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DIRECT NUMERICAL SIMULATION OF REACTING FLOWS

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The objectives of this work are (i) to to extend the technique of direct numerical simulations to turbulent, chemically reacting flows, (ii) to test the validity of the method by comparing computational results with laboratory data, and (iii) to use the simulations to gain a better understanding of the effects of turbulence on chemical reactions. In particular, we address the effects of both the large-scale structure and the smaller-scale turbulence on the overall reaction rates, examine the relationship between infinite reaction rate and finite reaction rate chemistry, and compare some of the results of our calculations with existing theories and laboratory data. The direct numerical simulation method involves the numerical solution of the detailed evolution of the complex turbulent velocity and concentration fields. Using very efficient numerical methods (e.g., pseudospectral methods), the fully nonlinear (possibly low-pass filtered) equations of motion are solved and no closure assumptions or turbulence models are used. Statistical data are obtained by performing spatial, temporal, and/or ensemble averages over the computed flow fields.

The scope of work to do this involved the following. First, existing computer codes were modified to treat the present problem. Next, extensive numerical testing of the computer codes was performed. Finally, in order to examine the effects of the mixing layer turbulence, both the large-scale structure and the smaller-scale turbulence, on the overall reaction rates, a sequence of three problems was computed: (i) reactions on a unidirectional (one-dimensional) mixing layer, (ii) reactions on a mixing layer experiencing large-scale, two-dimensional vortex rollup, and (iii) reactions on a three-dimensional turbulent mixing layer. The simulations of the two-dimensional mixing layer with vortex rollup are intended to model the large-scale structure in the mixing layer, whereas the three-dimensional simulations contain both the large-scale structure and the smaller-scale turbulence.

The numerical testing involved the comparison of computed results with exact solutions for a number of different cases. Both rigid body rotation and vortex rollup flow fields were used. The work greatly extended the results of Orszag (ref. 1) for the advection of a passive scalar on a rigidly rotating flow field (the color problem) to include also diffusion, chemical reaction, and more complex flows. We have found that high accuracy of the spectral methods observed in the advection case is also obtained when these further complications are present. Our results indicate that spectral numerical methods may prove to be useful in the future both for solving the model equations for combustor processes as well as for future studies of chemically reacting turbulent flows employing direct numerical simulations.

The approach of direct numerical simulations allowed extensive examination and interpretation of the reaction process. From the one-dimensional simulations, we found that we could easily compute finite reaction rates near the fast reaction limit, that the results were fairly insensitive to the initial conditions (for the class of initial conditions computed), and that the results were in reasonable agreement with theoretical predictions.

For the two-dimensional simulations, we found that in all of the cases computed, the vorticity field and the product field approximately coincided. From the computation of volume averages, we observed the enhancement of the overall reaction rate due to the vortex rollup. It also appeared that the merging of vortex cores was a more significant mechanism in increasing the overall reaction rate than the straining of the reaction interface. Significant species segregation was apparent, so that, for example, the product of the average concentrations was approximately equal to and opposite the correlation between the fluctuating concentrations. Some of the higher order correlations were also examined.

In the three-dimensional simulations, the contour plots indicated that the vortex rollup takes longer to develop, and the vortices and braids are not as distinct as in the two-dimensional case. Also, the vortices that develop are not strongly correlated laterally. Both the contour plots and the statistical results indicated that the spatial segregation was also not as strong as in the two-dimensional case, probably due to the weaker vortex rollup as well as the effects of smaller-scale, three-dimensional turbulence.

Comparisons were made between the simulation results and results using similarity theory. Approximately linear growth rates of various computed length scales, including the mean velocity half-width, the mean vorticity thickness, and the mean product thickness, were obtained and were in agreement with the theory. Similarity scaling was found to collapse quite well the results for the average reactant concentrations, the rms fluctuating reactant concentrations, the concentration correlations, the average product concentrations, and the rms fluctuating product concentrations.

Some limited comparisons were made with laboratory data. Computed profiles that were qualitatively similar to corresponding laboratory profiles were obtained for the average reactant concentrations, the rms fluctuating reactant concentrations, the average product concentrations, the rms fluctuating product concentrations, and the concentration correlations.

We have made some comparisons with existing theories. Donaldson and Hilst have suggested, in addition to using the equations for the average concentrations, including the equations for the concentration fluctuations and correlation (ref. 2). These equations can be closed by neglecting certain triple moments when compared to certain lower order terms. However, our results indicate that the triple moment terms are as important as other terms in the equations, so that an assumption of this type will probably lead to poor predictions. Mason and Spaulding have proposed a model for the mean reaction term, suggesting that it will be proportional to the average concentration of the lean species divided by a turbulent time scale (ref. 3). We have found that such an assumption will only be moderately successful if applied to our case. Finally, Toor has suggested estimating the concentration correlation of the reacting species in terms of that for the nonreacting case, which is much easier to model (ref. 4). Although this was proposed mainly for statistically homogeneous flows, we find that it is a reasonable approximation for our reacting flow simulations.

REFERENCES

1. Orszag, S. A.: Numerical Simulation of Incompressible Flows within Simple Boundaries: Accuracy. J. Fluid Mech., vol. 49, 1971, pp. 75-112.

2. Donaldson, C. duP.; and Hilst, G. R.: Effect of Inhomogeneous Mixing on Atmospheric Photochemical Reactions. Env. Sci. Tech., vol. 6, 1972, pp. 812-816.

3. Mason, H. B.; and Spaulding, D. B.: Prediction of Reaction RAtes in Turbulent Premixed Boundary Layer Flows. Proc. First Symp. (European) on Comb., 1973, pp. 601-606, Academic Press.

4. Toor, H. L.: Turbulent Mixing of Two Species With and Without Chemical Reactions. Ind. Eng. Chem. Fundam., vol. 8, 1969, pp. 655-659.

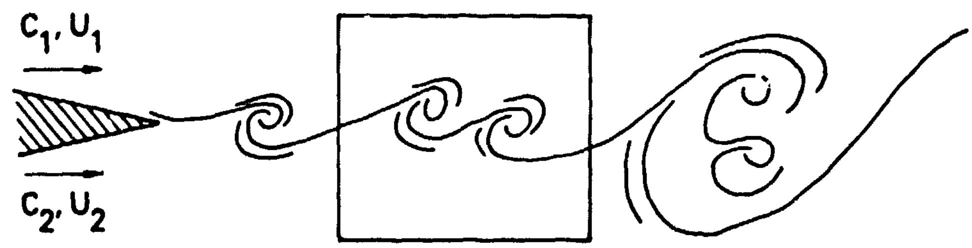
OBJECTIVES

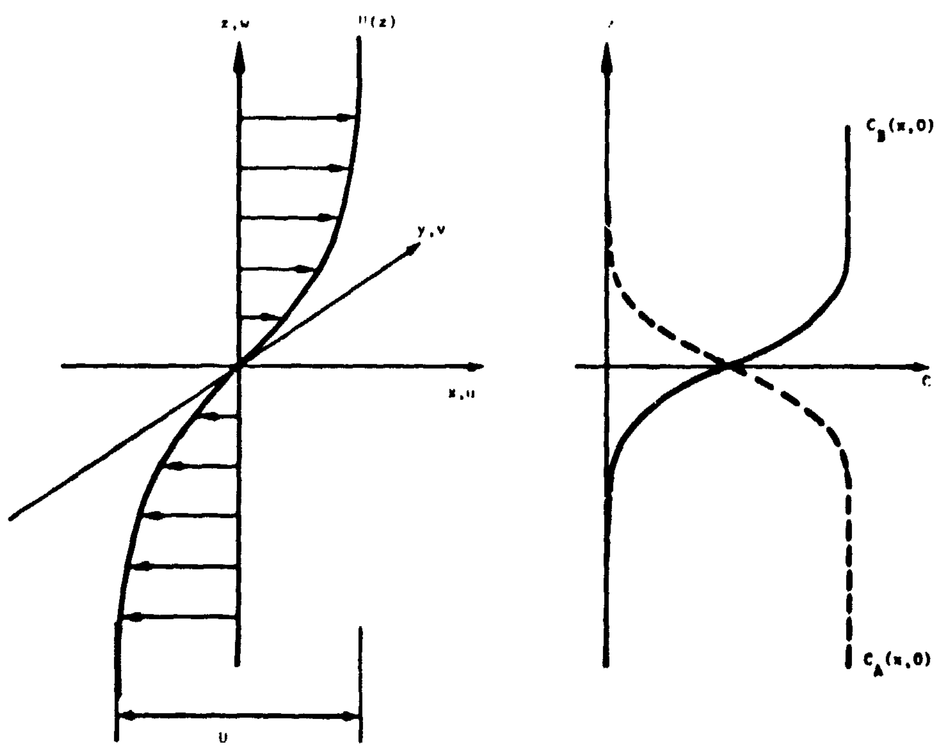
- Begin the Extension of Direct Numerical Simulations to Combustor Flows
  - Develop computational methodology
- Use Direct Numerical Simulations in Order to
  - Better understand the effects of turbulence on chemical reactions
  - Suggest model improvements
- Test Validity of the Method by Comparing Computational Results with Laboratory Data and Theoretical Models

PROBLEM CONSIDERED

- Temporally Growing, Three-Dimensional Mixing Layer
- Binary, Single-Step, Irreversible Chemical Reaction ($A + nB \rightarrow$ products) with negligible heat release
- Very Small Mach Number
- Initial Conditions – NonPremixed Species

PROBLEM CONSIDERED





Problem Geometry - Initial Conditions

SCOPE OF WORK

- Modify Existing Computer Codes to Treat the Present Problem
- Perform Numerical Testing of the Computer Codes
- Compute the Following Sequence of Problems
  - Unidirectional (one-dimensional) flow
  - Large-scale, two-dimensional vortex rollup
  - Three-dimensional turbulent mixing layer

EQUATIONS OF MOTION

- Conservation of Momentum

$$\frac{\partial}{\partial t} u_i + u_j \frac{\partial}{\partial x_j} u_i = -\frac{1}{\varrho} \frac{\partial}{\partial x_i} p + \nu \frac{\partial^2}{\partial x_j^2} u_i$$

- Conservation of Mass

$$\frac{\partial}{\partial x_i} u_i = 0$$

- Conservation of Species A and B

$$\frac{\partial}{\partial t} C_1 + u_j \frac{\partial}{\partial x_j} C_1 = -R_1 C_1 C_2 + D_1 \frac{\partial^2}{\partial x_j^2} C_1$$

$$\frac{\partial}{\partial t} C_2 + u_j \frac{\partial}{\partial x_j} C_2 = -R_2 C_1 C_2 + D_2 \frac{\partial^2}{\partial x_j^2} C_2$$

