 RHO3  1.6845E-3  MW3      28.0    HTF3      0.0
 RHO4  2.6665E-5  MW4      44.0    HTF4    -93.965
 RHO5  1.7965E-5  MW5      18.0    HTF5    -57.103
 RHO6      0.0    MW6       1.0    HTF6     51.631
 RHO7      0.0    MW7       2.0    HTF7      0.0
 RHO8      0.0    MW8      16.0    HTF8     58.989
 RHO9      0.0    MW9      14.0    HTF9    112.520
 RHO10     0.0    MW10     17.0    HTF10     9.289
 RHO11     0.0    MW11     28.0    HTF11   -27.200
 RHO12     0.0    MW12     30.0    HTF12    21.456
  NRK        4
 CF1   2.0000E10  EF1   1.5780E+4  ZF1        0.0
 CB1       0.0    EB1       0.0    ZB1        0.0
 AM1     40   619    0     0    0     0     0     0     0     0     0     0
 BM1     0     0     0   432  374     0     0     0     0     0     0     0
 AE1     0.250    1.500    0.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE1     0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 CF2   1.5587E14  EF2   6.7627E+4  ZF2        0.0
 CB2   7.5000E12  EB2       0.0    ZB2        0.0
 AM2     0     1     2     0     0     0     0     0     0     0     0     0
 BM2     0     0     0     0     0     0     0     0     2     0     0     2
 AE2     0.000    0.500    1.000    0.000    0.000    0.000    0.000    0.000
         0.000    0.000    0.000    0.000
 BE2     0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
         1.000    0.000    0.000    1.000
 CF3   2.6484E10  EF3   5.9418E+4  ZF3        1.0
 CB3   1.6000E+9  EB3   1.9678E+4  ZB3        1.0
```

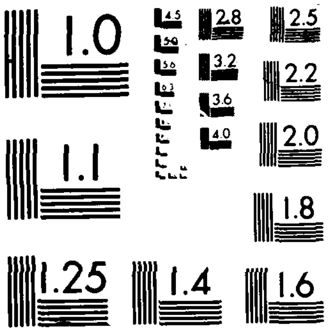
```
 AM3     0    2    1    0    0    0    0    0    0    0    0    0
 BM3     0    0    0    0    0    0    0    2    0    0    0    2
 AE3     0.000     1.000     0.500     0.000     0.000     0.000     0.000     0.000
         0.000     0.000     0.000     0.000
 BE3     0.000     0.000     0.000     0.000     0.000     0.000     0.000     1.000
         0.000     0.000     0.000     1.000
 CF4   2.1230E14 EF4    5.7020E+4 ZF4       0.0
 CB4      0.0      EB4      0.0      ZB4       0.0
 AM4     0    0    1    0    0    0    0    0    0    2    0    0
 BM4     0    0    0    0    0    2    0    0    0    0    0    2
 AE4     0.000     0.000     0.500     0.000     0.000     0.000     0.000     0.000
         0.000     1.000     0.000     0.000
 BE4     0.000     0.000     0.000     0.000     0.000     1.000     0.000     0.000
         0.000     0.000     0.000     1.000
  NRE        6
 AS1   0.990207   BS1     -51.7916   CS1     0.993074   DS1   -0.343428   ES1
0.0111668
 AN1     0    0    0    0    0    0    1    0    0    0    0    0
 BN1     0    0    0    0    0    2    0    0    0    0    0    0
 AS2   0.431310   BS2     -59.6554   CS2     3.503350   DS2   -0.340016   ES2
0.0158715
 AN2     0    1    0    0    0    0    0    0    0    0    0    0
 BN2     0    0    0    0    0    0    0    2    0    0    0    0
 AS3   0.794709   BS3   -113.2080    CS3     3.168370   DS3   -0.443814   ES3
0.0269699
 AN3     0    0    1    0    0    0    0    0    0    0    0    0
 BN3     0    0    0    0    0    0    0    0    2    0    0    0
 AS4  -0.652939   BS4      -9.8232   CS4     3.930330   DS4    0.163490
ES4  -0.0142865
 AN4     0    1    0    0    0    0    1    0    0    0    0    0
 BN4     0    0    0    0    0    0    0    0    0    2    0    0
 AS5   1.158882   BS5     -76.8472   CS5     8.532155   DS5   -0.868320   ES5
0.0463471
 AN5     0    1    0    0    2    0    0    0    0    0    0    0
 BN5     0    0    0    0    0    0    0    00    0    4    0    0
 AS6   0.980875   BS6      68.4453   CS6   -10.5938    DS6    0.574260
ES6  -0.0414570
 AN6     0    1    0    0    0    0    0    0    0    0    2    0
 BN6     0    0    0    2    0    0    0    0    0    0    0    0
```

A.5 Test Case Number 21

```
 TACOM DIESEL RUN MDM21-3
  NX         22
  NY          1
  NZ         18
  LWALL       1
  NCHOP       3
  LPR         2
  JSECTR      1
```

```
NCFILM 9999
NCTAP8 9999
NCLAST 9999
CAFILM   10.0
CAFIN    80.0
ANGMOM    1.0
CYL       1.0
DY        0.0
PGSSW     1.0
SAMPL     0.0
DTI       1.0E-5
DTMAX     1.0E-5
TLIMD     1.0
TWFIN    9.99E+9
FCHEM     0.25
STROKE   11.43
SQUISH    0.092
RPM     1.002E+3
ATDC    -90.0
CONROD   22.86
OFFSET    0.0
SWIRL    4.00
THSECT    0.5
THNOZL   12.5
SSSF      2.5
TEMPI   483.0
AO        0.0
BO        1.0
ANC4      0.05
ARTVIS    1.0
UVFREE    1.0
ADIA      0.0
CHARLF    2.0
ANUO      0.0
VISRAT-.66666667
RGAS   8.3143E+7
TCUT    800.0
TCUTE  1200.0
EPSCHM    0.02
OMGCHM    1.0
TKEI     0.02
ATKE     0.05
DTKE     1.0
AIRMU1  1.457E-5
AIRMU2  110.0
AIRLA1  252.0
AIRLA2  200.0
AIRDIF  2.341E-6
EXPDIF    0.6
TWALL   400.0
RPR       1.1
RSC       1.1
XIGNIT    0.0
```

AD-A175 155 A STOCHASTIC MIXING MODEL FOR PREDICTING EMISSIONS IN A 3/4
DIRECT INJECTION (U) MASSACHUSETTS INST OF TECH
CAMBRIDGE DEPT OF OCEAN ENGINEERIN A J BROWN SEP 86
UNCLASSIFIED N00228-85-G-3262 F/G 21/4 NL



MICROCOPY RESOLUTION TEST CHART

```
T1IGN    1.38E-2
T2IGN    1.52E-2
CA1IGN    -7.2
CA2IGN    -1.0
IIGNL1     0
IIGNR1     0
JIGNF1     0
JIGND1     0
KIGNB1     0
KIGNT1     0
IIGNL2     0
IIGNR2     0
JIGNF2     0
JIGND2     0
KIGNB2     0
KIGNT2     0
KWIKEQ     1
KOLIDE     1
EVAPP      1.0
T1INJ     -1.0
T2INJ     -1.0
CA1INJ  -15.0
CA2INJ     3.0
TSPMAS   0.05572
TNPARC  1000.0
RHOP     0.7452
TPI      350.0
VELINJ   1.66E+4
CONE     157.0
DCONE     12.5
TILT       0.0
SMR      9.5E-4
SURTEN    25.04
TCRIT    659.0
TURB       1.0
NPO       31
NUNIF      0
 1    1 0.0        0.4700
 2    1 0.2        0.4393
 3    1 0.4        0.4087
 4    1 0.6        0.3780
 5    1 0.8        0.3473
 6    1 1.0        0.3167
 7    1 1.2        0.2860
 8    1 1.4        0.2553
 9    1 1.6        0.2247
10    1 1.8        0.1940
11    1 2.0        0.1633
12    1 2.2        0.1327
13    1 2.4        0.1020
14    1 2.6        0.0713
15    1 2.8        0.0407
16    1 3.175      0.0
```

```
 16    2 3.4        0.0210
 16    3 3.6        0.0740
 16    4 3.8        0.1660
 16    5 4.05       0.3500
 16    6 4.22       0.5500
 16    7 4.334      0.7500
 16    8 4.401      0.9500
 16    9 4.445      1.2700
 17    9 4.6        1.27
 18    9 4.8        1.27
 19    9 5.0        1.27
 20    9 5.2        1.27
 21    9 5.4        1.27
 22    9 5.6        1.27
 23    9 5.715      1.27
 NSP        12
RHO1      0.0    MW1     148.6    HTF1    -26.614
RHO2  4.6302E-4  MW2      32.0    HTF2      0.0
RHO3  1.6374E-3  MW3      28.0    HTF3      0.0
RHO4  2.7885E-5  MW4      44.0    HTF4    -93.965
RHO5  1.8161E-5  MW5      18.0    HTF5    -57.103
RHO6      0.0    MW6       1.0    HTF6     51.631
RHO7      0.0    MW7       2.0    HTF7      0.0
RHO8      0.0    MW8      16.0    HTF8     58.989
RHO9      0.0    MW9      14.0    HTF9    112.520
RHO10     0.0    MW10     17.0    HTF10     9.289
RHO11     0.0    MW11     28.0    HTF11   -27.200
RHO12     0.0    MW12     30.0    HTF12    21.456
 NRK        4
CF1   2.0000E10 EF1   1.5780E+4 ZF1        0.0
CB1       0.0   EB1       0.0   ZB1        0.0
AM1     40  619     0     0     0     0     0     0     0     0     0     0
BM1      0    0     0   432   374     0     0     0     0     0     0     0
AE1     0.250   1.500   0.000   0.000   0.000   0.000   0.000   0.000
        0.000   0.000   0.000   0.000
BE1     0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
        0.000   0.000   0.000   0.000
CF2   1.5587E14 EF2   6.7627E+4 ZF2        0.0
CB2   7.5000E12 EB2       0.0   ZB2        0.0
AM2      0    1     2     0     0     0     0     0     0     0     0     0
BM2      0    0     0     0     0     0     0     0     2     0     0     2
AE2     0.000   0.500   1.000   0.000   0.000   0.000   0.000   0.000
        0.000   0.000   0.000   0.000
BE2     0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
        1.000   0.000   0.000   1.000
CF3   2.6484E10 EF3   5.9418E+4 ZF3        1.0
CB3   1.6000E+9 EB3   1.9678E+4 ZB3        1.0
AM3      0    2     1     0     0     0     0     0     0     0     0     0
BM3      0    0     0     0     0     0     0     2     0     0     0     2
AE3     0.000   1.000   0.500   0.000   0.000   0.000   0.000   0.000
        0.000   0.000   0.000   0.000
BE3     0.000   0.000   0.000   0.000   0.000   0.000   0.000   1.000
        0.000   0.000   0.000   1.000
```

```
 CF4   2.1230E14 EF4    5.7020E+4 ZF4        0.0
 CB4      0.0    EB4       0.0    ZB4        0.0
 AM4     0     0     1     0     0     0     0     0     0     2     0     0
 BM4     0     0     0     0     0     2     0     0     0     0     0     2
 AE4    0.000     0.000     0.500     0.000     0.000     0.000     0.000     0.000
        0.000     1.000     0.000     0.000
 BE4    0.000     0.000     0.000     0.000     0.000     1.000     0.000     0.000
        0.000     0.000     0.000     1.000
  NRE       6
 AS1   0.990207  BS1    -51.7916  CS1    0.993074  DS1   -0.343428  ES1
0.0111668
 AN1     0     0     0     0     0     0     1     0     0     0     0     0
 BN1     0     0     0     0     0     2     0     0     0     0     0     0
 AS2   0.431310  BS2    -59.6554  CS2    3.503350  DS2   -0.340016  ES2
0.0158715
 AN2     0     1     0     0     0     0     0     0     0     0     0     0
 BN2     0     0     0     0     0     0     0     2     0     0     0     0
 AS3   0.794709  BS3  -113.2080   CS3    3.168370  DS3   -0.443814  ES3
0.0269699
 AN3     0     0     1     0     0     0     0     0     0     0     0     0
 BN3     0     0     0     0     0     0     0     0     2     0     0     0
 AS4  -0.652939  BS4     -9.8232  CS4    3.930330  DS4    0.163490
ES4  -0.0142865
 AN4     0     1     0     0     0     0     1     0     0     0     0     0
 BN4     0     0     0     0     0     0     0     0     0     2     0     0
 AS5   1.158882  BS5    -76.8472  CS5    8.532155  DS5   -0.868320  ES5
0.0463471
 AN5     0     1     0     0     2     0     0     0     0     0     0     0
 BN5     0     0     0     0     0     0     0     0     0     4     0     0
 AS6   0.980875  BS6     68.4453  CS6  -10.5938    DS6    0.574260
ES6  -0.0414570
 AN6     0     1     0     0     0     0     0     0     0     0     2     0
 BN6     0     0     0     2     0     0     0     0     0     0     0     0
```

APPENDIX B

SMM FORTRAN CODE

```
C*****************************************************************
C
C SMM COMMON BLOCKS (SMMCOM.FOR)
C
      PARAMETER (NZONES=9,MAXELE=6000,NFLOW=9,NA=10)
      DIMENSION DTMIX(NA),NELS(NA),ZTIME(NA),TTBF(NA),
     1  TBF(NA),NNEVAP(NA),TMEVAP(NA),NELMIX(NA)
      REAL LLIMT
      LOGICAL SOOTON(NA)
      INTEGER IX,IY
      CHARACTER*12 FUEL,ID
      CHARACTER*30 NAME
      COMMON / FULAR / CATOM,DEL,PSI,PHICON
      COMMON /FULAR2/ ZH,ID,FUEL,HFG,TSAT,CPF,
     1  HEVAP,WTFUEL,SVFUEL,HFUEL,CTOF
      COMMON / ELEM / ELMM,NELS,NELAIR,NELTOT
      COMMON / CMBLIM / PHILOW,PHIHI,LLIMT,ULIMT
      COMMON / INTGRS/ IX,MAXITS,ITMAXV,NLINES,NAV,NAVP1,NCYC,NOLD
      COMMON /BASIC/ TIME,TIMMDM,CRANK,P,TFI,RHOL,TWALL,
     1  CBETA,CAD,CRANKD,DTKIN,FERMAX,NPRINT,ERMAX,VERMAX
      COMMON /DELT/ DT,DTMIX,DTPR,ZTIME,TIMEPR
      COMMON /SSOOT/ SOOTON,SOTSIZ,SOOTC,TSOOT
      COMMON /MDM1/ NAME,CA1INJ,CRKMAX,RPM,PSTART,EGR,SWIRL
      COMMON /OUT/ TBF,TMEVAP,TTBF
      COMMON /OUT2/ NNEVAP,DELTAP,NELMIX
C*****************************************************************
C*****************************************************************
C
C SMZ COMMON BLOCKS (SMZCOM.FOR)
C
C NOTE: ALWAYS APPEARS AFTER SMMCOM.FOR
C
      DIMENSION FM(NFLOW),FMV(NFLOW),FMBF(NFLOW)
      DIMENSION ZMEVAP(NA),ZVOL(NA),ZMVAP(NA),ZMFBRN(NA),
     1  ZQWALL(NA),ZBETA(NA),ZFMF(NA),ZMASSL(NA),ZTEMP(NA),ZNO(NA)
      DIMENSION DFM(NFLOW),DFMV(NFLOW),DFMBF(NFLOW)
      DIMENSION NP(NFLOW),NN(NFLOW)
      COMMON /FFLOW/ FM,FMV,FMBF,FML0
      COMMON /ZFLOW/ ZMEVAP,ZVOL,ZQWALL,ZBETA,ZFMF,ZNO,
     1              ZMASSL,ZMVAP,ZMFBRN,ZTEMP
      COMMON /DFLOW/ DFM,DFMV,DFMBF
      COMMON /ELEFLW/ NP,NN
      COMMON /SMZBAS/ PMDM
      COMMON /ZONES/ ZMA,ZMVA,ZMBFA
C*****************************************************************
C*****************************************************************
C
C     SUBROUTINE BTEMP
C
```

```
C     PURPOSE
C        GIVEN P, H, AND FR OF BURNED PRODUCTS, CALCULATES T
C
C     USAGE
C        CALL BTEMP  (TGUESS,FR,ENTHLP,T,N)
C
C     DESCRIPTION OF PARAMETERS (ALSO SEE SMM)
C        PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C        P          YES    NO       PRESSURE (ATM)
C        TGUESS     YES    NO       INITIAL GUESS FOR TEMPERATURE (K)
C        FR         YES    NO       FUEL FRACTION OF BURNED PRODUCTS
C        ENTHLP     YES    NO       ENTHALPY (CAL/G)
C        T          NO    YES       CALCULATED TEMPERATURE (K)
C        ERMAX      YES    NO       RELATIVE ERROR TOLERANCE (SEE
C        -----      ---    --       SUBROUTINES UTEMP AND BTEMP)
C        MAXITS     YES    NO       MAXIMUM NUMBER OF ITERATIONS (SEE
C        ------     ---    --       SUBROUTINES UTEMP AND BTEMP)
C        N          YES    NO       ELEMENT PROPERTY ARRAY
C                                     IDENTIFICATION NUMBER
C
C     SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED
C        BTHRMO
C
      SUBROUTINE BTEMP (TGUESS,FR,ENTHLP,T,N)
      INCLUDE 'SMMCOM.FOR'
      DIMENSION ELEMT(MAXELE,6)
      COMMON /ELEMT1/ ELEMT
      T=TGUESS
      DO 10 I=1,MAXITS
      CALL BTHRMO (P,T,FR,AHG,CSUBP,WT)
      TTOLD=T
      T=T+(ENTHLP-AHG)/(CSUBP)
      IF(ABS((T-TTOLD)/T).LE.ERMAX)GOTO 20
   10 CONTINUE
      CALL OUTPUT(6)
   20 ELEMT(N,5)=CSUBP
      ELEMT(N,6)=WT
      RETURN
      END
C*********************************************************************
C*********************************************************************
C
C     SUBROUTINE BTHRMO
C
C     PURPOSE
C        CALCULATES THERMODYNAMIC PROPERTIES OF BURNED PRODUCTS
C
C     DESCRIPTION OF PARAMETERS (ALSO SEE SMM)
C        PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C        P          YES    NO       PRESSURE (ATM)
C        T          YES    NO       TEMPERATURE (K)
C        FR         YES    NO       FUEL FRACTION OF BURNED PRODUCTS
C        H          NO     YES      ENTHALPY OF BURNED PRODUCTS (CAL/G)
C        CP         NO     YES      HEAT CAPACITY AT CONSTANT PRESSURE
C        --         ---    --       OF BURNED PRODUCTS (CAL/G K)
C        WT         NO     YES      MOLECULAR WEIGHT OF BURNED
```

```
C       —        —     ——       PRODUCTS (G/MOLE)
C
      SUBROUTINE BTHRMO (P,T,FR,H,CP,WT)
      COMMON/TABLE3/BHTBL(2688),BCTBL(2688),BWTBL(2688),BHFTBL(2688)
      COMMON/FULAR/CATOM,DEL,PSI,PHICON
      DIMENSION AP(7),AT(16),APHI(24)
      PARAMETER(RBAR=1.9869,PSCALE=.0242173)
      DATA AP /1.,5.,10.,20.,30.,60.,100./
      DATA AT /1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,
     &  2600.,2700.,2800.,2900.,3000.,3200.,3500./
      DATA APHI/0.0,0.3,0.4,0.5,0.6,0.7,0.8,0.85,0.9,0.95,1.0,1.05,1.1,
     &1.2,1.35,1.5,1.75,2.0,2.25,2.5,2.75,3.0,3.5,4.0/
      PHI=FR*PHICON/(1.-FR)
      PHIA=PHI
      PA=P
      TA=T
C
      IF(PA.LE.1.0)PA=1.
      IF(PA.GE.100.)PA=100.
      IF(TA.GE.3500.)TA=3500.
      IF(PHIA.LE.0.0)PHIA=0.
      IF(PHIA.GE.4.0)PHIA=4.0
C
      IF(TA.GE.1700.)GO TO 5
      CALL UTHRMO (P,T,FR,1.0,H,CP,WT)
      RETURN
C
    5 I=IFIX(TA/100.)-16
      IF(TA.GE.3200..AND.TA.LE.3500.)I=15
      IF(TA.GE.3000..AND.TA.LT.3200.)I=14
      TA1=AT(I)
      TA2=AT(I+1)
C
      J=6
      IF(PA.GE.60.)GO TO 10
      J=5
      IF(PA.GE.30.)GO TO 10
      J=IFIX(PA/10.)+2
      IF(PA.GE.10.)GO TO 10
      J=IFIX(PA/5.)+1
   10 PA1=AP(J)
      PA2=AP(J+1)
C
      K=23
      IF(PHIA.GE.3.5)GOTO 20
      K=IFIX((PHIA-3.0)/.5)+22
      IF(PHIA.GE.3.0.AND.PHIA.LT.4.0)GOTO 20
      K=IFIX((PHIA-1.5)/.25)+16
      IF(PHIA.GE.1.5.AND.PHIA.LE.3.0)GOTO 20
      K=IFIX((PHIA-1.2)/.15)+14
      IF(PHIA.GE.1.2.AND.PHIA.LE.1.5)GOTO 20
      K=13
      IF(PHIA.GE.1.1.AND.PHIA.LE.1.2)GOTO 20
      K=IFIX((PHIA-.9)/.05)+9
      IF(PHIA.GE.0.9.AND.PHIA.LE.1.1)GOTO 20
      K=IFIX((PHIA-.8)/.5)+7
      IF(PHIA.GE.0.8.AND.PHIA.LE.0.9)GOTO 20
      K=IFIX((PHIA-.6)/.1)+5
```

```
      IF(PHIA.GE.0.6.AND.PHIA.LE.0.8)GOTO 20
      K=IFIX((PHIA-.3)/.1)+2
      IF(PHIA.GE.0.3.AND.PHIA.LE.0.6)GOTO 20
      K=1
   20 PHI1=APHI(K)
      PHI2=APHI(K+1)
C
      IU1=J*384+K*16+I+1
      IU2=J*384+(K-1)*16+I+1
      IU3=J*384+(K-1)*16+I
      IU4=J*384+K*16+I
      IU5=(J-1)*384+K*16+I+1
      IU6=(J-1)*384+(K-1)*16+I+1
      IU7=(J-1)*384+(K-1)*16+I
      IU8=(J-1)*384+K*16+I
C
      R=(-PHI1+PHI+PHI-PHI2)/(PHI2-PHI1)
      S=(-TA1+T+T-TA2)/(TA2-TA1)
      V=(-PA1+P+P-PA2)/(PA2-PA1)
C
      H1=(1.+R)*(1.+S)*(1.+V)
      H2=(1.-R)*(1.+S)*(1.+V)
      H3=(1.-R)*(1.-S)*(1.+V)
      H4=(1.+R)*(1.-S)*(1.+V)
      H5=(1.+R)*(1.+S)*(1.-V)
      H6=(1.-R)*(1.+S)*(1.-V)
      H7=(1.-R)*(1.-S)*(1.-V)
      H8=(1.+R)*(1.-S)*(1.-V)
C
      H =.125*(H1*BHTBL(IU1)+H2*BHTBL(IU2)+
     &H3*BHTBL(IU3)+H4*BHTBL(IU4)+
     &H5*BHTBL(IU5)+H6*BHTBL(IU6)+
     &H7*BHTBL(IU7)+H8*BHTBL(IU8))
      CP=.125*(H1*BCTBL(IU1)+H2*BCTBL(IU2)+
     &H3*BCTBL(IU3)+H4*BCTBL(IU4)+
     &H5*BCTBL(IU5)+H6*BCTBL(IU6)+
     &H7*BCTBL(IU7)+H8*BCTBL(IU8))
      WT=.125*(H1*BWTBL(IU1)+H2*BWTBL(IU2)+
     &H3*BWTBL(IU3)+H4*BWTBL(IU4)+
     &H5*BWTBL(IU5)+H6*BWTBL(IU6)+
     &H7*BWTBL(IU7)+H8*BWTBL(IU8))
C
      RETURN
      END
C*******************************************************************
C*******************************************************************
C
C SUBROUTINE CMBUST(NZ,N,N2)
C
C PURPOSE
C        TO BURN ELEMENTS WHICH MEET COMBUSTION CRITERIA AND UPDATE
C          BURNED ELEMENT PROPERTIES.
C
C VARIABLES (SEE SMM)
C     N2     USED WHEN CALLED BY MIXING TO INDICATE BURNING FOR TWO C
ELEMENTS
C     N      ELEMENT PROPERTY ARRAY ID NUMBER
C
```

```
C
      SUBROUTINE CMBUST(NZ,N,N2)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION ELEMT(MAXELE,6)
      DIMENSION PREP(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT5/ PREP
      COMMON /ELEMT6/ NUM,TFMF
      IF(PREP(N).LT.1.)GO TO 100
      IF((TFMF(N).LT.LLIMT).OR.(TFMF(N).GT.ULIMT)) GO TO 100
      IF(ELEMT(N,3).GE.1.)GO TO 100
C
      BGFR=ELEMT(N,3)
      ELEMT(N,3)=1.
      ELEMT(N,1)=TFMF(N)
      CALL BTEMP(2100.,TFMF(N),ELEMT(N,4),ELEMT(N,2),N)
      IF(N2.GT.0)THEN
        TBF(NZ)=TBF(NZ)+2.*ELMM*(1.-BGFR)
      ELSE
        TBF(NZ)=TBF(NZ)+ELMM*(1.-BGFR)
      END IF
C
 100  RETURN
      END
C*********************************************************************
C*********************************************************************
C
C SUBROUTINE DISTRIB
C
C PURPOSE
C   CALCULATES DISTRIBUTION OF NUMBER OF ELEMENTS, TEMPERATURE, SOOT AND
C   NO AS A FUNCTION OF TFMF.  READS DISTRIBUTIONS FROM PREVIOUS RUNS
C   AND CALCULATES CUMMULATIVE DISTRIBTION.  TFMF RANGE 0.-.3 IS DIVIDED
C   INTO 30 INCREMENTS.
C
C VARIABLES AND ARRAYS (ALSO SEE SMM)
C
C   ND - DISTRIBUTION ID NUMBER
C   NOLD - NUMBER OF RUNS INCLUDED IN OLD CUMMULATIVE DISTRIBUTION
C   NNEW - NUMBER OF RUNS IN NEW CUMMULATIVE DISTRIBUTION
C   NELET - TOTAL NUMBER OF ELEMENTS IN ALL ZONES, ACTIVE AND INACTIVE
C   NZACT - NUMBER OF ZONES WITH AT LEAST ONE ELEMENT
C   NAIR - NUMBER OF AIR ZONE ELEMENTS, ACTIVE AND INACTIVE
C
      SUBROUTINE DISTRIB
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT6/ NUM,TFMF
      IF(NOLD.GT.0)READ(26,*)NOLD
      NNEW=NOLD+1
      WRITE(25,900)NNEW
      IF(NOLD.GT.0)READ(26,*)NZACT,NELET,NAIR
```

```
      NZACT=0
      NELET=0
      DO 100 NZ=1,NZONES
        IF(NELS(NZ).GT.0)NZACT=NZACT+1
        NELET=NELET+NELS(NZ)
 100  CONTINUE
      NELET=NELET+NELAIR
      NZACT=NZACT+1
      WRITE(25,*)NZACT,NELET,NELAIR
      DO 500 NZ=1,NA
        IF(NELS(NZ).LT.1.AND.NZ.NE.NA) GO TO 500
        IF(NOLD.GT.0)READ(26,*)NZOLD,CRANKO
 900    FORMAT(1X,I3)
        WRITE(25,901)NZ,CRANK
 901    FORMAT(1X,I2,2X,F6.2)
C
C SORT ELEMENTS INTO TFMF INCREMENTS
C
        DO 400 J=1,30
          FMFU=J*.01
          FMFL=(J-1)*.01
          FMFT=0.
          TT=0.
          TNO=0.
          TSOOT=0.
          XN=0.
C
C CALCULATE AVERAGE TEMP,NO,SOOT IN EACH INCREMENT
C
          IF(NZ.EQ.NA.AND.NELS(NA).LT.1)GO TO 310
          DO 300 L=1,NELS(NZ)
            I=NUM(NZ,L)
            IF(TFMF(I).LT.FMFL.OR.TFMF(I).GE.FMFU)GO TO 300
            XN=XN+1.
            FMFT=FMFT+TFMF(I)
            TT=TT+ELEMT(I,2)
            TNO=TNO+ELMT(I,1)
            TSOOT=TSOOT+ELMT(I,3)
 300      CONTINUE
          IF(XN.LE.0.)GO TO 310
          TT=TT/XN
          TNO=TNO*1.0E+06/XN
          IF(FMFT.LE.0.)GO TO 310
          TSOOT=TSOOT*100./(FMFT*ELMM*CTOF)
 310      FMFA=(FMFL+FMFU)/2.
          IF(NZ.EQ.NA.AND.J.EQ.1)THEN
            XN1=XN
            XN=NELAIR-NELS(NA)+XN1
            IF(XN.GT.0.)THEN
              TT=(TT*XN1+ZTEMP(NA)*(NELAIR-NELS(NA)))/XN
              TN0=TNO*XN1/XN
            ELSE
              XN=0.
            END IF
            XN1=0.
          END IF
          XNSQ=XN**2
C
```

```
C READ OLD CUMMULATIVE DISTRIBUTION AND CALCULATE NEW
C
          IF(NOLD.GT.0)READ(26,*)FMFA,XN1,XNSQ1,STDEV,TT1,TNO1,TSOOT1
          IF(XN1.GT.0.)THEN
            TT=(TT*XN+TT1*NOLD*XN1)/(XN+NOLD*XN1)
            TNO=(TNO*XN+TNO1*NOLD*XN1)/(XN+NOLD*XN1)
            TSOOT=(TSOOT*XN+TSOOT1*NOLD*XN1)/(XN+NOLD*XN1)
            XN=(XN+NOLD*XN1)/NNEW
            XNSQ=(XNSQ+NOLD*XNSQ1)/NNEW
          END IF
          STDEV=SQRT(ABS(XNSQ-XN**2))
C
C WRITE NEW CUMMULATIVE DISTRIBUTION
C
          WRITE(25,311)FMFA,XN,XNSQ,STDEV,TT,TNO,TSOOT
 311      FORMAT(1X,F6.4,3X,F6.1,3X,G10.4,3X,G10.4,3X,F6.1,3X,G10.4,
     1      3X,G10.4)
 400    CONTINUE
 500  CONTINUE
      RETURN
      END
C*****************************************************************
C*****************************************************************
C
C SUBROUTINE EVAP(NZ)
C
C PURPOSE
C       TO CREATE FUEL VAPOR ELEMENTS GENERATED BY EVAPORATION IN
C         EACH ZONE, MIX THEM WITH A RANDOM ELEMENT IN THE ZONE
C         AND CALCULATE THE PROPERTIES OF THE MIXED ELEMENTS.
C
C USAGE
C       CALL EVAP(NZ).  ALL DATA PASSED THROUGH COMMON.
C
C VARIABLES
C     (SEE SMM)
C
C ARRAYS
C     (SEE SMM)
C
      SUBROUTINE EVAP(NZ)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4),SVOLD(MAXELE)
      DIMENSION PREP(MAXELE),NEXT(MAXELE)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT4/ SVOLD
      COMMON /ELEMT5/ PREP
      COMMON /ELEMT6/ NUM,TFMF
      PARAMETER(RBAR=1.9869,CCAL=.02421725)
      NEVAP=IFIX(ZMEVAP(NZ)/ELMM)
      IF(NZ.EQ.NA)THEN
        IF(NEVAP.GT.NELAIR)NEVAP=NELAIR
      ELSE
        IF(NEVAP.GT.NELS(NZ))NEVAP=NELS(NZ)
      END IF
```

```
      IF(NEVAP.EQ.0)RETURN
      ZMVAP(NZ)=ZMEVAP(NZ)-NEVAP*ELMM
      DO 100 L=1,NEVAP
        NELTOT=NELTOT+1
        NELS(NZ)=NELS(NZ)+1
        NUM(NZ,NELS(NZ))=NUM(NA,NELTOT)
        I=NUM(NZ,NELS(NZ))
        IF(NZ.EQ.NA)THEN
          ENELS=FLOAT(NELAIR)-.01
          NELAIR=NELAIR+1
        ELSE
          ENELS=FLOAT(NELS(NZ)-1)-.01
        END IF
40      CALL RANDOM(IX,IY,YFL)
        IX=IY
        L2=IFIX(1.0+YFL*ENELS)
        IF(NZ.EQ.NA.AND.L2.EQ.NELS(NZ))GO TO 40
        IF(NZ.EQ.NA.AND.L2.GT.NELS(NZ))THEN
          NELS(NA)=NELS(NA)+1
          NELTOT=NELTOT+1
          NUM(NA,NELS(NA))=NUM(NA,NELTOT)
          J=NUM(NA,NELS(NA))
          ELEMT(J,1)=ZMBFA/(ZMA-ZMVA)
          ELEMT(J,2)=ZTEMP(NA)
          ELEMT(J,3)=(ZMA-ZMVA)/ZMA
          IF(ELEMT(J,3).LT.1.)THEN
            CALL UTHRMO(P,ELEMT(J,2),ELEMT(J,1),ELEMT(J,3),
     1        ELEMT(J,4),ELEMT(J,5),ELEMT(J,6))
          ELSE
            CALL BTHRMO(P,ELEMT(J,2),ELEMT(J,1),ELEMT(J,4),
     1        ELEMT(J,5),ELEMT(J,6))
          END IF
          ELMT(J,1)=0.
          ELMT(J,2)=0.
          ELMT(J,3)=0.
          ELMT(J,4)=TIME
          PREP(J)=0.
          SVOLD(J)=RBAR*ELEMT(J,2)/(ELEMT(J,6)*CCAL*P)
        ELSE
          J=NUM(NZ,L2)
          CALL PROP(TIME,NZ,J)
        END IF
        ELEMT(I,1)=ELEMT(J,1)
        ELEMT(I,3)=ELEMT(J,3)/2.
        ELEMT(I,4)=(ELEMT(J,4)+HFUEL+HEVAP)/2.
        TGUESS=(TSAT+ELEMT(J,2))/2.
        CALL UTEMP(TGUESS,ELEMT(I,1),ELEMT(I,3),ELEMT(I,4),
     1    ELEMT(I,2),I)
        ELMT(I,1)=ELMT(J,1)/2.
        ELMT(I,2)=ELMT(J,2)/2.
        ELMT(I,3)=ELMT(J,3)/2.
        PREP(I)=PREP(J)/2.
        CALL PREPUP(DTMIX(NZ)/2.,I)
        TFMF(I)=1.-ELEMT(I,3)*(1.-ELEMT(I,1))
        DO 50 K=1,6
          ELEMT(J,K)=ELEMT(I,K)
50      CONTINUE
        DO 60 K=1,4
```

