MONTE CARLO MODELING IN ELLIPTIC FLOWS

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A Monte Carlo method capable of predicting scalar (e.g. concentration) probability density functions (pdf's) in nonreacting and reacting elliptic flows is being developed. In particular, attention is being focused on a research combustor specifically designed to provide measurements of concentration and temperature pdf's in nonreacting and reacting flows. (e.g. 8).

The modeling technique being developed involves the coupling of a Monte Carlo coalescence/dispersion model (e.g. 2-7) with currently available codes (such as the finite-difference scheme described in (1)) for elliptic flow-field calculations. The latter provides solutions for the mean velocity, turbulent kinetic energy and dissipation rate. These serve as inputs to the Monte Carlo calculation procedure which is used to solve the transport equations for scalar pdf's.

The attraction of the Monte Carlo method is its practicability for multi-dimensional pdf's, while conventional finite-difference solutions of the pdf transport equations require prohibitive amounts of computer time (e.g. 2). This method also eliminates the necessity of assuming a shape for the pdf; instead, given an initial distribution function, the model allows for the temporal evolution of the pdf. Also, it can account for finite rate chemical reactions, which is essential for the successful prediction of pollutant formation rates and flame stability.

In the Monte Carlo calculation procedure, the composition distribution (due to concentration fluctuations) at a point in the flowfield is described by a statistical ensemble of computational elements which have a distribution in thermodynamic states. Each element has scalar properties associated with it so that its thermodynamic state is well defined. The number of such elements in a given state can vary because of turbulent mixing, chemical reactions, etc. Given such an ensemble of elements at every grid point in the flowfield, mean values of any scalar, as well as variance or higher moments can be obtained from instantaneous averaging over the ensemble population.

The effects of mixing, convection, diffusion, and chemical reaction on the scalar pdf's are incorporated into the calculation procedure as follows. The turbulent and moecular mixing processes are represented by allowing elements within each ensemble to mix with one another. These mixing interactions occur at discrete time intervals given by a mixing frequency which can be related to the local turbulent kinetic energy and dissipation rate (see reference 2 for details). The effects of turbulence on mixing and chemical reaction are thus introduced through the mixing frequency. During the time between mixing interactions, each element undergoes chemical

reaction at a rate specified by the user. Either an infinite rate assumption can be made or a chemical reaction mechanism and rate data specified. Since the processes of mixing and reaction are treated separately, the use of multiple finite rate reactions does not increase the complexity of the formulation. Also, the instantaneous reaction rate for each element is calculated, so the mean reaction rate can be obtained by simply averaging over the ensemble population. The transport processes of convection and diffusion are also treated separately; the former by transporting elements from one ensemble (i.e. grid point) to another at a rate governed by the local fluid velocity, and the latter by exchanging elements between ensembles at adjacent nodes at a rate governed by the local turbulent diffusivity.

The specification of initial ensembles at the grid points is as follows. For elliptic flows, properties at a point can be affected by values downstream. The calculation procedure will therefore involve iteration on some assumed initial distributions. The processes of convection, diffusion, mixing, and reaction will be simulated as described above. Also, the inlet flow conditions will specify ensembles along one axial location. The iteration will continue until the ensembles have become time stationary; a correct ensemble will then have been created at all spatial locations in the flowfield.

The ability of the Monte Carlo method to provide the coupling of finite rate fluid mechanic mixing and finite rate combustion chemistry is illustrated by presenting a coalescence/dispersion model developed for studies of ignition and blowout in a combustor primary zone. The use of the flame stability model (described in references 5-7) is demonstrated by generating lean ignition limits of premixed turbulent flames. The variations of the predicted lean ignition limit with reference velocity, inlet temperature, and pressure compare favorably with experimental trends and magnitudes.

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References

1) Lilley, D.G. and Rhode, D.L. (1982). NASA CR-3442.

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7) Radhakrishnan, K. and Pratt, D.T. (1982). AIAA Paper 82-1158.