- Initial Boundary Conditions

DIRECT NUMERICAL SIMULATIONS

- Compute the Solution of the Navier-Stokes Equations Numerically
- Initial Conditions (or Upstream Conditions)
  Random, turbulent-like – so that the flow field starts out as turbulent-like – or
  Small amplitude perturbations -- compute the flow through transition to turbulence
- Compute the Time Development of the Detailed Structure of the Flow Field
- No Reynolds Averaging
- Statistical Results are Obtained by Performing Spatial, Temporal, or Ensemble Averages over the Computed Flow Field
- Analogous to Laboratory Experiments

NUMERICAL METHODS

- Pseudo-Spectral Methods
  - Expand the dependent variables in fast-converging series

E. G.,

$$u(x) = \sum_{|k|<K} \hat{u}(k)e^{ikx}$$

- Resulting Equations

$$\frac{\partial}{\partial t}\hat{C}_1(\underset{\sim}{k},t) + \underbrace{i\sum_{\underset{\sim}{k}'} \hat{u}_j(\underset{\sim}{k}-\underset{\sim}{k}')k_j'\, \hat{C}_1(\underset{\sim}{k}')}_{\text{Convection}} = \underbrace{-R_1 \sum_{\underset{\sim}{k}'} \hat{C}_1(\underset{\sim}{k}-\underset{\sim}{k}')\hat{C}_2(\underset{\sim}{k}')}_{\text{Reaction}} \underbrace{- D_1 k^2 \hat{C}_1(\underset{\sim}{k})}_{\text{Diffusion}}$$

NUMERICAL TESTS

- Color Problem (Rigid Body Rotation of Passive Scalar)
  - Convection Alone (Orszag, Seinfeld et al.)
  - Convection Plus Reaction (Exact Solutions Available)
  - Convection Plus Diffusion (Exact Solutions Available)
- One-Dimensional, Diffusion-Reaction Problem
  - Test Against Exact Solutions
- Two-Dimensional Vortex Rollup
  - Convection, Diffusion, and Reaction
  - "Exact" Solution for $\theta = C_1 - C_2$ is Known from Previous Calculation

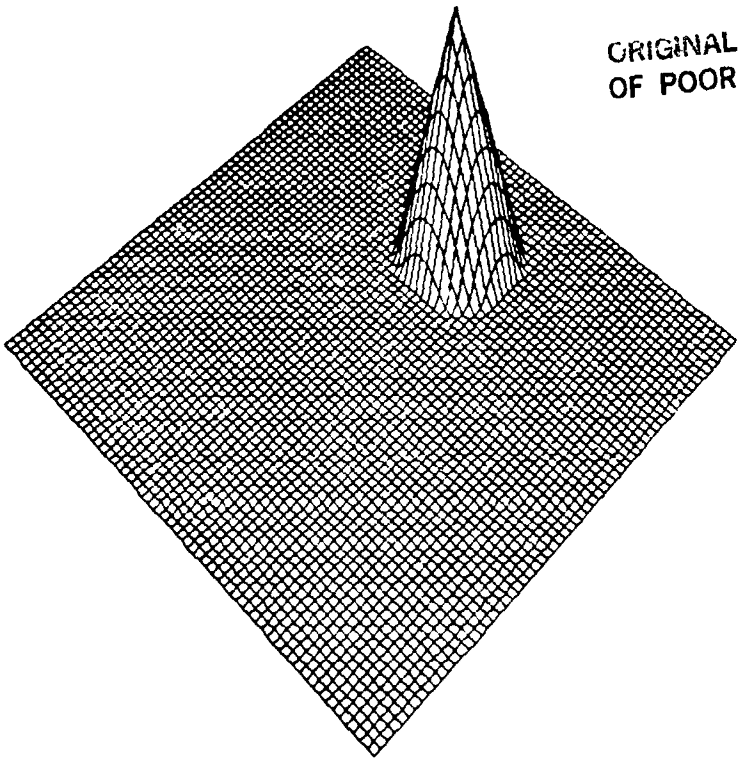
NUMERICAL TEST PROBLEMS

- Two Dimensional Rigid Rotation (Color Problem)
  - Initial condition: $C(x,z,0) = \exp\left(-\frac{x^2}{x_o^2} - \frac{z^2}{z_o^2}\right)$
- Analytical Solution for Identical Initial Concentration Fields (No Diffusion)

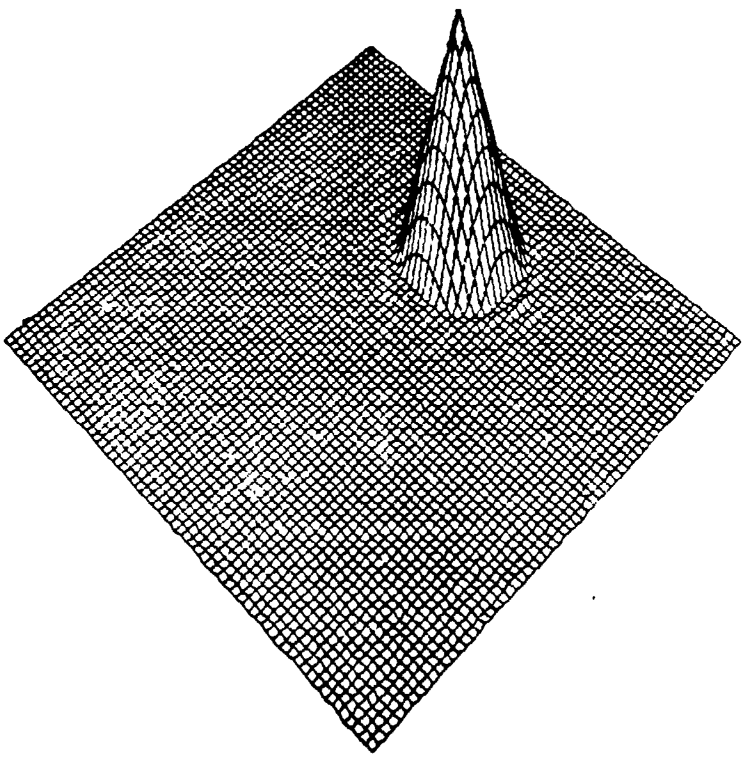
$$C(x',z',t) = \frac{C(x',z',0)}{1 + RtC(x',z',0)}$$

- Analytical Solution with Diffusion (No Reaction)

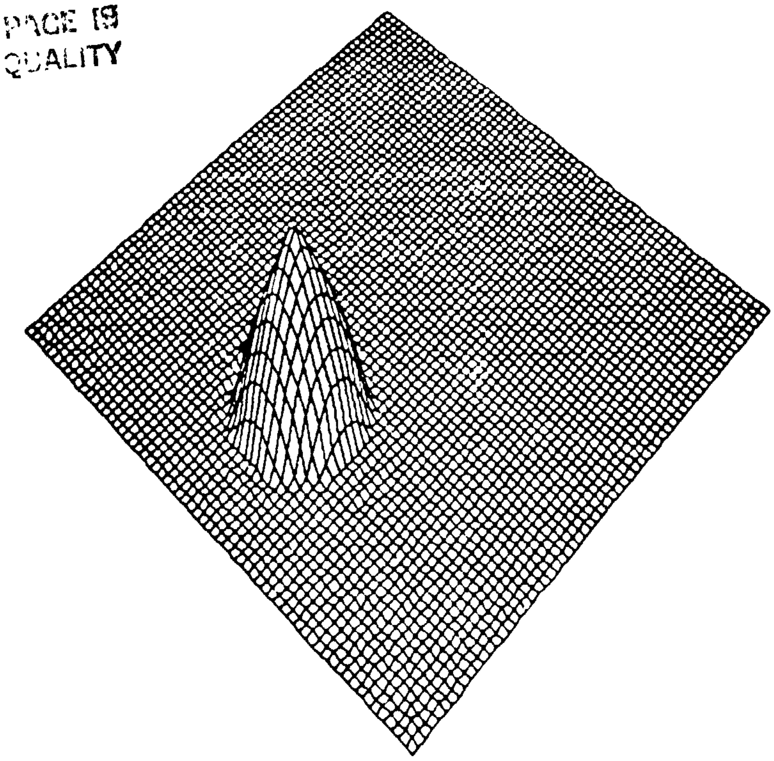
$$C(x',z',t) = \frac{1}{\sqrt{\left(1 + \frac{4Dt}{x_o^2}\right)\left(1 + \frac{4Dt}{z_o^2}\right)}} \exp\left[-\frac{x'^2/x_o^2}{\left(1 + \frac{4Dt}{x_o^2}\right)} - \frac{z'^2/z_o^2}{\left(1 + \frac{4Dt}{z_o^2}\right)}\right]$$



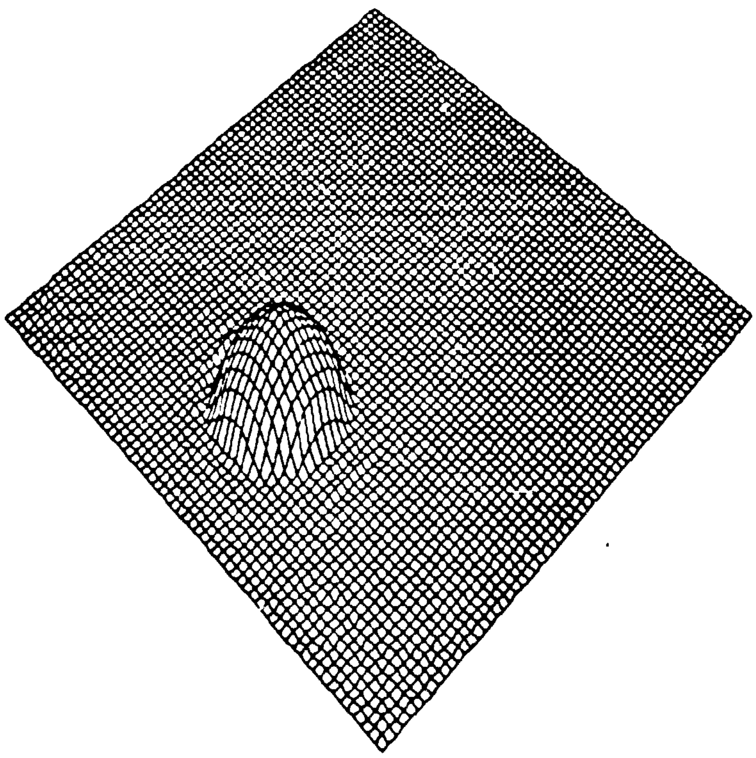
Initial Concentration Field for Color Problem Tests