```
          ELMT(J,K)=ELMT(I,K)
 60     CONTINUE
        PREP(J)=PREP(I)
        SVOLD(I)=SVFUEL
        TFMF(J)=TFMF(I)
 100  CONTINUE
      RETURN
      END
C*********************************************************************
C*********************************************************************
C
C SUBROUTINE FLOW
C
C PURPOSE
C
C        GIVEN INPUT FROM SMZ, TRANSFERS MASS ELEMENTS BETWEEN
C          ZONES.  CALCULATES DIFFERENCE FROM SPECIFIED MASS
C          FLOW FOR INCLUSION IN NEXT TIMESTEP. CALLS BOUNDARY
C          MIXING ROUTINES
C
      SUBROUTINE FLOW
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION FLM(NFLOW),FLMV(NFLOW),FLMBF(NFLOW),
     1  ELEMT(MAXELE,6),ELMT(MAXELE,4),SVOLD(MAXELE),
     2  PREP(MAXELE)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION NEXT1(MAXELE),NEXT2(MAXELE),NEXT3(MAXELE)
      DIMENSION NEXT4(MAXELE),NEXT5(MAXELE),NEXT6(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT4/ SVOLD
      COMMON /ELEMT5/ PREP
      COMMON /ELEMT6/ NUM,TFMF
      COMMON /SORT/ NEL1,NEL2,NEL3,NEXT1,NEXT2,NEXT3
      COMMON /SORTX/ NEL4,NEL5,NEL6,NEXT4,NEXT5,NEXT6
      PARAMETER (CCAL=.02421725,RBAR=1.9869)
C
      DO 850 NF=1,NFLOW
C
C INITIALIZE VARIABLES
C
 50   FLM(NF)=0.
      FLMV(NF)=0.
      FLMBF(NF)=0.
      NFP1=NF+1
      IF(NF.EQ.NFLOW) GO TO 600
      IF (NP(NF).LE.0.OR.NELS(NF).LE.0) GO TO 200
 55   IF (NP(NF).GE.NELS(NF)) THEN
C
C MOVE ALL ELEMENTS IN NF TO NFP1
C
        NP(NF)=NELS(NF)
        DO 100 K1=1,NELS(NF)
          K2=NELS(NFP1)+K1
          N1=NUM(NF,K1)
          NUM(NFP1,K2)=N1
C
```

```
C UPDATE FLOWS
C
 95        FLM(NF)=FLM(NF)+ELMM
           FLMV(NF)=FLMV(NF)+(1.-ELEMT(N1,3))*ELMM
           FLMBF(NF)=FLMBF(NF)+ELEMT(N1,1)*ELEMT(N1,3)*ELMM
 100     CONTINUE
         NELS(NFP1)=NELS(NFP1)+NELS(NF)
         NELS(NF)=0
       ELSE
C
C MOVE NP ELEMENTS FROM NF TO NFP1.  DETERMINE TYPE OF ELEMENT
C   NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR RICH
C   GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
         CALL SORT1(NF)
         DO 160 J=1,NP(NF)
           K2=NELS(NFP1)+J
C
C NEED FUEL VAPOR RICH ELEMENT
C
             IF((FMV(NF)-FLMV(NF)).GT.FERMAX.AND.(FMV(NF)-FLMV(NF))
     1        .GT.(FMBF(NF)-FLMBF(NF)).AND.NEL1.GT.0)THEN
               ENELS=FLOAT(NEL1)-.01
               CALL RANDOM(IX,IY,YFL)
               IX=IY
               J1=IFIX(1.0+YFL*ENELS)
               K1=NEXT1(J1)
               N1=NUM(NF,K1)
               NUM(NFP1,K2)=N1
C
C FILL SLOTS IN NF AND NEXT1
C
               NEXT1(J1)=NEXT1(NEL1)
               NEL1=NEL1-1
               IF(K1.EQ.NELS(NF))GO TO 152
               NUM(NF,K1)=NUM(NF,NELS(NF))
               IF(NEL1.GT.0)THEN
                 DO 151 L=1,NEL1
                   IF(NEXT1(L).EQ.NELS(NF))NEXT1(L)=K1
 151             CONTINUE
               END IF
 152           NELS(NF)=NELS(NF)-1
C
C NEED BURNED FUEL RICH ELEMENT
C
             ELSE IF((FMBF(NF)-FLMBF(NF)).GT.FERMAX.AND.NEL2.GT.0)THEN
               ENELS=FLOAT(NEL2)-.01
               CALL RANDOM(IX,IY,YFL)
               IX=IY
               J1=IFIX(1.0+YFL*ENELS)
               K1=NEXT2(J1)
               N1=NUM(NF,K1)
               NUM(NFP1,K2)=N1
C
C  FILL SLOT IN NF AND NEXT2
C
               NEXT2(J1)=NEXT2(NEL2)
               NEL2=NEL2-1
```

```
            IF(K1.EQ.NELS(NF))GO TO 154
            NUM(NF,K1)=NUM(NF,NELS(NF))
            IF(NEL2.GT.0)THEN
              DO 153 L=1,NEL2
                IF(NEXT2(L).EQ.NELS(NF))NEXT2(L)=K1
 153          CONTINUE
            END IF
 154        NELS(NF)=NELS(NF)-1
C
C NEED LEAN ELEMENT
C
        ELSE IF(NEL3.GT.0)THEN
            ENELS=FLOAT(NEL3)-.01
            CALL RANDOM(IX,IY,YFL)
            IX=IY
            J1=IFIX(1.0+YFL*ENELS)
            K1=NEXT3(J1)
            N1=NUM(NF,K1)
            NUM(NFP1,K2)=N1
C
C  FILL SLOT IN NF AND NEXT3
C
            NEXT3(J1)=NEXT3(NEL3)
            NEL3=NEL3-1
            IF(K1.EQ.NELS(NF))GO TO 156
            NUM(NF,K1)=NUM(NF,NELS(NF))
            IF(NEL3.GT.0)THEN
              DO 155 L=1,NEL3
                IF(NEXT3(L).EQ.NELS(NF))NEXT3(L)=K1
 155          CONTINUE
            END IF
 156        NELS(NF)=NELS(NF)-1
C
C OTHERWISE ANY RANDOM ELEMENT
C
        ELSE
          ENELS=FLOAT(NELS(NF))-.01
          CALL RANDOM(IX,IY,YFL)
          IX=IY
          K1=IFIX(1.0+YFL*ENELS)
          N1=NUM(NF,K1)
          NUM(NFP1,K2)=N1
          NUM(NF,K1)=NUM(NF,NELS(NF))
          NELS(NF)=NELS(NF)-1
        END IF
C
C       UPDATE FLOWS
C
          FLM(NF)=FLM(NF)+ELMM
          FLMV(NF)=FLMV(NF)+(1.-ELEMT(N1,3))*ELMM
          FLMBF(NF)=FLMBF(NF)+ELEMT(N1,1)*ELEMT(N1,3)*ELMM
 160    CONTINUE
        NELS(NFP1)=NELS(NFP1)+NP(NF)
      END IF
C
 200  IF(NN(NF).LE.0.OR.NELS(NFP1).LE.0)GO TO 790
      IF(NN(NF).GE.NELS(NFP1)) THEN
C
```

```
C MOVE ALL ELEMENTS FROM NFP1 TO NF
C
        NN(NF)=NELS(NFP1)
        DO 300 K2=1,NELS(NFP1)
          K1=NELS(NF)+K2
          N2=NUM(NFP1,K2)
          NUM(NF,K1)=N2
 245      FLM(NF)=FLM(NF)-ELMM
          FLMV(NF)=FLMV(NF)-(1.-ELEMT(N2,3))*ELMM
          FLMBF(NF)=FLMBF(NF)-ELEMT(N2,1)*ELEMT(N2,3)*ELMM
 300    CONTINUE
        NELS(NF)=NELS(NF)+NELS(NFP1)
        NELS(NFP1)=0
      ELSE
C
C MOVE NN ELEMENTS FROM ZONE NF+1 TO ZONE NF. DETERMINE TYPE OF
C   ELEMENT NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR RICH
C   GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
        CALL SORT2(NFP1)
        DO 360 J=1,NN(NF)
          K1=NELS(NF)+J
          IF((FMV(NF)-FLMV(NF)).LT.-FERMAX.AND.(FMV(NF)-FLMV(NF))
     1     .LT.(FMBF(NF)-FLMBF(NF)).AND.NEL4.GT.0)THEN
            ENELS=FLOAT(NEL4)-.01
            CALL RANDOM(IX,IY,YFL)
            IX=IY
            J2=IFIX(1.0+YFL*ENELS)
            K2=NEXT4(J2)
            N2=NUM(NFP1,K2)
            NUM(NF,K1)=N2
            NEXT4(J2)=NEXT4(NEL4)
            NEL4=NEL4-1
            IF(K2.EQ.NELS(NFP1))GO TO 302
            NUM(NFP1,K2)=NUM(NFP1,NELS(NFP1))
            IF(NEL4.GT.0)THEN
              DO 301 L=1,NEL4
                IF(NEXT4(L).EQ.NELS(NFP1))NEXT4(L)=K2
 301          CONTINUE
            END IF
 302        NELS(NFP1)=NELS(NFP1)-1
          ELSE IF((FMBF(NF)-FLMBF(NF)).LT.-FERMAX.AND.NEL5.GT.0)THEN
            ENELS=FLOAT(NEL5)-.01
            CALL RANDOM(IX,IY,YFL)
            IX=IY
            J2=IFIX(1.0+YFL*ENELS)
            K2=NEXT5(J2)
            N2=NUM(NFP1,K2)
            NUM(NF,K1)=N2
            NEXT5(J2)=NEXT5(NEL5)
            NEL5=NEL5-1
            IF(K2.EQ.NELS(NFP1))GO TO 304
            NUM(NFP1,K2)=NUM(NFP1,NELS(NFP1))
            IF(NEL5.GT.0)THEN
              DO 303 L=1,NEL5
                IF(NEXT5(L).EQ.NELS(NFP1))NEXT5(L)=K2
 303          CONTINUE
            END IF
```

```
304      NELS(NFP1)=NELS(NFP1)-1
        ELSE IF(NEL6.GT.0)THEN
         ENELS=FLOAT(NEL6)-.01
         CALL RANDOM(IX,IY,YFL)
         IX=IY
         J2=IFIX(1.0+YFL*ENELS)
         K2=NEXT6(J2)
         N2=NUM(NFP1,K2)
         NUM(NF,K1)=N2
         NEXT6(J2)=NEXT6(NEL6)
         NEL6=NEL6-1
         IF(K2.EQ.NELS(NFP1))GO TO 306
         NUM(NFP1,K2)=NUM(NFP1,NELS(NFP1))
         IF(NEL6.GT.0)THEN
          DO 305 L=1,NEL6
           IF(NEXT6(L).EQ.NELS(NFP1))NEXT6(L)=K2
305       CONTINUE
         END IF
306      NELS(NFP1)=NELS(NFP1)-1
        ELSE
         ENELS=FLOAT(NELS(NFP1))-.01
         CALL RANDOM(IX,IY,YFL)
         IX=IY
         K2=IFIX(1.0+YFL*ENELS)
         N2=NUM(NFP1,K2)
         NUM(NF,K1)=N2
         NUM(NFP1,K2)=NUM(NFP1,NELS(NFP1))
         NELS(NFP1)=NELS(NFP1)-1
        END IF
345     FLM(NF)=FLM(NF)-ELMM
        FLMV(NF)=FLMV(NF)-(1.-ELEMT(N2,3))*ELMM
        FLMBF(NF)=FLMBF(NF)-ELEMT(N2,1)*ELEMT(N2,3)*ELMM
C
360    CONTINUE
       NELS(NF)=NELS(NF)+NN(NF)
      END IF
      GO TO 790
600   IF(NP(NF).LE.0.OR.NELS(NF).LE.0) GO TO 770
      IF(NP(NF).GE.NELS(NF)) THEN
C
C MOVE ALL ELEMENTS FROM NF TO NA
C
       NP(NF)=NELS(NF)
       DO 700 K1=1,NELS(NF)
        N1=NUM(NF,K1)
        NELS(NA)=NELS(NA)+1
        NELAIR=NELAIR+1
        NUM(NA,NELS(NA))=N1
        FLM(NF)=FLM(NF)+ELMM
        FLMV(NF)=FLMV(NF)+(1.-ELEMT(N1,3))*ELMM
        FLMBF(NF)=FLMBF(NF)+ELEMT(N1,1)*ELEMT(N1,3)*ELMM
700    CONTINUE
       NELS(NF)=0
      ELSE
C
C MOVE NP ELEMENTS FROM NF TO NA.  DETERMINE TYPE OF ELEMENT
C   NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR RICH
C   GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
```

```
C
          CALL SORT1(NF)
          DO 760 J=1,NP(NF)
            NELS(NA)=NELS(NA)+1
            NELAIR=NELAIR+1
            IF((FMV(NF)-FLMV(NF)).GT.FERMAX.AND.NEL1.GT.0)THEN
              ENELS=FLOAT(NEL1)-.01
              CALL RANDOM(IX,IY,YFL)
              IX=IY
              J1=IFIX(1.0+YFL*ENELS)
              K1=NEXT1(J1)
              N1=NUM(NF,K1)
              NUM(NA,NELS(NA))=N1
              NEXT1(J1)=NEXT1(NEL1)
              NEL1=NEL1-1
              IF(K1.EQ.NELS(NF))GO TO 742
              NUM(NF,K1)=NUM(NF,NELS(NF))
              IF(NEL1.GT.0)THEN
                DO 741 L=1,NEL1
                  IF(NEXT1(L).EQ.NELS(NF))NEXT1(L)=K1
  741           CONTINUE
              END IF
  742         NELS(NF)=NELS(NF)-1
            ELSE IF((FMBF(NF)-FLMBF(NF)).GT.FERMAX.AND.NEL2.GT.0)THEN
              ENELS=FLOAT(NEL2)-.01
              CALL RANDOM(IX,IY,YFL)
              IX=IY
              J1=IFIX(1.0+YFL*ENELS)
              K1=NEXT2(J1)
              N1=NUM(NF,K1)
              NUM(NA,NELS(NA))=N1
              NEXT2(J1)=NEXT2(NEL2)
              NEL2=NEL2-1
              IF(K1.EQ.NELS(NF))GO TO 744
              NUM(NF,K1)=NUM(NF,NELS(NF))
              IF(NEL2.GT.0)THEN
                DO 743 L=1,NEL2
                  IF(NEXT2(L).EQ.NELS(NF))NEXT2(L)=K1
  743           CONTINUE
              END IF
  744         NELS(NF)=NELS(NF)-1
           ELSE IF(NEL3.GT.0)THEN
              ENELS=FLOAT(NEL3)-.01
              CALL RANDOM(IX,IY,YFL)
              IX=IY
              J1=IFIX(1.0+YFL*ENELS)
              K1=NEXT3(J1)
              N1=NUM(NF,K1)
              NUM(NA,NELS(NA))=N1
              NEXT3(J1)=NEXT3(NEL3)
              NEL3=NEL3-1
              IF(K1.EQ.NELS(NF))GO TO 746
              NUM(NF,K1)=NUM(NF,NELS(NF))
              IF(NEL3.GT.0)THEN
                DO 745 L=1,NEL3
                  IF(NEXT3(L).EQ.NELS(NF))NEXT3(L)=K1
  745           CONTINUE
              END IF
```

```
746        NELS(NF)=NELS(NF)-1
       ELSE
         ENELS=FLOAT(NELS(NF))-.01
         CALL RANDOM(IX,IY,YFL)
         IX=IY
         K1=IFIX(1.0+YFL*ENELS)
         N1=NUM(NF,K1)
         NUM(NA,NELS(NA))=N1
         NUM(NF,K1)=NUM(NF,NELS(NF))
         NELS(NF)=NELS(NF)-1
       END IF
         FLM(NF)=FLM(NF)+ELMM
         FLMV(NF)=FLMV(NF)+(1.-ELEMT(N1,3))*ELMM
         FLMBF(NF)=FLMBF(NF)+ELEMT(N1,1)*ELEMT(N1,3)*ELMM
760    CONTINUE
      END IF
C
C MOVE NN ELEMENTS FROM ZONE NA TO ZONE NA-1. DETERMINE TYPE OF
C   ELEMENT NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR RICH
C   GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
770   IF(NN(NF).LE.0.OR.ZMA.LE.0..OR.NELAIR.EQ.0)GO TO 790
      CALL SORT2(NA)
      DO 787 J=1,NN(NF)
        K1=NELS(NF)+1
        NELS(NF)=K1
        IF((FMV(NF)-FLMV(NF)).LT.-FERMAX.AND.NEL4.GT.0)THEN
          ENELS=FLOAT(NEL4)-.01
          CALL RANDOM(IX,IY,YFL)
          IX=IY
          J2=IFIX(1.0+YFL*ENELS)
          K2=NEXT4(J2)
          N2=NUM(NA,K2)
          NEXT4(J2)=NEXT4(NEL4)
          NEL4=NEL4-1
          IF(K2.EQ.NELS(NA))GO TO 782
          NUM(NA,K2)=NUM(NA,NELS(NA))
          IF(NEL4.GT.0)THEN
            DO 781 L=1,NEL4
              IF(NEXT4(L).EQ.NELS(NA))NEXT4(L)=K2
781         CONTINUE
          END IF
782       NELAIR=NELAIR-1
          NELS(NA)=NELS(NA)-1
        ELSE IF((FMBF(NF)-FLMBF(NF)).LT.-FERMAX.AND.NEL5.GT.0)THEN
          ENELS=FLOAT(NEL5)-.01
          CALL RANDOM(IX,IY,YFL)
          IX=IY
          J2=IFIX(1.0+YFL*ENELS)
          K2=NEXT5(J2)
          N2=NUM(NA,K2)
          NEXT5(J2)=NEXT5(NEL5)
          NEL5=NEL5-1
          IF(K2.EQ.NELS(NA))GO TO 784
          NUM(NA,K2)=NUM(NA,NELS(NA))
          IF(NEL5.GT.0)THEN
            DO 783 L=1,NEL5
              IF(NEXT5(L).EQ.NELS(NA))NEXT5(L)=K2
```

```
783         CONTINUE
          END IF
784       NELAIR=NELAIR-1
          NELS(NA)=NELS(NA)-1
        ELSE IF(NEL6.GT.0)THEN
          ENELS=FLOAT(NEL6)-.01
          CALL RANDOM(IX,IY,YFL)
          IX=IY
          J2=IFIX(1.0+YFL*ENELS)
          K2=NEXT6(J2)
          N2=NUM(NA,K2)
          NEXT6(J2)=NEXT6(NEL6)
          NEL6=NEL6-1
          IF(K2.EQ.NELS(NA))GO TO 786
          NUM(NA,K2)=NUM(NA,NELS(NA))
          IF(NEL6.GT.0)THEN
            DO 785 L=1,NEL6
              IF(NEXT6(L).EQ.NELS(NA))NEXT6(L)=K2
785         CONTINUE
          END IF
786       NELAIR=NELAIR-1
          NELS(NA)=NELS(NA)-1
        ELSE IF(NELS(NA).GT.0)THEN
          ENELS=FLOAT(NELS(NA))-.01
          CALL RANDOM(IX,IY,YFL)
          IX=IY
          K2=IFIX(1.0+YFL*ENELS)
          N2=NUM(NA,K2)
          NUM(NA,K2)=NUM(NA,NELS(NA))
          NELS(NA)=NELS(NA)-1
          NELAIR=NELAIR-1
        ELSE
C
C INACTIVE ELEMENTS ARE ASSIGNED MEAN AIR ZONE PROPERTIES.
C
          NELTOT=NELTOT+1
          N2=NUM(NA,NELTOT)
          NELAIR=NELAIR-1
          ELEMT(N2,1)=ZMBFA/(ZMA-ZMVA)
          ELEMT(N2,2)=ZTEMP(NA)
          ELEMT(N2,3)=(ZMA-ZMVA)/ZMA
          IF(ELEMT(N2,3).LT.1.)THEN
            CALL UTHRMO(P,ELEMT(N2,2),ELEMT(N2,1),ELEMT(N2,3),
     1        ELEMT(N2,4),ELEMT(N2,5),ELEMT(N2,6))
          ELSE
            CALL BTHRMO(P,ELEMT(N2,2),ELEMT(N2,1),ELEMT(N2,4),
     1        ELEMT(N2,5),ELEMT(N2,6))
          END IF
          ELMT(N2,1)=0.
          ELMT(N2,2)=0.
          ELMT(N2,3)=0.
          ELMT(N2,4)=TIME
          PREP(N2)=0.
          SVOLD(N2)=RBAR*ELEMT(N2,2)/(ELEMT(N2,6)*CCAL*P)
          TFMF(N2)=1.-ELEMT(N2,3)*(1.-ELEMT(N2,1))
        END IF
        NUM(NF,K1)=N2
        FLM(NF)=FLM(NF)-ELMM
```

```
        FLMV(NF)=FLMV(NF)-(1.-ELEMT(N2,3))*ELMM
        FLMBF(NF)=FLMBF(NF)-ELEMT(N2,1)*ELEMT(N2,3)*ELMM
 787  CONTINUE
C
C UPDATE RESIDUAL FLOWS
C
 790  DFM(NF)=FM(NF)-FLM(NF)
      DFMV(NF)=FMV(NF)-FLMV(NF)
      DFMBF(NF)=FMBF(NF)-FLMBF(NF)
C
C CALL BOUNDARY MIXING ROUTINES IF REQUIRED
C
      IF((ABS(DFMV(NF)).GT.FERMAX.OR.ABS(DFMBF(NF)).GT.FERMAX).AND.
     1  NF.NE.NFLOW.AND.NELS(NF).GT.1.AND.NELS(NFP1).GT.1)THEN
          CALL MIXINGB(NF)
      ELSE IF((ABS(DFMV(NF)).GT.FERMAX.OR.ABS(DFMBF(NF)).GT.FERMAX)
     1  .AND.NF.EQ.NFLOW.AND.NELS(NF).GT.1.AND.NELAIR.GT.0)THEN
          CALL MIXINGA
      END IF
C
 800  IF(ZVOL(NF).LE.0.)THEN
        DFM(NF)=0.
        DFMV(NF)=0.
        DFMBF(NF)=0.
      END IF
 850  CONTINUE
 900  RETURN
      END
C*********************************************************************
C*********************************************************************
C
C SUBROUTINE INPUT(N)
C
C PURPOSE
C   CALLED TO INPUT ENGINE PARAMETERS, SIMULATION PARAMETERS,
C   FUEL CHARACTERISTICS, COMBUSTION PARAMETERS, AND INPUT
C   FROM MULTIDIMENSIONAL MODEL.  ONLY INPUT NOT USING
C   THIS SUBROUTINE ARE TABLES OF THERMO DATA (TABLE).
C
C VARIABLES (ALSO SEE SMM)
C
C                CTOF - FUEL CARBON MASS PER UNIT FUEL MASS
C               CATOM - NUMBER OF CARBON ATOMS IN FUEL
C                DTPR - TIMESTEP FOR PRINTING OUTPUT
C                 CAD - CARNK ANGLE INCREMENT FOR PRINTING
C                             DISTRIBUTION
C               DTKIN - MINIMUM TIMESTEP FOR KINETIC UPDATE
C                ELMM - MASS OF AN INDIVIDUAL ELEMENT (GM)
C               ERMAX - ERROR CRITERION FOR TEMP ROUTINES
C                FUEL - CHARACTER VARIABLE - NAME OF FUEL
C                  ID - SIMULATION ID
C               IX,IY - RANDOM NUMBER SEEDS
C              MAXITS - MAXIMUM ITERATIONS FOR TEMP ROUTINES
C                NOLD - NUMBER OF PREVIOUS STOCHASTIC RUNS FOR
C                             AVERAGING
C              NZONES - NUMBER OF STOCHASTIC MIXING ZONES
C              TIMMDM - MDM CLOCK TIME
C               PHIHI - UPPER COMBUSTION LIMIT
```

```
C             PHILOW -  LOWER COMBUSTION LIMIT
C                PSI -  N2/O2 RATIO FOR AIR
C              SOOTC -  SOOT FORMATION CONSTANT
C              SOTON -  SOOT MODEL ON/OFF
C             SOTSIZ -  INITIAL SOOT PARTICLE RADIUS(cm)
C             VERMAX -  MAXIMUM ERROR SUBR VOL
C             WTFUEL -  FUEL MOLECULAR WEIGHT
C                 ZH -  NO. HYDROGEN ATOMS IN FUEL
C
      SUBROUTINE INPUT(N)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      PARAMETER(CCAL=.02421725)
      LOGICAL SOTON
      NAMELIST/INPUT1/ID,ELMM,DTPR,CAD,DTKIN,TWALL,CRKMAX,CBETA
     1 ,NPRINT,NOLD
      NAMELIST/INPUT2/CATOM,ZH,PSI,FUEL,TFI,RHOL,HFG,TSAT,
     1  CPF
      NAMELIST/INPUT3/ERMAX,IX,MAXITS,VERMAX,ITMAXV,FERMAX
      NAMELIST/INPUT4/PHILOW,PHIHI,SOTON,SOTSIZ,SOOTC,TSOOT
C
C********************************
C
C INPUT NR 1: DEFAULT RUN PARAMETERS (CALLED FROM SMM)
C
C  1.  OPERATING PARAMETERS
C
      IF(N.EQ.2)GO TO 200
      IF(N.EQ.3)GO TO 300
  100 ID = ' SMM 171-1 '
      ELMM = .0003
      DTPR = .0001
      CAD= 10.
      DTKIN=2.0E-05
      TWALL=400.
      CRKMAX=40.
      CBETA=.9
      NPRINT=3
      NOLD=0
C
      READ(10,INPUT1)
C
C  2.  FUEL CHARACTERISTICS
C
      CATOM = 10.8
      ZH    = 18.7
      PSI   = 3.773
      FUEL  = 'DIESEL'
      TFI   = 350.
      RHOL  = .7452
      HFG   = 43.246
      TSAT  = 550.
      CPF   = .46
C
      READ(10,INPUT2)
C
C  3.  SIMULATION CONTROL PARAMETERS
C
```

```
      ERMAX  = 0.002
      IX     = 20001
      MAXITS = 100
      VERMAX = 0.01
      ITMAXV = 100
      FERMAX = 1.E-4
C
      READ(10,INPUT3)
C
C  4. COMBUSTION/SOOT PARAMETERS
C
      PHILOW = 0.3
      PHIHI  = 4.0
      SOTON  = .TRUE.
      SOTSIZ = 2.0E-6
      SOOTC  = .001
      TSOOT  = 600.
C
      READ(10,INPUT4)
C
      DO 150 I=1,NZONES
       SOOTON(I)=SOTON
 150  CONTINUE
      GO TO 900
C
C INPUT NR 2.  READ INITIAL MDM OUTPUT.
C
 200  READ(11,901)NAME
      READ(11,902)CA1INJ,RPM
      READ(11,*)CA1INJ,SWIRL,EGR
      READ(11,*)NCYCLE
      READ(11,*)PSTART
      GO TO 900
C
C INPUT NR 3. READ MDM OUTPUT.
C
 300  READ(11,*)TIMMDM,PMDM
      READ(11,*)(FM(K),K=1,NFLOW)
      READ(11,*)(FMV(K),K=1,NFLOW)
      READ(11,*)FML0,(ZMASSL(K),K=1,NA)
      READ(11,*)(FMBF(K),K=1,NFLOW)
      READ(11,*)(ZTEMP(K),K=1,NA)
      READ(11,*)(ZNO(K),K=1,NA)
      READ(11,*)(ZMEVAP(K),K=1,NA)
      READ(11,*)(ZQWALL(K),K=1,NA)
      READ(11,*)(ZMFBRN(K),K=1,NA)
      READ(11,*)(ZVOL(K),K=1,NA)
      READ(11,*)(ZFMF(K),K=1,NA)
      READ(11,*)(ZBETA(K),K=1,NA)
      READ(11,*)ZMA,ZMVA,ZMBFA
C
      IF(ZTEMP(NA).LE.0..OR.ZMA.LT.ELMM)THEN
        NELS(NA)=0
        NELAIR=0
        ZMA=0.
      END IF
C
      DO 301 NZ=1,NZONES
```

```
        ZBETA(NZ)=CBETA*ZBETA(NZ)
 301  CONTINUE
C***************************
C
 900  RETURN
C
 901  FORMAT(A30)
 902  FORMAT(1X,F6.1,2X,F6.1)
C
      END
C********************************************************************
C********************************************************************
C   SUBROUTINE MIXING
C
C        PURPOSE
C
C          MIXES TWO RANDOMLY CHOSEN ELEMENTS TOGETHER, BURNS THEM IF
C          WITHIN LIMITS AND SEPARATES THEM, FORMING TWO IDENTICAL
C          ELEMENTS.
C
      SUBROUTINE MIXING(NZ)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4)
      DIMENSION PREP(MAXELE),SVOLD(MAXELE)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT4/ SVOLD
      COMMON /ELEMT5/ PREP
      COMMON /ELEMT6/ NUM,TFMF
      PARAMETER(RBAR=1.9869,CCAL=.02421725)
C
      ZTIME(NZ)=ZTIME(NZ)+DTMIX(NZ)
      NELMIX(NZ)=NELMIX(NZ)+2
C
C        TWO DIFFERENT ELEMENTS ARE CHOSEN AT RANDOM, AND THEIR
C        PROPERTIES ARE UPDATED.
C
C   FIRST ELEMENT IS SELECTED
C
   20 CALL RANDOM(IX, IY, YFL)
      IX=IY
      ENELS=FLOAT(NELS(NZ))-.01
      L1=IFIX(1.0 + YFL*ENELS)
C
C   SECOND ELEMENT IS CHOSEN WHICH IS DIFFERENT
C   FROM THE FIRST ONE
C
   30 CALL RANDOM(IX, IY, YFL)
      IX=IY
      L2=IFIX(1.0 + YFL*ENELS)
      IF(L1.EQ.L2) GO TO 30
C
      I=NUM(NZ,L1)
      CALL PROP(ZTIME(NZ),NZ,I)
      J=NUM(NZ,L2)
      CALL PROP(ZTIME(NZ),NZ,J)
```

```
C
C         DETERMINE THE TYPE OF MIX
C
C   1. BOTH BURNED, GO TO 90
C
      IF(ELEMT(I,3).EQ.1..AND.ELEMT(J,3).EQ.1.)GO TO 90
C
C   2. BOTH UNBURNED, GO TO 50
C
      IF(ELEMT(I,3).LT.1..AND.ELEMT(J,3).LT.1.)GO TO 50
C
C   3. ONE BURNED, ONE UNBURNED.
C
C     WHICH IS BURNED? CALCULATE A PREP TIME.
C
      IF(ELEMT(I,3).EQ.1.)THEN
        IB=I
      ELSE
        IB=J
      END IF
      CALL PREPUP(DTMIX(NZ),IB)
C
 40   ELEMT(I,1)=(ELEMT(I,1)*ELEMT(I,3) + ELEMT(J,1)
     1  *ELEMT(J,3))/(ELEMT(I,3) + ELEMT(J,3))
      TGUESS=(ELEMT(I,2) + ELEMT(J,2))/2.
      ELEMT(I,3)=(ELEMT(I,3) + ELEMT(J,3))/2.
      ELEMT(I,4)=(ELEMT(I,4) + ELEMT(J,4))/2.
      ELMT(I,1)=(ELMT(I,1) + ELMT(J,1))/2.
      ELMT(I,2)=(ELMT(I,2) + ELMT(J,2))/2.
      ELMT(I,3)=(ELMT(I,3) + ELMT(J,3))/2.
      PREP(I)=(PREP(I)+PREP(J))/2.
      CALL UTEMP(TGUESS,ELEMT(I,1),ELEMT(I,3),ELEMT(I,4),ELEMT(I,2),I)
      TFMF(I)=1.-ELEMT(I,3)*(1.-ELEMT(I,1))
      CALL CMBUST(NZ,I,J)
      GO TO 119
C
C 2. BOTH UNBURNED
C
 50   ELEMT(I,1)=(ELEMT(I,1)*ELEMT(I,3) + ELEMT(J,1)
     1  *ELEMT(J,3))/(ELEMT(I,3) + ELEMT(J,3))
      TGUESS=(ELEMT(I,2) + ELEMT(J,2))/2.
      ELEMT(I,3)=(ELEMT(I,3) + ELEMT(J,3))/2.
      ELEMT(I,4)=(ELEMT(I,4) + ELEMT(J,4))/2.
      ELMT(I,1)=(ELMT(I,1) + ELMT(J,1))/2.
      ELMT(I,2)=(ELMT(I,2) + ELMT(J,2))/2.
      ELMT(I,3)=(ELMT(I,3) + ELMT(J,3))/2.
      PREP(I)=(PREP(I)+PREP(J))/2.
      CALL UTEMP(TGUESS,ELEMT(I,1),ELEMT(I,3),ELEMT(I,4),ELEMT(I,2),I)
      TFMF(I)=1.-ELEMT(I,3)*(1.-ELEMT(I,1))
      CALL CMBUST(NZ,I,J)
      GO TO 119
C
C 3. MIXING OF TWO BURNED ELEMENTS
C
 90   ELEMT(I,1)=(ELEMT(I,1) + ELEMT(J,1))/2.
      TGUESS=(ELEMT(I,2) + ELEMT(J,2))/2.
      ELEMT(I,4)=(ELEMT(I,4) + ELEMT(J,4))/2.
      ELMT(I,1)=(ELMT(I,1) + ELMT(J,1))/2.
```

