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On Recontamination and Directional-Bias Problems in Monte Carlo Simulation of PDF Turbulence Models

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Turbulent combustion can not be simulated adequately by conventional moment closure turbulence models. The difficulty lies in the fact that the reaction rate is in general an exponential function of the temperature, and the higher order correlations in the conventional moment closure models of the chemical source term can not be neglected, making the applications of such models impractical. The probability density function (pdf) method offers an attractive alternative: in a pdf model, the chemical source terms are closed and do not require additional models.

The partial differential equation for the probability density function, $\tilde{P}$, can be written as

$$\bar{\rho}\partial_t\tilde{P} + \bar{\rho}\tilde{v}_\alpha\partial_\alpha\tilde{P} + \bar{\rho}\sum_{i=1}^{N}\partial_{\psi_i}\{w_i(\psi_1,\dots,\psi_N)\tilde{P}\}$$

$$= -\partial_\alpha(\bar{\rho} < v''_\alpha|\psi_i > \tilde{P}) - \bar{\rho}\sum_{i=1}^{N}\sum_{j=1}^{N}\partial^2_{\psi_i\psi_j}(< \epsilon_{ij}|\psi_k > \tilde{P})$$

where the terms represent the time derivative, mean convection, chemical reaction, turbulent convection, and molecular mixing, respectively. The fact that the pdf equation has a very large dimensionality renders finite difference schemes extremely demanding on computer memory and CPU time and thus impractical, if not entirely impossible. A logical alternative is the Monte Carlo scheme, wherein the number of computer operations increases only linearly with the increase of number of independent variables, as compared to the exponential increase in a conventional finite difference scheme.

A grid dependent Monte Carlo scheme following that of J.Y. Chen and W. Kollmann has been studied in the present work. In dealing with the convection and diffusion of the pdf, the pdf equation is discretized on a given grid, e.g.,

$$\tilde{P}_{x+dx,j} = \alpha_j\tilde{P}_{x,j+1} + \beta_j\tilde{P}_{x,j} + \gamma_j\tilde{P}_{x,j-1}$$

where

$$\alpha_j + \beta_j + \gamma_j = 1$$

However, if this is the only restriction satisfied by the numerical algorithm, the mass fractions may not be conserved due to re-contamination, and directional-bias also appears. These phenomena are illustrated in Figure 1: Consider a mixing layer; use white balls to represent contaminants in the upper stream and black balls to represent contaminants in the lower stream. As the two streams move toward right, the location of the white balls and black balls are interchanged randomly to simulate convection and diffusion. From Figure 1, it is clear that directional-bias caused by recontamination caused the center of the mixing layer to drift downward. (Directional-bias can be partially corrected by changing sweeping directions.) One also notices that after the first marching step, the conservation law is violated, reflected in the Figure as missing white or black balls.

It is found that in order to conserve the mass fractions absolutely, one needs to add further restriction to the scheme, namely

$$\alpha_j + \gamma_j = \alpha_{j-1} + \gamma_{j+1}$$

A new algorithm was devised that satisfies this restriction in the case of pure diffusion or uniform flow problems. Using the same example, it is shown that absolute conservation can be achieved. This result is shown in Figure 2. One can see that the diffusion process is symmetric, and the problem of directional-bias is eliminated.

Although for non-uniform flows absolute conservation seems impossible, the present scheme has reduced the error considerably.