Computed Concentration Field After One Revolution - No Diffusion or Reaction



Computed Concentration Field After One-Half Revolution - No Diffusion, R = 1.0



Computed Concentration Field After One-Half Revolution - No Diffusion, R = 4.0

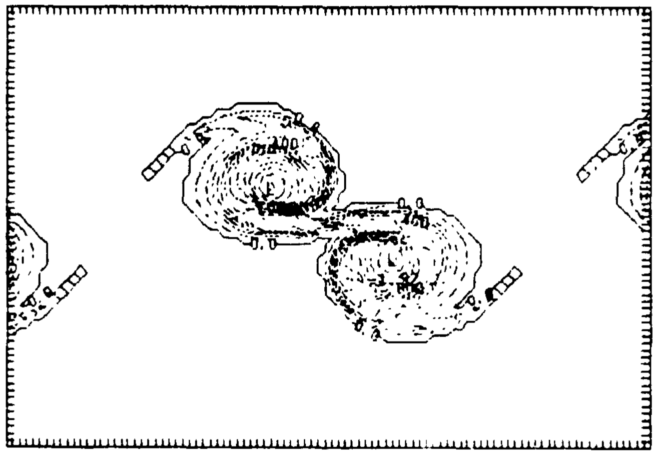


Figure 21a t = 12

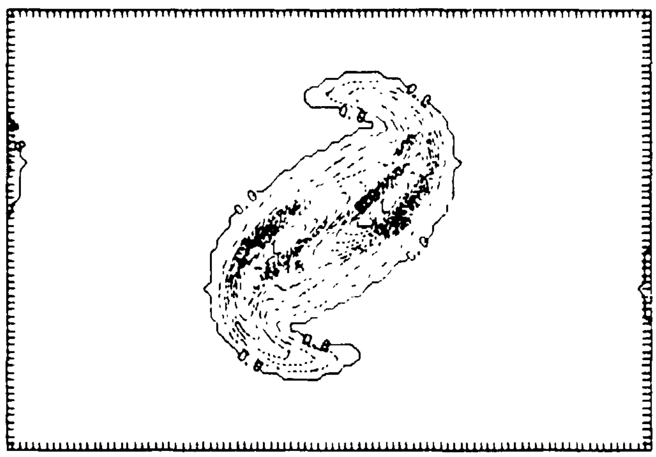


Figure 21b t = 24

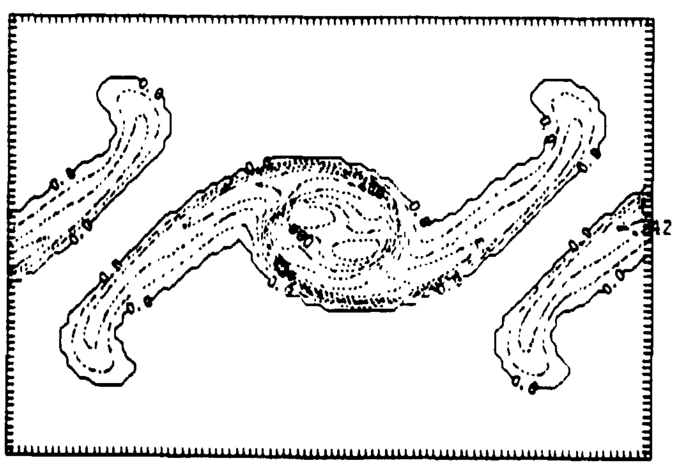


Figure 21c t = 36

Plots of Vorticity Contours for a Sequence of Times - Case 3 (Fundamental and Subharmonic Added Together Out-of-Phase)

TWO-DIMENSIONAL SIMULATIONS

- Case I: Most Unstable Mode Based Upon Linear Theory (Fundamental)
  - Results in a Single Rollup
- Case II: Subharmonic of the Most Unstable Mode
  - Results in a Single Rollup, of Approximately Twice the Size and Time Period
- Case III: Fundamental and Subharmonic 90° Out-of-Phase
  - Results in a Double Rollup

EQUATIONS (CONT.)

- Define Conserved Scalar $\theta = C_A - C_B$.

  Then θ satisfies

  $$\boxed{1}\ \frac{\partial \theta}{\partial t} + u \cdot \nabla \theta = D \frac{\partial^2}{\partial x_j^2} \theta \qquad \text{(No R dependence)}$$

  with initial conditions $\theta(t=0) = \theta(0) = C_A(0) - C_B(0)$

- Infinite Reaction Rate Limit

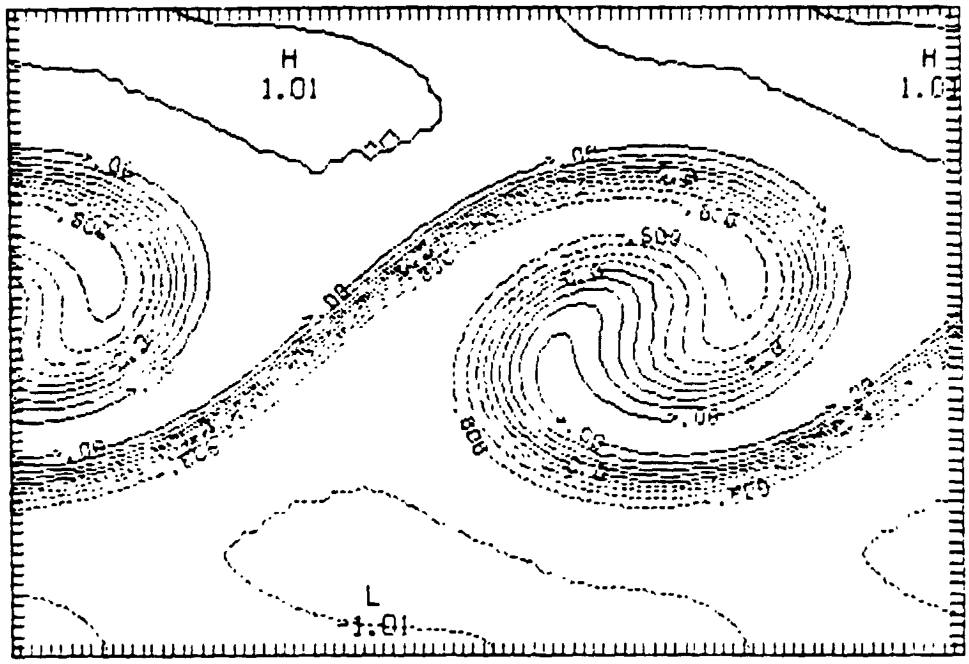
  $$C_1 = \begin{cases} \theta & \theta \geq 0 \\ 0 & \theta < 0 \end{cases} \qquad C_2 = \begin{cases} 0 & \theta > 0 \\ -\theta & \theta < 0 \end{cases}$$

  C_P can be obtained from conserved scalar

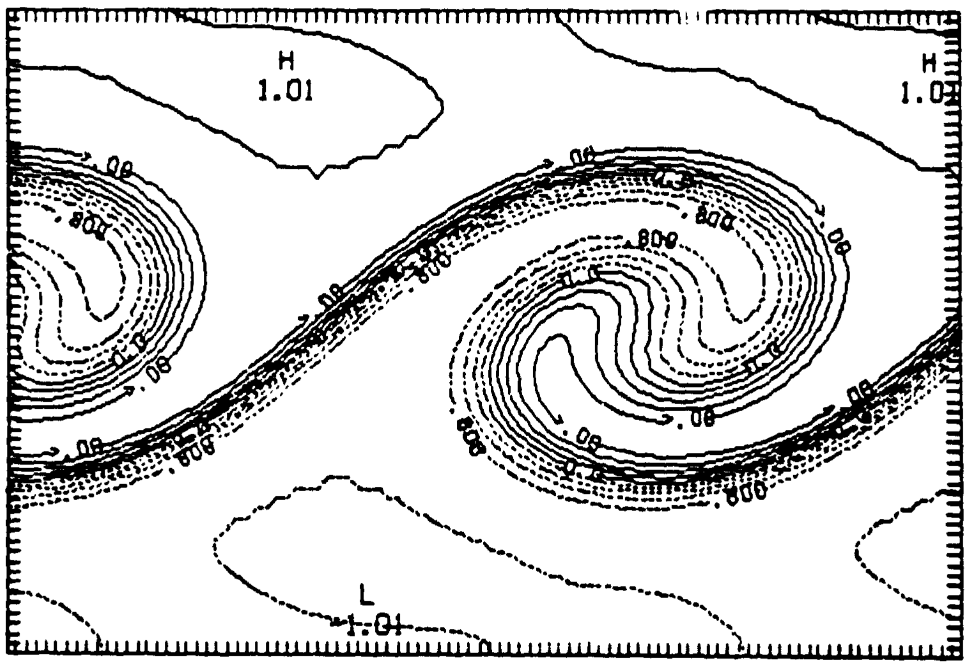
  $$\varnothing = C_P + C_A$$

  where $\varnothing$ also satisfies Equation $\boxed{1}$

  with initial conditions $\varnothing(t=0) = \varnothing(0) = C_A(0)$



Constant Contour Plot of Conserved Scalar Computed Indirectly from the Difference Between the Species Concentrations - t = 12



Constant Contour Plot of Conserved Scalar Computed Directly from the Difference Between the Species Concentrations - t = 12