```
      ELMT(I,2)=(ELMT(I,2) + ELMT(J,2))/2.
      ELMT(I,3)=(ELMT(I,3) + ELMT(J,3))/2.
      CALL BTEMP(TGUESS,ELEMT(I,1),ELEMT(I,4),ELEMT(I,2),I)
 110  TFMF(I)=ELEMT(I,1)
C
 119  DO 120 L=1,6
      ELEMT(J,L)=ELEMT(I,L)
  120 CONTINUE
      DO 130 L=1,3
      ELMT(J,L)=ELMT(I,L)
  130 CONTINUE
      PREP(J)=PREP(I)
      TFMF(J)=TFMF(I)
 200  RETURN
      END
C*************************************************************
C*************************************************************
C   SUBROUTINE MIXINGA
C
C         PURPOSE
C
C           THIS SUBROUTINE SIMULATES MIXING ACROSS THE BOUNDARY
C              BETWEEN ZONES NFLOW AND NA.
C
      SUBROUTINE MIXINGA
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4),SVOLD(MAXELE)
      DIMENSION PREP(MAXELE)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION NEXT1(MAXELE),NEXT2(MAXELE),NEXT3(MAXELE)
      DIMENSION NEXT4(MAXELE),NEXT5(MAXELE),NEXT6(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT4/ SVOLD
      COMMON /ELEMT5/ PREP
      COMMON /ELEMT6/ NUM,TFMF
      COMMON /SORT/ NEL1,NEL2,NEL3,NEXT1,NEXT2,NEXT3
      COMMON /SORTX/ NEL4,NEL5,NEL6,NEXT4,NEXT5,NEXT6
      PARAMETER(CCAL=.02421725,RBAR=1.9869)
C
      NF=NFLOW
      NFP1=NA
      CALL SORT1(NF)
      CALL SORT2(NFP1)
C
 20   NP(NF)=NP(NF)+1
      NN(NF)=NN(NF)+1
C
C   RANDOM ELEMENT IS CHOSEN FROM ZONE NFLOW.  DETERMINE TYPE OF
C     ELEMENT NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR
C     RICH GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
      IF(DFMV(NF).GT.FERMAX.AND.NEL1.GT.0)THEN
        ENELS1=FLOAT(NEL1)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS1)
```

```
        L1=NEXT1(LX)
        NEXT1(LX)=NEXT1(NEL1)
        NEL1=NEL1-1
      ELSE IF(DFMBF(NF).GT.FERMAX.AND.NEL2.GT.0)THEN
        ENELS1=FLOAT(NEL2)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS1)
        L1=NEXT2(LX)
        NEXT2(LX)=NEXT2(NEL2)
        NEL2=NEL2-1
      ELSE IF(NEL3.GT.0)THEN
        ENELS1=FLOAT(NEL3)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS1)
        L1=NEXT3(LX)
        NEXT3(LX)=NEXT3(NEL3)
        NEL3=NEL3-1
      ELSE
        GO TO 200
      END IF
      I=NUM(NF,L1)
C
C   SECOND RANDOM ELEMENT IS CHOSEN FROM ZONE NF+1. DETERMINE TYPE
C     OF ELEMENT NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR
C     RICH GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
      IF(DFMV(NF).LT.-FERMAX.AND.NEL4.LT.0)THEN
        ENELS2=FLOAT(NEL4)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS2)
        L2=NEXT4(LX)
        NEXT4(LX)=NEXT4(NEL4)
        NEL4=NEL4-1
        J=NUM(NFP1,L2)
      ELSE IF(DFMBF(NF).LT.-FERMAX.AND.NEL5.GT.0)THEN
        ENELS2=FLOAT(NEL5)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS2)
        L2=NEXT5(LX)
        NEXT5(LX)=NEXT5(NEL5)
        NEL5=NEL5-1
        J=NUM(NFP1,L2)
      ELSE IF(NEL6.GT.0)THEN
        ENELS2=FLOAT(NEL6)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS2)
        L2=NEXT6(LX)
        NEXT6(LX)=NEXT6(NEL6)
        NEL6=NEL6-1
        J=NUM(NFP1,L2)
      ELSE
C
C   INACTIVE ELEMENTS ARE ASSIGNED MEAN AIR ZONE PROPERTIES
```

```
C                    AND BECOME ACTIVE ELEMENTS.
C
          IF(NELS(NA).GE.IFIX(ZMA/ELMM))GO TO 200
          NELS(NA)=NELS(NA)+1
          NELTOT=NELTOT+1
          J=NUM(NA,NELTOT)
          L2=NELS(NA)
          ELEMT(J,1)=ZMBFA/(ZMA-ZMVA)
          ELEMT(J,2)=ZTEMP(NA)
          ELEMT(J,3)=(ZMA-ZMVA)/ZMA
          IF(ELEMT(J,3).LT.1.)THEN
            CALL UTHRMO(P,ELEMT(J,2),ELEMT(J,1),ELEMT(J,3),
     1        ELEMT(J,4),ELEMT(J,5),ELEMT(J,6))
          ELSE
            CALL BTHRMO(P,ELEMT(J,2),ELEMT(J,1),ELEMT(J,4),
     1        ELEMT(J,5),ELEMT(J,6))
          END IF
          ELMT(J,1)=0.
          ELMT(J,2)=0.
          ELMT(J,3)=0.
          ELMT(J,4)=TIME
          PREP(J)=0.
          SVOLD(J)=RBAR*ELEMT(J,2)/(ELEMT(J,6)*P*CCAL)
          TFMF(J)=1.-ELEMT(J,3)*(1.-ELEMT(J,1))
        END IF
C
C   CALCULATE FLOWS
C
 60     DFMV(NF)=DFMV(NF)-ELMM*(ELEMT(J,3)-ELEMT(I,3))
        DFMBF(NF)=DFMBF(NF)-ELMM*(ELEMT(I,1)*ELEMT(I,3)-
     1    ELEMT(J,1)*ELEMT(J,3))
C
C   EXCHANGE ELEMENTS BETWEEN ZONES
C
        NUM(NA,L2)=I
        NUM(NF,L1)=J
C
        IF(ABS(DFMV(NF)).GT.FERMAX.OR.ABS(DFMBF(NF)).GT.FERMAX)THEN
          GO TO 20
        ELSE
          GO TO 300
        END IF
 200    DFMV(NF)=DFMV(NF)-ELMM*(ELEMT(J,3)-ELEMT(I,3))
        DFMBF(NF)=DFMBF(NF)-ELMM*(ELEMT(I,1)*ELEMT(I,3)-
     1    ELEMT(J,1)*ELEMT(J,3))
 300    RETURN
        END
C**********************************************************************
C**********************************************************************
C   SUBROUTINE MIXINGB(NF)
C
C        PURPOSE
C
C          THIS SUBROUTINE SIMULATES MIXING ACROSS THE BOUNDARY
C             BETWEEN TWO MIXING ZONES.
C          IT EXCHANGES TWO RANDOMLY CHOSEN ELEMENTS ACROSS THE
C             BOUNDARY.
C
```

```
      SUBROUTINE MIXINGB(NF)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION NEXT1(MAXELE),NEXT2(MAXELE),NEXT3(MAXELE)
      DIMENSION NEXT4(MAXELE),NEXT5(MAXELE),NEXT6(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT6/ NUM,TFMF
      COMMON /SORT/ NEL1,NEL2,NEL3,NEXT1,NEXT2,NEXT3
      COMMON /SORTX/ NEL4,NEL5,NEL6,NEXT4,NEXT5,NEXT6
      NFP1=NF+1
      CALL SORT1(NF)
      CALL SORT2(NFP1)
C
C
C         TWO DIFFERENT ELEMENTS ARE CHOSEN AT RANDOM, ONE FROM
C           EACH ZONE.
C
C   FIRST RANDOM ELEMENT IS SELECTED FROM ZONE NF.  DETERMINE TYPE
C     OF ELEMENT NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR
C     RICH GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
 20   NP(NF)=NP(NF)+1
      NN(NF)=NN(NF)+1
      IF(DFMV(NF).GT.FERMAX.AND.NEL1.GT.0)THEN
        ENELS1=FLOAT(NEL1)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS1)
        L1=NEXT1(LX)
        NEXT1(LX)=NEXT1(NEL1)
        NEL1=NEL1-1
      ELSE IF(DFMBF(NF).GT.FERMAX.AND.NEL2.GT.0)THEN
        ENELS1=FLOAT(NEL2)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS1)
        L1=NEXT2(LX)
        NEXT2(LX)=NEXT2(NEL2)
        NEL2=NEL2-1
      ELSE IF(NEL3.GT.0)THEN
        ENELS1=FLOAT(NEL3)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS1)
        L1=NEXT3(LX)
        NEXT3(LX)=NEXT3(NEL3)
        NEL3=NEL3-1
      ELSE
        GO TO 200
      END IF
      I=NUM(NF,L1)
C
C   SECOND RANDOM ELEMENT IS CHOSEN FROM ZONE NF+1. DETERMINE TYPE
C     OF ELEMENT NEEDED AND SELECT RANDOM ELEMENT FROM FUEL VAPOR
C     RICH GROUP, BURNED FUEL RICH GROUP, OR LEAN GROUP.
C
```

```
      IF(DFMV(NF).LT.-FERMAX.AND.NEL4.LT.0)THEN
        ENELS2=FLOAT(NEL4)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS2)
        L2=NEXT4(LX)
        NEXT4(LX)=NEXT4(NEL4)
        NEL4=NEL4-1
      ELSE IF(DFMBF(NF).LT.-FERMAX.AND.NEL5.GT.0)THEN
        ENELS2=FLOAT(NEL5)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS2)
        L2=NEXT5(LX)
        NEXT5(LX)=NEXT5(NEL5)
        NEL5=NEL5-1
      ELSE IF(NEL6.GT.0)THEN
        ENELS2=FLOAT(NEL6)-.01
        CALL RANDOM(IX,IY,YFL)
        IX=IY
        LX=IFIX(1.0+YFL*ENELS2)
        L2=NEXT6(LX)
        NEXT6(LX)=NEXT6(NEL6)
        NEL6=NEL6-1
      ELSE
        GO TO 200
      END IF
        J=NUM(NFP1,L2)
C
C CALCULATE FLOWS
C
 60   DFMV(NF)=DFMV(NF)-ELMM*(ELEMT(J,3)-ELEMT(I,3))
      DFMBF(NF)=DFMBF(NF)-ELMM*(ELEMT(I,1)*ELEMT(I,3)-
     1  ELEMT(J,1)*ELEMT(J,3))
C
C EXCHANGE ELEMENTS BETWEEN ZONES
C
      NUM(NFP1,L2)=I
      NUM(NF,L1)=J
C
      IF(ABS(DFMV(NF)).GT.FERMAX.OR.ABS(DFMBF(NF)).GT.FERMAX)THEN
        GO TO 20
      ELSE
        GO TO 300
      END IF
 200  DFMV(NF)=DFMV(NF)-ELMM*(ELEMT(J,3)-ELEMT(I,3))
      DFMBF(NF)=DFMBF(NF)-ELMM*(ELEMT(I,1)*ELEMT(I,3)-
     1  ELEMT(J,1)*ELEMT(J,3))
 300  RETURN
      END
C*******************************************************************
C*******************************************************************
C SUBROUTINE OUTPUT(N)
C
C PURPOSE
C       HANDLES ALL OUTPUT FOR PROGRAM SMM
C
C VARIABLES
```

```
C
C      Y(1)   -  AVERAGE TEMPERATURE OF ENSEMBLE
C      Y(2)   -  AVERAGE GAS TEMPERATURE OF ENSEMBLE
C      Y(3)   -  AVERAGE SPECIFIC VOLUME
C      Y(4)   -  AVERAGE SPECIFIC VOLUME OF GASEOUS ELEMENTS
C      Y(5)   -  AVERAGE FUEL MASS FRACTION
C      Y(6)   -  AVERAGE FUEL MASS FRACTION OF GASEOUS ELEMENTS
C      Y(7)   -  AVERAGE FUEL MASS FRACTION OF BURNED ELEMENTS
C      Y(8)   -  AVERAGE TEMPERATURE OF BURNED ELEMENTS
C      NOX    -  NO EMISSIONS (PPM)
C      TMOLS  -  TOTAL NO. OF MOLES
C
C
C
      SUBROUTINE OUTPUT(N)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4)
      DIMENSION TAV(NA),FFUEL(NA),TBFX(NA)
      DIMENSION TAVX(NA),DFMVX(NFLOW),DFMBFX(NFLOW),FFUELX(NA)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT6/ NUM,TFMF
      REAL NOX,Y(9),YT(9),MGAS,MBURN,MTOT
      PARAMETER(CCAL=.02421725,RBAR=1.9869)
C
C OUTPUT NR 1 - PRINTOUT INPUT DATA
      IF(N.EQ.1) GO TO 100
C
C OUTPUT NR 2 - INTERMEDIATE RESULTS
      IF(N.EQ.2) GO TO 200
C
C OUTPUT NR 5 - VOLUME OUT OF TOLERANCE
      IF(N.EQ.5) GO TO 500
C
C OUTPUT NR 6 - BTEMP DID NOT CONVERGE
      IF(N.EQ.6) GO TO 600
C
C OUTPUT NR 9 - UTEMP DID NOT CONVERGE
      IF(N.EQ.9) GO TO 650
C
C OUTPUT NR 8 - FINAL
      IF(N.EQ.8) GO TO 200
C
C***********************************
C
C OUTPUT NR 1: PRINTOUT INPUT DATA
C
C   SET UP TITLE PAGE
C
 100  WRITE(14,908)
      WRITE(14,900)
      DO 110 I=1,10
        WRITE(14,901)
 110  CONTINUE
      WRITE(14,902)
      DO 111 I=1,5
```

```
        WRITE(14,901)
 111  CONTINUE
      WRITE(14,903)
      DO 112 I=1,4
        WRITE(14,901)
 112  CONTINUE
      WRITE(14,9031)ID
      DO 1121 I=1,13
        WRITE(14,901)
 1121 CONTINUE
      WRITE(14,904)
      WRITE(14,905)
      WRITE(14,906)
      DO 113 I=1,12
        WRITE(14,901)
 113  CONTINUE
      WRITE(14,907)
C
C   SET UP INPUT DATA PAGE
C
      IPAGE=1
      WRITE(14,908)
      WRITE(14,909)IPAGE
      WRITE(14,910)ID
C
C PRINT OUT INPUT DATA AND SELECTED CALCULATIONS
C
      WRITE(14,912)
      WRITE(14,913)
      WRITE(14,914)NAME
      WRITE(14,915)RPM
      WRITE(14,916)CA1INJ
      WRITE(14,917)CRKMAX
      WRITE(14,918)
      WRITE(14,919)FUEL
      WRITE(14,920)CATOM,DEL
      WRITE(14,921)PSI
      WRITE(14,922)
      WRITE(14,923)ELMM
      WRITE(14,924)VERMAX,ERMAX
      WRITE(14,925)MAXITS,ITMAXV
      WRITE(14,926)IX
      WRITE(14,927)NA
      WRITE(14,928)DTPR
      WRITE(14,9281)DTKIN
C
      IPAGE=IPAGE+1
C
      WRITE(14,908)
      WRITE(14,909)IPAGE
      WRITE(14,910)ID
C
      WRITE(14,929)
      WRITE(14,930)PHIHI,PHILOW
      WRITE(14,931)SOTSIZ
      WRITE(14,932)SOOTON(2)
      WRITE(14,933)SOOTC
      WRITE(14,9333)CBETA
```

```
      NLINES=9
      GO TO 899
C
C***********************************
C
C OUTPUT NR 2: INTERMEDIATE RESULTS
C
C   OUTPUT CALCULATIONS
C
 200  TSOOT=0.
      TNOX=0.
      TWT=0.
      TMGAS=0.
      TMTOT=0.
      TMBURN=0.
      TTMOLS=0.
      TTMEVAP=0.
      TOTBF=0.
      TBFMDM=0.
      TMASSL=0.
      FFUEL1=0.
      FFUEL2=0.
      DO 205 J=1,9
        YT(J)=0.
 205  CONTINUE
C
C CALCULATE OUTPUT FOR EACH ZONE EXCEPT NA
C
      DO 250 NZ=1,NZONES
        MBURN=0
        MGAS=NELS(NZ)*ELMM+ZMVAP(NZ)
        DO 210 J=1,9
          Y(J)=0.
 210    CONTINUE
        SOOT=0.
        TMOLS=0.
        NOX=0.
        IF(MGAS.LE.0..OR.NELS(NZ).LT.1)GO TO 250
        IF(NLINES.GE.9.AND.NPRINT.NE.2.AND.NPRINT.NE.3) THEN
          IPAGE=IPAGE+1
          WRITE(14,908)
          WRITE(14,937)ID,IPAGE
          WRITE(14,938)
          NLINES=0
        END IF
        DO 212 LI=1,NELS(NZ)
          I=NUM(NZ,LI)
          SV=RBAR*ELEMT(I,2)/(P*CCAL*ELEMT(I,6))
          UFMF=1.0-ELEMT(I,3)
          Y(2)=Y(2)+ELEMT(I,2)*ELMM
          Y(4)=Y(4)+SV*ELMM
          Y(6)=Y(6)+(1.-ELEMT(I,3)*(1.-ELEMT(I,1)))*ELMM
          Y(9)=Y(9)+UFMF*ELMM
          IF(ELEMT(I,3).LT.1.) GO TO 212
          MBURN=MBURN+ELMM
          Y(7)=Y(7)+ELEMT(I,1)*ELMM
          Y(8)=Y(8)+ELEMT(I,2)*ELMM
 212    CONTINUE
```

```
      Y(1)=Y(2)+ZMASSL(NZ)*TFI
      Y(3)=Y(4)+ZMASSL(NZ)/RHOL
      Y(6)=Y(6)+ZMVAP(NZ)
      Y(5)=Y(6)+ZMASSL(NZ)
      Y(9)=Y(9)+ZMVAP(NZ)
      DO 215 J=1,9
        YT(J)=YT(J)+Y(J)
 215  CONTINUE
      MTOT=MGAS+ZMASSL(NZ)
      Y(1)=Y(1)/MTOT
      Y(3)=Y(3)/MTOT
      Y(5)=Y(5)/MTOT
      Y(2)=Y(2)/MGAS
      IF(NZ.EQ.1)T1=Y(2)
      IF(NZ.EQ.2)T2=Y(2)
      Y(4)=Y(4)/MGAS
      Y(6)=Y(6)/MGAS
      Y(9)=Y(9)/MGAS
      IF(MBURN.EQ.0.) GO TO 216
      Y(7)=Y(7)/MBURN
      Y(8)=Y(8)/MBURN
C
C
 216  DO 220 LI=1,NELS(NZ)
        I=NUM(NZ,LI)
        TMOLS=TMOLS+ELMM/ELEMT(I,6)
        NOX=NOX+ELMT(I,1)*ELMM
        SOOT=SOOT+ELMT(I,3)
  220 CONTINUE
C
      WTMOL=NELS(NZ)*ELMM/TMOLS
      TWT=TWT+NELS(NZ)*ELMM
      TTMOLS=TTMOLS+TMOLS
      TSOOT=TSOOT+SOOT
      TNOX=TNOX+NOX
      NOX=NOX*1.0E+06/MGAS
      SOOT=(SOOT/(MTOT*Y(5)*CTOF))*100.
      FFUEL(NZ)=Y(6)
      TAV(NZ)=Y(2)
      PHIAV=PHICON*Y(5)/(1. - Y(5))
      PHIGAS=PHICON*Y(6)/(1. - Y(6))
      PHIBRN=PHICON*Y(7)/(1. - Y(7))
      IF(NPRINT.NE.2.AND.NPRINT.NE.3)THEN
      WRITE(14,939)NZ,CRANK,Y(1),Y(2),Y(3),Y(4),PHIAV,PHIGAS,P
      WRITE(14,940)NCYC,Y(8),Y(9),NOX,ELMM,PHIBRN,PMDM
      WRITE(14,9401)DTMIX(NZ),NELS(NZ),ZMASSL(NZ),SOOT,WTMOL,
     1   TMEVAP(NZ),TTBF(NZ),TBF(NZ)
      END IF
      TMASSL=TMASSL+ZMASSL(NZ)
      TMTOT=TMTOT+MTOT
      TMGAS=TMGAS+MGAS
      NLINES=NLINES+1
  250 CONTINUE
      DO 251 NZ=1,NZONES
        TTMEVAP=TTMEVAP+TMEVAP(NZ)
        TOTBF=TOTBF+TBF(NZ)
        TBFMDM=TBFMDM+TTBF(NZ)
  251 CONTINUE
```

```
C
C CALCULATE OUTPUT FOR ALL ZONES INCLUDING 1
C
      ZMA=ZMA-DFM(NFLOW)
      ZMVA=ZMVA-DFMV(NFLOW)
      ZMBFA=ZMBFA-DFMBF(NFLOW)
      TMASSL=TMASSL+ZMASSL(NA)
      UBFMFA=ZMVA
      TTMEVAP=TTMEVAP+TMEVAP(NA)
      IF((ZMA.LE.0..OR.NELS(NA).EQ.0).AND.TMTOT.GT.0.)THEN
        YT(1)=YT(1)/TMTOT
        YT(2)=YT(2)/TMGAS
        YT(3)=YT(3)/TMTOT
        YT(4)=YT(4)/TMGAS
        YT(5)=(TTMEVAP+TMASSL)/TMTOT
        YT(6)=TTMEVAP/TMGAS
        YT(9)=(YT(9)+UBFMFA)/TMGAS
        TWTMOL=TWT/TTMOLS
        TSOOT=(TSOOT/(TMTOT*YT(5)*CTOF))*100.
        TNOX=TNOX*1.0E+6/TMGAS
      ELSE
        TMTOT=TMTOT+ZMA+ZMASSL(NA)
        TMGAS=TMGAS+ZMA
        TMOLSA=0.
        NOX=0.
        SOOT=0.
        DO 255 LI=1,NELS(NA)
          I=NUM(NA,LI)
          NOX=NOX+ELMT(I,1)*ELMM
          SOOT=SOOT+ELMT(I,3)
 255    CONTINUE
        BGFRA=1.-ZMVA/ZMA
        FRA=ZMBFA/(ZMA-ZMVA)
        IF(BGFRA.LT.1.) THEN
          CALL UTHRMO(P,ZTEMP(NA),FRA,BGFRA,HAIR,CPAIR,WTAIR)
        ELSE
          CALL BTHRMO(P,ZTEMP(NA),FRA,HAIR,CPAIR,WTAIR)
        END IF
        TMOLSA=ZMA/WTAIR
        SVAIR=RBAR*ZTEMP(NA)/(P*CCAL*WTAIR)
 270    YT(1)=(YT(1)+ZTEMP(NA)*ZMA+TFI*ZMASSL(NA))/TMTOT
        YT(2)=(YT(2)+ZTEMP(NA)*ZMA)/TMGAS
        YT(3)=(YT(3)+SVAIR*ZMA+ZMASSL(NA)/RHOL)/TMTOT
        YT(4)=(YT(4)+SVAIR*ZMA)/TMGAS
        YT(5)=(TTMEVAP+TMASSL)/TMTOT
        YT(6)=(TTMEVAP)/TMGAS
        YT(9)=(YT(9)+UBFMFA)/TMGAS
        TTMOLS=TTMOLS+TMOLSA
        TWTMOL=(TWT+ZMA)/TTMOLS
        TSOOT=((TSOOT+SOOT)/(TMTOT*YT(5)*CTOF))*100.
        TNOX=(TNOX+NOX)*1.0E+06/TMGAS
        TOTBF=TOTBF+TBF(NA)
        TBFMDM=TBFMDM+TTBF(NA)
      END IF
      PHIAV=PHICON*YT(5)/(1.-YT(5))
      PHIGAS=PHICON*YT(6)/(1.-YT(6))
      IF(NPRINT.NE.2.AND.NPRINT.NE.3)THEN
      WRITE(14,941)CRANK,YT(1),YT(2),YT(3),YT(4),PHIAV,PHIGAS,P
```

```
      WRITE(14,942)NCYC,YT(9),TNOX,TMTOT,PHIBRN,PMDM
      WRITE(14,9421)TMASSL,TSOOT,TWTMOL,TTMEVAP,TBFMDM,TOTBF
      END IF
      IF(NPRINT.NE.5)THEN
        IF(NAV.GT.0.AND.NOLD.GT.0)THEN
          READ(20,*)CRANK,(TAVX(L),L=1,NZONES)
          READ(21,*)CRANK,(DFMVX(L),DFMBFX(L),L=1,NFLOW)
          READ(22,*)CRANK,(FFUELX(L),L=1,NZONES)
          READ(23,*)CRANK,(TBFX(L),L=1,NZONES)
        END IF
        WRITE(15,9422)CRANK,((NAV*TAVX(L)+TAV(L))/NAVP1,L=1,NZONES)
        WRITE(16,9425)CRANK,((NAV*DFMVX(L)+DFMV(L))/NAVP1,(NAV*
     1   DFMBFX(L)+DFMBF(L))/NAVP1,L=1,NFLOW)
        WRITE(17,9424)CRANK,((NAV*FFUELX(L)+FFUEL(L))/NAVP1,L=1,NZONES)
        WRITE(18,9424)CRANK,((NAV*TBFX(L)+TBF(L))/NAVP1,L=1,NZONES)
      END IF
      WRITE(9,9423)CRANK,P,YT(2),TNOX,TSOOT,TOTBF
      PTEMP=P
      IF(NAV.GT.0.AND.NOLD.GT.0)THEN
        READ(24,*)CRANK,PX,YTX,TNOXX,TSOOTX,TOTBFX
        PTEMP=(NAV*PX+P)/NAVP1
        YT(2)=(NAV*YTX+YT(2))/NAVP1
        TNOX=(NAV*TNOXX+TNOX)/NAVP1
        TSOOT=(NAV*TSOOTX+TSOOT)/NAVP1
        TOTBF=(NAV*TOTBFX+TOTBF)/NAVP1
      END IF
      WRITE(19,9423)CRANK,PTEMP,YT(2),TNOX,TSOOT,TOTBF
      IF(N.EQ.8) GO TO 800
      NLINES=NLINES+1
      GO TO 899
C
C ****************************************
C
C OUTPUT NR 5: VOLUME OUT OF TOLERANCE
 500  WRITE(13,945) NCYC,TIME,CRANK,VOLERR
      GO TO 899
C
C ****************************************
C
C OUTPUT NR 6: BTEMP DID NOT CONVERGE
 600  WRITE(13,946) NCYC,CRANK
      GO TO 899
C
C ****************************************
C
C OUTPUT NR 9: UTEMP DID NOT CONVERGE
 650  WRITE(13,9461) NCYC,CRANK
      GO TO 899
C
C ****************************************
C
C OUTPUT NR 8: FINAL
 800  WRITE(14,948) NCYC,TIME,CRANK
C
C ****************************************
C
 899  RETURN
C
```

```
C FORMAT STATEMENTS *********************
C
  900 FORMAT(//,7X,110('*'))
  901 FORMAT(7X,'*',108X,'*')
  902 FORMAT(7X,'*',42X,'MIT SLOAN AUTOMOTIVE LAB',42X,'*')
  903 FORMAT(7X,'*',29X,'STOCHASTIC MIXING MODEL ENGINE COMBUS',
     &'TION SIMULATION',27X,'*')
 9031 FORMAT(7X,'*',47X,A15,46X,'*')
  904 FORMAT(7X,'*',6X,'VERSION 1.0',91X,'*')
  905 FORMAT(7X,'*',6X,'AUGUST 1985 ',90X,'*')
  906 FORMAT(7X,'*',6X,'A.J. BROWN     ',87X,'*')
  907 FORMAT(7X,110('*'))
  908 FORMAT('1')
  909 FORMAT(//,31X,'— STOCHASTIC MIXING MODEL ENGINE COMBU',
     &'STION SIMULATION —',21X,'PAGE ',I1)
  910 FORMAT(///,5X,' SIMULATION ID: ',A15)
  912 FORMAT(///,49X,21('-'),/,49X,'I N P U T     D A T A',
     &/,49X,21('-'))
  913 FORMAT(//,10X,100('-'),/,5X,'I.   OPERATING CONDITIONS')
  914 FORMAT(/,14X,'MULTIDIMENSIONAL MODEL —>',8X,A30)
  915 FORMAT(/,14X,'ENGINE SPEED (RPM) —>',8X,F6.1)
  916 FORMAT(/,14X,'INJECTION CRANK ANGLE (ATDC) —>',8X,F6.1)
  917 FORMAT(/,14X,'END CRANK ANGLE (ATDC) —>'8X,F6.1)
  918 FORMAT(//,10X,100('-'),/,5X,'II.  FUEL AND AIR')
  919 FORMAT(/,14X,'FUEL TYPE —>',15X,A12)
  920 FORMAT(/,14X,'SPECIFICATIONS —>',10X,'CARBON ATOMS: ',
     &  1P E9.2,6X,'C/H RATIO: ',1P E10.3)
  921 FORMAT(/,14X,'NITROGEN/OXYGEN RATIO —>',2X,1P E10.3)
  922 FORMAT(//,10X,100('-'),/,5X,'III.  SIMULATION CONTROL')
  923 FORMAT(/,14X,'ELEMENT MASS (g) —>',8X,1P E10.3)
  924 FORMAT(/,14X,'ERROR TOLERANCES (rel) —>',8X,'VOLUME:',
     &  1P E10.3,6X,'ENTHALPY (for temp calc): ',1P E10.3)
  925 FORMAT(/,14X,'MAXIMUM NUMBER OF ITERATIONS —>',2X,
     & 'TEMPERATURE SUBROUTINES:',1X,I3,2X,'VOLUME SUBROUTINE:',1X,I3)
  926 FORMAT(/,14X,'RANDOM NUMBER SEED     —>',6X,I9)
  927 FORMAT(/,14X,'NUMBER OF ZONES        —>',6X,I2)
  928 FORMAT(/,14X,'PRINTOUT TIMESTEP (s) —>',6X,1P E10.3)
 9281 FORMAT(/,14X,'KINETIC UPDATE TIMESTEP (s) —>',6X,1P E10.3)
  929 FORMAT(//,10X,100('-'),/,5X,'IV.   ASSUMED INPUT VALUES')
  930 FORMAT(/,14X,'LIMITS OF COMBUSTION (phi) —>',4X,'UPPER: ',F6.4,
     &  6X,'LOWER: ',F6.5)
  931 FORMAT(/,14X,'INITIAL SOOT SIZE UPON FORMATION (cm) —>',2X,
     &1P E10.3)
  932 FORMAT(/,14X,'SOOT MODEL IS ON            —>',2X,L1)
  933 FORMAT(/,14X,'SOOT FORMATION RATE FACTOR —>',2X,G10.3)
 9333 FORMAT(/,14X,'CBETA  —>',2X,F5.2)
  937 FORMAT(29X,'— STOCHASTIC MIXING MODEL ENGINE COMBUSTION '
     1  'SIMULATION —',9X,A12,2X,'PAGE ',I2,///)
  938 FORMAT(7X,'ZONE',3X,'CRANK(ATDC)',4X,'TAVE(K)',5X,'TGAVE(K)',
     1  6X,'SVAVE(CC/G)',3X,'SVGAVE(CC/G)',4X,'PHIAV',6X,'PHIGAS',
     2  9X,'P(ATM)',/,14X,'NCYC',11X,'TBURN(K)',4X,'UBFMF',9X,
     3  'NOX(PPM)',7X,'ELMM(G)',4X,'PHIBURN',8X,'PMDM',
     4  /,14X,'DTMIX(S)',7X,'NELS',8X,'ZMASSL(G)',5X,'SOOT(%C)',6X,
     5  'WTMOL',11X,'MEVAP(G)',4X,'TBFMDM(G)',5X,'TBF(G)')
  939 FORMAT(//,8X,I2,4X,F7.2,8X,F7.2,5X,3(F7.2,7X),F6.2,6X,F5.2,
     1  10X,F6.2)
  940 FORMAT(13X,I4,12X,F7.2,5X,G12.5,2X,G12.5,2X,G12.5,2X,
     1  F4.2,10X,F6.2)
```

```
9401 FORMAT(13X,G12.5,4X,I4,8X,G12.5,2X,G12.5,2X,G12.5,2X,G12.5,
    1  2X,G9.2,2X,G9.2)
 941 FORMAT(//,8X,'ALL',3X,F7.2,8X,F7.2,5X,3(F7.2,7X),1X,F5.2,7X,
    1  F4.2,10X,F6.2)
 942 FORMAT(13X,I4,24X,G12.5,2X,G12.5,2X,G12.5,2X,F4.2,10X,F6.2)
9421 FORMAT(41X,G12.5,2X,G12.5,2X,G12.5,2X,G12.5,2X,G9.2,2X,G9.2)
9422 FORMAT(1X,F6.2,10F7.1)
9423 FORMAT(1X,F6.2,F6.2,F7.1,1X,G9.3,1X,G9.3,1X,G9.3)
9424 FORMAT(1X,F6.2,10G9.2)
9425 FORMAT(1X,F6.2,9G10.2,/,7X,9G10.2)
 943 FORMAT(4X,'ERROR 3: NCYC=',I4,3X,'TIME=',F6.4,3X,'CRANK=',F6.2,
    1  3X,'NZ=',I2,3X,'ZMASSL=',G10.3)
 944 FORMAT(4X,'ERROR 4: NCYC=',I4,3X,'TIME=',F6.4,3X,'CRANK=',F6.2,
    1  3X,'NZ=',I2,3X,'ZMASSL=',G10.3,3X,'ZMEVAP=',G10.3)
 945 FORMAT(4X,'ERROR 5: NCYC=',I4,3X,'TIME=',F6.4,3X,'CRANK=',F6.2,
    1  3X,'VOLERR=',G10.3)
 946 FORMAT(4X,'ERROR 6:(BTEMP)  NCYC=',I4,3X,'CRANK=',F6.2)
9461 FORMAT(4X,'ERROR 9:(UTEMP)  NCYC=',I4,3X,'CRANK=',F6.2)
 948 FORMAT(//,7X,'THE END: NCYC=',I4,3X,'TIME=',F6.4,3X,'CRANK=',
    1  F6.2)
      END
C****************************************************************
C****************************************************************
C
C  SUBROUTINE PREPUP(DTUP,N)
C
C  PURPOSE
C    UPDATES ELEMENT IGNITION PREPARATION
C
C  PARAMETERS
C    DELAY   -   IGNITION DELAY TIME
C    PREP    -   INTEGRATED IGNITION PREPARATION
C    DTUP      -   TIME INTERVAL FOR UPDATE
C
C
      SUBROUTINE PREPUP(DTUP,N)
      INCLUDE 'SMMCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),PREP(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT5/ PREP
      PARAMETER(A=3.45E-3,E=2100.,C=1.02)
C
      DELAY=A*EXP(E/ELEMT(N,2))/(P**C)
      PREP(N)=PREP(N)+DTUP/DELAY
C
      RETURN
      END
C*****************************************************************
C*****************************************************************
C SUBROUTINE PROP(TIMUP,NZ,N)
C
C PURPOSE
C
C       TO UPDATE ELEMENT PROPERTIES EVERY DTKIN OR BEFORE MIXING.
C       TO CALCULATE THE FORMATION OF NO AND THE FORMATION/
C       OXIDATION OF SOOT.(AS SPECIFIED)
C
C METHOD
```