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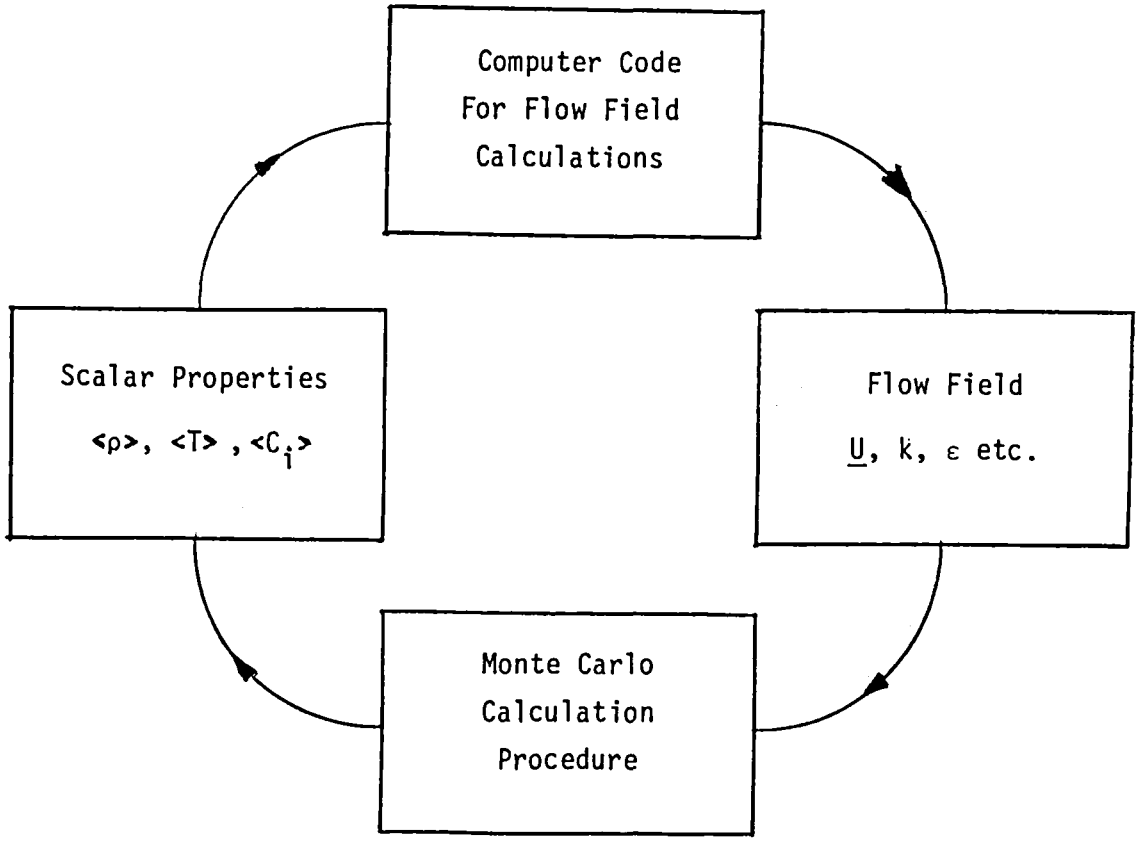
9) Westbrook, C.K. and Dryer, F.L. (1981). Combustion Science & Technology, 27, p.31.

Method

Combine existing computer codes for elliptic flow field calculations with a Monte Carlo method to simulate the transport equations for scalar probability density functions.



Solution Technique For Elliptic Flows

Interative as follows:

Assume initial ensemble (and hence, pdf's) at all grid points.

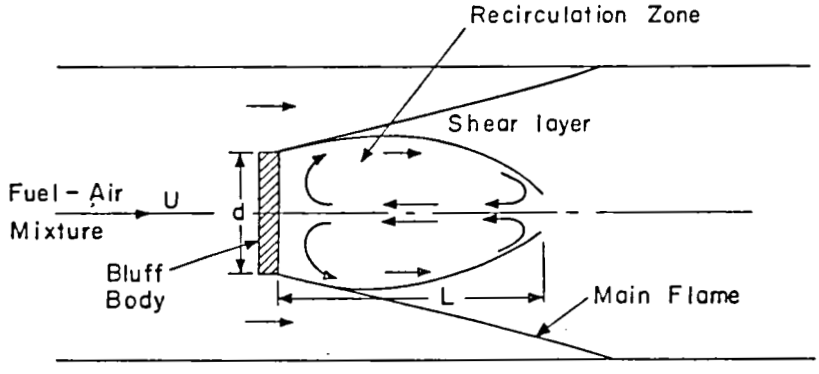
Calculate $< \rho >$, $< T >$, etc.

Solve for flow velocity, turbulent kinetic energy and dissipation rates at all grid points.

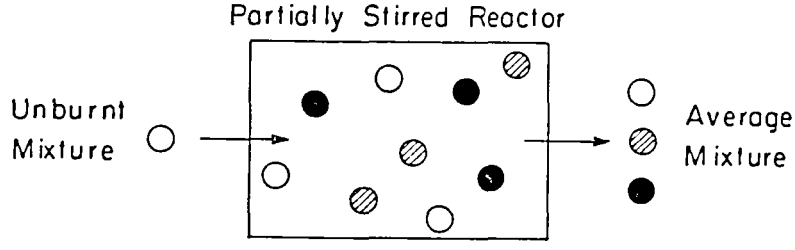
Generate new pdf's at all grid points.

Check if new pdf's agree with old values.