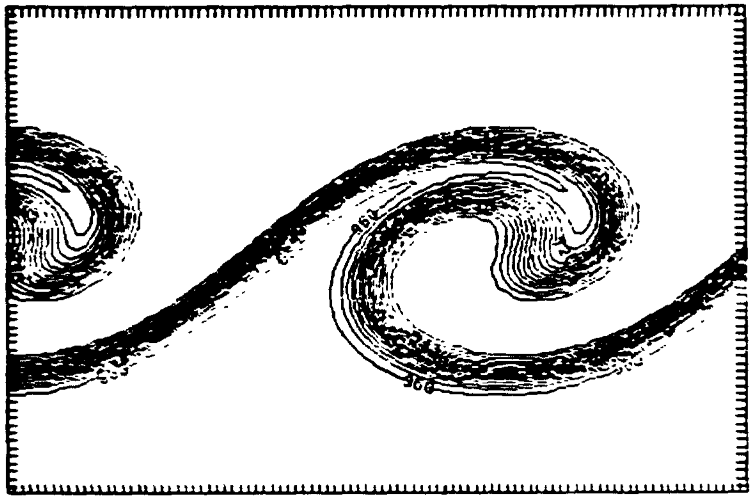


Figure 23a Species A

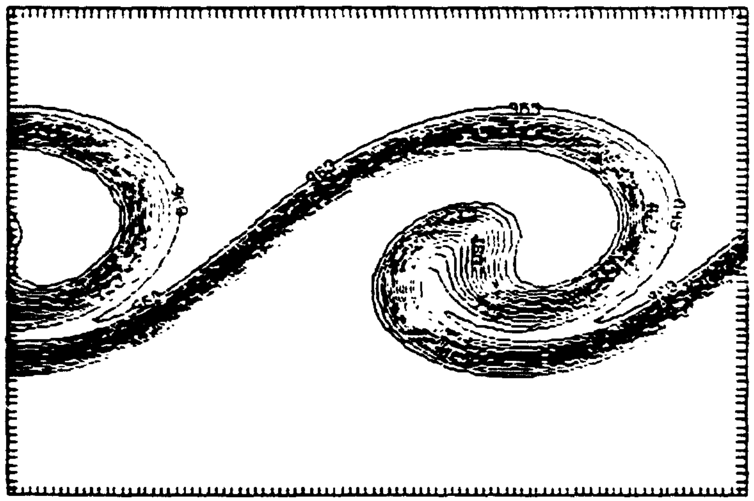


Figure 23b Species B

Plots of Concentration Contours for Species A and B at t = 12 for Case 1 (Fundamental Mode Alone) - Two-Dimensional Simulations

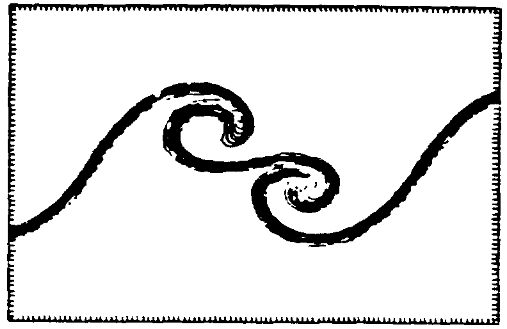


Figure 28a t = 12

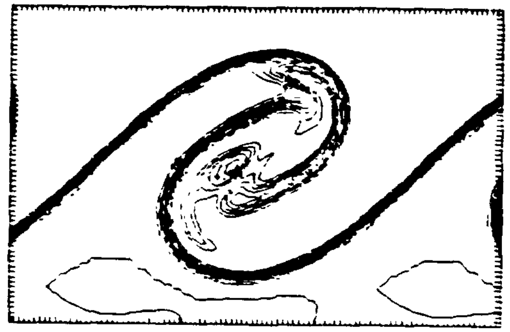


Figure 28b t = 24

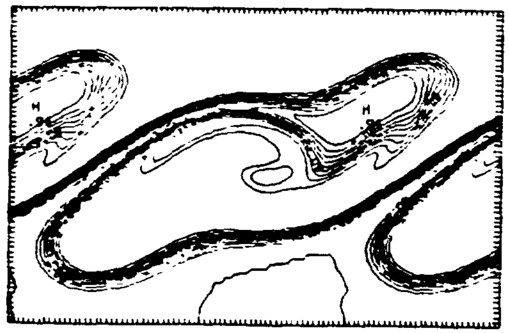
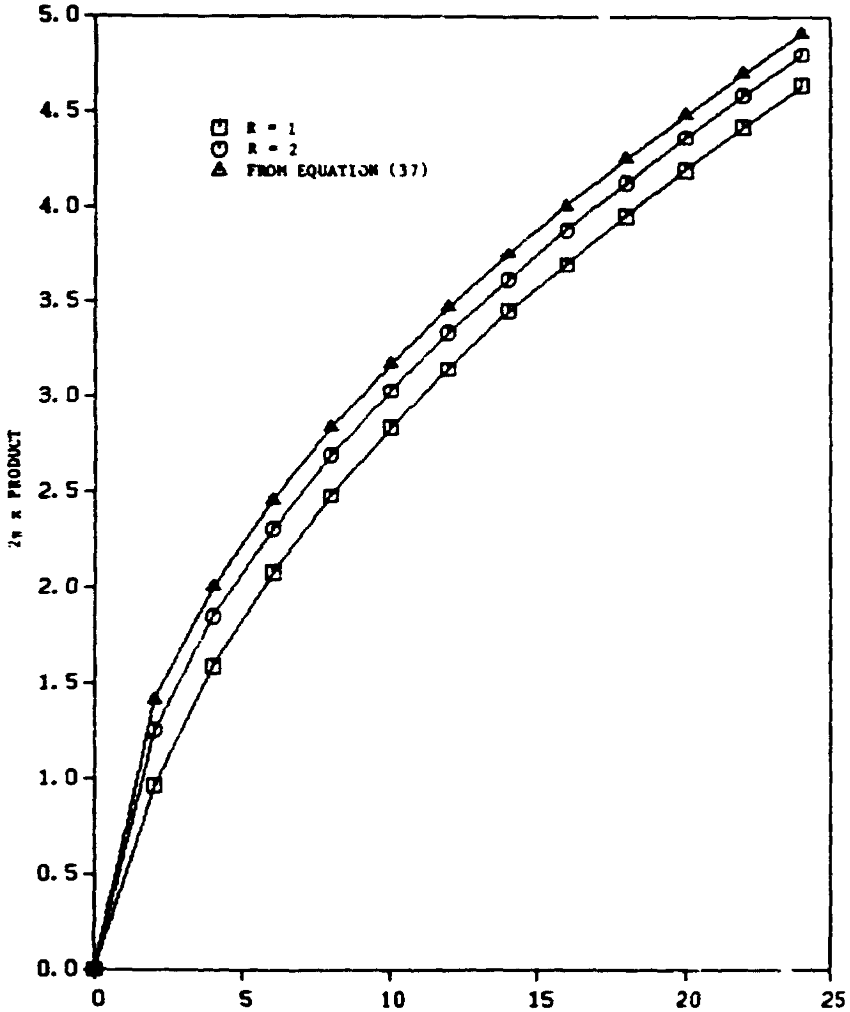
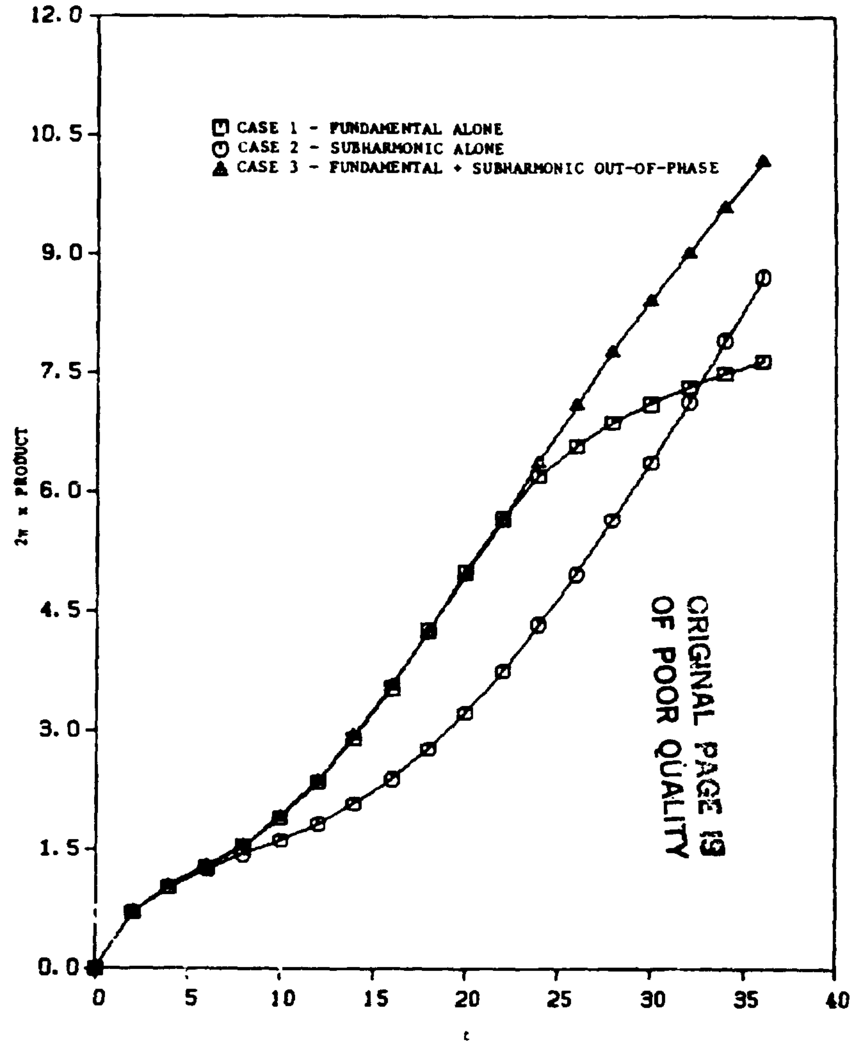