```
C
C        NO FORMATION IS CALCULATED VIA THE ZELDOVICH MECHANISM
C        AND SOOT OXIDATION IS CALCULATED BY THE NAGLE AND
C        STRICKLAND-CONSTABLE RELATION.
C
      SUBROUTINE PROP(TIMUP,NZ,N)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4),PREP(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT5/ PREP
      PARAMETER(RHO=1.8,CONSNO=4.56E15,CCAL=.02421725,RBAR=1.9869)
C
C
C UPDATE PROPERTIES
C
      DTPROP=TIMUP-ELMT(N,4)
      IF(DTPROP.LE.0.)GO TO 400
      ELMT(N,4)=TIMUP
      IF(ELEMT(N,3).LT.1.) THEN
        CALL PREPUP(DTPROP,N)
        CALL CMBUST(NZ,N,0)
        WTBG=ELEMT(N,6)*WTFUEL*ELEMT(N,3)/(WTFUEL-
     1    ELEMT(N,6)*(1.-ELEMT(N,3)))
        CALL SPECO2(P,ELEMT(N,2),ELEMT(N,1),O2)
        O2=O2*ELEMT(N,3)*ELEMT(N,6)/WTBG
        IF(SOOTON(NZ)) CALL SOOT(DTPROP,O2,N)
      ELSE
        CALL SPECO2(P,ELEMT(N,2),ELEMT(N,1),O2)
        PREP(N)=0.
      END IF
      IF(ELEMT(N,2).LE.1700.) GO TO 300
C
C NO FORMATION CALCULATIONS
C
      SV=RBAR*ELEMT(N,2)/(P*CCAL*ELEMT(N,6))
      CALL SPECNO (P,ELEMT(N,2),ELEMT(N,1),U1,U2,U3)
      ALFA=ELMT(N,1)*ELEMT(N,6)/(U1*30.)
      BETA=82.05*ELEMT(N,2)*82.05*ELEMT(N,2)/(P*P)
      DNODT=CONSNO*EXP(-38000./ELEMT(N,2))*(1.-ALFA*ALFA)*
     & U2*SV/((1.+ALFA*U3)*BETA)
      ELMT(N,1)=ELMT(N,1)+DNODT*DTPROP*ELEMT(N,3)
      IF(ELMT(N,1).LT.0.)ELMT(N,1)=0.
C
C SOOT OXIDATION CALCULATIONS
C
 300  IF(ELMT(N,3) .LE. 0.) GO TO 340
      IF(ELMT(N,2) .LE. 0.) GO TO 340
      IF(ELEMT(N,2).LT.TSOOT)GO TO 400
      SKA=20.*EXP(-15100./ELEMT(N,2))
      SKB=4.46E-3*EXP(-7650./ELEMT(N,2))
      SKT=1.51E5*EXP(-48800./ELEMT(N,2))
      SKZ=21.3*EXP(2060./ELEMT(N,2))
      U4PPC=O2*P
      SXX=1./(1.+SKT/(SKB*U4PPC))
      WXX=12.*(SKA*U4PPC/(1.+SKZ*U4PPC))*SXX+SKB*U4PPC*(1.-SXX)
      DSOXDT=ELMT(N,2)*WXX
```

```
C
C SOOT MASS CHANGE
C
      OLD=ELMT(N,3)
      ELMT(N,3)=ELMT(N,3)-DTPROP*DSOXDT
      IF(ELMT(N,3) .GT. 0.)GO TO 350
 340  ELMT(N,3)=0.
      ELMT(N,2)=0.
      GO TO 400
C
C SOOT SURFACE AREA CHANGE
C
 350  ELMT(N,2)=ELMT(N,2)*((ELMT(N,3)/OLD)**.666666)
C
C
 400  RETURN
      END
C*********************************************************************
C*********************************************************************
C
C SUBROUTINE QWALL(NZ)
C
C PURPOSE
C         DISTRIBUTES ZQWALL TO EACH ELEMENT IN THE ZONE
C           ACCORDING TO (T-TWALL) AND SURFACE AREA
C
C VARIABLES
C
      SUBROUTINE QWALL(NZ)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      REAL XSVDT(MAXELE),ELEMT(MAXELE,6)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT6/ NUM,TFMF
      PARAMETER(RBAR=1.9869,CCAL=.02421725)
      IF(ZQWALL(NZ).EQ.0.) GO TO 300
      DEN=0.
      TTHIRD=2./3.
      DO 100, LN=1,NELS(NZ)
        N=NUM(NZ,LN)
        SV=RBAR*ELEMT(N,2)/(P*CCAL*ELEMT(N,6))
        XSVDT(N)=(SV**TTHIRD)*(ELEMT(N,2)-TWALL)
        DEN=DEN+XSVDT(N)
 100  CONTINUE
      DO 200, LN=1,NELS(NZ)
        N=NUM(NZ,LN)
        ELEMT(N,4)=ELEMT(N,4)+ZQWALL(NZ)*XSVDT(N)/(DEN*ELMM)
 200  CONTINUE
 300  RETURN
      END
C*********************************************************************
C*********************************************************************
C
C     SUBROUTINE RANDOM
C
C     PURPOSE
C        COMPUTES UNIFORMLY DISTRIBUTED RANDOM NUMBERS BETWEEN
```

```
C         0 AND 1.0 AND RANDOM INTEGERS BETWEEN ZERO AND 2**31.
C         EACH ENTRY USES AS INPUT AN INTEGER RANDOM NUMBER AND
C         PRODUCES A NEW INTEGER AND REAL RANDOM NUMBER
C
C
C      DESCRIPTION OF PARAMETERS
C         PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C         IX          YES    NO       FOR THE FIRST ENTRY THIS MUST
C         —           ——     —        CONTAIN ANY ODD INTEGER NUMBER WITH
C         —           ——     —        NINE OR LESS DIGITS. AFTER THE FIRST
C         —           ——     —        ENTRY IX SHOULD BE THE PREVIOUS
C         —           ——     —        VALUE OF IY COMPUTED BY THIS
C         —           ——     —        SUBROUTINE.
C         IY          NO     YES      A RANDOM NUMBER BETWEEN 0 AND 2**31
C         YFL         NO     YES      A RANDOM NUMBER BETWEEN 0 AND 1.0
C
C
C      REMARKS
C         NONE
C
C      SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED
C         NONE
C
C      METHOD
C         SEE IBM MANUAL C20-8011, RANDOM NUMBER
C         GENERATION AND TESTING
C
      SUBROUTINE RANDOM(IX,IY,YFL)
      INTEGER*4 IX,IY
      IY=IX*65539
      IF(IY)1,2,2
    1 IY=IY+2147483647+1
    2 YFL=IY
      YFL=YFL*0.465661E-9
      RETURN
      END
C*****************************************************************
C*****************************************************************
C
C PROGRAM SMM
C
C PURPOSE
C
C              FUNCTION AS THE PRIMARY CONTROL PROGRAM FOR A
C              STOCHASTIC MIXING MODEL TO CALCULATE EMISSIONS IN A
C              DIESEL ENGINE.  INITIALIZES VARIABLES
C              CALLS INPUT AND OUTPUT, DOES PRELIMINARY CALCULATIONS
C              AND CONTROLS PROGRAM EXECUTION AND EVENT TIMING.
C
C LOGICAL UNITS:
C
C     INPUT    OUTPUT                CONTENT
C
C                 9      PRIMARY SINGLE RUN OUTPUT FILE
C      10                NAMELIST
C      11                MDM DATA
C      12                THERMO DATA
```

```
C                  13       ERRORS
C                  14       FANCY SINGLE RUN OUTPUT
C        20        15       MEAN ZONE TEMPERATURES (MULTIPLE RUN AVERAGE)
C        21        16       FLOW ERRORS (MULTIPLE RUN AVERAGE)
C        22        17       ZONE FUEL FRACTIONS (MULTIPLE RUN AVERAGE)
C        23        18       ZONE BURNED FUEL (MULTIPLE RUN AVERAGE)
C        24        19       PRIMARY OUTPUT (MULTIPLE RUN AVERAGE)
C        26        25       DISTRIBUTIONS (MULTIPLE RUN AVERAGE)
C
C VARIABLES
C
C              CA1INJ -  CRANK ANGLE START OF INJECTION (ATDC)
C                 CAD -  CRANK ANGLE BETWEEN DISTRIBUTION OUTPUTS
C               CATOM -  NUMBER OF CARBON ATOMS IN FUEL
C               CBETA -  SCALING CONSTANT FOR MIXING INTENSITY
C                  CP -  SPECIFIC HEAT (cal/g-k)
C                 CPF -  FUEL SPECIFIC HEAT (cal/g-K)
C               CRANK -  CRANK ANGLE (DEGREES ATDC)
C              CRANKD -  CRANK OF PREVIOUS DISTRIBUTION OUTPUT (ATDC)
C              CRKMAX -  CRANK ANGLE END OF RUN (ATDC)
C                CTOF -  FUEL CARBON MASS PER UNIT FUEL MASS
C                  DT -  BASIC TIMESTEP (s)
C                 DEL -  FUEL C:H RATIO
C              DELTAP -  SMM PRESSURE DIFFERENCE SINCE LAST MDM
C                          UPDATE(atm)
C                DTPR -  TIMESTEP FOR PRINTING OUTPUT(s)
C               DTKIN -  MINIMUM TIME BETWEEN CHEMISTRY UPDATES (S)
C                 CAD -  CRANK ANGLE INCREMENT FOR DISTRIBUTION OUTPUT
C                ELMM -  ELEMENT MASS (g)
C               ERMAX -  ERROR CRITERION FOR TEMP ROUTINES (fraction)
C              FERMAX -  FLOW ERROR TOLERANCE (g)
C                FML0 -  LIQUID FUEL INJECTED DURING MDM TIMESTEP (g)
C                FUEL -  CHARACTER VARIABLE CONTAINING NAME OF FUEL
C               HEVAP -  FUEL SENSIBLE+LATENT HEAT OF EVAPORATION(cal/g)
C                 HFG -  FUEL LATENT HEAT (cal/g)
C               HFUEL -  FUEL VAPOR ENTHALPY AT TSAT (cal/g)
C                  ID -  CHARACTER VARIABLE, SPECIFIED SIMULATION ID
C              ITMAXV -  MAX ITERATIONS FOR VOLUME CONSERVATION ROUTINE
C               IX,IY -  RANDOM NUMBER SEEDS
C               LLIMT -  LOWER LIMIT OF COMBUSTION (FMF)
C              MAXITS -  MAXIMUM NUMBER OF ITERATIONS FOR TEMP ROUTINES
C                NAME -  NAME OF MDM RUN USED
C                  NA -  TOTAL NUMBER OF ZONES OR NUMBER OF AIR ZONE
C                 NAV -  NUMBER OF SMM RUNS USED FOR AVERAGING
C                NCYC -  NUMBER OF MDM UPDATES
C              NELAIR -  NUMBER OF ELEMENTS IN AIR ZONE(ACTIVE+INACTIVE)
C              NELTOT -  TOTAL NUMBER OF ACTIVE ELEMENTS (ALL ZONES)
C                  NF -  ZONE FLOW NUMBER
C              NLINES -  NUMBER OF LINES IN OUTPUT PAGE
C              NPRINT -  SPECIFIES OUTPUT FORMAT
C                          NPRINT=1 - WRITES ALL OUTPUT FILES
C                          NPRINT=2 - WRITES LOGICAL UNITS 15-19
C                          NPRINT=3 - WRITES 15-19,25
C                          NPRINT=4 - WRITES 13-19,25
C                          NPRINT=5 - WRITES 13,14,19
C
C                  NZ -  ZONE NUMBER
C              NZONES -  NUMBER OF SMM ZONES NOT INCLUDING AIR ZONE
```

```
C                  P -  SMM PRESSURE (atm)-CALCULATED
C               PMDM -  MDM INPUT PRESSURE (ATM)
C                PHI -  FUEL-AIR EQUIVALENCE RATIO
C             PHICON -  STOICHIOMETRIC AIR - FUEL RATIO
C              PHIHI -  PHI UPPER COMBUSTION LIMIT
C             PHILOW -  PHI LOWER COMBUSTION LIMIT
C                PSI -  N2/O2 RATIO FOR INLET AIR
C             PSTART -  PRESSURE AT CRANK=CA1INJ (atm)
C               RHOL -  FUEL DENSITY (g/cc)
C                RPM -  ENGINE SPEED
C             SOTSIZ -  INITIAL SOOT PARTICLE RADIUS FOR FORMATION (cm)
C              SOOTC -  SOOT FORMATION RATE CORRECTION FACTOR
C             SVFUEL -  FUEL VAPOR SPECIFIC VOLUME AT TSAT (cc/g)
C                TFI -  FUEL TEMPERATURE AT INJECTION (K)
C               TIME -  CUMULATIVE SMM CLOCK TIME (s)
C             TIMEPR -  TIME OF PREVIOUS BASIC PRINTOUT (s)
C             TIMMDM -  TIME END OF NEXT MDM CYCLE (s)
C             TMPROP -  TIME ROUTINE PROP LAST CALLED (s)
C              TSOOT -  MIN TEMP FOR SOOT OXIDATION (K)
C               TSAT -  FUEL SATURATION TEMPERATURE AT P=50ATM (K)
C              TWALL -  CYLINDER WALL TEMPERATURE (K)
C              ULIMT -  UPPER LIMIT OF COMBUSTION (FMF)
C             VERMAX -  MAX VOLUME ERROR IN VOL ROUTINE (FRAC)
C             WTFUEL -  FUEL MOLECULAR WEIGHT (g/gmol)
C                 ZH -  NO. OF HYDROGEN ATOMS IN THE FUEL
C                ZMA -  AIR ZONE TOTAL MASS (g)
C               ZMVA -  AIR ZONE FUEL VAPOR MASS (g)
C              ZMBFA -  AIR ZONE BURNED FUEL MASS (g)
C
C ARRAYS
C
C            DFM(NF) -  RESIDUAL FLOW MASS (g) ADDED TO FM NEXT DT
C          DFMBF(NF) -  RESIDUAL FLOW BURNED FUEL MASS (g)
C           DFMV(NF) -  RESIDUAL FLOW FUEL VAPOR MASS (g)
C          DTMIX(NZ) -  TIME STEP BETWEEN MIXING FOR ZONE NZ (S)
C             FM(NF) -  TOTAL MASS FLOW (g)
C           FMBF(NF) -  BURNED FUEL MASS FLOW (g)
C            FMV(NF) -  FUEL VAPOR MASS FLOW (g)
C         NELMIX(NZ) -  NUMBER OF ELEMENTS MIXED IN ZONE NZ LAST
C                        TIMESTEP
C           NELS(NZ) -  NUMBER OF ACTIVE ELEMENTS IN ZONE NZ
C
C    NOTE: ELEMENTS IN THE AIR ZONE DO NOT BECOME ACTIVE UNTIL THEY ARE
C          REQUIRED FOR SOME SMM PROCESS, IE. MIXING, EVAPORATION,
C          FLOW.  THIS REDUCES RUN TIME BY NOT MIXING ELEMENTS THAT
C          AREN'T DOING ANYTHING. NELS(NA) = ACTIVE AIR ZONE ELEMENTS.
C          NELAIR = TOTAL AIR ZONE ELEMENTS.
C
C             NN(NF) -  NUMBER OF MASS FLOW ELEMENTS IN NEGATIVE
C                        DIRECTION
C             NP(NF) -  NUMBER OF MASS FLOW ELEMENTS IN POSITIVE
C                        DIRECTION
C          NUM(NZ,N) -  PROPERTY ARRAY NUMBER FOR ELEMENT N IN ZONE NZ
C         SOOTON(NZ) -  IF 'TRUE' SOOT MODEL ON IN ZONE NZ
C            TBF(NZ) -  TOTAL BURNED FUEL FOR ZONE NZ IN SMM
C             TBFMDM -  TOTAL BURNED FUEL ALL MDM ZONES (g)
C              TOTBF -  TOTAL BURNED FUEL ALL SMM ZONES (g)
C           TTBF(NZ) -  TOTAL BURNED FUEL FOR ZONE NZ IN MDM (g)
```

```
C           TTMEVAP -  TOTAL FUEL MASS EVAPORATED ALL ZONES (g)
C           TFMF(I) -  TOTAL FUEL MASS FRACTION FOR STORAGE ARRAY I
C        ZBETA(NZ) -  ZONE MIXING INTENSITY (1/s)
C         ZFMF(NZ) -  ZONE MEAN TOTAL FUEL MASS FRACTION
C       ZMEVAP(NZ) -  TOTAL FUEL MASS EVAPORATED IN ZONE NZ (g)
C          ZMV(NZ) -  ZONE FUEL VAPOR MASS (g)
C       ZMFBRN(NZ) -  MDM TOTAL BURNED FUEL ZONE NZ DURING TIMESTEP(g)
C        ZMVAP(NZ) -  RESIDUAL EVAPORATED FUEL IN ZONE NZ (g)
C          ZNO(NZ) -  MDM TOTAL NO IN ZONE NZ (g)
C       ZQWALL(NZ) -  ZONE WALL HEAT TRANSFER DURING TIMESTEP (cal)
C        ZTEMP(NZ) -  MDM MEAN ZONE TEMPERATURE ZONE NZ (K)
C        ZTIME(NZ) -  TIME OF LAST MIXING IN ZONE NZ (S)
C         ZVOL(NZ) -  ZONE VOLUME (cc)
C
C
C   PROPERTIES OF EACH ELEMENT ARE STORED IN THESE ARRAYS:
C        I=PROPERTY ARRAY ID. I IS RELATED TO AN ELEMENT NUMBER BY
C          I=NUM(NZ,N).  THIS MAPPING PROVIDES EFFICIENT MIXING
C          AND FLOW PROPERTY EXCHANGES AND REDUCES PAGE FAULTING.
C
C  ELEMT(I,1)   -    FUEL FRACTION OF BURNT FRACTION
C  ELEMT(I,2)   -    TEMPERATURE (K)
C  ELEMT(I,3)   -    BURNT GAS FRACTION (BGFR; INCLUDES AIR)
C  ELEMT(I,4)   -    SPECIFIC STANDARD ENTHALPY (CAL/G) 298K DATUM
C  ELEMT(I,5)   -    SPECIFIC HEAT [CP] (CAL/G-K)
C  ELEMT(I,6)   -    MOLECULAR WEIGHT
C  ELMT(I,1)    -    NITRIC OXIDE MASS FRACTION
C  ELMT(I,2)    -    EFFECTIVE AREA OF SOOT (CM**2)
C  ELMT(I,3)    -    MASS OF SOOT (G)
C  ELMT(I,4)    -    TIME OF LAST KINETIC UPDATE (SEC)
C
C SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        ERRSET (VAX/VMS ERROR CONTROL ROUTINE),EXIT (VAX/VMS FILE
C          CLOSING ROUTINE),INPUT,MIXING,OUTPUT,SMZ,TABLE,UTHRMO
C
C WRITTEN BY A.J.BROWN
C
      PROGRAM SMM
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      CHARACTER*12 IDX
      COMMON /ELEMT6/ NUM,TFMF
      PARAMETER(RBAR=1.9869,CCAL=.02421725)
C
C READ IN PROGRAM BASIC DATA
C
      CALL INPUT(1)
C
      CALL TABLE
C
      CALL ERRSET(70,.TRUE.,.FALSE.,.FALSE.,.FALSE.,15)
C
C PRELIMINARY CALCULATIONS
C
      DEL=CATOM/ZH
      PHICON=(32.+28.013*PSI)*(DEL+.25)/(12.0*DEL+1.008)
      LLIMT=PHILOW/(PHILOW+PHICON)
```

```
      ULIMT=PHIHI/(PHIHI+PHICON)
      CTOF = 12./(12. + 1.008/DEL)
      CALL UTHRMO(50.,TSAT,0.,0.,HFUEL,CP,WTFUEL)
      SVFUEL=TSAT*RBAR/(50.*CCAL*WTFUEL)
      HEVAP=-HFG-CPF*(TSAT-TFI)
C
C INPUT BASIC MDM DATA
C
      CALL INPUT(2)
C
C PRINT OUT TITLE PAGE, INPUT DATA AND RESULTS OF PRELIMINARY
C   CALCULATIONS
C
      IF(NPRINT.EQ.4.OR.NPRINT.EQ.5)CALL OUTPUT(1)
C
C PRINTOUT HEADINGS FOR VARIOUS OUTPUT FILES
C READ NUMBER OF RUNS INCLUDED IN OUTPUT AVERAGES
C
      IF(NPRINT.EQ.1)THEN
        DO 50 L=1,NZONES
          WRITE(L,1001)ID
 50     CONTINUE
      END IF
      ND=IFIX((CRKMAX-CA1INJ)/CAD)
      WRITE(9,1002)ID
      WRITE(19,1002)ID
      NAV=0
      IF(NOLD.GT.0)READ(24,1002)IDX
      IF(NOLD.GT.0)READ(24,*)NAV
      NAVP1=NAV+1
      WRITE(19,*)NAVP1
      IF(NPRINT.NE.5)THEN
        WRITE(15,1003)ID
        WRITE(16,1004)ID
        WRITE(17,1005)ID
        WRITE(18,1006)ID
      END IF
      IF((NPRINT.EQ.3.OR.NPRINT.EQ.4).AND.NOLD.GT.0)THEN
        WRITE(25,1000)NAME
        WRITE(25,*)CA1INJ,SWIRL,EGR
        WRITE(25,*)ND
        READ(26,1000)NAME
        READ(26,*)CA1INJ,SWIRL,EGR
        READ(26,*)ND
      ELSE IF(NPRINT.EQ.3.OR.NPRINT.EQ.4)THEN
        WRITE(25,1000)NAME
        WRITE(25,*)CA1INJ,SWIRL,EGR
        WRITE(25,*)ND
      END IF
 1000 FORMAT(A30)
      IF(NPRINT.NE.5.AND.NAV.NE.0)THEN
        READ(20,1007)IDX
        READ(21,1008)IDX
        READ(22,1009)IDX
        READ(23,1010)IDX
      END IF
      IF(NPRINT.NE.2.AND.NPRINT.NE.3)WRITE(13,1002)ID
 1001 FORMAT(30X,A15,/,30X,'ZONE DATA',/,1X,'CRANK',3X,
```

```
     1   'NELS',3X,'NP',4X,'NN',4X,'NEVAP',2X,'NMIX',6X,
     2   'DELP(%)')
 1002 FORMAT(30X,A15,/)
 1003 FORMAT(30X,A15,/,25X,'ZONE AVERAGE TEMPERATURES')
 1007 FORMAT(30X,A15,/)
 1004 FORMAT(30X,A15,/,27X,'ZONE FUEL FLOW ERRORS')
 1008 FORMAT(30X,A15,/)
 1005 FORMAT(30X,A15,/,30X,'ZONE AVERAGE FMF')
 1009 FORMAT(30X,A15,/)
 1006 FORMAT(30X,A15,/,30X,'ZONE FUEL BURNED')
 1010 FORMAT(30X,A15,/)
C*******************
C
C SET CLOCKS AND INITIAL PRESSURE, INITIALIZE VARIABLES.
C
      TIME=(CA1INJ+90.)/(RPM*6.)
      TIMMDM=TIME
      TIMEPR=TIME
      CRANKD=CA1INJ
      DT=0.
      DO 150 NZ=1,NA
        TMEVAP(NZ)=0.
        TBF(NZ)=0.
        TTBF(NZ)=0.
        ZTIME(NZ)=TIME
        ZMVAP(NZ)=0.
 150  CONTINUE
      DO 160 NF=1,NFLOW
        DFM(NF)=0.
        DFMV(NF)=0.
        DFMBF(NF)=0.
        NELS(NF)=0
 160  CONTINUE
      NELS(NA)=0
      P=PSTART
      PMDM=PSTART
      NCYC=0
      DO 170 N=1,MAXELE
        NUM(NA,N)=N
 170  CONTINUE
      NELTOT=0
C
C BEGIN SIMULATION ****************************************************
C
 200  TIME=TIME+DT
      IF(TIME.GE.TIMMDM) THEN
        TIME=TIMMDM
        CRANK=TIME*RPM*6.-90.
        CALL SMZ
C
C WRITE FLOW ELEMENT EXCHANGE ***
C
        IF(NPRINT.EQ.1)THEN
        DO 2110 NZ=1,NZONES
          IF(ZVOL(NZ).EQ.0.)GO TO 2110
          WRITE(NZ,2101) CRANK,NELS(NZ),NP(NZ),NN(NZ),
     1      NNEVAP(NZ),NELMIX(NZ),DELTAP
 2101     FORMAT(1X,F6.2,2X,I4,2X,I4,3X,I4,3X,I4,2X,I4,3X,G12.3)
```

```
          NNEVAP(NZ)=0
          NELMIX(NZ)=0
 2110   CONTINUE
        DELTAP=0.
        END IF
C**********
C
C TIME TO EXIT?
C
 2111   IF(CRANK.GT.CRKMAX)GO TO 300
      END IF
C
C MIX ZONES
C
 205  DO 210 NZ=1,NA
        IF(NELS(NZ).LT.2) GO TO 210
        IF(TIME.GE.(ZTIME(NZ)+DTMIX(NZ))) CALL MIXING(NZ)
 210  CONTINUE
      GO TO 200
 300  CALL EXIT
      END
C***********************************************************************
C***********************************************************************
C
C SUBROUTINE SMZ
C
C PURPOSE
C
C        COMPLETES PREVIOUS CYCLE. STARTS NEXT.
C        CALLS MDM INPUT.  CONTROLS FLOW OF
C        ELEMENTS TO THE SMZ'S.  HANDLES CONSERVATION OF COMPONENT
C        MASS, ENERGY AND VOLUME. CALCULATES ZONE MIXING TIMES.
C
C
C VARIABLES AND ARRAYS (SEE SMM)
C
      SUBROUTINE SMZ
C
C DECLARATIONS AND COMMON BLOCKS
C
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      PARAMETER(CCAL=.02421725)
      DIMENSION ELMT(MAXELE,4),ELEMT(MAXELE,6)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      COMMON /ELEMT6/ NUM,TFMF
C
C IF THIS IS THE START OF CYCLE 1?
C
      IF(NCYC.EQ.0)THEN
        CALL INPUT(3)
        NCYC=1
        NELAIR=IFIX(ZMA/ELMM)+1
        GO TO 191
      END IF
C
```

```
C FINISH CYCLE
C
C
C CALCULATE HEAT TRANSFER FOR EACH ELEMENT.
C
      DO 100 NZ=1,NZONES
        IF(NELS(NZ).LT.1)GO TO 100
        CALL QWALL(NZ)
        DO 50 LI=1,NELS(NZ)
          I=NUM(NZ,LI)
C
C UPDATE SOOT, NO, PREP, COMBUSTION.
C
          IF((TIME-ELMT(I,4)).LT.DTKIN)GO TO 50
          CALL PROP(TIME,NZ,I)
 50     CONTINUE
 100  CONTINUE
C
C UPDATE PREP AND COMBUSTION FOR ACTIVE AIR ZONE ELEMENTS
C
      DO 105 LI=1,NELS(NA)
        I=NUM(NA,LI)
        DTPROP=TIME-ELMT(I,4)
        IF(DTPROP.LT.DTKIN)GO TO 105
        ELMT(I,4)=TIME
        CALL PREPUP(DTPROP,I)
        CALL CMBUST(NA,I,0)
 105  CONTINUE
C
C CONSERVE VOLUME. CALCULATE NEW TEMPERATURES AND PRESSURE.
C
      CALL VOL
C
C****************
C
C UPDATE TOTALS
C
      DO 110 NZ=1,NA
        TTBF(NZ)=TTBF(NZ)+ZMFBRN(NZ)
 110  CONTINUE
C
C TIME TO EXIT?
C
      IF(CRANK.LE.CRKMAX) GO TO 150
      IF(NPRINT.EQ.4.OR.NPRINT.EQ.5)CALL OUTPUT(8)
      RETURN
C
C TIME TO WRITE OUTPUT?
C
 150  IF(TIME.LT.(TIMEPR+DTPR)) GO TO 155
      TIMEPR=TIME
      CALL OUTPUT(2)
C
C TIME TO WRITE DISTRIBUTION?
C
 155  IF(CRANK.LT.(CRANKD+CAD).OR.NPRINT.EQ.2.OR.
     1  NPRINT.EQ.5)GO TO 190
      CRANKD=CRANK
```

```
      CALL DISTRIB
C
C END OF CYCLE *******
C
C*****************************************************
C
C START NEW CYCLE ****
C
  190 CALL INPUT(3)
      NCYC=NCYC+1
C
C CALCULATE NET FLOWS IN EACH DIRECTION.
C
  191 DO 200 NF=1,NFLOW
        FM(NF)=FM(NF)+DFM(NF)
        DFM(NF)=0.
        FMV(NF)=FMV(NF)+DFMV(NF)
        DFMV(NF)=0.
        FMBF(NF)=FMBF(NF)+DFMBF(NF)
        DFMBF(NF)=0.
  200 CONTINUE
      DO 250 NF=1,NFLOW
        IF(ZVOL(NF).LE.0.)THEN
          NP(NF)=NELS(NF)
          NN(NF)=0.
        ELSE IF(FM(NF).GT.0.) THEN
          NP(NF)=IFIX(FM(NF)/ELMM)
          NN(NF)=0
        ELSE IF(FM(NF).LT.0.) THEN
          NP(NF)=0
          NN(NF)=IFIX(-FM(NF)/ELMM)
        ELSE
          NP(NF)=0
          NN(NF)=0
        END IF
  250 CONTINUE
C
      CALL FLOW
C
C EVAPORATE THE FUEL.  ADD VAPOR ELEMENTS TO THE ZONES.
C
      DO 300 NZ=1,NA
C
C CLEAN UP THE CLOSING OF A ZONE
C
        IF(ZVOL(NZ).LE.0..AND.NZ.NE.NA)THEN
          ZMEVAP(NZ+1)=ZMEVAP(NZ+1)+ZMEVAP(NZ)
          ZMVAP(NZ+1)=ZMVAP(NZ+1)+ZMVAP(NZ)
          ZMEVAP(NZ)=0.
          ZMVAP(NZ)=0.
          GO TO 300
        END IF
C
C UPDATE EVAPORATION
C
        TMEVAP(NZ)=TMEVAP(NZ)+ZMEVAP(NZ)
        NNEVAP(NZ)=IFIX(TMEV[illegible]LMM)-IFIX((TMEVAP(NZ)-
     1   ZMEVAP(NZ))/ELMM)
```

```
        ZMEVAP(NZ)=ZMEVAP(NZ)+ZMVAP(NZ)
        ZMVAP(NZ)=0.
C
C ADD VAPOR ELEMENTS TO ZONES
C
        IF(NZ.EQ.NA)THEN
          NELX=NELAIR
        ELSE
          NELX=NELS(NZ)
        END IF
        IF(ZMEVAP(NZ).GT.ELMM.AND.NELX.GT.1)THEN
          CALL EVAP(NZ)
        ELSE
          ZMVAP(NZ)=ZMEVAP(NZ)
        END IF
 300  CONTINUE
C
C CALCULATE NEW DTMIX
C
      DT=TIMMDM-TIME
      DO 400 NZ=1,NA
        IF(NELS(NZ).LT.0)NELS(NZ)=0
        IF(ZBETA(NZ).LE.0.)GO TO 400
        IF(NELS(NZ).LT.2)GO TO 400
        DTMIX(NZ)=1./(ZBETA(NZ)*NELS(NZ))
        DT=AMIN1(DT,DTMIX(NZ))
 400  CONTINUE
      RETURN
      END
C*********************************************************************
C*********************************************************************
C   SUBROUTINE SOOT(DTPROP,O2,I) - WANG MODEL
C
C        PURPOSE
C
C             TO CALCULATE THE FORMATION OF SOOT DUE TO PYROLYSIS OF
C             FUEL VAPOR.
C
C        METHOD
C
C             THE SOOT FORMATION RATE IS CALCULATED VIA THE RELATIONS
C             OF WANG,MATULA,AND FARMER DEVELOPED FOR SYNTHETIC FUELS.
C             (20TH SYMPOSIUM ON COMBUSTION. THE COMBUSTION INSTITUTE,
C             1981. PG. 1149.)
C             IMPORTANT PARAMETERS ARE  [HC],  [O2], AND TEMPERATURE.
C
C
C VARIABLES
C
C             (SEE SMM)
C             UFUELF - UNBURNED FUEL FRACTION
C             FUELC  - FUEL CARBON IN ELEMENT (g)
C             HCCONC - UNBURNED FUEL CONCENTRATION, C2H2, G-MOLE/CC
C             O2CONC - UNBURNED OXYGEN CONCENTRATION, G-MOLE/CC
C             DSFDT  - SOOT MASS FORMATION RATE, G/S
C             MFORM  - SOOT MASS FORMED THIS CALCULATION, G
C             RUNIV  - UNIVERSAL GAS CONSTANT (cal/gmole-K)
C
```