Schematic of Bluff Body Stabilized Flame



Simulation of Recirculation Zone



Monte Carlo Mixing Interaction

Element	i	j	i	j
Burnt Fraction	B_i	B_j	$(B_i + B_j)/2$	

Model Parameters and Relations

Mixing Frequency

$$\beta = c_{\beta} \, (P_j/ML^2)^{1/3}$$

Inflow Time

$$\tau_i = (V/\dot{m}_i \bar{v})$$

Residence Time

$$\tau = (V/\dot{m}_e \bar{v})$$

Chemical Kinetics

Two Step Mechanism

$$C_3H_8 + 3.5\ O_2 \rightarrow 3\ CO + 4\ H_2O$$

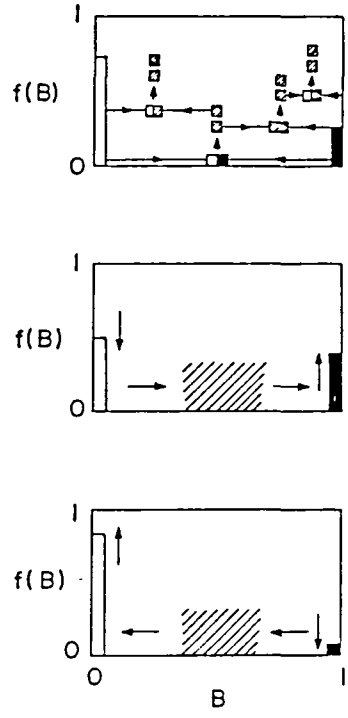
$$CO + 0.5\ O_2 \rightleftarrows CO_2$$

Reaction Rates from Westbrook and Dryer (1981)
Preexponential Constants Adjusted

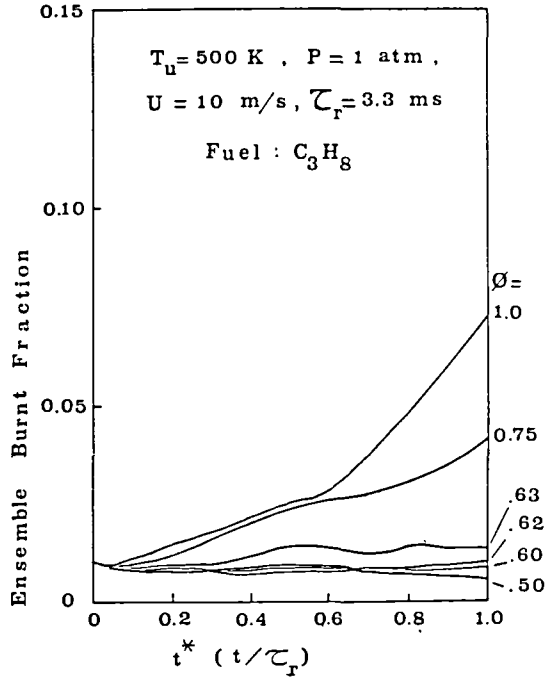
Ensemble Property

$$\bar{z} = \frac{1}{N} \Sigma z_i$$

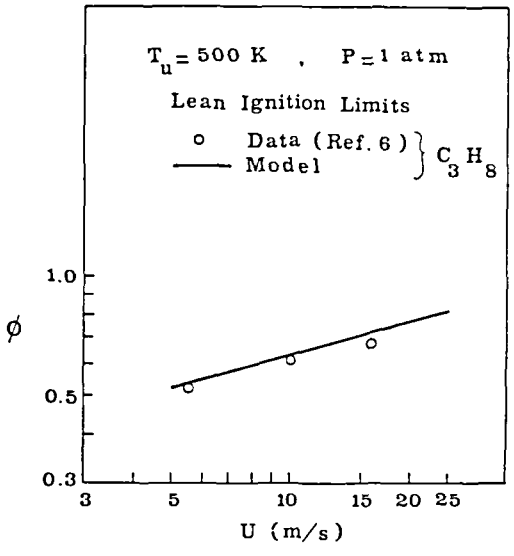
Example : Ignition



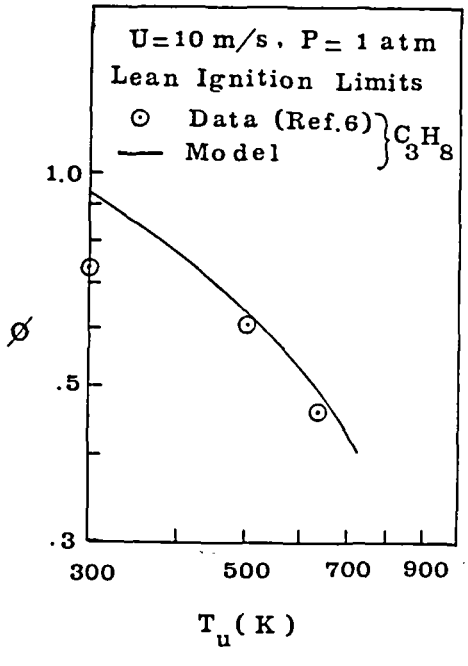
EXAMPLE:LEAN IGNITION LIMIT



Variations of Limits with Velocity



Variations of Limits
with Inlet Temperature



Variation of Predicted Limit with Pressure