Figure 28c t = 36

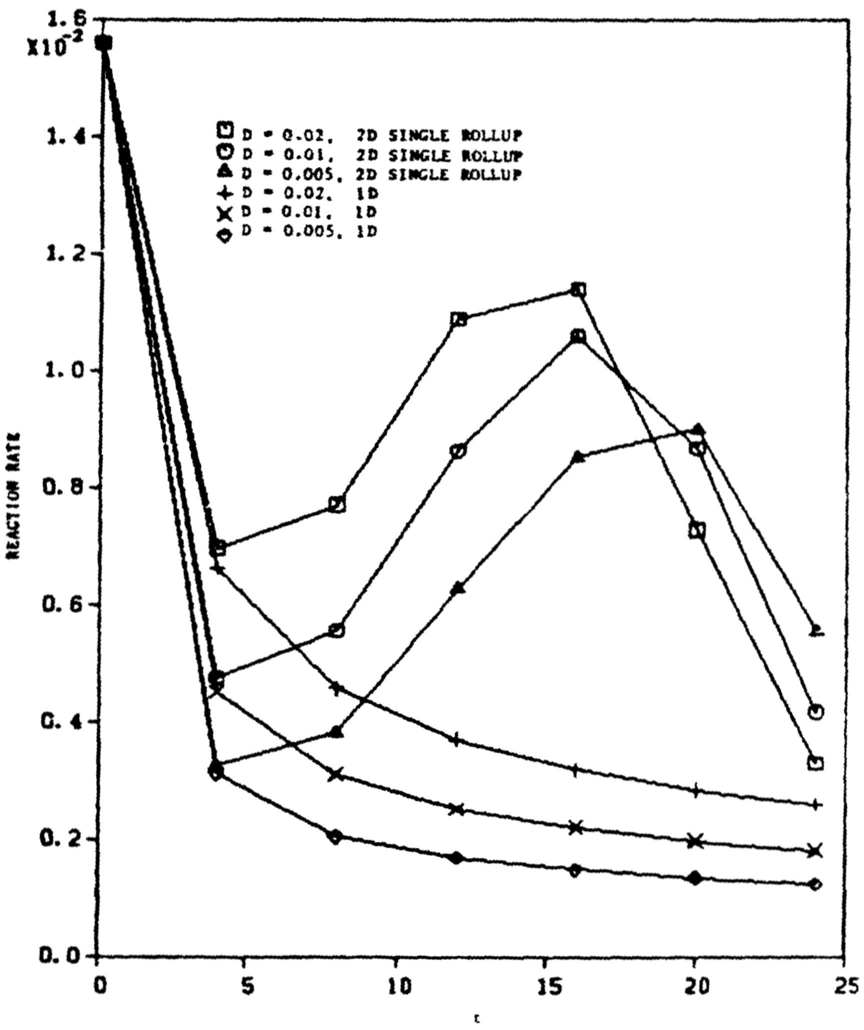
Plots of Concentration Contours for Species A for a Sequence of Times for Case 3 (Fundamental and Subharmonic Added Together Out-of-Phase) - Two-Dimensional Simulations



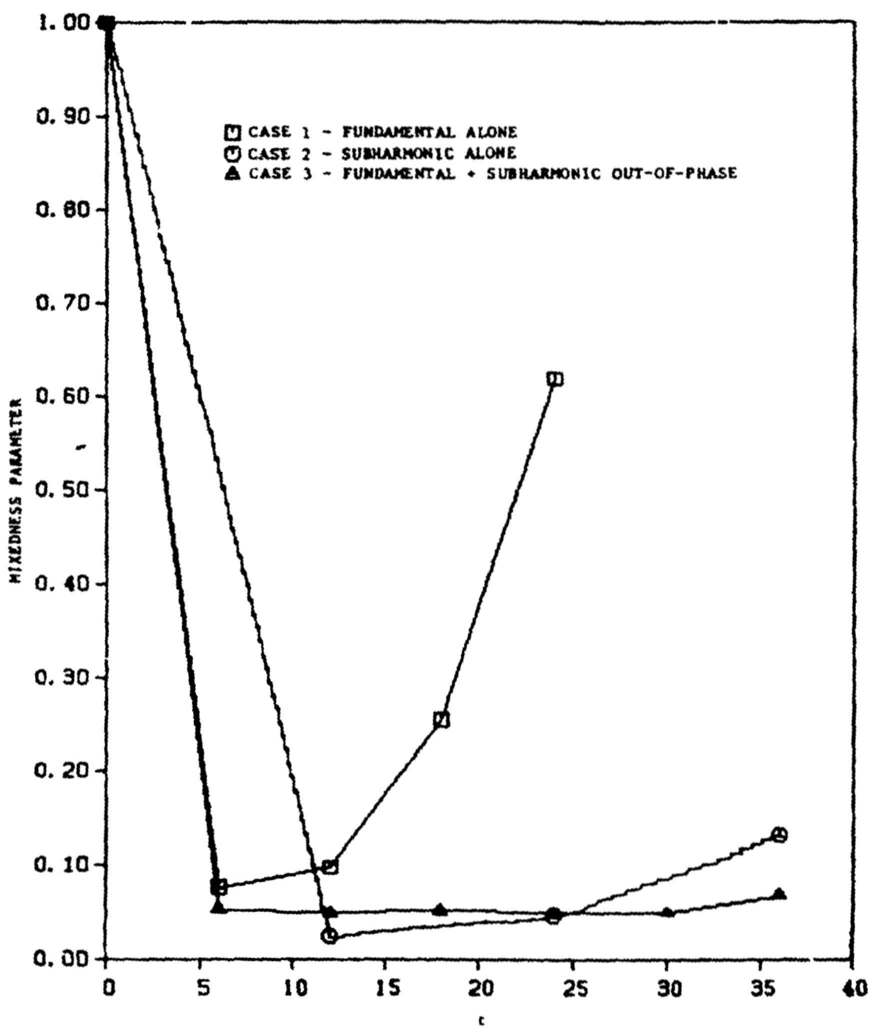
Total Product Versus Time for Two Different Values of the Reaction Rate Coefficient R - One-Dimensional Simulations. Also Shown Is the Infinite Reaction Rate Solution [Equation (37)]



Total Product Versus Time - Two-Dimensional Simulations



Total Reaction Rate Versus Time for Different Diffusivities - One- and Two-Dimensional Simulations



Mixedness Parameter Versus Time - Two-Dimensional Simulations

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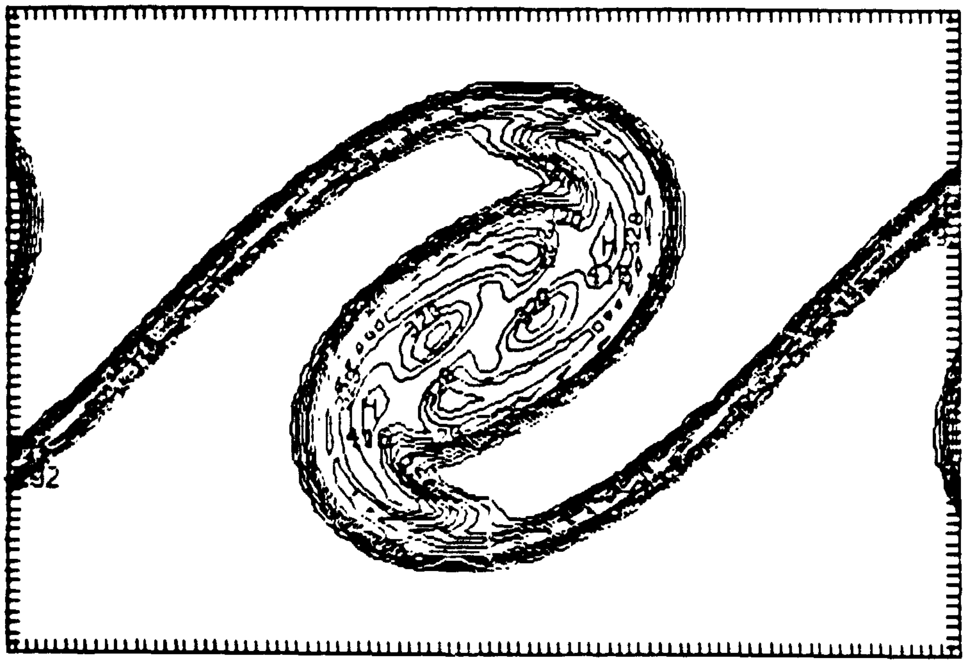

Plot of Product Concentration Contours at t = 24 for Case 3 (Fundamental and Subharmonic Added Together Out-of-Phase) - Two-Dimensional Simulations

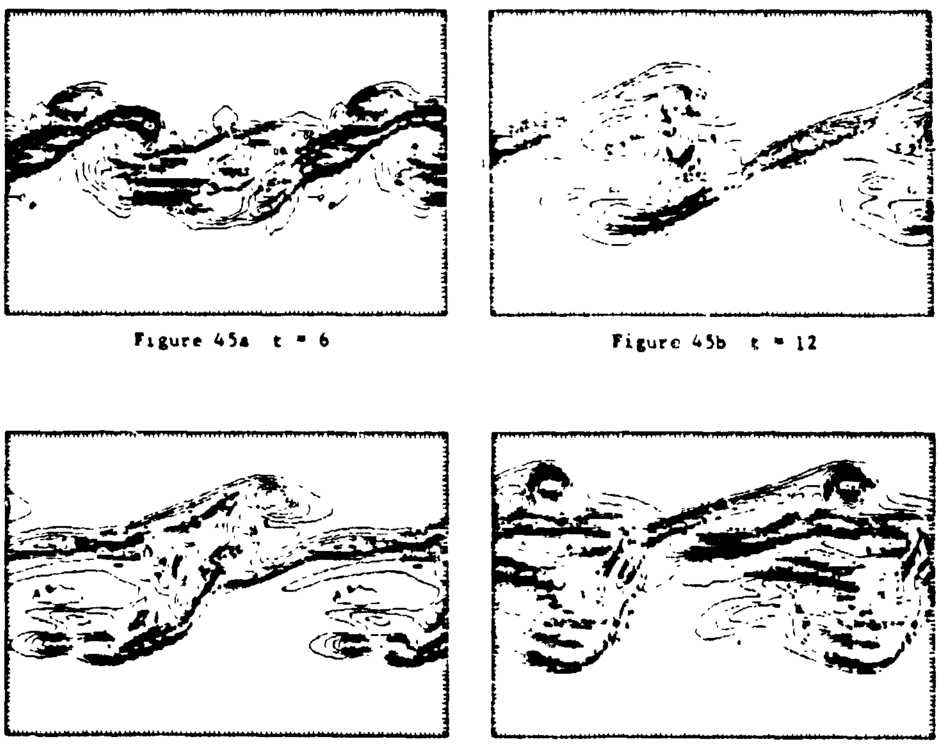

Figure 45a t = 6

Figure 45b t = 12

Figure 45c t = 18

Figure 45d t = 24

Plots of Lateral (y) Vorticity Contours for a Sequence of Times in an x-z Plane Located a Lateral Distance $L_y/2$ from that Depicted in Figure 44 - Single Rollup Case, Three-Dimensional Simulations, Run JN20B