```
C ARRAYS
C             (SEE SMM)
C
C COMMENTS
C
C          PRODUCTION OF MORE SOOT THAN THERE IS FUEL CARBON IN
C          A GIVEN ELEMENT IS NOT ALLOWED.
C
      SUBROUTINE SOOT(DTPROP,O2,I)
      INCLUDE 'SMMCOM.FOR'
      REAL MFORM
      DIMENSION ELEMT(MAXELE,6),ELMT(MAXELE,4)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT2/ ELMT
      PARAMETER(RHO=1.8,RUNIV=1.98,CCAL=.0242)
C
C SOOT FORMATION RATE CALCULATIONS
C
      IF(ELEMT(I,2) .LE. 300.)GO TO 120
      UFUELF=1.-ELEMT(I,3)
      FUELC=UFUELF*ELMM*CTOF-ELMT(I,3)
      IF(FUELC.LE.0.)FUELC=0.
      SV=RUNIV*ELEMT(I,2)/(P*CCAL*ELEMT(I,6))
      HCCONC=UFUELF/(SV*WTFUEL)
      O2CONC=O2/(ELEMT(I,6)*SV)
      TM=1800.
      IF(ELEMT(I,2).LE.TM)THEN
        GAMMA=0.
      ELSE
        GAMMA=1.
        TGAM=1./ELEMT(I,2)-1./TM
      END IF
      XCONC=1./(ELEMT(I,6)*SV)-HCCONC-O2CONC
      DSFDT=SOOTC*5.55E16*EXP(-41800./(RUNIV*ELEMT(I,2))-
     1        GAMMA*48100.*TGAM/RUNIV)*((1.54*HCCONC)**2.59)*
     2        (XCONC**.13)/(O2CONC**.71)
      DSFDTMX=SOOTC*1.04E13*EXP(-29700./(RUNIV*ELEMT(I,2))+
     1        GAMMA*39700.*TGAM/RUNIV)*((1.54*HCCONC)**1.48)*
     2        (XCONC**.24)
      IF(DSFDT.GT.DSFDTMX)DSFDT=DSFDTMX
C
C          SOOT MASS CHANGE
C
      MFORM=DSFDT*DTPROP*ELMM*SV
      IF(MFORM.LE.0.) GO TO 120
      IF(MFORM.LE.FUELC) GO TO 30
      MFORM = FUELC
 30   ELMT(I,3)=ELMT(I,3)+MFORM
C
C          SOOT SURFACE AREA CHANGE
C
      ELMT(I,2)=ELMT(I,2)+3.*MFORM/(RHO*SOTSIZ)
 120  RETURN
      END
C*****************************************************************
C*****************************************************************
C
C SUBROUTINE SORT1
```

```
C
C PURPOSE
C   SORTS ZONE ELEMENTS INTO 3 GROUPS: THOSE CONTAINING FUEL
C     VAPOR, THOSE WITH SIGNIFICANT BURNED FUEL AND OTHER. FOR
C     ZONE NF OR NZ.
C
C VARIABLES AND ARRAYS (ALSO SEE SMM)
C   NEL1 - NUMBER OF ELEMENTS IN GROUP 1
C   NEL2 - NUMBER OF ELEMENTS IN GROUP 2
C   NEL3 - NUMBER OF REMAINING ELEMENTS
C   NEXT1 - ARRAY OF ELEMENTS IN GROUP 1
C   NEXT2 - ARRAY OF ELEMENTS IN GROUP 2
C   NEXT3 - ARRAY OF OTHER ELEMENTS
C   TFMFS - LOWER LIMIT FOR MASS FRACTION OF BURNED FUEL IN GROUP 2.
C           STOICHIOMETRIC TFMF EXCEPT FOR VERY LEAN ZONES WHERE
C           TFMFS IS SET TO LLIMT.
C
      SUBROUTINE SORT1(NZ)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION NEXT1(MAXELE),NEXT2(MAXELE),NEXT3(MAXELE)
      DIMENSION ELEMT(MAXELE,6)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT6/ NUM,TFMF
      COMMON /SORT/ NEL1,NEL2,NEL3,NEXT1,NEXT2,NEXT3
      NEL1=0
      NEL2=0
      NEL3=0
      TFMFS=1./(1.+PHICON)
      IF(ZFMF(NZ).LT.TFMFS)TFMFS=LLIMT
      IF(NELS(NZ).LE.0)GO TO 500
 200  DO 400 L=1,NELS(NZ)
        L1=NUM(NZ,L)
        IF(TFMF(L1).GT.ULIMT)THEN
          NEL1=NEL1+1
          NEXT1(NEL1)=L
        ELSE IF(ELEMT(L1,3)*ELEMT(L1,1).GT.TFMFS)THEN
          NEL2=NEL2+1
          NEXT2(NEL2)=L
        ELSE
          NEL3=NEL3+1
          NEXT3(NEL3)=L
        END IF
 400  CONTINUE
 500  RETURN
      END
C**************************************************************
C**************************************************************
C
C SUBROUTINE SORT2
C
C PURPOSE
C   SORTS ZONE ELEMENTS INTO 3 GROUPS: THOSE CONTAINING FUEL
C     VAPOR, THOSE WITH SIGNIFICANT BURNED FUEL AND OTHER. FOR
C     ZONE NFP1.
C
C VARIABLES AND ARRAYS (ALSO SEE SMM)
```

```
C   NEL4 - NUMBER OF ELEMENTS IN GROUP 1
C   NEL5 - NUMBER OF ELEMENTS IN GROUP 2
C   NEL6 - NUMBER OF REMAINING ELEMENTS
C   NEXT4 - ARRAY OF ELEMENTS IN GROUP 1
C   NEXT5 - ARRAY OF ELEMENTS IN GROUP 2
C   NEXT6 - ARRAY OF OTHER ELEMENTS
C   TFMFS - LOWER LIMIT FOR MASS FRACTION OF BURNED FUEL IN GROUP 2.
C           STOICHIOMETRIC TFMF EXCEPT FOR VERY LEAN ZONES WHERE
C           TFMFS IS SET TO LLIMT.
C
C
      SUBROUTINE SORT2(NZ)
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      DIMENSION NEXT4(MAXELE),NEXT5(MAXELE),NEXT6(MAXELE)
      DIMENSION ELEMT(MAXELE,6)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT6/ NUM,TFMF
      COMMON /SORTX/ NEL4,NEL5,NEL6,NEXT4,NEXT5,NEXT6
      NEL4=0
      NEL5=0
      NEL6=0
      TFMFS=1./(1.+PHICON)
      IF(ZFMF(NZ).LT.TFMFS)TFMFS=LLIMT
      IF(NELS(NZ).LE.0)GO TO 500
 200  DO 400 L=1,NELS(NZ)
        L1=NUM(NZ,L)
        IF(TFMF(L1).GT.ULIMT)THEN
          NEL4=NEL4+1
          NEXT4(NEL4)=L
        ELSE IF(ELEMT(L1,3)*ELEMT(L1,1).GT.TFMFS)THEN
          NEL5=NEL5+1
          NEXT5(NEL5)=L
        ELSE
          NEL6=NEL6+1
          NEXT6(NEL6)=L
        END IF
 400  CONTINUE
 500  RETURN
      END
C*****************************************************************
C*****************************************************************
C
C     SUBROUTINE SPECNO
C
C     PURPOSE
C        CALCULATES EQUILIBRIUM SPECIES CONCENTRATION NEEDED FOR
C        NO  CALCULATION
C
C     DESCRIPTION OF PARAMETERS
C        PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C        P          YES    NO       PRESSURE (ATM)
C        T          YES    NO       TEMPERATURE (K)
C        FR         YES    NO       FUEL FRACTION OF BURNED PRODUCTS
C        U1         NO     YES      EQUILIBRIUM MOLE FRACTION
C        __         __     ___      OF (NO)
```

```
C        U2          NO      YES       EQUILIBRIUM MOLE FRACTION
C        --          --      ---       OF  (O)*(N2)
C        U3          NO      YES       K1=R1/(R2+R3)    (SEE REPORT)
C
C
      SUBROUTINE SPECNO (P,T,FR,U1,U2,U3)
      COMMON/FULAR/CATOM,DEL,PSI,PHICON
      COMMON/TABLE5/A(2592),B(2592),C(2592)
      DIMENSION AP(6),AT(16),APHI(27)
      DATA AP /1.,10.,30.,50.,75.,100./
      DATA AT /1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,
     1  2600.,2700.,2800.,2900.,3000.,3200.,3500./
      DATA APHI /0.0,.2,.4,.6,.8,.9,.95,1.,1.05,1.1,1.2,1.3,1.4,1.5,
     1  1.6,1.8,2.,2.2,2.4,2.6,2.8,3.,3.2,3.4,3.6,3.8,4./
C
      PA=P
      TA=T
      PHI=PHICON*FR/(1.0-FR)
      PHIA=PHI
C
      IF(PA.LE.1.0)PA=1.0
      IF(PA.GE.100.)PA=100.
      IF(TA.LE.1700.)TA=1700.
      IF(TA.GE.3500.)TA=3500.
      IF(PHIA.LE.0.0)PHIA=0.0
      IF(PHIA.GE.4.0)PHIA=4.0
C
      I=1
      IF(PA.LT.10.)GO TO 10
      I=2
      IF(PA.LT.30.)GO TO 10
      I=3
      IF(PA.LT.50.)GO TO 10
      I=4
      IF(PA.LT.75.)GO TO 10
      I=5
   10 PA1=AP(I)
      PA2=AP(I+1)
C
      J=IFIX(PHIA/.2)+1
      IF(PHIA.LT..9)GOTO 20
      J=6
      IF(PHIA.LT.0.95)GOTO 20
      J=IFIX((PHIA-.95)/.05)+7
      IF(PHIA.LT.1.1)GOTO 20
      J=IFIX((PHIA-1.1)/.1)+10
      IF(PHIA.LT.1.6)GOTO 20
      J=IFIX((PHIA-1.6)/.2)+15
      IF(PHIA.LT.4.0)GOTO 20
      J=26
   20 PHI1=APHI(J)
      PHI2=APHI(J+1)
C
      K=IFIX((TA-1700.)/100.)+1
      IF(TA.GE.3000..AND.TA.LT.3200.)K=14
      IF(TA.GE.3200..AND.TA.LE.3500.)K=15
   30 TA1=AT(K)
      TA2=AT(K+1)
```

```
C
      IU1=I*432+J*16+K+1
      IU2=I*432+(J-1)*16+K+1
      IU3=I*432+(J-1)*16+K
      IU4=I*432+J*16+K
      IU5=(I-1)*432+J*16+K+1
      IU6=(I-1)*432+(J-1)*16+K+1
      IU7=(I-1)*432+(J-1)*16+K
      IU8=(I-1)*432+J*16+K
C
      R=(-PHI1+PHI+PHI-PHI2)/(PHI2-PHI1)
      S=(-TA1+TA+TA-TA2)/(TA2-TA1)
      V=(-PA1+PA+PA-PA2)/(PA2-PA1)
C
      H1=(1.+R)*(1.+S)*(1.+V)
      H2=(1.-R)*(1.+S)*(1.+V)
      H3=(1.-R)*(1.-S)*(1.+V)
      H4=(1.+R)*(1.-S)*(1.+V)
      H5=(1.+R)*(1.+S)*(1.-V)
      H6=(1.-R)*(1.+S)*(1.-V)
      H7=(1.-R)*(1.-S)*(1.-V)
      H8=(1.+R)*(1.-S)*(1.-V)
C
      U1=0.125*(H1*A(IU1)+H2*A(IU2)+H3*A(IU3)+H4*A(IU4)+
     &H5*A(IU5)+H6*A(IU6)+H7*A(IU7)+H8*A(IU8))
      U1=EXP(U1)
      U2=0.125*(H1*B(IU1)+H2*B(IU2)+H3*B(IU3)+H4*B(IU4)+
     &H5*B(IU5)+H6*B(IU6)+H7*B(IU7)+H8*B(IU8))
      U2=EXP(U2)
      U3=0.125*(H1*C(IU1)+H2*C(IU2)+H3*C(IU3)+H4*C(IU4)+
     &H5*C(IU5)+H6*C(IU6)+H7*C(IU7)+H8*C(IU8))
      U3=EXP(U3)
C
      RETURN
      END
C*****************************************************************
C*****************************************************************
C
C     SUBROUTINE SPECO2
C
C     PURPOSE
C        CALCULATES EQUILIBRIUM SPECIES CONCENTRATION OF
C        OXYGEN MOLECULE IN BURNED PRODUCTS OF COMBUSTION
C
C     DESCRIPTION OF PARAMETERS
C        PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C        P          YES    NO       PRESSURE (ATM)
C        T          YES    NO       TEMPERATURE (K)
C        FR         YES    NO       FUEL FRACTION OF BURNED PRODUCTS
C        U4         NO     YES      EQUILIBRIUM MOLE FRACTION
C        -          -      -        OF (O2)
C
      SUBROUTINE SPECO2 (P,T,FR,U4)
      COMMON/FULAR/CATOM,DEL,PSI,PHICON
      COMMON/TABLE6/D(2592),E(2592)
      DIMENSION AP(6),AT(16),APHI(27)
      DATA AP /1.,10.,30.,50.,75.,100./
```

```
      DATA AT /1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,
     1  2600.,2700.,2800.,2900.,3000.,3200.,3500./
      DATA APHI /0.0,.2,.4,.6,.8,.9,.95,1.,1.05,1.1,1.2,1.3,1.4,1.5,
     1  1.6,1.8,2.,2.2,2.4,2.6,2.8,3.,3.2,3.4,3.6,3.8,4./
C
      PA=P
      TA=T
      PHI=PHICON*FR/(1.0-FR)
      PHIA=PHI
C
      IF(PA.LE.1.0)PA=1.0
      IF(PA.GE.100.)PA=100.
      IF(TA.LE.1700.)TA=1700.
      IF(TA.GE.3500.)TA=3500.
      IF(PHIA.LE.0.0)PHIA=0.0
      IF(PHIA.GE.4.0)PHIA=4.0
C
      I=1
      IF(PA.LT.10.)GO TO 10
      I=2
      IF(PA.LT.30.)GO TO 10
      I=3
      IF(PA.LT.50.)GO TO 10
      I=4
      IF(PA.LT.75.)GO TO 10
      I=5
   10 PA1=AP(I)
      PA2=AP(I+1)
C
      J=IFIX(PHIA/.2)+1
      IF(PHIA.LT.0.9)GOTO 20
      J=6
      IF(PHIA.LT.0.95)GOTO 20
      J=IFIX((PHIA-.95)/.05)+7
      IF(PHIA.LT.1.1)GOTO 20
      J=IFIX((PHIA-1.1)/.1)+10
      IF(PHIA.LT.1.6)GOTO 20
      J=IFIX((PHIA-1.6)/.2)+15
      IF(PHIA.LT.4.0)GOTO 20
      J=26
   20 PHI1=APHI(J)
      PHI2=APHI(J+1)
C
      K=IFIX((TA-1700.)/100.)+1
      IF(TA.GE.3000..AND.TA.LT.3200.)K=14
      IF(TA.GE.3200..AND.TA.LE.3500.)K=15
   30 TA1=AT(K)
      TA2=AT(K+1)
C
      IU1=I*432+J*16+K+1
      IU2=I*432+(J-1)*16+K+1
      IU3=I*432+(J-1)*16+K
      IU4=I*432+J*16+K
      IU5=(I-1)*432+J*16+K+1
      IU6=(I-1)*432+(J-1)*16+K+1
      IU7=(I-1)*432+(J-1)*16+K
      IU8=(I-1)*432+J*16+K
C
```

```
      R=(-PHI1+PHI+PHI-PHI2)/(PHI2-PHI1)
      S=(-TA1+TA+TA-TA2)/(TA2-TA1)
      V=(-PA1+PA+PA-PA2)/(PA2-PA1)
C
      H1=(1.+R)*(1.+S)*(1.+V)
      H2=(1.-R)*(1.+S)*(1.+V)
      H3=(1.-R)*(1.-S)*(1.+V)
      H4=(1.+R)*(1.-S)*(1.+V)
      H5=(1.+R)*(1.+S)*(1.-V)
      H6=(1.-R)*(1.+S)*(1.-V)
      H7=(1.-R)*(1.-S)*(1.-V)
      H8=(1.+R)*(1.-S)*(1.-V)
C
      U4=0.125*(H1*D(IU1)+H2*D(IU2)+H3*D(IU3)+H4*D(IU4)+
     &H5*D(IU5)+H6*D(IU6)+H7*D(IU7)+H8*D(IU8))
      U4=EXP(U4)
C
      RETURN
      END
C*****************************************************************
C*****************************************************************
C
C     SUBROUTINE TABLE
C
C     PURPOSE
C        READS AND STORES A TABLE OF THERMODYNAMIC PROPERTIES OF
C        UNBURNED MIXTURE AND BURNED PRODUCTS AS WELL AS EQUILIBRIUM
C        SPECIES CONCENTRATION OF BURNED PRODUCTS.
C
      SUBROUTINE TABLE
      COMMON/FULAR/CATOM,DEL,PSI,PHICON
      COMMON/TABLE1/UHTBL(96),UCTBL(96),UWTBL(96),UHFTBL(96)
      COMMON/TABLE3/BHTBL(2688),BCTBL(2688),BWTBL(2688),BHFTBL(2688)
      COMMON/TABLE5/A(2592),B(2592),C(2592)
      COMMON/TABLE6/D(2592),E(2592)
C
      READ(12,10)(UHTBL(I),I=1,96)
      READ(12,20)(UCTBL(I),I=1,96)
      READ(12,30)(UWTBL(I),I=1,96)
      READ(12,10)(UHFTBL(I),I=1,96)
   10 FORMAT(2X,10F7.1)
   20 FORMAT(2X,10F7.3)
   30 FORMAT(2X,10F7.2)
C
      READ(12,10)(BHTBL(I),I=1,2688)
      READ(12,20)(BCTBL(I),I=1,2688)
      READ(12,30)(BWTBL(I),I=1,2688)
      READ(12,10)(BHFTBL(I),I=1,2688)
      READ(12,40)(A(I),I=1,2592)
      READ(12,40)(B(I),I=1,2592)
      READ(12,40)(C(I),I=1,2592)
      READ(12,40)(D(I),I=1,2592)
      READ(12,40)(E(I),I=1,2592)
   40 FORMAT(5(1E14.7,1X))
      RETURN
      END
C*****************************************************************
C*****************************************************************
```

```
C
C     SUBROUTINE UTEMP
C
C     PURPOSE
C        GIVEN P, H, FR, AND BGFR OF UNBURNED MIXTURE, CALCULATES T
C
C     DESCRIPTION OF PARAMETERS
C        PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C        TGUESS     YES    NO       INITIAL GUESS FOR TEMPERATURE (K)
C        FR         YES    NO       SEE REMARKS
C        BGFR       YES    NO       SEE REMARKS
C        ENTHLP     YES    NO       ENTHALPY (CAL/G)
C        T          NO     YES      CALCULATED TEMPERATURE (K)
C        ERMAX      YES    NO       RELATIVE ERROR TOLERANCE (SEE
C        ------     ---    --       SUBROUTINES UTEMP AND BTEMP)
C        MAXITS     YES    NO       MAXIMUM NUMBER OF ITERATIONS (SEE
C        -------    ---    --       SUBROUTINES UTEMP AND BTEMP)
C        N          YES    NO       ELEMENT PROPERTY ARRAY
IDENTIFICATION
C                                          NUMBER
C        NZ         YES    NO       ZONE IDENTIFICATION NUMBER
C        WTBG        NO    YES      MOLECULAR WT OF BURNED GAS
C
C     REMARKS
C        1.-BGFR                    = FRACTION OF FUEL VAPOR IN THE
C        -------                    MIXTURE
C        FR                         = FUEL FRACTION OF BURNED PRODUCTS
C        --                         IN MIXTURE TIMES MASS FRACTION OF
C        --                         BURNED PRODUCTS IN THE MIXTURE,
C        --                         THEN, DIVIDED BY "BGFR".
C        --                         "BGFR".
C     FOR EXAMPLE:
C     1)  FOR PURE AIR              FR=0.0    AND    BGFR=1.0
C     2)  FOR PURE FUEL VAPOR       FR=0.0    AND    BGFR=0.0
C     3)  FOR A MIXTURE OF
C         10% FUEL VAPOR AND
C         20% BURNED PRODUCTS WITH
C         FUEL FRACTION OF 0.08 AND
C         70% AIR                   FR=.20*.08/(.20+.70)=0.0155   AND
C                                   BGFR=.20+.70=.90
C         THEREFORE                 FR=0.0155 AND    BGFR=0.90
C
C
      SUBROUTINE UTEMP (TGUESS,FR,BGFR,ENTHLP,T,N)
      INCLUDE 'SMMCOM.FOR'
      DIMENSION ELEMT(MAXELE,6)
      COMMON /ELEMT1/ ELEMT
      T=TGUESS
      DO 10 I=1,MAXITS
      CALL UTHRMO (P,T,FR,BGFR,AHG,CSUBP,WT)
      TTOLD=T
      T=T+(ENTHLP-AHG)/(CSUBP)
      IF(ABS((T-TTOLD)/T).LE.ERMAX)GOTO 20
   10 CONTINUE
      CALL OUTPUT(9)
   20 ELEMT(N,5)=CSUBP
      ELEMT(N,6)=WT
```

```
      RETURN
      END
C*********************************************************************
C*********************************************************************
C
C     SUBROUTINE UTHRMO
C
C     PURPOSE
C        CALCULATES THERMODYNAMIC PROPERTIES OF UNBURNED MIXTURE
C
C     USAGE
C        CALL UTHRMO (P,T,FR,BGFR,H,CP,WT)
C
C     DESCRIPTION OF PARAMETERS
C        PARAMETER  INPUT  OUTPUT   DESCRIPTION
C
C        P          YES    NO       PRESSURE (ATM)
C        T          YES    NO       TEMPERATURE (K)
C        FR         YES    NO       SEE REMARKS
C        BGFR       YES    NO       SEE REMARKS
C        H          NO     YES      ENTHALPY OF MIXTURE (CAL/G)
C        CP         NO     YES      HEAT CAPACITY AT CONSTANT PRESSURE
C        —          ——     —        OF MIXTURE (CAL/G K)
C        WT         NO     YES      MOLECULAR WEIGHT OF MIXTURE (G/MOLE)
C
C
C     REMARKS
C        1.-BGFR                    = FRACTION OF FUEL VAPOR IN THE
C        ———————                    MIXTURE
C        FR                         = FUEL FRACTION OF BURNED PRODUCTS
C        —                          IN MIXTURE TIMES MASS FRACTION OF
C        —                          BURNED PRODUCTS IN THE MIXTURE,
C        —                          THEN, DIVIDED BY "BGFR".
C        —                          "BGFR".
C     FOR EXAMPLE:
C     1)  FOR PURE AIR              FR=0.0    AND     BGFR=1.0
C     2)  FOR PURE FUEL VAPOR       FR=0.0    AND     BGFR=0.0
C     3)  FOR A MIXTURE OF
C         10% FUEL VAPOR AND
C         20% BURNED PRODUCTS WITH
C         FUEL FRACTION OF 0.08 AND
C         70% AIR                   FR=.20*.08/(.20+.70)=0.0155   AND
C                                   BGFR=.20+.70=.90
C         THEREFORE                 FR=0.0155 AND     BGFR=0.90
C
C
C     SUBROUTINE AND FUNCTION SUBPROGRAMS REQUIRED
C        BTHRMO
C
      SUBROUTINE UTHRMO (P,T,FR,BGFR,H,CP,WT)
      COMMON/TABLE1/UHTBL(96),UCTBL(96),UWTBL(96),UHFTBL(96)
      COMMON/FULAR/CATOM,DEL,PSI,PHICON
      DIMENSION AT(8),APHI(12),FCF(6)
      DATA AT /300.,500.,700.,900.,1100.,1300.,1500.,1700./
      DATA APHI/0.0,0.8,.9,1.0,1.1,1.2,1.5,2.,2.5,3.,3.5,4./
C
C
C-----------------------------------------------------------------------
```

```
C  THE FOLLOWING DATA IS GOOD FOR DIESEL (C10.8 H18.7) ONLY.
C  STANDARD ENTHALPY, 298K DATUM.
C
      DATA FCF/-9.1063,246.97,-143.74,32.329,.0518,-50.128/
      DATA WTV/148.6/
C
C-----------------------------------------------------------------------
C
C
C
      PHI=FR*PHICON/(1.-FR)
      PHIA=PHI
      VA=1.-BGFR
      TA=T
C
      IF(PHIA.LE.0.0)PHIA=0.
      IF(PHIA.GE.4.0)PHIA=4.0
      IF(TA.LE.300.)TA=300.
      IF(TA.GT.1700.)GO TO 30
C
      I=IFIX((TA-300.)/200.)+1
      IF(TA.GE.1500.)I=7
      IF(TA.LT.500.)I=1
      TA1=AT(I)
      TA2=AT(I+1)
C
      K=11
      IF(PHIA.GE.3.5)GOTO 20
      K=IFIX((PHIA-1.5)/.5)+7
      IF(PHIA.GE.1.5.AND.PHIA.LT.3.5)GOTO 20
      K=6
      IF(PHIA.GE.1.2.AND.PHIA.LT.1.5)GOTO 20
      K=IFIX((PHIA-0.8)/.1)+2
      IF(PHIA.GE..8.AND.PHIA.LT.1.2)GOTO 20
      K=1
   20 PHI1=APHI(K)
      PHI2=APHI(K+1)
C
      IU1=K*8+I+1
      IU2=(K-1)*8+I+1
      IU3=(K-1)*8+I
      IU4=K*8+I
C
      R=(-PHI1+PHI+PHI-PHI2)/(PHI2-PHI1)
      S=(-TA1+T+T-TA2)/(TA2-TA1)
C
      H1=(1.+R)*(1.+S)
      H2=(1.-R)*(1.+S)
      H3=(1.-R)*(1.-S)
      H4=(1.+R)*(1.-S)
C
      HU=.25*(H1*UHTBL(IU1)+H2*UHTBL(IU2)+
     &H3*UHTBL(IU3)+H4*UHTBL(IU4))
      CPU=.25*(H1*UCTBL(IU1)+H2*UCTBL(IU2)+
     &H3*UCTBL(IU3)+H4*UCTBL(IU4))
      WTU=.25*(H1*UWTBL(IU1)+H2*UWTBL(IU2)+
     &H3*UWTBL(IU3)+H4*UWTBL(IU4))
      GO TO 40
```

```
   30 CALL BTHRMO (P,T,FR,HU,CPU,WTU,SVU)
   40 ST=T/1000.
      HV=(((FCF(4)/4.*ST+FCF(3)/3.)*ST+FCF(2)/2.)*ST+
     &FCF(1))*ST-FCF(5)/ST+FCF(6)
      CPV=((FCF(4)*ST+FCF(3))*ST+FCF(2))*ST+FCF(1)+FCF(5)/(ST*ST)
      HV=1000.*HV/WTV
      CPV=CPV/WTV
C
      H=HU*BGFR+HV*VA
      CP=CPU*BGFR+CPV*VA
      WT=WTU*WTV/(WTU*VA + WTV*BGFR)
      RETURN
      END
C**************************************************************
C**************************************************************
C
C SUBROUTINE VOL
C
C PURPOSE
C         CALCULATES PRESSURE AND ELEMENT TEMPERATURES TO MEET
C         TOTAL VOLUME CONSTRAINT.
C
C VARIABLES - SEE SMM
C
C ARRAYS - SEE SMM
C
C
C
      SUBROUTINE VOL
      INCLUDE 'SMMCOM.FOR'
      INCLUDE 'SMZCOM.FOR'
      DIMENSION ELEMT(MAXELE,6),SVOLD(MAXELE),TNEW(MAXELE)
      DIMENSION NUM(NA,MAXELE),TFMF(MAXELE)
      COMMON /ELEMT1/ ELEMT
      COMMON /ELEMT4/ SVOLD
      COMMON /ELEMT6/ NUM,TFMF
      PARAMETER(RBAR=1.9869,CCAL=.02421725,GAMMA=1.35)
      PNEW=P
      ITER=1
      TOTVOL=0.
      DO 50 NZ=1,NZONES
        IF(NELS(NZ).LT.1)GO TO 50
        TOTVOL=TOTVOL+ZVOL(NZ)
 50   CONTINUE
      TOTVOL=TOTVOL+ZVOL(NA)
 60   DELP=PNEW-P
      VOLNEW=0
      VOLAIR=ZVOL(NA)*(PMDM/PNEW)**(1./GAMMA)
C
      DO 100 NZ=1,NZONES
        IF(NELS(NZ).LT.1) GO TO 100
        DO 70 LN=1,NELS(NZ)
          N=NUM(NZ,LN)
          R=RBAR/ELEMT(N,6)
          DEN=1.-.5*R*DELP/(ELEMT(N,5)*PNEW)
          TNEW(N)=(ELEMT(N,2)+.5*DELP*CCAL*SVOLD(N)/ELEMT(N,5))/DEN
          VOLNEW=VOLNEW+TNEW(N)*R*ELMM/(PNEW*CCAL)
 70     CONTINUE
```