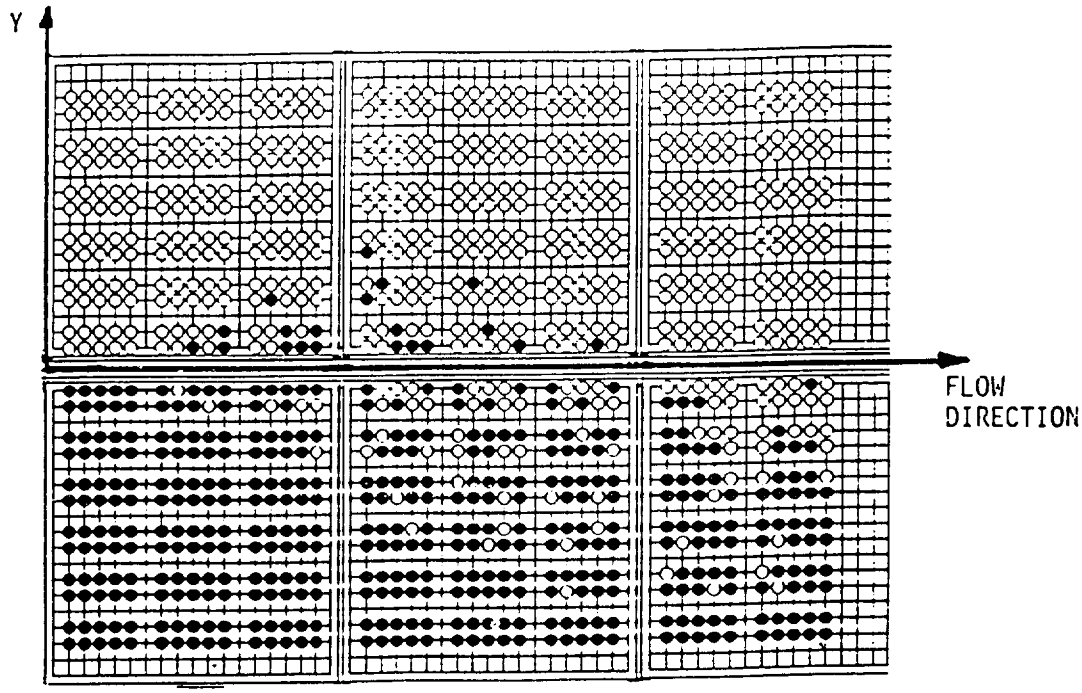

Figure 1. Illustration of directional-bias and recontamination problems in Monte Carlo simulation.

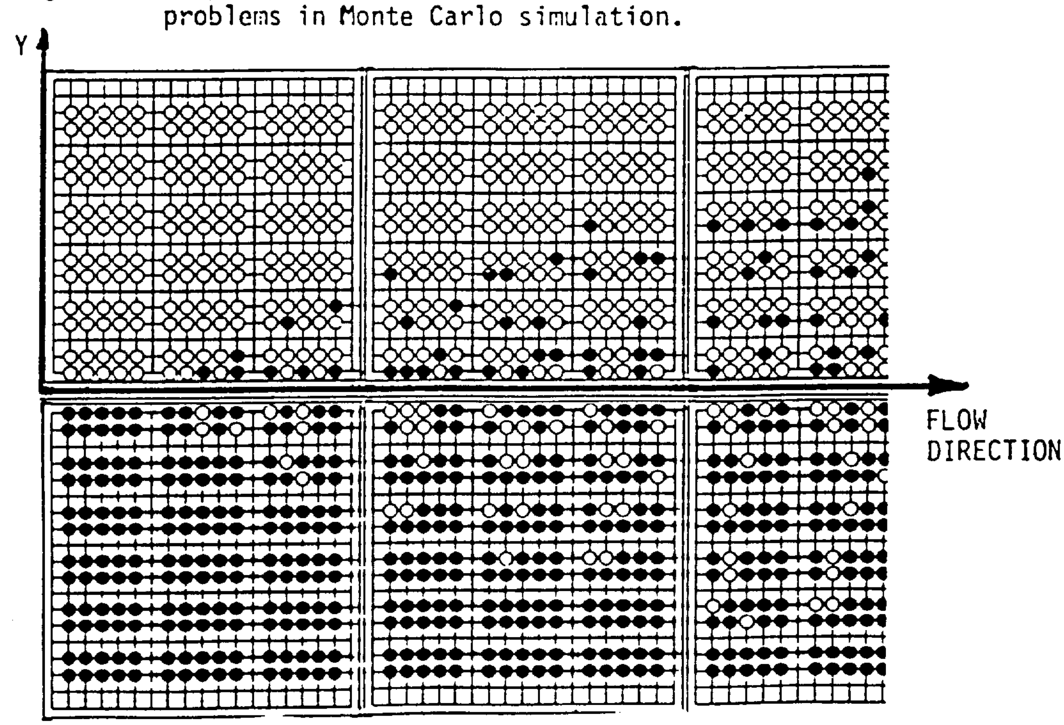

Figure 2. Solution obtained by using additional constraint in the solution procedure.