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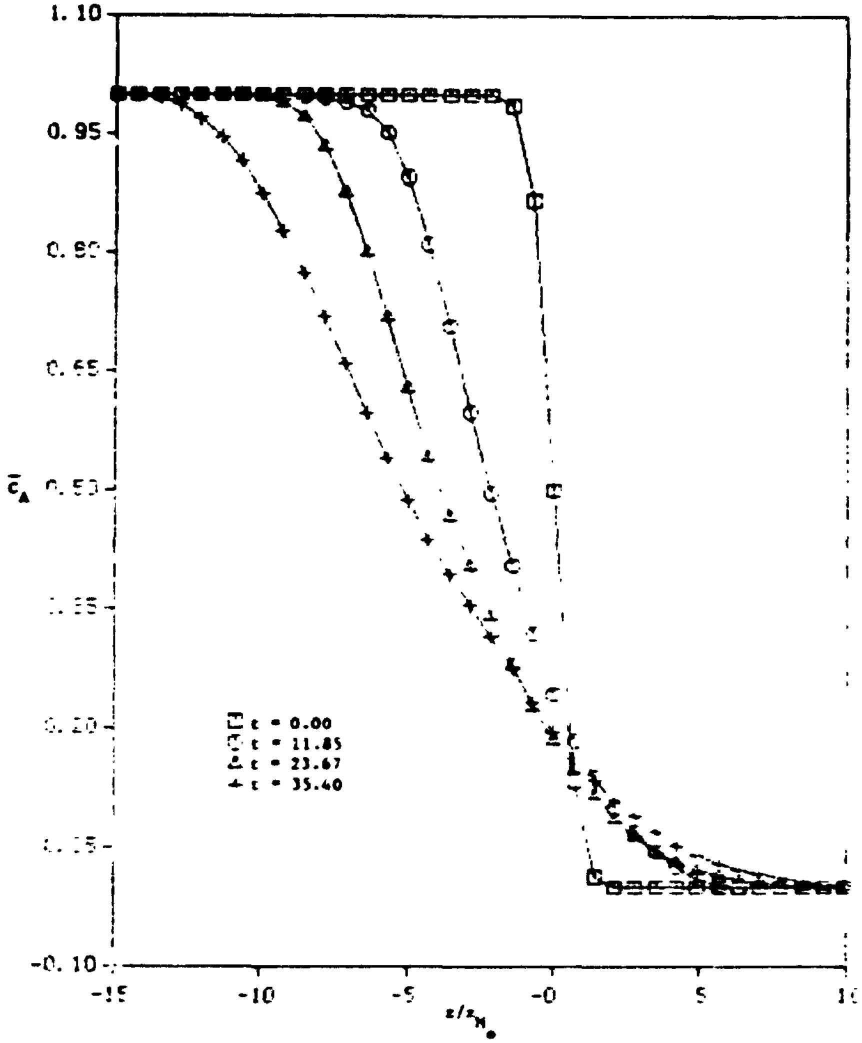
Figure 46a t = 6

Figure 46b t = 12

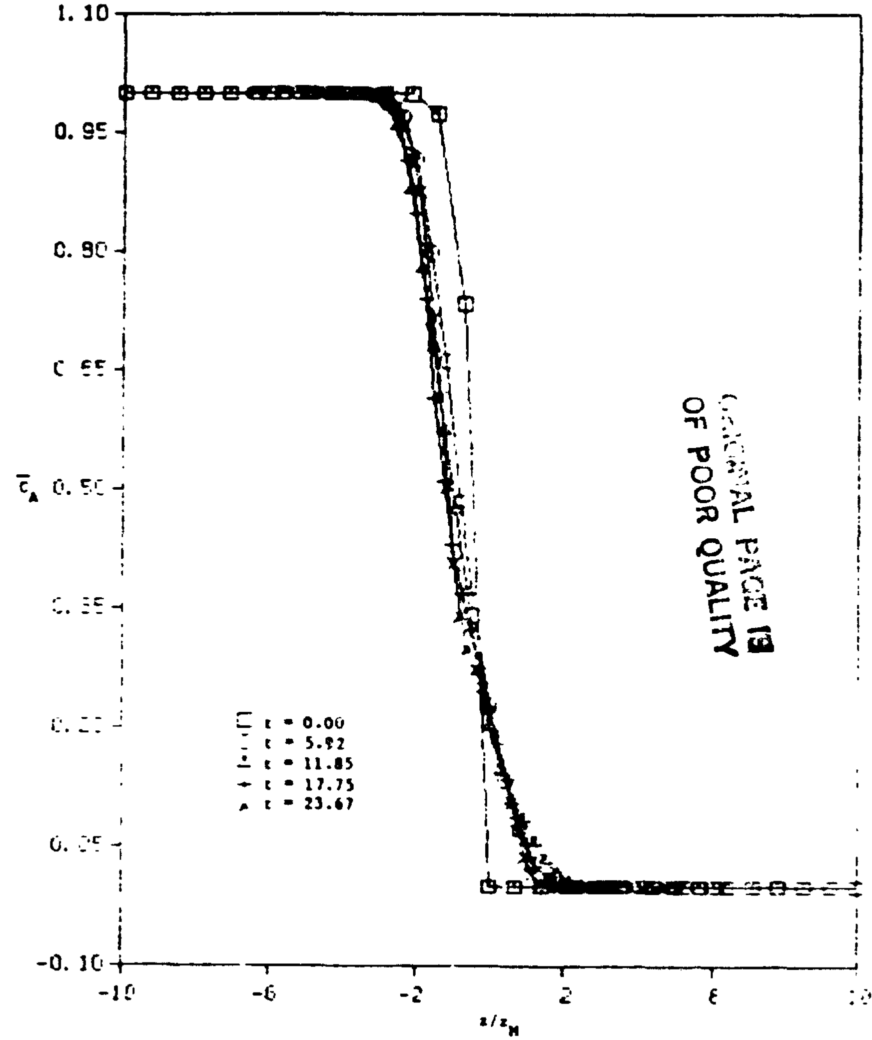
Figure 46c t = 18

Figure 46d t = 24

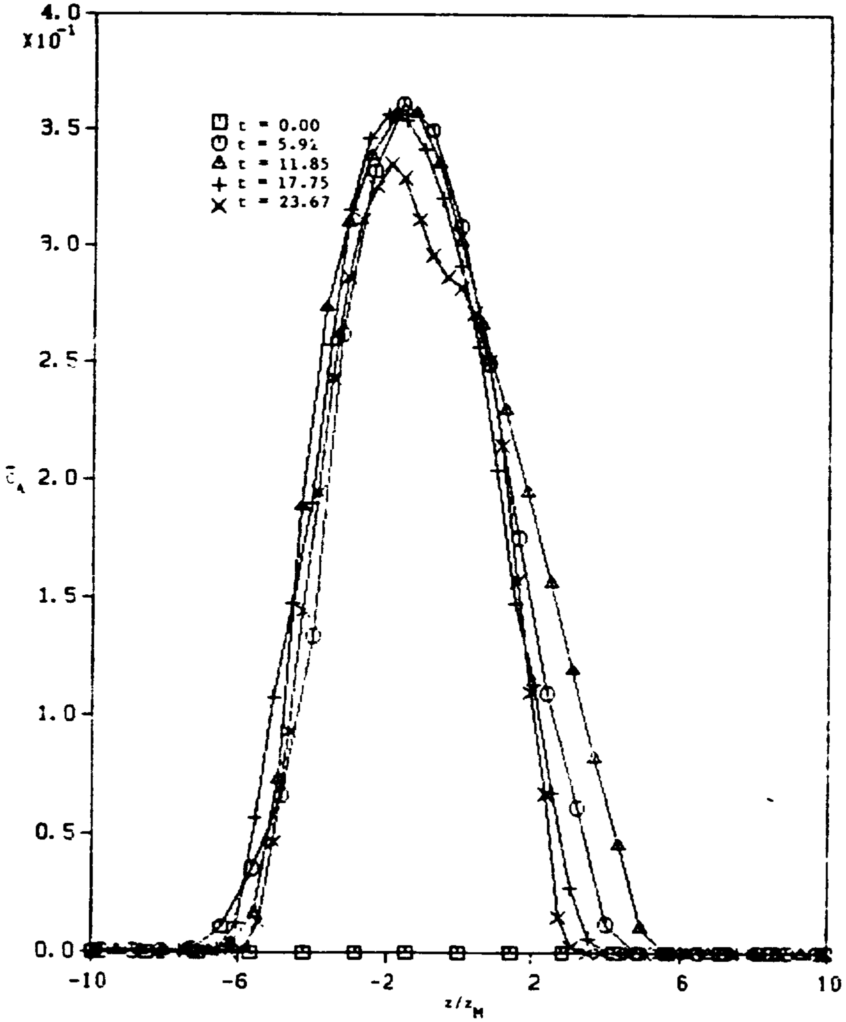
Plots of Concentration Contours for Species B for a Sequence of Times in the Same x-z Plane as for Figure 44 - Single Rollup Case, Three-Dimensional Simulations



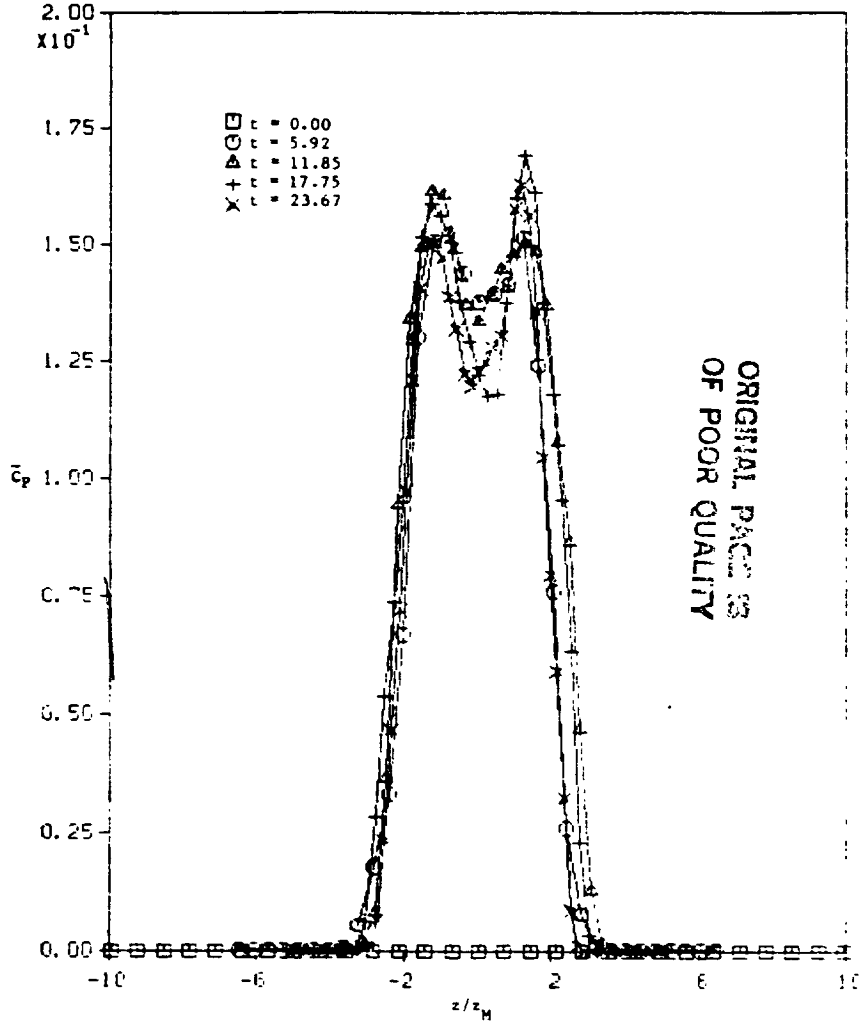
Average Concentration of Species A Versus z for a Sequence of Times - Realization II, Double Rollup Case, Three-Dimensional Simulations