```
 100  CONTINUE
      VOLNEW=VOLNEW+VOLAIR
      VOLERR=ABS(VOLNEW/TOTVOL-1.)
      IF(VOLERR.LE.VERMAX) GO TO 140
      IF(ITER.GT.ITMAXV) THEN
        CALL OUTPUT(5)
        GO TO 140
      END IF
      PNEW=(VOLNEW/TOTVOL)*PNEW
      ITER=ITER+1
      GO TO 60
C
C  UPDATE AIR ZONE ACTIVE ELEMENTS
C
 140  IF(NELS(NA).LE.0)GO TO 200
      DO 150 LN=1,NELS(NA)
        N=NUM(NA,LN)
        R=RBAR/ELEMT(N,6)
        DEN=1.-.5*R*DELP/(ELEMT(N,5)*PNEW)
        ELEMT(N,2)=(ELEMT(N,2)+.5*DELP*CCAL*SVOLD(N)/
     1                  ELEMT(N,5))/DEN
        IF(ELEMT(N,3).LT.1.)THEN
          CALL UTHRMO(P,ELEMT(N,2),ELEMT(N,1),
     1     ELEMT(N,3),ELEMT(N,4),ELEMT(N,5),ELEMT(N,6))
        ELSE
          CALL BTHRMO(P,ELEMT(N,2),ELEMT(N,1),
     1     ELEMT(N,4),ELEMT(N,5),ELEMT(N,6))
        END IF
        SVOLD(N)=RBAR*ELEMT(N,2)/(P*CCAL*ELEMT(N,6))
 150  CONTINUE
 200  DO 300 NZ=1,NZONES
        IF(NELS(NZ).LT.1)GO TO 300
C
C UPDATE PROPERTIES AFTER CORRECTING VOLUME
C
        DO 250 LN=1,NELS(NZ)
          N=NUM(NZ,LN)
          ELEMT(N,2)=TNEW(N)
          IF(ELEMT(N,3).LT.1.)THEN
            CALL UTHRMO(P,ELEMT(N,2),ELEMT(N,1),
     1       ELEMT(N,3),ELEMT(N,4),ELEMT(N,5),ELEMT(N,6))
          ELSE
            CALL BTHRMO(P,ELEMT(N,2),ELEMT(N,1),
     1       ELEMT(N,4),ELEMT(N,5),ELEMT(N,6))
          END IF
          SVOLD(N)=RBAR*ELEMT(N,2)/(P*CCAL*ELEMT(N,6))
 250    CONTINUE
 300  CONTINUE
 400  DELTAP=DELP*100./P
      P=PNEW
      RETURN
      END
C********************************************************************
```

APPENDIX C

STOCHASTIC MIXING MODEL DETAILS

C.1 Slow Reaction Chemistry

The requirement for including the effect of turbulent fluctuations in modeling slow reaction rates can be demonstrated using a simple second order reaction: (see Section 2.2.1 for nomenclature)

$$a_1\chi_1 + a_2\chi_2 \xrightarrow{k_f} \text{products} \qquad (C.1)$$

Equations (2.9) and (2.10) reduce to:

$$\dot{\omega} = k_f\,(\rho\sigma_1)^{a_1'}\,(\rho\sigma_2)^{a_2'} \qquad (C.2)$$

$$k_f = A_f\,T^{\zeta_f}\exp(-E_f^+/T) \qquad (C.3)$$

where:

$$\rho\sigma_1 = \rho_1/W_1 \qquad \rho\sigma_2 = \rho_2/W_2 \qquad \rho = PW/RT$$

If:

$$a_1' = 1 \qquad a_2' = 1$$

Equation (C.2) becomes:

$$\dot{\omega} = k_f\rho^2\sigma_1\sigma_2 = A_f T^{\zeta_f - 2}(PW/R)^2\sigma_1\sigma_2\,\exp[-E_f^+/T] \qquad (C.4)$$

Applying a Reynold's decomposition with:

$$T = \bar{T} + T' \qquad \sigma_1 = \bar{\sigma}_1 + \sigma_1' \qquad \sigma_2 = \bar{\sigma}_2 + \sigma_2'$$

results in:

$$\dot{\omega} = A_f \, (\bar{T}+T')^{\zeta_f - 2} (PW/R)^2 (\bar{\sigma}_1 + \sigma_1')(\bar{\sigma}_2 + \sigma_2') \exp[-E_f^+/(\bar{T}+T')] \qquad (C.5)$$

Following the expansion scheme of Borghi [39], by applying series expansions for exp(x) and $(1+x)^\alpha$ and time averaging, Equation (C.5) may be rewritten as:

$$\bar{\dot{\omega}} = A_f \, (PW/R)^2 \, \bar{T}^{\zeta_f - 2} \bar{\sigma}_1 \bar{\sigma}_2 \exp[-E_f^+/\bar{T}] \cdot \tilde{X} \qquad (C.6)$$

where:

$$\tilde{X} = 1 + \frac{\overline{\sigma_1' \sigma_2'}}{\overline{\sigma_1 \sigma_2}} + \left[\frac{P_2 + Q_2 + P_1 Q_1}{\bar{T}^2}\right] \overline{T'^2} + (P_1 + Q_1)\left[\frac{\overline{T' \sigma_1'}}{\bar{T}\bar{\sigma}_1} + \frac{\overline{T' \sigma_2'}}{\bar{T}\bar{\sigma}_2}\right] + P_1 \frac{\overline{T' \sigma_1' \sigma_2'}}{\bar{T}\bar{\sigma}_1 \bar{\sigma}_2}$$

$$+ P_2\left[\frac{\overline{T' T' \sigma_1'}}{\bar{T}^2 \bar{\sigma}_1} + \frac{\overline{T' T' \sigma_2'}}{\bar{T}^2 \bar{\sigma}_2}\right] + (P_3 + Q_3)\frac{\overline{T'^3}}{\bar{T}^3} + \ldots\ldots \qquad (C.7)$$

and:

$$P_n = \sum_{k=1}^{n} (-1)^{n-k} \frac{(n-1)!}{(n-k)![(k-1)!]^2 k} (E_f^+/\bar{T})^k$$

$$Q_n = \frac{(\zeta_f - 2)(\zeta_f - 1)\ldots\ldots(\zeta_f + 1 + n)}{n!}$$

Equation (C.6) is identical to the rate of reaction expression written in terms of local mean properties, but multiplied by a correction factor, X. This correction term is exact, assuming that pressure fluctuations and changes in molecular weight are not significant and that (T'/T)<1.

When turbulent fluctuations go to zero the value of X goes to 1. Terms containing products of fluctuation terms are dependent on the correlation of these fluctuations and X may be greater or less than one as a result of these correlation terms. If the activation energy E_f is high or the mean temperature T is low, P_n will increase very rapidly with n while Q_n decreases with n. This results in a correction term very different from one when slow reactions or low mean temperatures exist. For reactions with low activation energy or high mean temperatures the value of X is very nearly one and mean temperatures and concentrations may be used to calculate reaction rates with reasonable accuracy.

There are no simple methods for incorporating the effect of turbulent fluctuations on slow reaction chemistry into a computational reacting-flow model. Two approaches, probability density function (PDF) models and stochastic models have been used with some success in particular applications. The PDF approach uses a joint PDF to describe the chemical, thermodynamic and flow properties. This PDF contains all the information required to describe the reactive flow. Working from the basic turbulent flow conservation equations a single equation for this joint PDF can be derived. Using a Monte Carlo solution method, Pope [40] was able to solve this equation for some very simple geometries. The complexity and unsteadiness of diesel combustion makes this approach impractical for our application. Stochastic mixing models provide a less complete, but more computationally efficient method of dealing with this problem.

C.2 The Random Coalescence Model

In order to model more complex chemistry and include the effect of turbulent fluctuations within reasonable computational limits some compromises must be made in dealing with the flow details. The use of stochastic phenomenalogical models has gained broad·acceptance for steady flow chemical reactors, especially when some details of the flow and mixing are already known.

The development of these models has occurred gradually. Pratt [41] provides an excellent overview of this development. Danckwerts [42] and Zweitering [43] introduced the concept of "population balance" modeling in which the flow is described as an ensemble of fluid particles. Entry of reactant particles into the reactor is called a "birth" event and exit from the reactor is a "death" event. The time a particle spends in the reactor from birth to death is the particle "residence time". Two types of mixing may occur in these models.

1. Macromixing or backmixing is the large scale mixing of elements of different "ages" within a flow. It is typical of a recirculating flow. At any point within the flow particles have a distribution of ages. Macromixing is often characterized by a residence time distribution (RTD) which refers to the distribution of particle ages at exit. Macromixing does not consider mixing on a molecular level.

2. Micromixing or stream mixing refers to the mixing of particles on a molecular level.

Until the coalescence and dispersion model proposed by Curl [1], early applications of these concepts were limited to the extremes of perfect micromixing or no micromixing and perfect macromixing or no macromixing. Two examples of these are:

1. A plug flow reactor (PFR) in which groups of particles that enter together stay together (no macromixing). These groups of particles are either homogeneous on a molecular level (perfectly micromixed) or unmixed on a molecular level.

2. A perfectly sttirred reactor (PSR) where the flow is homogeneous in terms of particle age distribution (perfectly macromixed), and either homogeneous or unmixed on a molecular level.

Curl's model allowed for finite rate micromixing. His model assumed that initially segregated parcels are continuously fed into a perfectly stirred reactor (perfectly macromixed) having a constant parcel population. Randomly selected pairs of parcels are mixed on a molecular level (coalesced) according to a prescribed mixing rate and then separated again into two parcels of equal average intensive properties (dispersed). Finite rate batch chemistry proceeds continuously in each parcel during the time interval between mixings. Curl derived a differential equation based on this process to describe the concentration probability density function. Monte Carlo solutions of this equation for perfectly stirred reactors, plug flow reactors with finite rate micromixing, and series combinations of plug flow and perfectly stirred reactors have gained widespread use. [44,45,46] In our application various zones within the flow are assumed to be perfectly stirred reactors (perfectly macromixed) and finite rate micromixing within these zones is achieved using this technique.

The mixing rate specified in Curl's model represents the number of pairs of parcels mixed per unit time or the reciprocal of the characteristic micromixing time. An expression for the mixing rate, $\beta(t)$, was derived by Corrsin in an analysis of the exponential decay of concentration fluctuations in isotropic turbulence. [47] Despite Corrsin's rather restrictive assumptions, his results have been shown to work for more general reactive flows as long as the mixing rate is adequately large. [48,49]

For a single phase turbulent reacting flow with constant diffusivity and density, the species conservation equation, Equation (2.2), in indical notation is:

$$\frac{\partial \rho_m}{\partial t} + u_j \frac{\partial \rho_m}{\partial x_j} = D\nabla^2 \rho_m + \dot{\rho}_m^C \qquad \text{(C.8)}$$

Applying Reynold's decomposition and time averaging, assuming homogeneous isotropic turbulence, this becomes:

$$\frac{d\bar{\rho}_m}{dt} = \dot{\rho}_m^C \qquad \text{(C.9)}$$

where:

$$\rho_m = \bar{\rho}_m + \rho_m'$$

Subtracting (C.9) from (C.8), multiplying by ρ_m' and again time averaging results in:

$$\frac{d\overline{\rho_m'^2}}{dt} = -2D[\overline{\left(\frac{\partial \rho_m'}{\partial x_j}\right)\left(\frac{\partial \rho_m'}{\partial x_j}\right)} + 2\overline{\rho_m^{C'}\rho_m'} \qquad \text{(C.10)}$$

For isotropic turbulence:

$$\overline{\left(\frac{\partial \rho_m'}{\partial x_j}\right)\left(\frac{\partial \rho_m'}{\partial x_j}\right)} = 3\,\overline{\left(\frac{\partial \rho_m'}{\partial x}\right)^2} \qquad \text{(C.11)}$$

For fluctuations in concentration:

$$\lambda_m^2 = \left[\overline{\rho_m'^2} \,/\, \left(\overline{\frac{\partial \rho_m'}{\partial x}} \right)^2 \right] \tag{C.12}$$

is analogous to the Taylor microscale:

$$\lambda_T^2 = \left[\overline{u'^2} \,/\, \left(\overline{\frac{\partial u'}{\partial x}} \right)^2 \right]$$

where:

$$\frac{\lambda_T^2}{\lambda_m^2} = Sc$$

Substituting these expressions into Equation (C.10) yields:

$$\frac{d\overline{\rho_m'^2}}{dt} = -6\nu \frac{\rho_m'^2}{\lambda_T^2} + 2\overline{\rho_m^{C'} \rho_m'} \tag{C.13}$$

Considering only the effect due to mixing:

$$\frac{d\overline{\rho_m'^2}}{dt} = -6\nu \frac{\overline{\rho_m'^2}}{\lambda_T^2} = -\beta \overline{\rho_m'^2} \tag{C.14}$$

This differential equation represents an exponential decay of the species density turbulent variance:

$$\overline{\rho_m'^2}(t) = \overline{\rho_{mo}'^2} \exp(-\beta t) \qquad (C.15)$$

Although the coalescence/dispersion model is not intended to represent the details of the actual mixing process it does predict this same exponential decay.

Following the above analysis, the mixing rate for our coalescence/dispersion model may be expreessed in terms of physical turbulent flow properties:

$$\beta(t) = \frac{6\nu}{\lambda_T^2} = 6\nu \; \overline{\left(\frac{\partial u'}{\partial x} \right)^2} \Big/ \; \overline{u'^2} \approx \frac{\overline{u'}}{L} = \frac{50 \; C_\beta \mu_T}{\rho L^2} \qquad (C.16)$$

where L is equal to the subgid scale length. For our analysis, turbulent viscosity, μ_T, and the subgrid scale characteristic length are calculated as part of KIVA's multi-dimensional solution so that the mixing rate of each stochastic mixing zone may be calculated by the MDM. With a scaling factor of 50.0 included in Equation (C.16), a value of C_β near unity best reproduces the MDM results.

APPENDIX D

NASA PROGRAM INPUT

D.1 Equilibrium Data Input

Program SMM requires tables of composition and thermodynamic properties for the burned fuel mixture in order to calculate the thermodynamic state of elements, NO production and oxidation, and soot oxidation. For high temperatures, the burned gas mixture is assumed to be at equilibrium. For temperatures below 1700K, thermodynamic properties are calculated assuming that the mixture composition is frozen at 1700K. The NASA Equilibrium Code [50] is used to generate tables of composition and properties as a function of temperature (300K-3500K), pressure (1atm -100atm), and total equivalence ratio (0-4.0). Changes to the NASA Code and supplementary programs are listed in APPENDIX D.2. Standard enthalpy with a 298K datum is used for all calculations. Thermodynamic properties calculated are: standard enthalpy, specific heat at constant pressure, molecular weight and heat of formation at 298K. Compositions calculated are: U1, U2, U3, K1, K2, [O_2], [OH], and [CO]. (See Equation 3.16) The diesel fuel used is $C_{10.8}H_{18.7}$. Running command files NASA1, NASA2, NASA3, NASA4A, NASA4B, TABLE1, TABLE2 AND TABLE3, in that order, will generate the NASA Tables, file TBL1T7.DAT. Subroutine BTHRMO calculates the thermodynamic properties of burned elements and the burned gas fraction (BGFR) of unburned elements by interpolation in the NASA

Tables.

Subroutine UTHRMO calculates the thermodynamic properties of elements containing a mixture of unburned fuel vapor and burned gas. (BGFR<1.) An unburned element is assumed to consist of equilibrium burned gas (BGFR), whose properties are calculated by Subroutine BTHRMO, and unburned fuel vapor, whose properties are calculated using empirical expressions. Coefficients for calculating fuel vapor enthalpy and specific heat are from Reference [16].

D.2 FORTRAN Code

```
C*** NASA.FOR UPDATE ****************** MLS 12/83,AJB 6/85 *******
      DIMENSION ZEXTRA(10), YOUT(10,13)
      COMMON/SH/SENSH(13),ENTLPY
C************************************ MLS 12/83, AJB 6/85***********
      DATA ZEXTRA/4HCO2 ,4HH2O ,4HCO  ,4HH2  ,4HO2  ,4HN2  ,4HNO  ,
     &            4HO   ,4HN   ,4HOH  /
C*************************************** MLS 12/83, AJB 6/85********
      IF(CHFROZ) THEN
        CALL CHFRZN(NS,EQRAT)
        GO TO 4
      END IF
      IF(.NOT.THMON)GO TO 4
      CALL SHCALC(NS,NPT)
      DO 910 I=1,NPT
      WRITE(10,900) PPP(I), TTT(I), EQRAT, ENTLPY(I),SPHEAT(I),WM(I),
     1  SENSH(I)
  900 FORMAT(1X,1F10.1,1F10.1,1F10.2,1F12.1,1F10.3,1F10.2,1F12.1)
  910 CONTINUE
C******************************** MLS 12/83, AJB 6/85***************
      IF(CHFROZ.OR.THMON)GO TO 3000
      DO 1003 K=1,10
     DO 1002 I=1,NS
     IF(SUB(I,1).NE.ZEXTRA(K)) GO TO 1002
       DO 1001 I2=1,NPT
            YOUT(K,I2)=EN(I,I2)/TOTN(I2)
 1001       CONTINUE
         GO TO 1003
 1002     CONTINUE
 1003 CONTINUE
C
      DO 1009 I=1,NPT
       WRITE(11,1110) PPP(I), TTT(I), EQRAT, (YOUT(K,I), K=1,6)
       WRITE(12,1120) PPP(I), TTT(I), EQRAT, (YOUT(K,I), K=7,10)
```

```
 1009 CONTINUE
C
 1110 FORMAT(1X,1F10.1,1F10.1,1F10.2,6(2X,G12.5))
 1120 FORMAT(1X,1F10.1,1F10.1,1F10.2,4(2X,G12.5))
C*** CHFRZN.FOR ***********************************************
C
C SUBROUTINE CHFRZN(NS,EQRAT)
C
C PURPOSE
C        TO CALCULATE PROPERTIES OF BURNED MIXTURE WHOSE
C        COMPOSITION IS FROZEN AT 1700K.
C        INTENDED TO BE USED AS A SUBROUTINE OF
C        THE NASA CODE.
C
C ARRAYS
C        HFORM  -  HEAT OF FORMATION AT 298K(cal/g)
C        H      -  STANDARD ENTHALPY(cal/g) AT 298K DATUM
C        CP     -  SPECIFIC HEAT(cal/g-K)
C
C
      SUBROUTINE CHFRZN(NS,EQRAT)
      DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN,DELH
      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
     1  GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),
     2  TTT(13),VLM(13),TOTN(13)
      COMMON/SPECES/COEF(2,7,300),S(300),H0(300),DELN(300),DUMMY(300),
     1 EN(300,13),ENLN(300),A(20,300),SUB(300,3),IUSE(300),TEMP(150,2)
      R=1.9872
      NPT=1
      TT=298.15
      K=2
      HFORM=0.
C
C NOTE: THE HEAT OF FORMATION IS THE SAME AT ALL TEMPERATURES SINCE
C         THE COMPOSITION IS FROZEN BELOW 1700K.
C
      DO 400 J=1,NS
        HFORM=HFORM+(((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT
     1  +COEF(K,3,J)/3.)*TT+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+
     2  COEF(K,6,J)/TT)*EN(J,NPT)*TT*R
 400  CONTINUE
      DO 500 NT=1,8
        TT=100.+NT*200.
        H=0.
        CP=0.
        DO 100 J=1,NS
          K=1
          IF(TT.LE.1000.) K=2
          KK=0
          IF(COEF(K,1,J).NE.0.)GO TO 75
          KK=K
          K=1
```

```
            IF(KK.EQ.1)K=2
 75         H=H+(((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT+
     1        COEF(K,3,J)/3.)*TT+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+
     2        COEF(K,6,J)/TT)*R*TT*EN(J,NPT)
            CP=CP+((((COEF(K,5,J)*TT+COEF(K,4,J))*TT+
     1        COEF(K,3,J))*TT+COEF(K,2,J))*TT+COEF(K,1,J))*R*EN(J,NPT)
 100      CONTINUE
          WRITE(10,900)PPP(NPT),TT,EQRAT,H,CP,WM(NPT),HFORM
 500    CONTINUE
 900    FORMAT(1X,2F10.1,F10.2,F12.1,F10.3,F10.2,F12.1)
        RETURN
        END
C*** SHCALC.FOR ************************************************
C
C SUBROUTINE SHCALC(NS,NPT)
C
C PURPOSE
C          CALCULATES HEAT OF FORMATION BASED ON 298K DATUM FROM
C          STANDARD OR ASSIGNED ENTHALPY AS CALCULATED IN THE NASA
C          EQUILIBRIUM CODE. INTENDED TO BE USED AS A SUBROUTINE OF
C          THE NASA CODE.
C
C ARRAYS
C          SENSH   -  HT OF FORMATION AT 298K FOR MIXTURE COMPOSTION
C                       AT BURNED TEMPERATURE AND PRESSURE (CAL/G)
C          DELH    -  SPECIES HEAT OF FORMATION AT 298K (CAL/G)
C
        SUBROUTINE SHCALC(NS,NPT)
        DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN
        DOUBLE PRECISION DELH
        COMMON/SPECES/COEF(2,7,300),S(300),HO(300),DELN(300),DUMMY(300),
       1 EN(300,13),ENLN(300),A(20,300),SUB(300,3),IUSE(300),TEMP(150,2)
        COMMON/SH/SENSH(13),ENTLPY(13)
        DIMENSION DELH(300)
        R=1.9872
        TT=298.15
        DO 100 J=1,NS
          K=2
 50       DELH(J)=((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT+COEF(K,3,J)/
     1       3.)*TT+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+COEF(K,6,J)/TT
 100    CONTINUE
        DO 300 N=1,NPT
          SENSH(N)=0.
          DO 200 J=1,NS
            D=DELH(J)*EN(J,N)*TT*R
            SENSH(N)=SENSH(N)+D
 200      CONTINUE
 300    CONTINUE
        RETURN
        END
C*** NASA1.COM *****************************************************
$!     COMMAND PROCEDURE TO RUN NASA
$!
```

```
$ ON WARNING THEN EXIT
$ ON CONTROL_Y THEN EXIT
$!
$ DEFINE FOR003 [BROWN.NASA]NL;
$ DEFINE FOR004 [BROWN.NASA]NASA.DAT
$ DEFINE FOR005 [BROWN.NASA]NASA1.INP
$ DEFINE FOR006 [BROWN.NASA]NL;
$ DEFINE FOR010 [BROWN.NASA]NASA1.OUT
$!
$ RUN [BROWN.NASA]NASA
$!
$ EXIT
C*** NASA1.INP *******************************************************
REACTANTS
C 10.8   H 18.7                              100.    -53570.  G298.15  F
.69
N 1.561760 .41959 AR.009324C .000300         100.    -28.2    G298.15  0

NAMELIST
 $INPT2
    TP=.TRUE.
    P=60.
    ERATIO=.TRUE.
    MIX=1.0E-2,.8,.9,1.0,1.1,1.2,1.5,2.0,2.5,3.0,3.5,4.0
    T=1700.
    KASE=4
    TRNSPT=.FALSE.
    CHFROZ=.TRUE.
 $END
STOP
C*** NASA2.COM ******************************************************
$!     COMMAND PROCEDURE TO RUN NASA
$!
$ ON WARNING THEN EXIT
$ ON CONTROL_Y THEN EXIT
$!
$ DEFINE FOR003 [BROWN.NASA]NL;
$ DEFINE FOR004 [BROWN.NASA]NASA.DAT
$ DEFINE FOR005 [BROWN.NASA]NASA2.INP
$ DEFINE FOR006 [BROWN.NASA]NL;
$ DEFINE FOR010 [BROWN.NASA]NASA2.OUT
$!
$ RUN [BROWN.NASA]NASA
$!
$ EXIT
C*** NASA2.INP *****************************************************
REACTANTS
C 10.8   H 18.7                              100.    -53570.  G298.15  F
.69
N 1.561760 .41959 AR.009324C .000300         100.    -28.2    G298.15  0
```

```
NAMELIST
 $INPT2
    TP=.TRUE.
    P=1.,5.,10.,20.,30.,60.,100.
    ERATIO=.TRUE.
    MIX=.01,.3,.4,.5,.6,.7,.8,.85,.9
    T=1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,2600.,
        2700.,2800.,2900.,3000.,3200.,3500.
    KASE=1
    TRNSPT=.FALSE.
    CHFROZ=.FALSE.
 $END
STOP
C*** NASA3.COM ****************************************************
$!    COMMAND PROCEDURE TO RUN NASA
$!
$ ON WARNING THEN EXIT
$ ON CONTROL_Y THEN EXIT
$!
$ DEFINE FOR003 [BROWN.NASA]NL;
$ DEFINE FOR004 [BROWN.NASA]NASA.DAT
$ DEFINE FOR005 [BROWN.NASA]NASA3.INP
$ DEFINE FOR006 [BROWN.NASA]NL;
$ DEFINE FOR010 [BROWN.NASA]NASA3.OUT
$!
$ RUN [BROWN.NASA]NASA
$!
$ EXIT
C*** NASA3.INP ********************************************************
REACTANTS
C 10.8   H 18.7                         100.    -53570.  L298.15  F
.69
N 1.561760 .41959 AR.009324C .000300    100.    -28.2    G298.15  0

NAMELIST
 $INPT2
    TP=.TRUE.
    P=1.,5.,10.,20.,30.,60.,100.
    ERATIO=.TRUE.
    MIX=.95,1.0,1.05,1.1,1.2,1.35,1.5,1.75,2.0,2.25,2.5,2.75,3.0,3.5,4.0
    T=1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,2600.,
        2700.,2800..,2900.,3000.,3200.,3500.
    KASE=1
    TRNSPT=.FALSE.
    CHFROZ=.FALSE.
 $END
STOP
C*** NASA4A.COM ***************************************************
$!    COMMAND PROCEDURE TO RUN NASA
$!
$ ON WARNING THEN EXIT
$ ON CONTROL_Y THEN EXIT
```

```
$!
$ DEFINE FOR003 [BROWN.NASA]NL;
$ DEFINE FOR004 [BROWN.NASA]NASA.DAT
$ DEFINE FOR005 [BROWN.NASA]NASA4A.INP
$ DEFINE FOR006 [BROWN.NASA]NL;
$ DEFINE FOR011 [BROWN.NASA]NAS4A1.OUT
$ DEFINE FOR012 [BROWN.NASA]NAS4A2.OUT
$!
$ RUN [BROWN.NASA]NASA
$!
$ EXIT
C*** NASA4A.INP *******************************************************
REACTANTS
C 10.8   H 18.7                                  100.    -53570.  L298.15  F
.69
N 1.561760 .41959 AR.009324C .000300             100.    -28.2    G298.15  0

NAMELIST
 $INPT2
    TP=.TRUE.
    P=1.,10.,30.,50.,75.,100.
    ERATIO=.TRUE.
    MIX=.01,.2,.4,.6,.8,.9,.95,1.0,1.05,1.1,1.2,1.3,1.4,1.5,1.6
    T=1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,2600.,2700.,
       2800.,2900.,3000.,3200.,3500.
    KASE=1
    TRNSPT=.FALSE.
    CHFROZ=.FALSE.
    THMON=.FALSE.
    TRACE=1.E-20
 $END
STOP
C*** NASA4B.COM ************************************************
$!     COMMAND PROCEDURE TO RUN NASA
$!
$ ON WARNING THEN EXIT
$ ON CONTROL_Y THEN EXIT
$!
$ DEFINE FOR003 [BROWN.NASA]NL;
$ DEFINE FOR004 [BROWN.NASA]NASA.DAT
$ DEFINE FOR005 [BROWN.NASA]NASA4B.INP
$ DEFINE FOR006 [BROWN.NASA]NL;
$ DEFINE FOR011 [BROWN.NASA]NAS4B1.OUT
$ DEFINE FOR012 [BROWN.NASA]NAS4B2.OUT
$!
$ RUN [BROWN.NASA]NASA
$!
$ EXIT
C*** NASA4B.INP ******************************************************
```

```
REACTANTS
C 10.8   H 18.7                             100.    -53570.  L298.15  F
.69
N 1.561760 .41959 AR.009324C .000300        100.    -28.2    G298.15  0

NAMELIST
 $INPT2
    TP=.TRUE.
    P=1.,10.,30.,50.,75.,100.
    ERATIO=.TRUE.
    MIX=1.8,2.0,2.2,2.4,2.6,2.8,3.0,3.2,3.4,3.6,3.8,4.0
    T=1700.,1800.,1900.,2000.,2100.,2200.,2300.,2400.,2500.,2600.,2700.
       ,2800.,2900.,3000.,3200.,3500.
    KASE=1
    TRNSPT=.FALSE.
    CHFROZ=.FALSE.
    THMON=.FALSE.
    TRACE=1.E-20
 $END
STOP
C*** TABLE1.FOR ****************************************************
C
C THIS PROGRAM CALCULATES TABLE COEFICIENTS FROM NASA DATA
C  FOR TEMPERATURES BELOW 1700K WHERE THE CHEMISTRY IS FROZEN.
C  IT SHOULD BE THE FIRST RUN INPUT INTO TBL1T7.DAT.
C
      PROGRAM TABLE1
      DIMENSION H(96),CP(96),WM(96),SH(96)
      OPEN (UNIT=3, FILE='[BROWN.SMM]TBL1T7.DAT', STATUS='NEW')
      OPEN (UNIT=10, FILE='[BROWN.NASA]NASA1.OUT', STATUS='OLD')
      DO 100 N=1,96
        READ(10,901) X1,X2,X3,H(N),CP(N),WM(N),SH(N)
 100  CONTINUE
      WRITE(3,910) (H(N),N=1,96)
      WRITE(3,920) (CP(N),N=1,96)
      WRITE(3,930) (WM(N),N=1,96)
      WRITE(3,910) (SH(N),N=1,96)
      CLOSE (UNIT=3)
      CLOSE (UNIT=10)
      STOP
 901  FORMAT(1X,2F10.1,F10.2,F12.1,F10.3,F10.2,F12.1)
 910  FORMAT(2X,10F7.1)
 920  FORMAT(2X,10F7.3)
 930  FORMAT(2X,10F7.2)
      END
C*** TABLE2.FOR ****************************************************
C
C THIS IS THE SECOND PROGRAM FOR PROCESSING NASA TO TABLE DATA.
C   IT IS FOR BURNED PRODUCTS THERMO DATA. T>1700K.
      PROGRAM TABLE2
      DIMENSION H(24,7,16),CP(24,7,16),WM(24,7,16),SH(24,7,16)
```

```
      OPEN (UNIT=3, FILE='[BROWN.SMM]TBL1T7.DAT', STATUS='OLD' '
     1  ACCESS='APPEND')
      OPEN (UNIT=10, FILE='[BROWN.NASA]NASA2.OUT', STATUS='OLD')
      OPEN (UNIT=11, FILE='[BROWN.NASA]NASA3.OUT', STATUS='OLD')
      DO 100 I=1,9
        DO 100 J=1,7
          DO 100 K=1,16
            READ(10,901) X1,X2,X3,H(I,J,K),CP(I,J,K),WM(I,J,K),
     1        SH(I,J,K)
 100  CONTINUE
      DO 200 I=10,24
        DO 200 J=1,7
          DO 200 K=1,16
            READ(11,901) X1,X2,X3,H(I,J,K),CP(I,J,K),WM(I,J,K),
     1        SH(I,J,K)
 200  CONTINUE
      WRITE(3,910) (((H(I,J,K),K=1,16),I=1,24),J=1,7)
      WRITE(3,920) (((CP(I,J,K),K=1,16),I=1,24),J=1,7)
      WRITE(3,930) (((WM(I,J,K),K=1,16),I=1,24),J=1,7)
      WRITE(3,910) (((SH(I,J,K),K=1,16),I=1,24),J=1,7)
      CLOSE (UNIT=3)
      CLOSE (UNIT=10)
      CLOSE (UNIT=11)
      STOP
 901  FORMAT(1X,2F10.1,F10.2,F12.1,F10.3,F10.2,F12.1)
 910  FORMAT(2X,10F7.1)
 920  FORMAT(2X,10F7.3)
 930  FORMAT(2X,10F7.2)
      END
C*** TABLE3.FOR ***************************************************
      PROGRAM TABLE3
      DIMENSION A(27,6,16),B(27,6,16),C(27,6,16),D(27,6,16),
     1  E(27,6,16),F(27,6,16)
      REAL KK,K1,K2,K3
      OPEN (UNIT=3, FILE='[BROWN.SMM]TBL1T7.DAT', STATUS='OLD',
     1  ACCESS='APPEND')
      OPEN (UNIT=10, FILE='[BROWN.NASA]NAS4A1.OUT', STATUS='OLD')
      OPEN (UNIT=11, FILE='[BROWN.NASA]NAS4A2.OUT', STATUS='OLD')
      OPEN (UNIT=12, FILE='[BROWN.NASA]NAS4B1.OUT', STATUS='OLD')
      OPEN (UNIT=13, FILE='[BROWN.NASA]NAS4B2.OUT', STATUS='OLD')
      K3=4.1E13
      DO 100 I=1,15
        DO 100 J=1,6
          DO 100 K=1,16
            READ(10,901) X1,T,X2,XCO2,XH2O,XCO,XH2,XO2,XN2
            READ(11,902) X1,X2,X3,XNO,XO,XN,XOH
            A(I,J,K)=ALOG(XNO)
            XX=XO*XN2
            B(I,J,K)=ALOG(XX)
            K1=(7.6E+13)*EXP(-38000./T)
            K2=(1.5E+9)*EXP(-19500./T)
            KK=K1*XN2*XO/(K2*XN*XO2+K3*XN*XOH)
            C(I,J,K)=ALOG(KK)
```

```
          D(I,J,K)=ALOG(XO2)
          E(I,J,K)=ALOG(XOH)
          F(I,J,K)=ALOG(XCO)
  100 CONTINUE
      DO 200 I=16,27
        DO 200 J=1,6
          DO 200 K=1,16
          READ(12,901) X1,T,X2,XCO2,XH2O,XCO,XH2,XO2,XN2
          READ(13,902) X1,X2,X3,XNO,XO,XN,XOH
          A(I,J,K)=ALOG(XNO)
          XX=XO*XN2
          B(I,J,K)=ALOG(XX)
          K1=(7.16E+13)*EXP(-38000./T)
          K2=(1.5E+9)*EXP(-19500./T)
          KK=K1*XN2*XO/(K2*XN*XO2+K3*XN*XOH)
          C(I,J,K)=ALOG(KK)
          D(I,J,K)=ALOG(XO2)
          E(I,J,K)=ALOG(XOH)
          F(I,J,K)=ALOG(XCO)
  200 CONTINUE
      WRITE(3,910) (((A(I,J,K),K=1,16),I=1,27),J=1,6)
      WRITE(3,910) (((B(I,J,K),K=1,16),I=1,27),J=1,6)
      WRITE(3,910) (((C(I,J,K),K=1,16),I=1,27),J=1,6)
      WRITE(3,910) (((D(I,J,K),K=1,16),I=1,27),J=1,6)
      WRITE(3,910) (((E(I,J,K),K=1,16),I=1,27),J=1,6)
      WRITE(3,910) (((F(I,J,K),K=1,16),I=1,27),J=1,6)
      CLOSE (UNIT=3)
      CLOSE (UNIT=10)
      CLOSE (UNIT=11)
      CLOSE (UNIT=12)
      CLOSE (UNIT=13)
      STOP
  901 FORMAT(1X,2F10.1,F10.2,6(2X,G12.5))
  902 FORMAT(1X,2F10.1,F10.2,4(2X,G12.5))
  910 FORMAT(5(1E14.7,1X))
      END
C*****************************************************************
```

APPENDIX E

CHANGES TO KIVA FORTRAN CODE

```
C************* SMM INPUT AND NRL MOD*********************************
*I,DEFINE.29
C *********************************************************************
C +++ KIVA UPDATE DECK
C +++ MODIFIED FOR GENERATING INPUT TO STOCHASTIC MIXING MODEL BY ALAN
C +++ BROWN, MIT, 121185. FURTHER MODIFIED FOR USE ON NAVAL RESEARCH
C +++ LAB, WASHINGTON VAX/CRAY SYSTEM.
C
C USE OF INPUT VARIABLE LPR:
C   LPR=1  LONG PRINT
C   LPR=2  MDMOUT (OUTPUT FOR SMM)
C   LPR=3  PLOTDAT (GRAPHICS OUTPUT)
C   LPR=4  MDMOUT AND PLOTDAT
C   LPR=0  NONE OF THE ABOVE
C
C *********************************************************************
*D,COMD.7,8
      PARAMETER (NV=1200,LNXPYP=60,LNSP=12,LNRK=4,LNRE=6,NPAR=1000,
     1 LP=40,LCHOP=25,LVAP=67,NZMDM=10)
*I,COMD.26
      COMMON /LC8/ AAA8(1),BMV(NV),QCOMB(NV),QWALL(NV),DMEVAP(NV),
     1 TMFBRN(NZMDM),TMEVAP(NZMDM),TQCOMB(NZMDM),TQWALL(NZMDM),
     2 ZMOLD(NZMDM),ZMLOLD(NZMDM),ZMVOLD(NZMDM),ZMBFO(NZMDM),
     3 ZVOLO(NZMDM),TIMMDM,NCALL,ZZZ8
*D,KIVA.1,2
      PROGRAM KIVA
      OPEN(UNIT=4,FILE='MDMOUT',STATUS='NEW')
      OPEN(UNIT=5,FILE='ITAPE',STATUS='OLD')
      OPEN(UNIT=7,FILE='RDUMP',STATUS='OLD')
      OPEN(UNIT=8,FILE='WDUMP',STATUS='NEW')
      OPEN(UNIT=9,FILE='PLOTDAT',STATUS='NEW')
      OPEN(UNIT=12,FILE='KIVAOUT',STATUS='NEW')
*D,KIVA.29,30
      IF(NRK.GT.0.AND.T.GE.T1IGN) CALL CHEM
      IF(NRE.EQ.6.AND.T.GE.T1IGN) CALL CHMQGM
*D,BEGIN.5,16
*D,BEGIN.19,59
      NWLCM=LOC(ZZZ1)-LOC(AAA1)+1
      DO 10 N=1,NWLCM
   10 AAA1(N)=0.
      NWLCM=LOC(ZZZ2)-LOC(AAA2)+1
```

