Numerical Solution of the Continuity Equation

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In treating the transient flow of a compressible fluid in a closed vessel, certain difficulties were experienced in solving the continuity equation. Because this equation is frequently encountered in chemical applications, and because of the popularity of numerical methods, it is believed that readers will be interested in both the problem and its solution. The storage of a gas during a space mission served as the basis for the problem. Due to continual heat flow into the system, the gas pressure increases with time. It was required to find the rate of pressure increase. In solving the problem, the energy, continuity, and momentum equations were considered. Richtmyer (*1*, pp. 171 and 194) presented difference forms for treating the problem.

For one-dimensional motion in a closed vessel, the continuity equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \qquad (1)$$

The interval $0 \leq x \leq L$ is subdivided into n equal increments, each of width Δx, as usual. Richtmyer (*1*), in his excellent test on numerical methods, describes an efficient mesh. The function $u(x, t)$ is evaluated at boundaries between Δx segments, while the function $\rho(x, t)$ is evaluated on centers of the Δx segments. Thus subscripts on u and ρ designate position by

$$u_i \cong u\,((i-1)\,\Delta x, t),\; i = 1, 2, \ldots n + 1 \qquad (2)$$

$$u_o = u_{n+1} = 0$$

$$\rho_i \cong \rho((i - 1/2)\,\Delta x, t),\; i = 1, 2, \ldots n \qquad (3)$$

Richtmyer (*1*, p. 194) presented an explicit technique for solving Equation (1). For reasons of stability it is necessary to shift between forward and backward differences of $u(\partial\rho/\partial x)$ depending upon the sign of u. We assume here that the $u(x, t)$ function is known over the mesh—for example by solving the momentum equation by the method of Richtmyer (*1*, p. 194). From the point of view of a total material balance this technique is unacceptable.

In forming a material balance, it is natural to use

$$\int_0^L \rho dx \cong \sum_{i=1}^{n} \rho_i \,\Delta x = \text{a constant} \qquad (4)$$

For the above cited explicit technique, it is easy to show that Equation (4) is not satisfied for arbitrary distributions of u_i. Failure to satisfy (4) is not a trivial matter. In reactor design, for example, calculation of transient pressures is of interest. But accumulation or loss of material by successive violation of (4) would introduce spurious pressure changes.

Although mesh refinement would reduce the error of Richtmyer's method, economic considerations suggest that other methods of solving the continuity equation should be examined.

Roberts and Weiss (*2*) also recognized this problem in their study of convective difference schemes. These authors presented several explicit schemes for approximating the continuity equation. Difference schemes which satisfied (4) were said to be conservative. In certain applications the use of implicit methods may be advantageous because of stability considerations.

To approximate (1)and also to satisfy (4), the following implicit method is proposed:

$$\rho'_i - \rho_i = -s\,[u'_{i+1}\,(\rho'_{i+1} + \rho'_i) - u'_i\,(\rho'_i + \rho'_{i-1})] \qquad (5)$$

where the prime designates time level $t + \Delta t$. By regrouping (5), the following expression results:

$$-s\; u_i'\,\rho'_{i-1} + (1 - s\,(u'_{i+1} - u_i'))\,\rho'_i + s\,u'_{i+1}\,\rho'_{i+1} = \rho_i \qquad (6)$$

The system of n equations, each of the form of (6), is efficiently solved by the method of Peaceman and Rachford (*3*).

Now it will be shown that solutions of (6) satisfy (4). If A is the square matrix of coefficients formed by writing (6) n times, it may be shown that each column of A has a sum unity. It follows that each column of the inverse of A also has a sum unity. Thus at each computation step

$$\sum_{i=1}^{n} \rho_i' = \sum_{i=1}^{n} \rho_i \qquad (7)$$

Except for small round-off errors, the mass in the closed system is constant, and this result applies regardless of the mesh size.

The proposed method for approximating the continuity equation is consistent, stable, easy to solve, and satisfies the total material balance equation.

NOTATION

L = slab width
u = velocity
x = length
s = $0.5\;\Delta t/\Delta x$
ρ = density

LITERATURE CITED

1. Richtmyer, R. D., "Difference Methods for Initial-Value Problems," Interscience, New York (1957).
2. Roberts, K. V., and N. O. Weiss, *Math. Comp.*, **20**, 272-279 (1966).
3. Peaceman, D. W., and H. H. Rachford, *J. Soc. Ind. Appl. Math.*, **3**, 28-41 (1955).