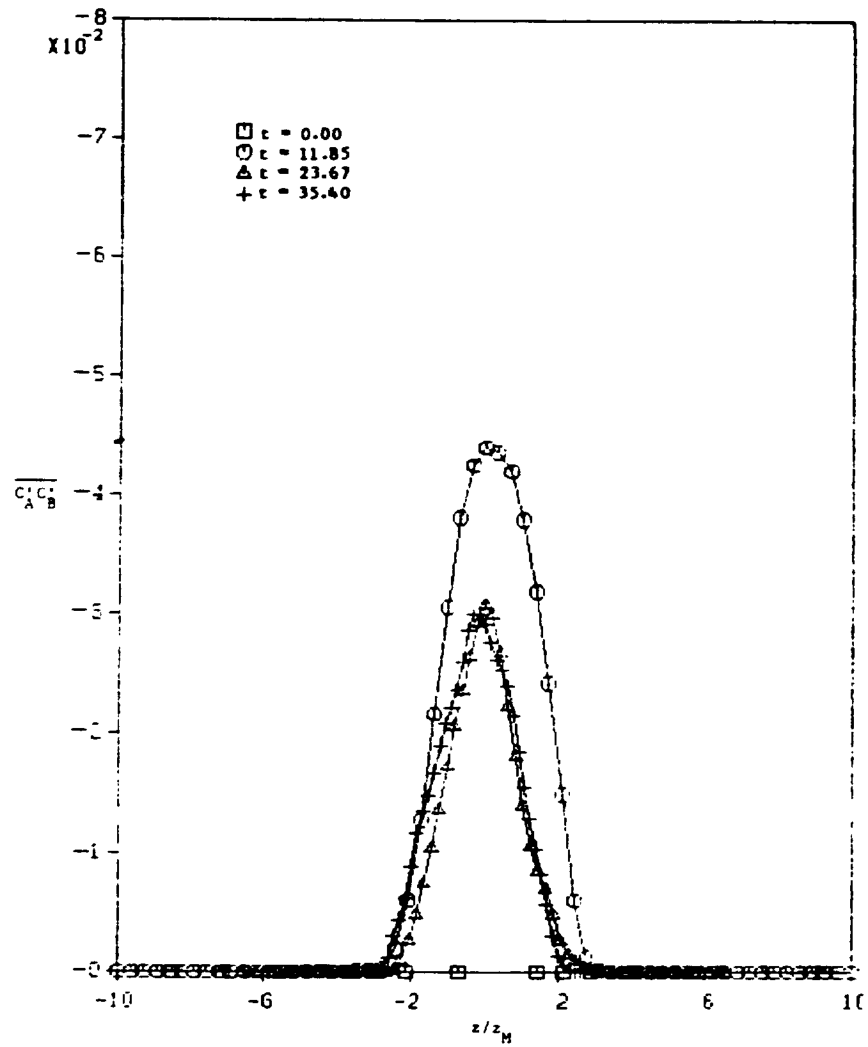
Similarity Plots of $\bar{C}_A/C_A$, Versus z/z_M (= $z/z_{1/2}$) for Various Times - Single Rollup Case, Infinite Reaction Rate, Three-Dimensional Simulations



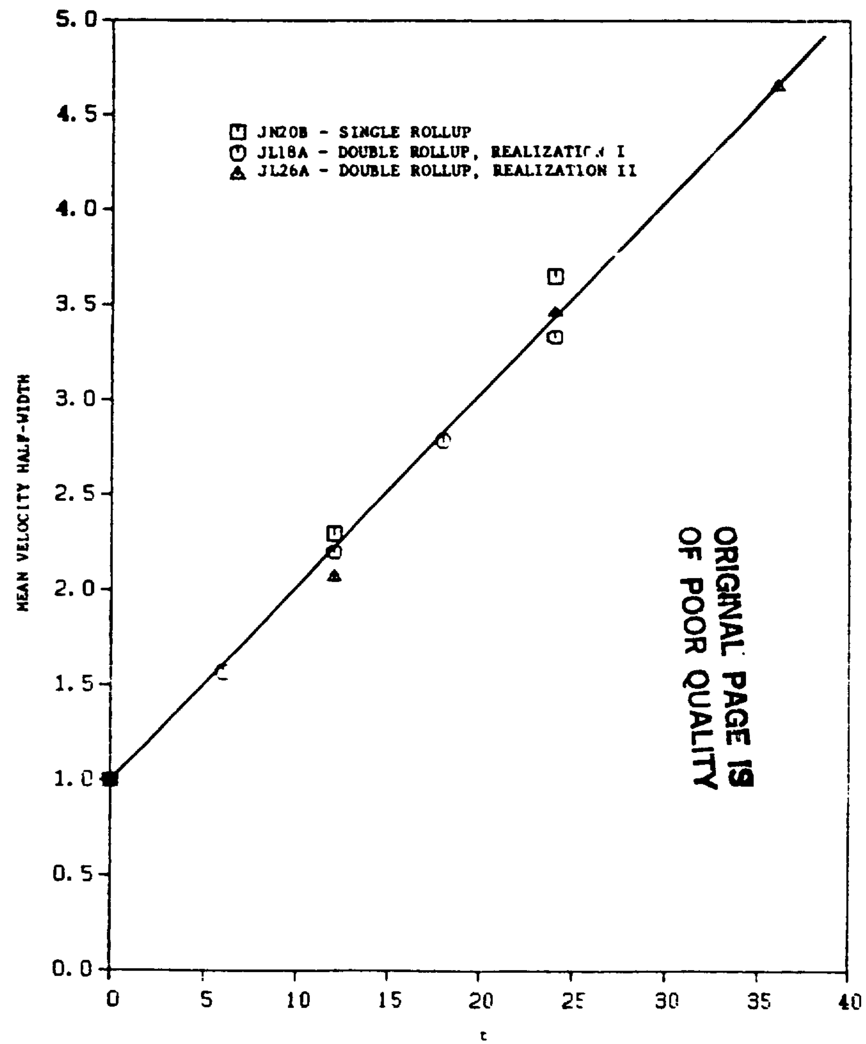
Similarity Plots of $\bar{C}_A/C_{A\infty}$ Versus z/z_M ($= z/z_{1/2}$) for Various Times - Single Rollup Case, Infinite Reaction Rate, Three-Dimensional Simulations



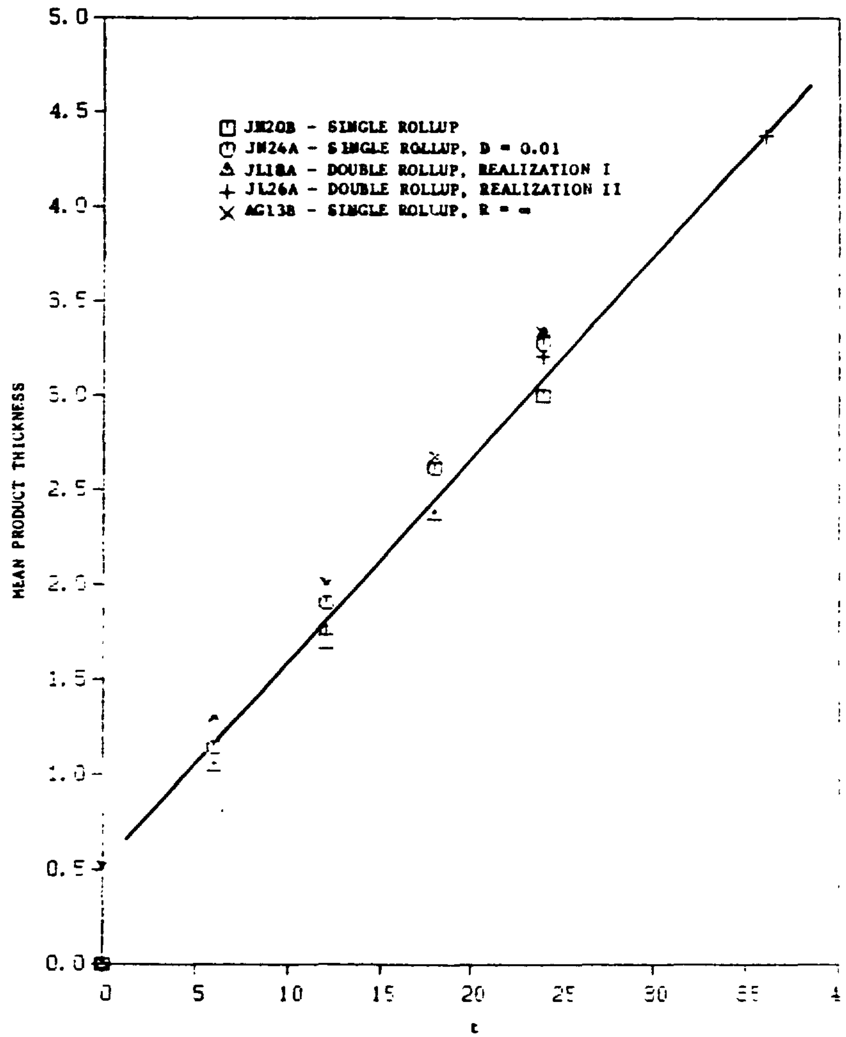
Similarity Plots of $\bar{C}_P/C_{A\infty}$ Versus z/z_M ($= z/z_{1/2}$) for Various Times - Single Rollup Case, Infinite Reaction Rate, Three-Dimensional Simulations