```
      DO 20 N=1,NWLCM
   20 AAA2(N)=0.
      NWLCM=LOC(ZZZ3)-LOC(AAA3)+1
      DO 30 N=1,NWLCM
   30 AAA3(N)=0.
      NWLCM=LOC(ZZZ4)-LOC(AAA4)+1
      DO 40 N=1,NWLCM
   40 AAA4(N)=0.
      NWLCM=LOC(ZZZ5)-LOC(AAA5)+1
      DO 50 N=1,NWLCM
   50 AAA5(N)=0.
      NWLCM=LOC(ZZZ6)-LOC(AAA6)+1
      DO 60 N=1,NWLCM
   60 AAA6(N)=0.
      NWLCM=LOC(ZZZ7)-LOC(AAA7)+1
      DO 70 N=1,NWLCM
   70 AAA7(N)=0.
      NWLCM=LOC(ZZZ8)-LOC(AAA8)+1
      DO 80 N=1,NWLCM
   80 AAA8(N)=0.
*I,CHEM.15
      BMV(I4)=0.
      QCOMB(I4)=0.
*I,CHEM.18
      SPDV=SPD(I4,1)
      SIEBEG=SIE(I4)
*I,CHEM.81
      BMV(I4)=VOL(I4)*(SPDV-SPD(I4,1))
      QCOMB(I4)=VOL(I4)*RO(I4)*(SIE(I4)-SIEBEG)
*D,CHEMEQ.1,133
*I,CHMQGM.33
      SIEBEG=SIE(I4)
*D,CHMQGM.125
*I,CHMQGM.143
      QCOMB(I4)=QCOMB(I4)+VOL(I4)*RO(I4)*(SIE(I4)-SIEBEG)
*D,CHOP.18
*D,CHOP.21
*D,CHOP.233
*I,EVAP.116
      DMEVAP(I4)=DMTOT(I4)
*I,FULOUT.9
      IF((LPR.NE.3).AND.(LPR.NE.4))GO TO 100
*D,FULOUT.18,19
  100 IF(LPR.EQ.1) CALL LNGPRT
*D,INJECT.70,72
  130 WRITE(12,200) T,NCYC
      CALL EXIT
*D,LAWALL.11
      DO 181 I=1,NX
      IF(F(I4).EQ.0.) GO TO 1801
      SIEOLD=SIE(I4)
*D,LAWALL.260
  180 QWALL(I4)=VOL(I4)*RO(I4)*(SIE(I4)-SIEOLD)
```

```
 1801 I4=I4+1
  181 CONTINUE
C*******************************************************************
*DECK MDMOUT
C
C SUBROUTINE MDMOUT
C
C PURPOSE
C
C         TO BE INCLUDED AS A SUBROUTINE IN KIVA.  WRITE NECESSARY
C         MDM DATA TO A TAPE FOR PROCESSING AND USE AS INPUT TO A
C         STOCHASTIC MIXING MODEL FOR PREDICTING EMISSIONS.
 C
C
      SUBROUTINE MDMOUT
C
C DECLARATION STATEMENTS AND COMMON BLOCKS
C
*CALL COMD
*CALL PART
      DIMENSION CELLM(NV),CMV(NV),CML(NV),CMBF(NV),CVOL(NV),CTEMP(NV),
     1  CQCOMB(NV),CBMV(NV),CMEVAP(NV),CQWALL(NV),CNO(NV),
     2  CAMU(NV)
      REAL MLIQ(NV)
      PARAMETER(CPE=2.389E-08)
      DIMENSION ZLLIMT(NZMDM),ZULIMT(NZMDM)
      DIMENSION ZM(NZMDM),ZML(NZMDM),ZMV(NZMDM),ZMBF(NZMDM),
     1  ZMFBRN(NZMDM),ZMEVAP(NZMDM),ZVOL(NZMDM),ZTEMP(NZMDM),
     2  ZQWALL(NZMDM),ZAMU(NZMDM),ZQCOMB(NZMDM),ZFMF(NZMDM),
     3  ZBETA(NZMDM),ZNO(NZMDM)
      DATA (ZLLIMT(L),L=1,NZMDM) /.2,.16,.12,.1,.08,.06,.04,.02,
     1  .005,0.0/
      DATA (ZULIMT(L),L=1,NZMDM) /1.0,.2,.16,.12,.1,.08,.06,.04,
     1  .02,.005/
C
      CPE2D=CPE*FAC2D
C
C           THESE CALCULATIONS ASSUME A HYDROCARBON REACTION
C             MECHANISM WITH THE FOLLOWING CHEMICAL SPECIES INVOLVED:
C             1-DIESEL, 2-02, 3-N2, 4-CO2, 5-H20, 6-H, 7-H2, 8-0, 9-N
C             10-OH, 11-CO, 12-NO
C
      IF((T-TIMMDM).LT.1.0E-05.AND.NCALL.GT.0)GO TO 200
C
      PAV=0.
      NC=0
C
      IF(NCALL.EQ.0)THEN
        CA1INJ=ATDC+T1INJ*RPM*6.
        WRITE(4,999)(NAME(N),N=1,10),CA1INJ,RPM
      END IF
  999 FORMAT(10A8,/,1X,F6.1,2X,F6.1)
```

```
C
C SUM ALL FLUID PARTICLES IN A CELL FOR THE CELL FLUID MASS
C
      DO 50 I4=1,IJKVEC
        MLIQ(I4)=0.
 50   CONTINUE
      IF(NP.LE.0)GO TO 101
      DO 100 N=1,NP
        I4=I4P(N)
        MLIQ(I4)=MLIQ(I4)+PI403R*PARTN(N)*RADP(N)**3
 100  CONTINUE
C
C CALCULATE ALL CELL PROPERTIES AT START OF INJECTION AND EVERY
C  DTMDM.
C
 101  DO 150 I4=1,IJKVEC
          IF(F(I4).LT..9) GO TO 150
          NC=NC+1
          CVOL(NC)=FAC2D*VOL(I4)
          CELLM(NC)=CVOL(NC)*RO(I4)
          CML(NC)=MLIQ(I4)*FAC2D
          CMV(NC)=CVOL(NC)*SPD(I4,1)
          CMBF(NC)=CVOL(NC)*(.273*SPD(I4,4)+.112*SPD(I4,5)+
     1     SPD(I4,6)+SPD(I4,7)+.059*SPD(I4,10)+.429*SPD(I4,11))
          CTEMP(NC)=CELLM(NC)*TEMP(I4)
C
C PRESSURE IN DYNES/CM**2
C
          PAV=PAV+P(I4)
C
C   ENERGY PROPERTIES MUST BE CONVERTED FROM ERGS TO CAL.
C
          CMEVAP(NC)=FAC2D*DMEVAP(I4)
          DMEVAP(I4)=0.
          CQWALL(NC)=CPE2D*QWALL(I4)
          CQCOMB(NC)=CPE2D*QCOMB(I4)
          CAMU(NC)=AMU(I4)*CVOL(NC)
          CBMV(NC)=FAC2D*BMV(I4)
          CNO(NC)=CVOL(NC)*SPD(I4,12)
 150  CONTINUE
C
C CONVERT PRESSURE UNITS TO ATM.
C
      PAV=PAV/(NC*1.01325E+06)
C
C INITIALIZE ZONE PROPERTIES.
C
      DO 160 NNZ=1,NZMDM
        ZM(NNZ)=0.
        ZML(NNZ)=0.
        ZMV(NNZ)=0.
        ZNO(NNZ)=0.
        ZMBF(NNZ)=0.
```

```
        ZVOL(NNZ)=0.
        ZTEMP(NNZ)=0.
        ZAMU(NNZ)=0.
        ZMFBRN(NNZ)=0.
        ZMEVAP(NNZ)=0.
        ZQWALL(NNZ)=0.
        ZQCOMB(NNZ)=0.
 160  CONTINUE
      NCELL=NC
      GO TO 250
C
C CALCULATE AND UPDATE CUMULATIVE ZONE PROPERTIES EVERY MDM
C  CYCLE.
C
 200  NC=0
      DO 240 I4=1,IJKVEC
             IF(F(I4).LT..9)GO TO 240
             NC=NC+1
C
C TO CALCULATE FMF
C
             CELLM(NC)=VOL(I4)*RO(I4)*FAC2D
             CMV(NC)=VOL(I4)*SPD(I4,1)*FAC2D
             CMBF(NC)=VOL(I4)*FAC2D*(.273*SPD(I4,4)+.112*SPD(I4,5)+
     1        SPD(I4,6)+SPD(I4,7)+.059*SPD(I4,10)+.429*SPD(I4,11))
C
C CUMULATIVE CELL PROPERTIES
C
             CBMV(NC)=FAC2D*BMV(I4)
             CMEVAP(NC)=FAC2D*DMEVAP(I4)
             DMEVAP(I4)=0.
             CQCOMB(NC)=CPE2D*QCOMB(I4)
             CQWALL(NC)=CPE2D*QWALL(I4)
 240  CONTINUE
C
C INITIALIZE CUMULATIVE ZONE PROPERTIES.
C
      DO 245 NNZ=1,NZMDM
        ZMFBRN(NNZ)=0.
        ZMEVAP(NNZ)=0.
        ZQWALL(NNZ)=0.
        ZQCOMB(NNZ)=0.
 245  CONTINUE
      NCELL=NC
C
C CALCULATE ZONE PROPERTIES
C
 250  DO 300 NC=1,NCELL
        IF(CELLM(NC).EQ.0.)GO TO 300
        FMF=(CMV(NC)+CMBF(NC))/CELLM(NC)
        DO 260 NNZ=1,NZMDM
          IF((FMF.GE.ZLLIMT(NNZ)).AND.(FMF.LT.ZULIMT(NNZ)))THEN
            NNNZ=NNZ
```

```
            GO TO 270
          END IF
 260    CONTINUE
 270    IF((T-TIMMDM).LT.1.0E-05.AND.NCALL.GT.0)GO TO 280
C
C INSTANTANEOUS ZONE PROPERTIES
C
        ZM(NNNZ)=ZM(NNNZ)+CELLM(NC)
        ZML(NNNZ)=ZML(NNNZ)+CML(NC)
        ZMV(NNNZ)=ZMV(NNNZ)+CMV(NC)
        ZMBF(NNNZ)=ZMBF(NNNZ)+CMBF(NC)
        ZNO(NNNZ)=ZNO(NNNZ)+CNO(NC)
        ZVOL(NNNZ)=ZVOL(NNNZ)+CVOL(NC)
        ZTEMP(NNNZ)=ZTEMP(NNNZ)+CTEMP(NC)
        ZAMU(NNNZ)=ZAMU(NNNZ)+CAMU(NC)
C
C CUMULATIVE ZONE PROPERTIES
C
 280    ZMFBRN(NNNZ)=ZMFBRN(NNNZ)+CBMV(NC)
        ZMEVAP(NNNZ)=ZMEVAP(NNNZ)+CMEVAP(NC)
        ZQWALL(NNNZ)=ZQWALL(NNNZ)+CQWALL(NC)
        ZQCOMB(NNNZ)=ZQCOMB(NNNZ)+CQCOMB(NC)
 300  CONTINUE
C
      DO 350 NNZ=1,NZMDM
C
C SUM CUMULATIVE PROPERTIES
C
        TMFBRN(NNZ)=TMFBRN(NNZ)+ZMFBRN(NNZ)
        TMEVAP(NNZ)=TMEVAP(NNZ)+ZMEVAP(NNZ)
        TQWALL(NNZ)=TQWALL(NNZ)+ZQWALL(NNZ)
        TQCOMB(NNZ)=TQCOMB(NNZ)+ZQCOMB(NNZ)
        IF((T-TIMMDM).LT.1.0E-05.AND.NCALL.GT.0)GO TO 350
C
C CALCULATE ZONE MEAN FMF,TEMP AND BETA EVERY DTMDM
C
        IF(ZM(NNZ).EQ.0.)THEN
          ZFMF(NNZ)=0.
          ZBETA(NNZ)=0.
          ZTEMP(NNZ)=0.
          GO TO 350
        END IF
        IF(CHARL.EQ.0.)THEN
          ZBETA(NNZ)=0.
          GO TO 340
        END IF
        ZBETA(NNZ)=ZAMU(NNZ)/(ZM(NNZ)*CHARL**2)
 340    ZFMF(NNZ)=(ZMV(NNZ)+ZMBF(NNZ))/ZM(NNZ)
        ZTEMP(NNZ)=ZTEMP(NNZ)/ZM(NNZ)
 350  CONTINUE
C
      IF((T-TIMMDM).LT.1.0E-05.AND.NCALL.GT.0)GO TO 800
C
```

```
      TIMMDM=T
      WRITE(4,904)TIMMDM,PAV
 904  FORMAT(1X,E13.5,1X,F8.4)
      WRITE(4,906)(ZM(K),K=1,NZMDM)
      WRITE(4,906)(ZML(K),K=1,NZMDM)
      WRITE(4,906)(ZMV(K),K=1,NZMDM)
      WRITE(4,906)(ZMBF(K),K=1,NZMDM)
      WRITE(4,906)(ZTEMP(K),K=1,NZMDM)
      WRITE(4,906)(TQCOMB(K),K=1,NZMDM)
      WRITE(4,906)(TMEVAP(K),K=1,NZMDM)
      WRITE(4,906)(TQWALL(K),K=1,NZMDM)
      WRITE(4,906)(TMFBRN(K),K=1,NZMDM)
      WRITE(4,906)(ZNO(K),K=1,NZMDM)
      WRITE(4,906)(ZVOL(K),K=1,NZMDM)
      WRITE(4,906)(ZFMF(K),K=1,NZMDM)
      WRITE(4,906)(ZBETA(K),K=1,NZMDM)
 906  FORMAT(1X,6E13.4)
C
      IF(NCALL.EQ.0)GO TO 800
C
C ZERO CUMULATIVE PROPERTIES AFTER WRITING (EVERY DTMDM),
C   BUT NOT AT START OF INJECTION.
C
      DO 700 NNZ=1,NZMDM
        TMFBRN(NNZ)=0.
        TMEVAP(NNZ)=0.
        TQCOMB(NNZ)=0.
        TQWALL(NNZ)=0.
 700  CONTINUE
C
 800  NCALL=NCALL+1
      RETURN
      END
*MOVEDK MDMOUT:LNGPRT
C*********************************************************************
*D,NEWCYC.6
*D,NEWCYC.53,56
  100 IF(MOD(NCYC,10).EQ.0) WRITE(12,200) NCYC,CRANK,T,DT,NS,
     1  NVS,GRIND,IDSP(1),TSPM(1),PM,AVP,PGS,IDDT
      IF(T.GE.T1INJ.AND.(LPR.EQ.2.OR.LPR.EQ.4)) CALL MDMOUT
*D,NEWCYC.60
*D,NEWCYC.69,76
*D,NEWCYC.85,86
      CALL EXIT
*D,PFIND.239,241
      CALL EXIT
*D,PRES.106,108
 200  WRITE(12,900)T,NCYC,NSUB
      CALL EXIT
*I,RINPUT.4
      DATA (RERF(K),K=1,21) / 0.,.04434039,.08885599,.1337269,.1791435,
     1  .2253121,.2724627,.3208583,.3708072,.4226803,.4769363,.5341591,
     2  .5951161,.6608545,.7328691,.8134198,.9061939,1.017902,1.163087,
```

```
     3  1.385904,2. /
C******** DIESEL FUEL MOD *********************************************
C
C  UPDATE TO CONVERT PHYSICAL PROPERTIES OF FUEL IN KIVA
C                TO DIESEL C10.8H18.7
C
C    ENTHALPY DATA FROM HEYWOOD/LORUSSO/ROSSINI: INTERPOLATED
C    ABOVE 1500K. FOR DIESEL MIX.
C
C    REMAINING DATA FROM VERGAFTIK PP. 284-285: PROPERTIES FOR
C    DODECANE ARE USED FOR LATENT HEAT, VAPOR PRESSURE,
C    TCRIT,SURFACE TENSION, AND DENSITY.
C
C    FOR DODECANE:   TCRIT=659K
C                    SURTEN AT 298K = 25.04 (CGS)
C                    LIQUID DENSITY AT 298K = .7452
C +++
C +++ INPUT LABELS TO IDENTIFY THE SPECIES
C +++
*D,RINPUT.8,23
      DATA (IDSP(N),N=1,12) /8H  DIESEL,8H      O2,8H      N2,
     1                       8H     CO2,8H     H2O,8H       H,
     2                       8H      H2,8H       O,8H       N,
     3                       8H      OH,8H      CO,8H      NO/
C +++
C +++ ENTHALPIES OF THE PURE SPECIES ARE FROM THE JANNAF TABLES.
C +++ INTERVALS ARE T=100(N-1),
C +++ UNITS ARE KCAL/MOLE. 1=DIESEL(C10.8H18.7), 2=O2, 3=N2, 4=CO2,
C +++ 5=H2O, 6=H, 7=H2, 8=O, 9=N, 10=OH, 11=CO, 12=NO
C +++
      DATA (HK(N,1),N=1,51) /0.0,1.24,2.49,6.98,13.13,20.73,29.6,
     1 39.57,50.46,62.14,74.5,87.41,100.81,114.63,128.82,143.36,
     2 157.89,172.43,186.97,201.5,216.04,230.58,245.11,259.65,
     3 274.19,288.72,303.26,317.8,332.33,346.87,361.41,375.95,
     4 390.48,405.02,419.56,434.09,448.63,463.17,477.7,492.24,
     5 506.78,521.31,535.85,550.39,564.92,579.46,594.,608.53,
     6 623.07,637.61,652.14/
*D,RINPUT.90,106
C
C +++
C +++ INPUT THE LATENT HEAT OF THE LIQUID, ALSO AT INTERVALS T=100(N-1).
C +++ DODECANE LATENT HEAT VALUES IN RANGE 300-600K (ERGS/G)
C
      DATA (HLATO(N),N=1,51) /5.160E9,4.64E9,4.12E9,3.6E9,
     1 3.08E9,2.56E9,9.4E8,44*0.0/
C +++
C +++ INPUT THE LIQUID VAPOR PRESSURE IN DYNES AT INTERVALS T=10(N-1).
C +++
      DATA (PVAP(N),N=1,LVAP) /27*0.0,1.23,3.73,9.73,2.37E2,
     1  5.32E2,1.11E3,2.19E3,4.07E3,7.24E3,1.23E4,2.02E4,
     2  3.2E4,4.91E4,7.34E4,1.07E5,1.52E5,2.13E5,2.91E5,
     3  3.917E5,5.186E5,6.765E5,8.706E5,1.106E6,1.389E6,1.73E6,
     4  2.1227E6,2.571E6,3.093E6,3.695E6,4.386E6,5.176E6,6.07E6,
```

```
     5  7.087E6,8.228E6,9.505E6,1.093E7,1.251E7,1.427E7,1.62E7,
     6  1.813E7/
C**********************************************************************
*I,RINPUT.118
      NZMAX=NZ
*D,RINPUT.176,177
*D,RINPUT.217
*D,RINPUT.264
*D,RINPUT.362,376
*D,RINPUT.387,392
  204 WRITE(12,440)
      GO TO 209
  205 WRITE(12,430)
      GO TO 209
  206 WRITE(12,460)
  209 CALL EXIT
*D,SETUP.290
*D,STATE.44,46
  100 WRITE(12,110) T,NCYC,I,J,K,I4,TEMP(I4),SIE(I4),IT,CRANK
      CALL EXIT
*D,TAPERD.9,10
*D,TAPERD.14,31
      NWSCM=LOC(ZZ)-LOC(AA)+1
      READ(7) (AA(N),N=1,NWSCM)
      IF(NTD.NE.NDUMP) GO TO 40
      NWLCM=LOC(ZZZ1)-LOC(AAA1)+1
      READ(7) (AAA1(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ2)-LOC(AAA2)+1
      READ(7) (AAA2(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ3)-LOC(AAA3)+1
      READ(7) (AAA3(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ4)-LOC(AAA4)+1
      READ(7) (AAA4(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ5)-LOC(AAA5)+1
      IF(NP.GT.0) READ(7) (AAA5(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ6)-LOC(AAA6)+1
      IF(NP.GT.0) READ(7) (AAA6(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ7)-LOC(AAA7)+1
      IF(NP.GT.0) READ(7) (AAA7(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ8)-LOC(AAA8)+1
      READ(7) (AAA8(N),N=1,NWLCM)
      WRITE(12,100) NDUMP,T,NCYC,CRANK
*D,TAPERD.35,38
*D,TAPERD.45,47
 40   WRITE(12,110)NDUMP,NTD
      CALL EXIT
*D,TAPEWR.10,33
      NWSCM=LOC(ZZ)-LOC(AA)+1
      WRITE(8) (AA(N),N=1,NWSCM)
      NWLCM=LOC(ZZZ1)-LOC(AAA1)+1
      WRITE(8) (AAA1(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ2)-LOC(AAA2)+1
      WRITE(8) (AAA2(N),N=1,NWLCM)
```

```
      NWLCM=LOC(ZZZ3)-LOC(AAA3)+1
      WRITE(8) (AAA3(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ4)-LOC(AAA4)+1
      WRITE(8) (AAA4(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ5)-LOC(AAA5)+1
      IF(NP.GT.0) WRITE(8) (AAA5(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ6)-LOC(AAA6)+1
      IF(NP.GT.0) WRITE(8) (AAA6(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ7)-LOC(AAA7)+1
      IF(NP.GT.0) WRITE(8) (AAA7(N),N=1,NWLCM)
      NWLCM=LOC(ZZZ8)-LOC(AAA8)+1
      WRITE(8) (AAA8(N),N=1,NWLCM)
      WRITE(12,100) NDUMP,T,NCYC,CRANK
      NDUMP=NDUMP-1
*D,TIMSTP.69,71
*D,TIMSTP.79,81
      CALL EXIT
*DECK CBRT
      FUNCTION CBRT(A)
      THIRD=1./3.
      CBRT=A**THIRD
      RETURN
      END
*MOVEDK VSTRES:CBRT
C********* HEAT FLUX MOD*******************************************
*D,LAWALL.101
      FLUX=2.0*CP*(TBAR-TWALL)*ABS(TAUW/VEL)
*D,LAWALL.178
      FLUX=2.0*CP*(TBAR-TWALL)*ABS(TAUW/VEL)
*D,LAWALL.258
      FLUX=2.0*CP*(TBAR-TWALL)*ABS(TAUW/VEL)
C********* FUEL SPRAY CONSTANT DIFFUSIVITY MOD ************************
*IDENT TKEFUDRR
*D,PMOVTV.40,PMOVTV.45
      IF(IMOM.GT.99999 .OR. TURBT(N).GT.T)GOTO 30
      QT=.1*(U(IMOM)*U(IMOM)+V(IMOM)*V(IMOM)+W(IMOM)*W(IMOM))
      TEDDYSZ=169.5/(SQRT(QT)+1.E-10)
      TSC1=TEDDYSZ/(SQRT(QT)+1.E-10)
      VRELED=SQRT((UN(IMOM)-UP(N))**2+(VN(IMOM)-VP(N))**2
     1            +(WN(IMOM)-WP(N))**2)
      TSC2=TEDDYSZ/(VRELED+1.E-10)
C******** PARTICLE DIFFUSION MOD *************************************
*IDENT PARDIF
*D,PMOVTV.48
      IF(TSCALE.GE.DT)GO TO 25
      RELVEL(N)=SQRT((UN(IMOM)-UP(N))**2+(VN(IMOM)-VP(N))**2+
     1  (WN(IMOM)-WP(N))**2)
      I4=I4P(N)
      VRELT=RELVEL(N)
      TG=TP(N)+THIRD*(TEMP(I4)-TP(N))
      VISCP=AIRMU1*TG*SQRT(TG)/(TG+AIRMU2)
      REYP=AMAX1(1.0E-10,2.0*RO(I4)*RADP(N)*VRELT/VISCP)
      CD=CVMGT(.424,24./REYP*(1.0+SIXTH*REYP**TWOTHD),REYP.GT.1000.)
```

```
      DRAGDT=.375*RO(I4)*VRELT*CD*DT/(RHO*RADP(N))
      ATD=DRAGDT/DT*TSCALE
      EXPATD=EXP(ATD)
      EXPMATD=1./EXPATD
      EXP2ATD=EXPATD**2
      TERM1=(1.-EXPMATD)**4
      TERM2=EXP2ATD/(EXP2ATD-1.)
      DTOTD=DT/TSCALE
      EXPATD=EXP(DRAGDT)
      TERM3=DTOTD-(1.-1./EXPADT**2)/(1.-EXPMATD**2)
      TERM4=(ATD-1.+EXPMATD)**2*DTOTD
      FSUBX=SQRT(TERM1*TERM2*TERM3+TERM4)
      FSUBXO=DRAGDT-1.+1./EXPADT
      TURVEL=TURVEL*FSUBX/FSUBXO
*I,PMOVTV.63
      IF(TSCALE.LT.DT) GO TO 40
C******* ENHANCED DIFFUSIVITY MOD***************************
*D,TIMSTP.8
      IF(T.LT.T2IGN)GO TO 4
      IF(RPR.LT.3.)RPR=RPR+.01
      IF(RSC.LT.3.)RSC=RSC+.01
      IF(ATKE.LT..6)ATKE=ATKE+.003
      IF(AO.LT.1.0)THEN
        AO=AO+.005
        AOME=AO
        AOMOM=AO
      END IF
      IF(BO.GT.0)BO=BO-.005
 4    DTCON=1.E+20
C*****************************************************
```

APPENDIX F

PROCESSING PROGRAM (PRCMDM1)

```
C************************************************
      PROGRAM PRCMDM1
C
C  PROGRAM PRCMDM1
C
C  WRITTEN BY: A.J.BROWN
C
C  REDUCES 10 ZONE RAW DATA FROM KIVA TO 10 ZONE SMM INPUT.
C
C
      PARAMETER(NF=9,NZ=10,NZP1=11)
      DIMENSION ZQCOMB(NZ),ZMEVAP(NZ),ZQWALL(NZ),ZVOL(NZ),ZFMF(NZ),
     2  ZBETA(NZ),ZMFBRN(NZ),ZM(NZ),ZNO(NZ),ZML(NZ),ZMV(NZ),
     3  ZMBF(NZ),ZTEMP(NZ)
      DIMENSION ZMOLD(NZ),ZMLOLD(NZ),ZMVOLD(NZ),ZMBFO(NZ),
     1  ZVOLO(NZ)
      DIMENSION FM(NF),FML(NF),FMV(NF),FMBF(NF),B(NZ)
      CHARACTER*30 NAME
      READ(11,901)NAME,CA1INJ,RPM
      WRITE(4,901)NAME,CA1INJ,RPM
      READ(12,*)CA1INJ,SWIRL,EGR,T2IGN
      WRITE(4,*)CA1INJ,SWIRL,EGR
      READ(12,*)N
      N1=N-1
      WRITE(4,*)N1
      DO 50 I=1,NZ
       B(I)=0.
 50   CONTINUE
      DO 100 I=1,N
        READ(11,905)T,P
        READ(11,906)(ZM(K),K=1,NZ)
        READ(11,906)(ZML(K),K=1,NZ)
        READ(11,906)(ZMV(K),K=1,NZ)
        READ(11,906)(ZMBF(K),K=1,NZ)
        READ(11,906)(ZTEMP(K),K=1,NZ)
        READ(11,906)(ZQCOMB(K),K=1,NZ)
        READ(11,906)(ZMEVAP(K),K=1,NZ)
        READ(11,906)(ZQWALL(K),K=1,NZ)
        READ(11,906)(ZMFBRN(K),K=1,NZ)
        READ(11,906)(ZNO(K),K=1,NZ)
        READ(11,906)(ZVOL(K),K=1,NZ)
        READ(11,906)(ZFMF(K),K=1,NZ)
        READ(11,906)(ZBETA(K),K=1,NZ)
C
C READ ZBETA'S WITHOUT ENHANCED DIFFUSIVITY
C
        IF(T.GE.T2IGN) READ(15,*)(ZBETA(K),K=1,NZ)
```

```
      DO 110 L=1,1 0
        IF(ZM(L).LE.0.)THEN
          ZNO(L)=0.
        ELSE
          ZNO(L)=ZNO(L)/ZM(L)
        END IF
        ZBETA(L)=50.*ZBETA(L)
 110  CONTINUE
C
      DO 120 L=1,10
        IF(ZBETA(L).GT.1.E4)ZBETA(L)=1.E4
        IF(ZBETA(L).LE.0.)ZBETA(L)=B(L)
        B(L)=ZBETA(L)
 120  CONTINUE
C
      IF(I.EQ.1)GO TO 200
      FM(1)=ZMOLD(1)-ZM(1)+ZMEVAP(1)
      FMV(1)=ZMVOLD(1)-ZMV(1)+ZMEVAP(1)-ZMFBRN(1)
      FMBF(1)=ZMBFO(1)-ZMBF(1)+ZMFBRN(1)
      DO 150 L=2,9
        FM(L)=ZMOLD(L)-ZM(L)+ZMEVAP(L)+FM(L-1)
        FMV(L)=ZMVOLD(L)-ZMV(L)+ZMEVAP(L)-ZMFBRN(L)+FMV(L-1)
        FMBF(L)=ZMBFO(L)-ZMBF(L)+ZMFBRN(L)+FMBF(L-1)
 150  CONTINUE
      FML(9)=ZML(10)-ZMLOLD(10)+ZMEVAP(10)
      DO 160 L=8,1,-1
        FML(L)=ZML(L+1)-ZMLOLD(L+1)+ZMEVAP(L+1)+FML(L+1)
 160  CONTINUE
      FMLO=ZML(1)-ZMLOLD(1)+ZMEVAP(1)+FML(1)
C
      WRITE(4,910)T,P
      WRITE(4,906)(FM(L),L=1,9)
      WRITE(4,906)(FMV(L),L=1,9)
      WRITE(4,906)FMLO,(ZML(L),L=1,10)
      WRITE(4,906)(FMBF(L),L=1,9)
      WRITE(4,906)(ZTEMP(L),L=1,10)
      WRITE(4,906)(ZNO(L),L=1,10)
      WRITE(4,906)(ZMEVAP(L),L=1,10)
      WRITE(4,906)(ZQWALL(L),L=1,10)
      WRITE(4,906)(ZMFBRN(L),L=1,10)
      WRITE(4,906)(ZVOL(L),L=1,10)
      WRITE(4,906)(ZFMF(L),L=1,10)
      WRITE(4,906)(ZBETA(L),L=1,10)
      WRITE(4,908)ZM(10),ZMV(10),ZMBF(10)
C
 200  DO 250 J=1,10
        ZMOLD(J)=ZM(J)
        ZMLOLD(J)=ZML(J)
        ZMVOLD(J)=ZMV(J)
        ZMBFO(J)=ZMBF(J)
        ZVOLO(J)=ZVOL(J)
 250  CONTINUE
      IF(I.GT.1)GO TO 100
      WRITE(4,902)P
```

```
  100 CONTINUE
C
  901 FORMAT(A30,/,1X,F6.1,2X,F6.1)
  902 FORMAT(1X,F8.4)
  905 FORMAT(1X,E13.5,1X,F8.4)
  906 FORMAT(1X,6E13.4)
  908 FORMAT(1X,3E13.4)
  910 FORMAT(1X,E13.5,1X,F8.4)
C
      CALL EXIT
      END
C**************************************************************
```

APPENDIX G

ENGINE TEST DATA

RUN # 17
DATE: 9/9/80

LAB. CONDITIONS:
Patm (psia) 14.39
Pboost desire (psia) 6.91
Tdry bulb (°F) 73
Twet bulb (°F) 51
ω (lbm_{H_2O}/lbm_{air}) 0.003

FUEL:
H/C 1.7817
F/A|s 0.0690767
TRIGGER -168°

TEST DESCRIPTION:
with 8-hole nozzle, retarded injection timing and optimum swirl dump at different degree crank angle
NO_x correction = 7.34

ENGINE CONDITIONS:
INJ. TIMING -15°
NOZZLE TYPE 8-hole
SHROUD POSITION 160"
SWIRL RATIO 2.46
$P_{up\ stream\ orifice}$ (psia) 55.4
P_{boost} (psia) 6.9
$P_{exh.\ surge}$ (psia) 10
$\dot{M}_{air}$ (lbm/min)(dry) 1.7912
FUEL TIME (sec) 1724
FUEL WT. (gm) 80.15
$\dot{M}_{fuel}$ (lbm/min) 0.0615
F/A 0.0313
ϕ 0.4570
ENGINE SPEED (rpm) 1001

TEMPERATURE:
INT. at reg (°F) 80.6
INT. at head (°F) 150.8
EXH. at head (°F) 725
EXH. at surge (°F) 426.2
COOLANT out (°F) 186.8
COOLANT block (°F) 186.8
OIL (°F) 168.8
EGR (%) 0
% CO_2 In air
% CO_2 In exh.
% CO_2 In Int

PERFORMANCE:
BRAKE LOAD (lbf) 21.8
MOTOR LOAD (lbf) 12.8
VOL. EFF. (%) 92.27
BMEP (psia) 80.4137
BHP (hp) 7.2739
BSFC (lbm/hp-hr) 0.5072
FMEP (psia) 47.2154
FHP (hp) 4.2709
IMEP (psia) 127.6292
IHP (hp) 11.5449
ISFC (lbm/hp-hr) 0.3196
PEAK PRES. (psia) 1047.3
SMOKE (BOSCH NO.) 4.2

EXH NO (ppm) 842
EXH NO_x (ppm) 855
BSNO (lbm/hp-hr) 3.713×10^{-6}
BSNO$_x$ (lbm/hp-hr) 3.799×10^{-6}
DISK/TRACK 9/6-2

P_1 3 in Hg
T_1 33°C
(before dumping)

	1	2	3	4	5	6	7			
$DUMP_{desire}$ (°ca)	45	30	15	20	TDC	-18	24			
$DUMP_{actual}$ (°ca)	63	25	8	18	-1	-12				
NO (ppm)	107	88.5	33.9	54.2	7.3	1.8	842			
NO_x (ppm)	109	95.3	38.7	60.6	11.5	3.3	855			
DISK/TRACK	9/1-1	9/7-1	9/3-1	8/1-1	9/8-2	8/1-2				

Figure G-1 Run 17 Test Data

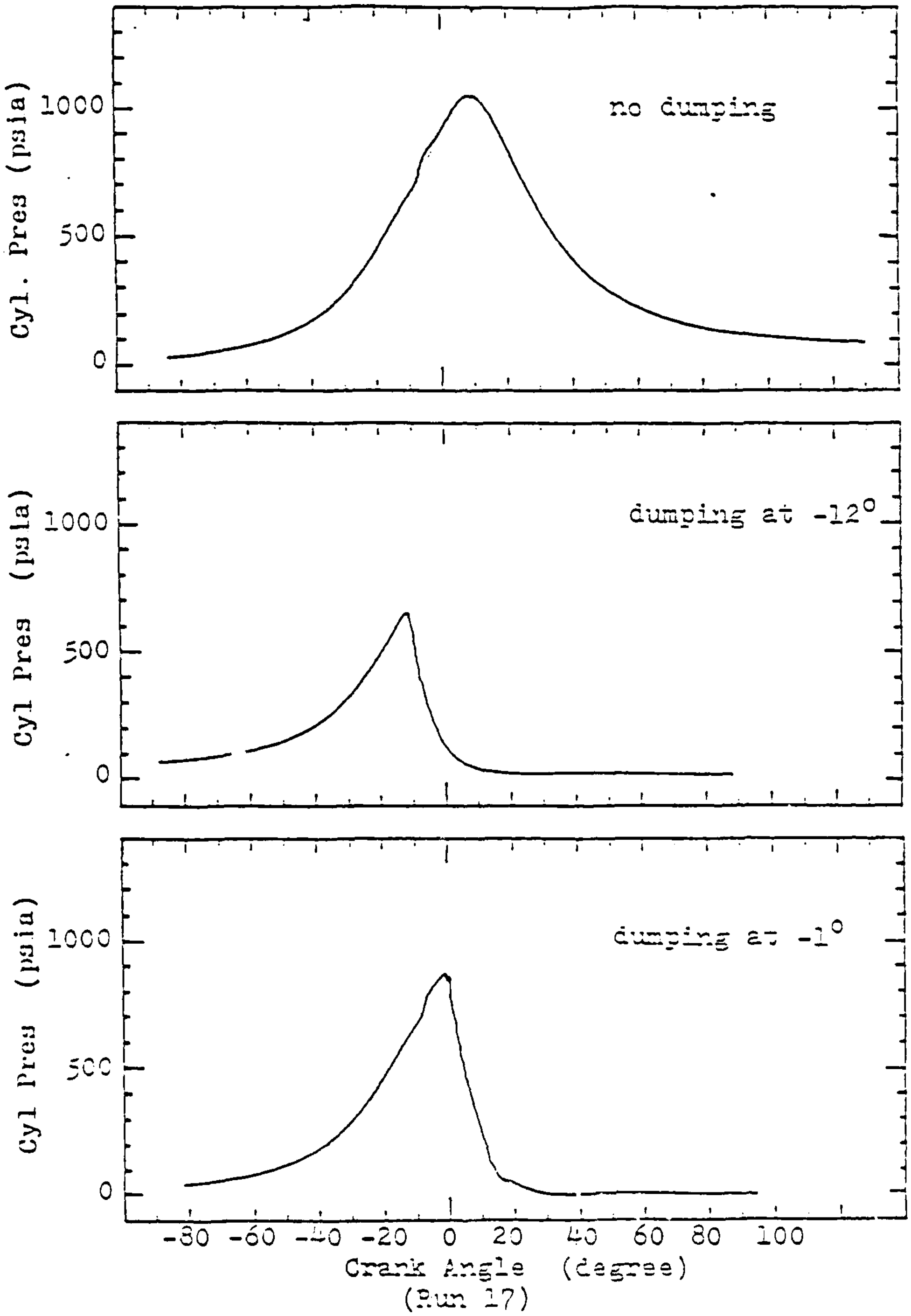
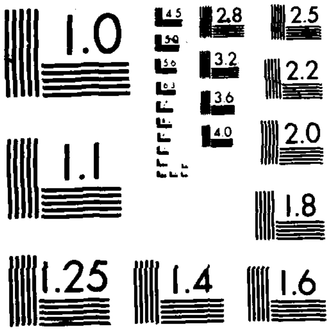


Figure G-2 Run 17 Pressure Traces

AD-A175 155 A STOCHASTIC MIXING MODEL FOR PREDICTING EMISSIONS IN A 4/4
DIRECT INJECTION (U) MASSACHUSETTS INST OF TECH
CAMBRIDGE DEPT OF OCEAN ENGINEERIN A J BROWN SEP 86
UNCLASSIFIED N00228-85-G-3262 F/G 21/4 NL



CROCOPY RESOLUTION TEST CHART

RUN # 18   DATE: 9/10/80

LAB. CONDITIONS:	
Patm (psia)	14.3
Pboost desire (psia)	6.87
Tdry bulb (°F)	74.5
Twet bulb (°F)	52
ω (lbm$_{H_2O}$/lbm$_{air}$)	0.0032

FUEL:	
H/C	1.7817
F/A|s	0.0690767
TRIGGER	-168°

TEST DESCRIPTION:

At retarded injection timing
Run at high swirl, no EGR

NO$_x$ correction = 6.99

ENGINE CONDITIONS:	
INJ. TIMING	-15°
NOZZLE TYPE	8-hole
SHROUD POSITION	110°
SWIRL RATIO	4
Pup stream orifice (psia)	54.4
Pboost (psia)	6.88
Pexh. surge (psia)	10.5
Ṁair (lbm/min)(dry)	1.7688
FUEL TIME (sec)	173.26
FUEL WT. (gm)	80.15
Ṁ fuel (lbm/min)	0.0612
F/A	0.0346
φ	0.5008
ENGINE SPEED (rpm)	1001

TEMPERATURE:		
INT. air	reg (°F)	78.8
	head (°F)	152.6
EXH. air	head (°F)	703.4
	surge (°F)	404.6
COOLANT	out (°F)	185.
	block (°F)	183.2
OIL	(°F)	170.6
EGR (%)		0
% CO$_2$ in air		
% CO$_2$ in exh.		
% CO$_2$ in inl		

PERFORMANCE:	
BRAKE LOAD (lbf)	19.9
MOTOR LOAD (lbf)	12.8
VOL. EFF. (%)	91.3262
BMEP (psia)	73.4051
BHP (hp)	6.64
BSFC (lbm/hp-hr)	0.5529
FMEP (psia)	47.2159
FHP (hp)	4.2709
IMEP (psia)	120.6205
IHP (hp)	10.9109
ISFC (lbm/hp-hr)	0.3365
PEAK PRES. (psia)	1052.16
SMOKE (BOSCH NO)	4.3

EXH NO (ppm)	625
EXH NO$_x$ (ppm)	610
BSNO (lbm/hp-hr)	
BSNO$_x$ (lbm/hp-hr)	
DISK/TRACK	8/5-1,2
P$_1$	3 in Hg
T$_1$	32 °C

	1	2	3	4	5	6	7 Exh			
DUMP$_{desire}$ (°ca)	40	25	25	5	-10	-25				
DUMP$_{actual}$ (°ca)	47	16	26	5	-7	-18				
NO (ppm)	78.4	56.4	68.3	21.3	5.6	1.3	625			
NO$_x$ (ppm)	80.1	59.4	71.7	27.5	7.3	3.4	610			
DISK/TRACK	8/2-1	8/2-2	8/3-1	8/3-2	8/4-1	8/4-2				

Figure G-3 Run 18 Test Data

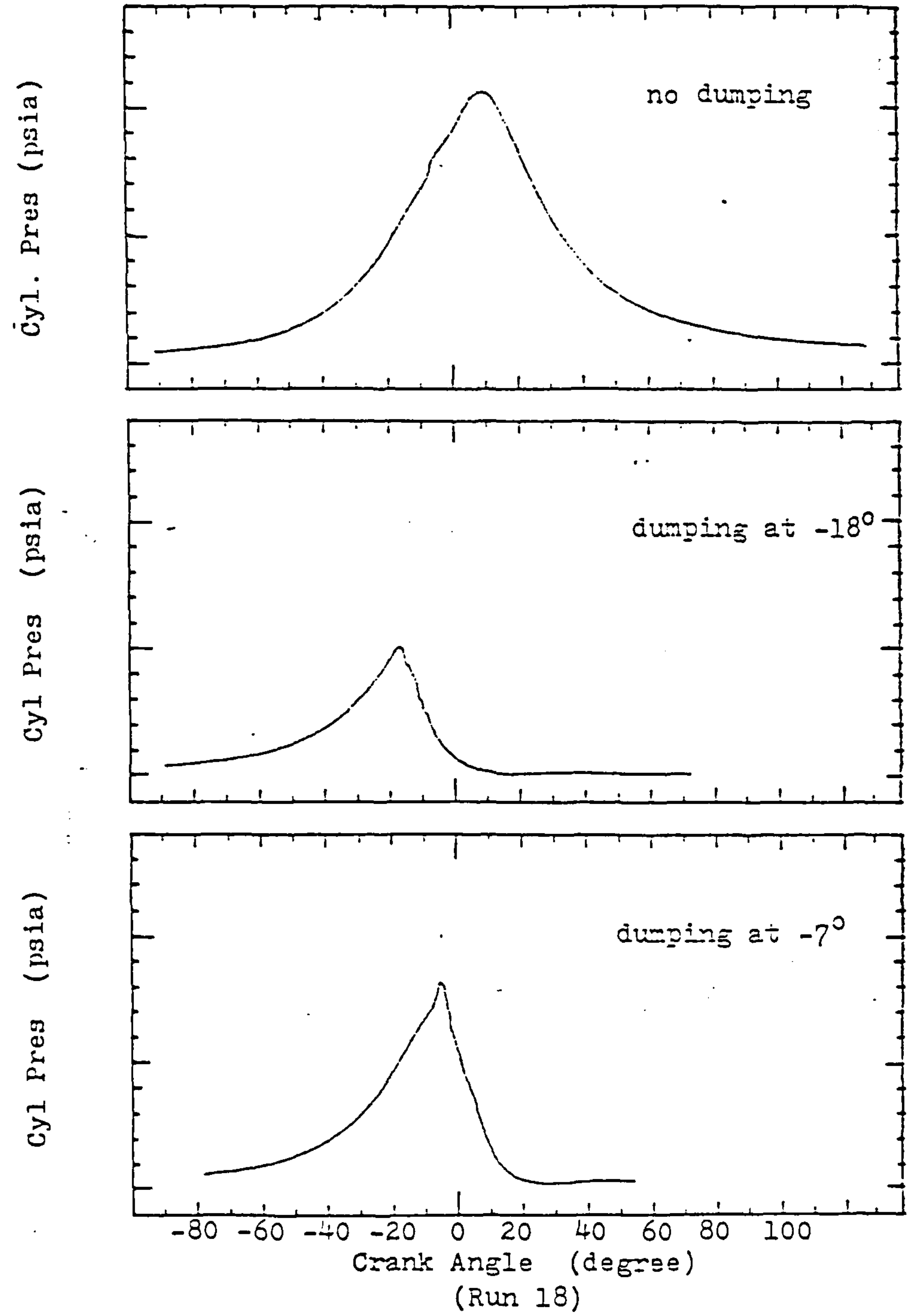


Figure G-4 Run 18 Pressure Traces

RUN #: 19 DATE: 9/17/80

LAB. CONDITIONS:

Patm (psia)	14.29
Pboost desire (psia)	7.01
Tdry bulb (°F)	69.5
Twet bulb (°F)	52
ω (lbm$_{H_2O}$/lbm$_{air}$)	0.0013

FUEL:

H/C 1.7817

F/A|s 0.0690767

TRIGGER -168°

TEST DESCRIPTION:

For 8 hole nozzle run at optimum injection timing and optimum swirl, No EGR

NO_x correction factor = 9.40

ENGINE CONDITIONS:

INJ. TIMING	-25°
NOZZLE TYPE	8-hole
SHROUD POSITION	160°
SWIRL RATIO	2.46
Pup stream orifice (psia)	55.2
Pboost (psia)	7.01
Pexh. surge (psia)	9.8
$\dot{M}$air (lbm/min)(dry)	1.7864
FUEL TIME (sec)	171.25
FUEL WT. (gm)	80.15
$\dot{M}$ fuel (lbm/min)	0.0619
F/A	0.0347
φ	0.5016
ENGINE SPEED (rpm)	998

TEMPERATURE:

INT. at	reg (°F)	77
	head (°F)	150.8
EXH. at	head (°F)	696.2
	surge (°F)	410.6
COOLANT	out (°F)	183.2
	block (°F)	181.4
OIL	(°F)	168.8
EGR (%)		0
% CO_2 in air		
% CO_2 in exh.		
% CO_2 in int		

PERFORMANCE:

BRAKE LOAD (lbf)	22.0
MOTOR LOAD (lbf)	12.7
VOL. EFF. (%)	92.418
BMEP (psia)	81.1514
BHP (hp)	7.3187
BSFC (lbm/hp-hr)	0.5075
FMEP (psia)	46.8465
FHP (hp)	4.2249
IMEP (psia)	127.9979
IHP (hp)	11.5435
ISFC (lbm/hp-hr)	0.3218
PEAK PRES. (psia)	1343.68
SMOKE (Bosch)	3.3

EXH NO (ppm)	1600
EXH NO_x (ppm)	1700
BSNO (lbm/hp-hr)	
BSNO$_x$ (lbm/hp-hr)	
DISK/TRACK	5/3-1,2
P_i	3 in Hg
T_i	33 °C

	1	2	3	4	5	6	7	8 s/l		
DUMP$_{desire}$ (°ca)	45	25	18	10	10	-15	-20			
DUMP$_{actual}$ (°ca)	53.5	22	16	-2	5	-8	-11			
NO (ppm)	215	226	171	55	117	20	4.5	1600		
NO_x (ppm)	218	232	177	62	121	22	4.0	1700		
DISK/TRACK	8/6-1	8/7-1	8/7-2	8/8-1	8/8-2	7/1-1	7/1-2			

Figure G-5 Run 19 Test Data

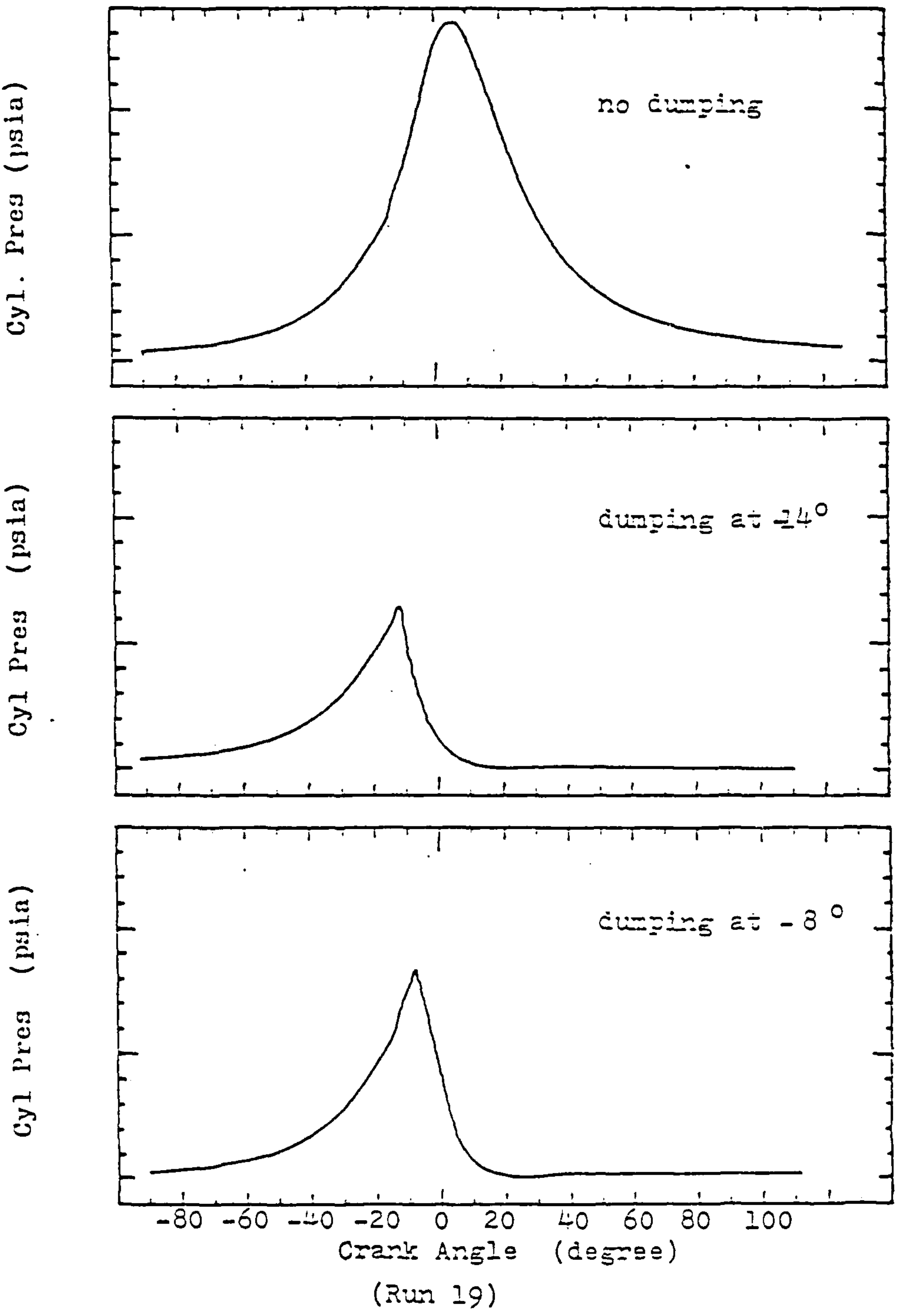
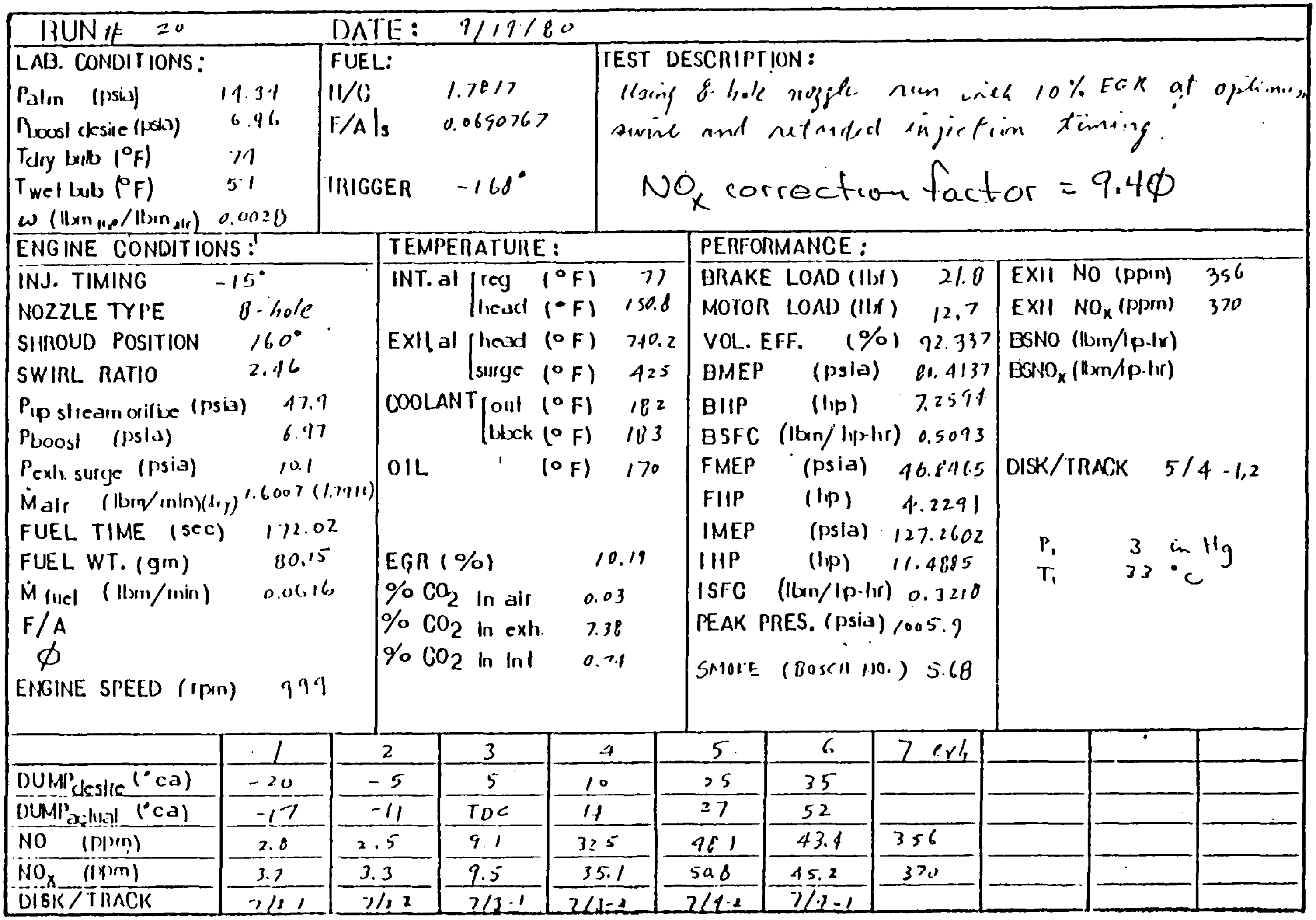


Figure G-6 Run 19 Pressure Traces



RUN # 20
DATE: 9/19/80

LAB. CONDITIONS:
Patm (psia) 14.34
Pboost desire (psia) 6.96
Tdry bulb (°F) 79
Twet bulb (°F) 51
ω (lbm$_{H_2O}$/lbm$_{air}$) 0.0028

FUEL:
H/C 1.7817
F/A|s 0.0690767

TRIGGER -168°

TEST DESCRIPTION:
Using 8-hole nozzle run with 10% EGR at optimum swirl and retarded injection timing.

NO$_x$ correction factor = 9.40

ENGINE CONDITIONS:
INJ. TIMING -15°
NOZZLE TYPE 8-hole
SHROUD POSITION 160°
SWIRL RATIO 2.46
Pup stream orifice (psia) 47.9
Pboost (psia) 6.97
Pexh. surge (psia) 10.1
Ṁair (lbm/min)(dry) 1.6007 (1.7911)
FUEL TIME (sec) 172.02
FUEL WT. (gm) 80.15
Ṁ fuel (lbm/min) 0.0616
F/A
φ
ENGINE SPEED (rpm) 999

TEMPERATURE:
INT. at [reg (°F) 77
INT. at [head (°F) 150.8
EXH at [head (°F) 740.2
EXH at [surge (°F) 425
COOLANT [out (°F) 182
COOLANT [block (°F) 183
OIL (°F) 170

EGR (%) 10.19
% CO$_2$ in air 0.03
% CO$_2$ in exh. 7.38
% CO$_2$ in inl 0.74

PERFORMANCE:
BRAKE LOAD (lbf) 21.8
MOTOR LOAD (lbf) 12.7
VOL. EFF. (%) 92.337
BMEP (psia) 81.4137
BHP (hp) 7.2594
BSFC (lbm/hp-hr) 0.5093
FMEP (psia) 46.8465
FHP (hp) 4.2291
IMEP (psia) 127.2602
IHP (hp) 11.4885
ISFC (lbm/hp-hr) 0.3210
PEAK PRES. (psia) 1005.9
SMOKE (BOSCH NO.) 5.68

EXH NO (ppm) 356
EXH NO$_x$ (ppm) 370
BSNO (lbm/hp-hr)
BSNO$_x$ (lbm/hp-hr)

DISK/TRACK 5/4-1,2

P$_1$ 3 in Hg
T$_1$ 33 °C

	1	2	3	4	5	6	7 cyl			
DUMP$_{desire}$ (°ca)	-20	-5	5	10	25	35				
DUMP$_{actual}$ (°ca)	-17	-11	TDC	14	27	52				
NO (ppm)	2.8	2.5	9.1	32.5	48.1	43.4	356			
NO$_x$ (ppm)	3.7	3.3	9.5	35.1	50.8	45.2	370			
DISK/TRACK	7/1-1	7/1-2	7/3-1	7/3-2	7/4-2	7/4-1				

Figure G-7 Run 20 Test Data

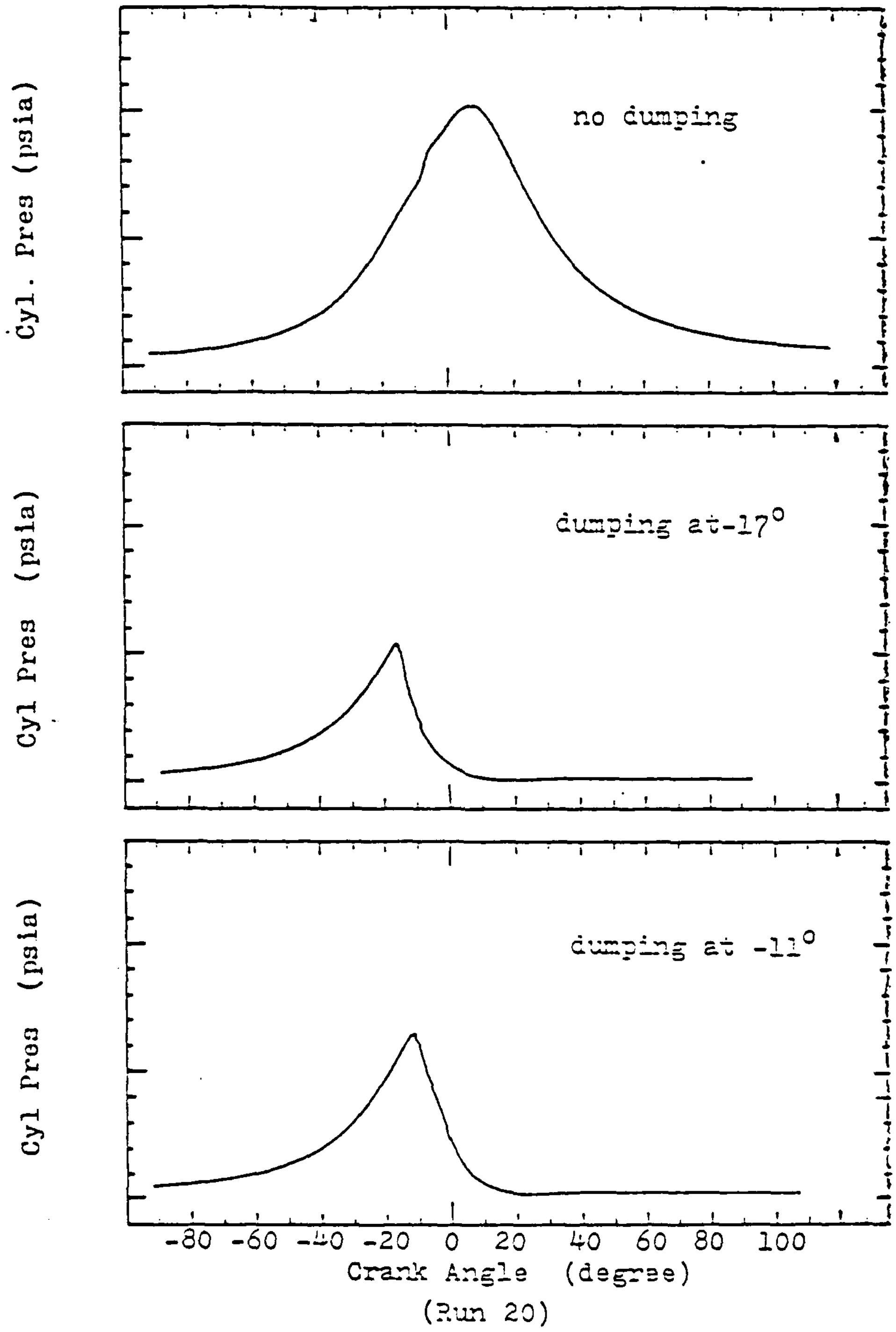


Figure G-8 Run 20 Pressure Traces

RUN # 21 DATE: 7/26/80

LAB. CONDITIONS:

P_{atm} (psia) 14.48
$P_{boost\ desire}$ (psia) 6.82
$T_{dry\ bulb}$ (°F) 70
$T_{wet\ bulb}$ (°F) 49
ω (lbm_{H_2O}/lbm_{air}) 0.0027

FUEL:

H/C 1.7817
$F/A|_s$ 0.0690767

TRIGGER -168°

TEST DESCRIPTION:

with 8-hole nozzle run at retarded timing, high swirl and 10% EGR

NO_x correction factor = 9.46

ENGINE CONDITIONS:

INJ. TIMING -15°
NOZZLE TYPE 8-hole
SHROUD POSITION 110°
SWIRL RATIO 4
$P_{up\ stream\ orifice}$ (psia) 49.8
P_{boost} (psia) 6.8
$P_{exh.\ surge}$ (psia) 10
$\dot{M}_{air}$ (lbm/min)(dry) 1.5522 (1.7692)
FUEL TIME (sec) 112.1
FUEL WT. (gm) 80.15
$\dot{M}_{fuel}$ (lbm/min) 0.0615
F/A
ϕ
ENGINE SPEED (rpm) 1002

TEMPERATURE:

INT. at reg (°F) 75.3
INT. at head (°F) 150.8
EXH. at head (°F) 701.6
EXH. at surge (°F) 393.8
COOLANT out (°F) 183.2
COOLANT block (°F) 186.8
OIL (°F) 167

EGR (%) 10.7
% CO_2 in air 0.03
% CO_2 in exh. 7.11
% CO_2 in Int 0.75

PERFORMANCE:

BRAKE LOAD (lbf) 17.6
MOTOR LOAD (lbf) 12.6
VOL. EFF. (%) 91.042
BMEP (psia) 64.9111
BHP (hp) 5.8784
BSFC (lbm/hp-hr) 0.6281
FMEP (psia) 46.4776
FHP (hp) 0.2089
IMEP (psia) 111.3987
IHP (hp) 10.0868
ISFC (lbm/hp-hr) 0.3660
PEAK PRES. (psia) 1016.6

SMOKE (BOSCH NO.) 695

EXH NO (ppm) 290
EXH NO_x (ppm) 300
BSNO (lbm/hp-hr)
$BSNO_x$ (lbm/hp-hr)

DISK/TRACK 7/5-2
7/5-1 (NO EGR)

P_i 3 in Hg
T_i 33 °C

	1	2	3	4	5	6				
$DUMP_{desire}$ (°ca)	35	25	15	10	-10					
$DUMP_{actual}$ (°ca)	41	20	9	2	-12					
NO (ppm)	35.1	34.1	25.3	13.9	9.5	290				
NO_x (ppm)	37.5	36.8	26.5	15.8	4.3	300				
DISK/TRACK	7/6-1	7/6-2	7/7-2	7/7-1	7/8-1					

Figure G-9 Run 21 Test Data

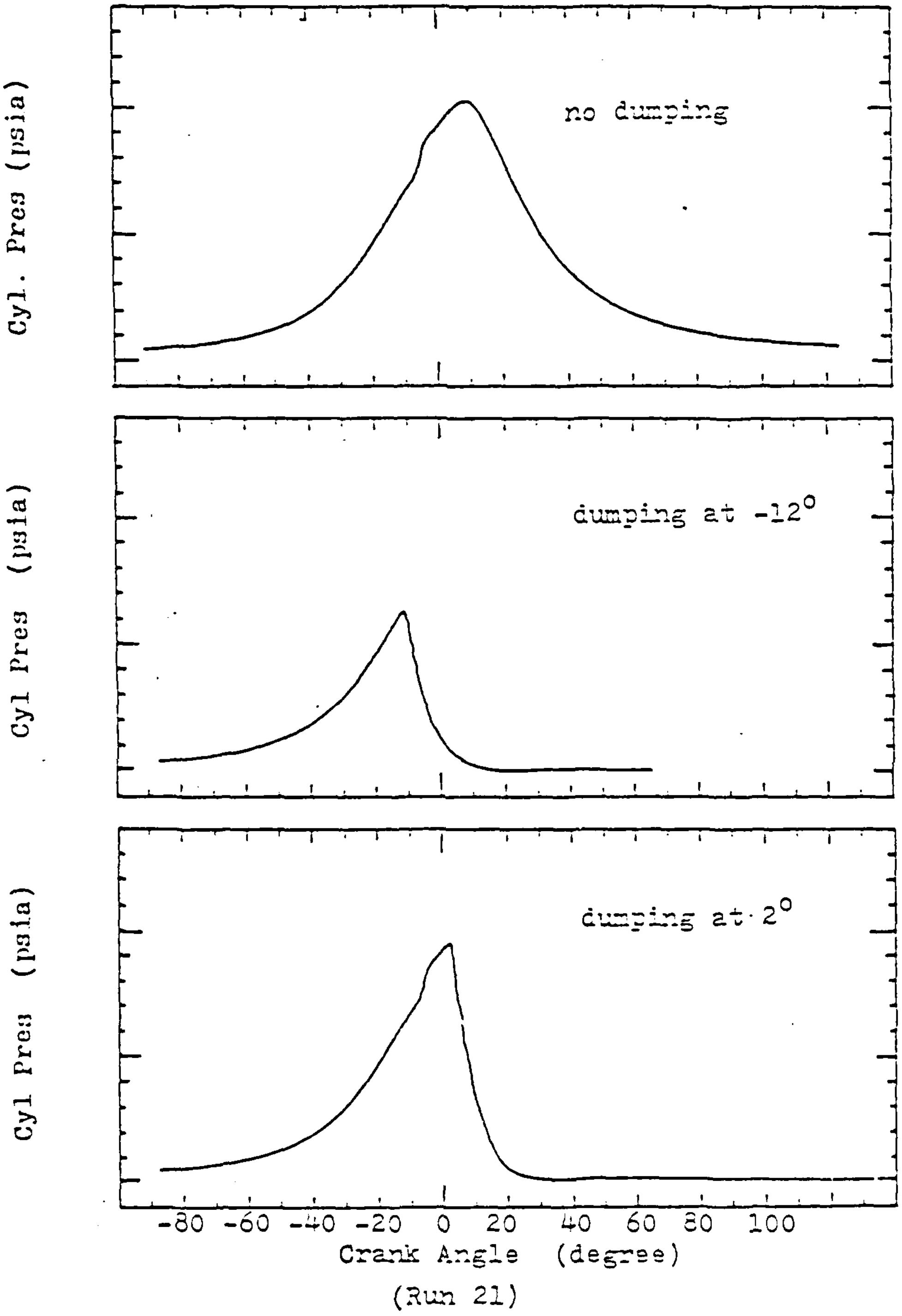


Figure G-10 Run 21 Pressure Traces

END

2-87

DTIC