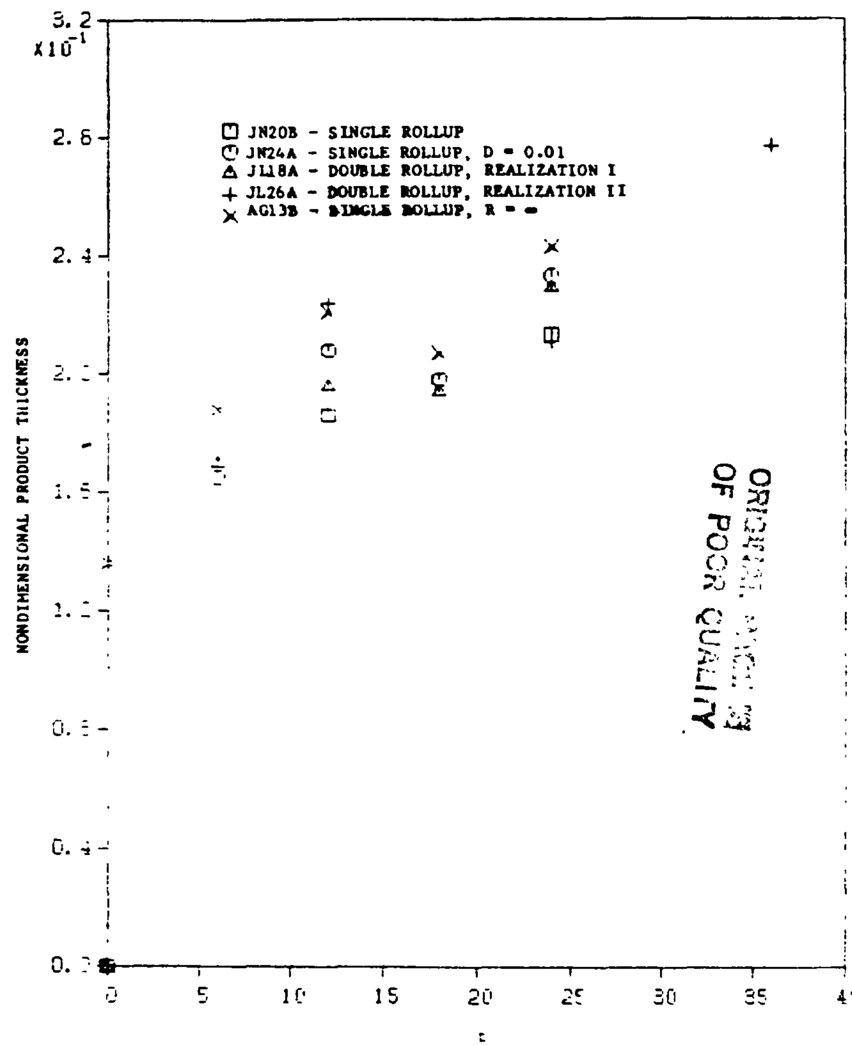
Similarity Plots of $\overline{C_A'C_B'}/C_{A\infty}^2$ Versus z/z_M (= $z/z_{1/2}$) for Various Times - Double Rollup Case, Finite Reaction Rate, Three-Dimensional Simulations



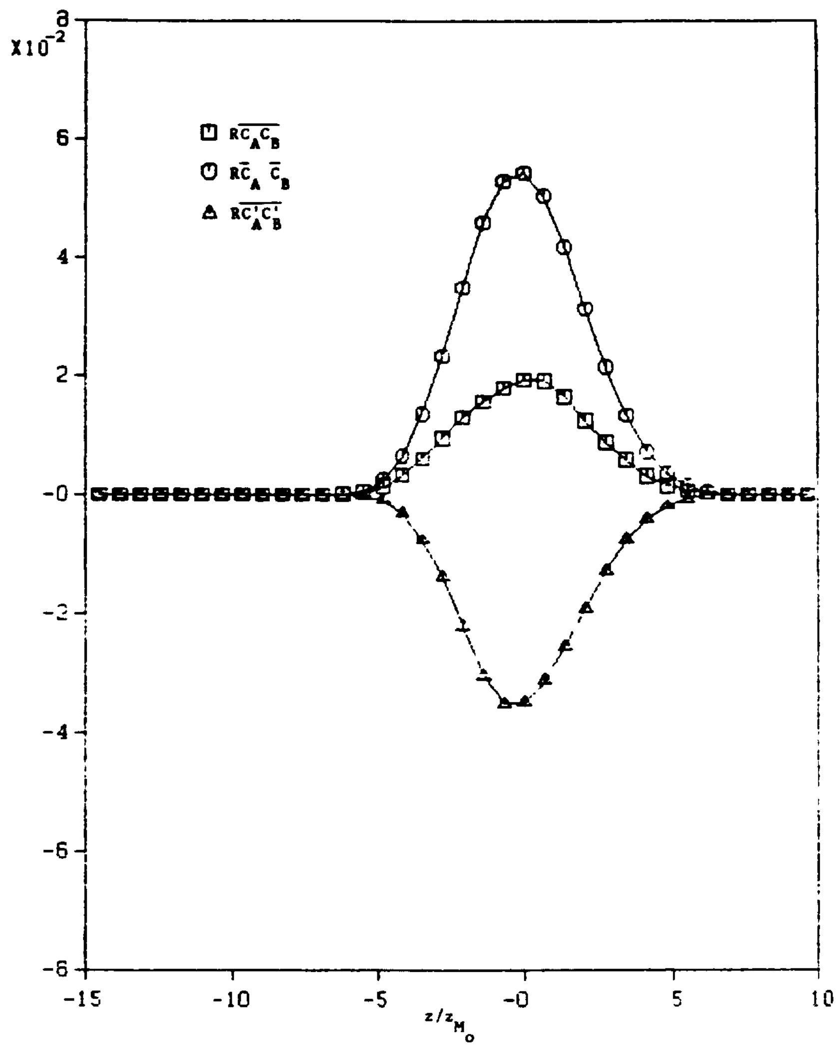
Mean Velocity Half-Width, z_M (= $z_{1/2}$), Versus Time - Three-Dimensional Simulations



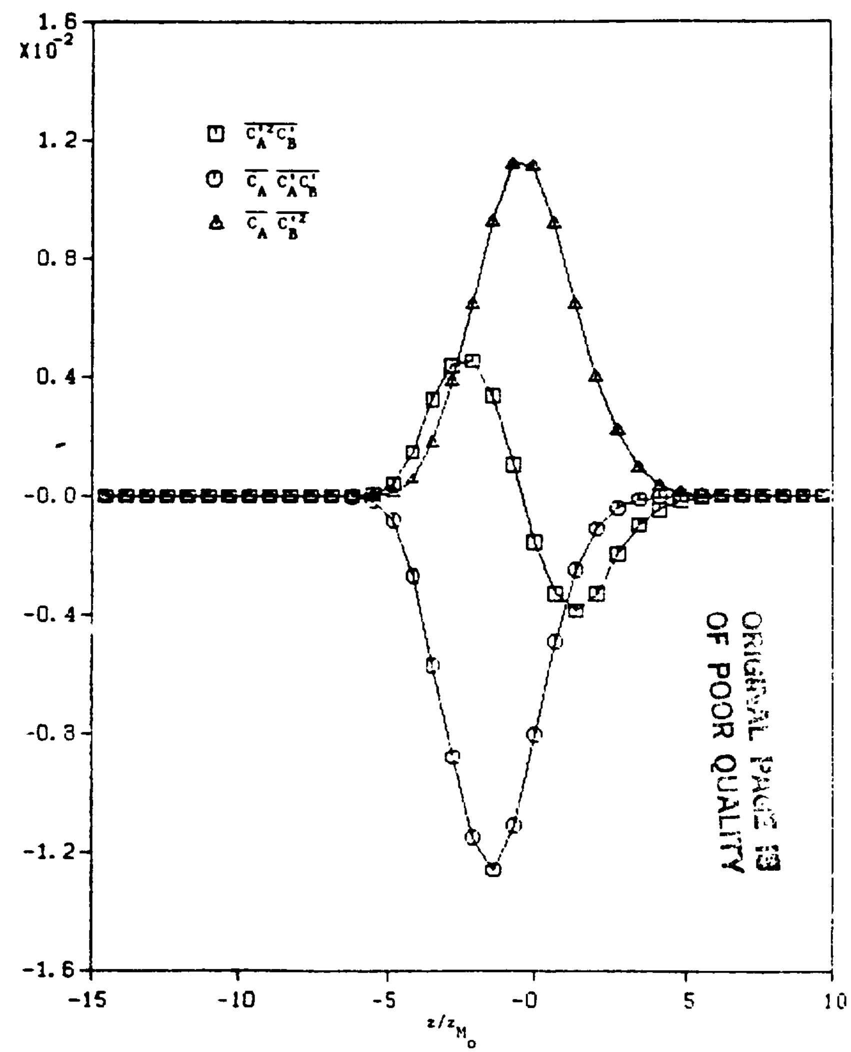
Mean Product Thickness, zp, Versus Time - Three-Dimensional Simulations



Nondimensional Product Thickness Versus Time - Three-Dimensional Simulations



Average of the Product of the Concentrations, the Product of the Averages, and the Concentration Correlation Versus z at t = 12 - Realization I, Double Rollup Case, Three-Dimensional Simulations



Various Concentration Moments Versus z at t = 12 - Realization I, Double Rollup Case, Three-Dimensional Simulations

CONCLUSIONS

- Color Problem Tests Showed That
  - Spectral methods produced high accuracy solutions in the presence of advection, reaction, and diffusion
  - Weak spatial filter insured numerical stability
- One-Dimensional Simulations Showed That
  - Calculations close to the infinite reaction rate can be done
  - Results were fairly insensitive to initial conditions
  - Results were in reasonable agreement with theoretical predictions
- Two-Dimensional Simulations Showed That
  - Reaction zone was significantly stretched by vortex rollup
  - Vorticity and product fields coincided
  - Significant species segregation and "flame shortening" effects were present

CONCLUSIONS (CONT.)

- Three-Dimensional Simulations Showed That
  - Good agreement with self-similarity theory was obtained
  - Technique can treat entire range of reaction rates – from very slow to infinite
  - Computed profiles qualitatively similar to profiles from laboratory data
  - Quantitative comparisons will be made soon
  - Nondimensional product thickness was 0.22 – compared to values of 0.3 to 0.35 from laboratory data
  - No adjustable parameters are used
  - Some presently used estimates of correlation products can be significantly in error