

# A Numerical Solution Procedure for One-Dimensional Multiphase Flow

A.V. Jones

*Commission of the European Communities, J.R.C. Ispra Establishment,  
Department A, I-21020 Ispra, Italy*

A. Prosperetti

*Università degli Studi di Milano, Dipartimento di Fisica, Via Celoria 16,  
I-20133 Milano, Italy*

## Abstract

Many of the flows involving two or more fluids encountered in reactor technology and safety analysis can be treated as one-dimensional in a first approximation. The multifield codes commonly used to calculate such flows use semi-implicit numerical procedures but there is a recent trend towards more fully implicit schemes because of their potential for higher accuracy and greater stability. This paper presents a highly implicit solution procedure for the 6-equation model and compares its predictions in two test problems with analytical results and with a semi-implicit code. It is concluded that for one-dimensional problems fully implicit schemes have significant advantages.

## 1. Introduction

Flows in which several materials or phases are present and move with differing velocities are common in reactor technology and are frequently met with in reactor safety analysis. A high proportion of these flows can be treated using one-dimensional multifield models, and techniques for the discretisation and numerical solution of the PDEs of such models are now well known. Examples of codes adopting this approach are PHOENICS [1], KFIX [2], SIMMER [3] and CATHARE [4]. The earlier codes tend to use the semi-implicit solution procedure proposed by Harlow and Amsden [5] while there is a more recent trend towards schemes involving increased implicitness. More highly implicit schemes offer the possibility of better accuracy and may allow the use of larger timesteps. To assess the potential of one such scheme a very highly implicit code, SRIGHT, has been implemented at the JRC Ispra. This paper presents the equations and solution procedure of the new code, applies the code to two specimen problems and makes some preliminary judgements of the benefits to be gained from increasing implicitness. It is concluded that these benefits are significant especially as regards accuracy.

## 2. Space Discretisation of the Field Equations

The SRIGHT code actually includes in its field equations several gas phase components and the possibility of heat and mass transfer between the phases. It also has quite sophisticated material equations of state allowing for variable specific and latent heats and the calculation of correctly averaged mean properties for a gas phase consisting of a mixture of constituents. To simplify the presentation we present the equations to which the SRIGHT model

would reduce in the case of the combined flow of a non-evaporating liquid and an incompressible gas with constant material properties and without exchange of heat.

The conservation equations are discretised on the standard ICE [6] staggered grid which we take to be uniform, with spacing  $\Delta X$ . Upwinding is used throughout and it is convenient to employ the symbol  $\langle \rangle$ , defining

$$\langle v_j f_j \rangle_{i+\frac{1}{2}} = (v_j)_{i+\frac{1}{2}} \begin{cases} f_i & v_j \geq 0 \\ f_{i+1} & v_j < 0 \end{cases} \quad (1)$$

where  $f_j$  is any magnitude associated with phase  $j$  and the subscript  $i$  refers to the  $i^{\text{th}}$  cell. The semi-discretised continuity equations are with this notation

$$\frac{\partial}{\partial t} (\alpha_j \rho_j)_{i+\frac{1}{2}} = -(\Delta x)^{-1} [\langle \alpha_j \rho_j v_j \rangle_{i+\frac{1}{2}} - \langle \alpha_j \rho_j v_j \rangle_{i-\frac{1}{2}}]_{i,j=L,G} \quad (2)$$

The energy equations are discretised in a similar way, while the discretisation of the momentum equations is slightly different because the velocities are defined on the cell boundaries. As a slight extension of the notation (1) we define

$$\langle \alpha_j \rho_j v_j^2 \rangle = \frac{1}{2} \left( v_{j,i-\frac{1}{2}} + v_{j,i+\frac{1}{2}} \right) \cdot \begin{cases} (\alpha_j \rho_j v_j)_{i-\frac{1}{2}} & v_j \geq 0 \\ (\alpha_j \rho_j v_j)_{i+\frac{1}{2}} & v_j < 0 \end{cases} \quad (3)$$

in which the  $(\alpha_j \rho_j v_j)_{i+\frac{1}{2}}$  are obtained by averaging of the cell centre values. The momentum equations in space-discretised form are then

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_j \rho_j v_j)_{i+\frac{1}{2}} = & -(\Delta x)^{-1} [\langle \alpha_j \rho_j v_j^2 \rangle_{i+1} - \langle \alpha_j \rho_j v_j^2 \rangle_i - \alpha_j]_{i+\frac{1}{2}} (p_{i+1} - p_i)] + \\ & + (\alpha_j \rho_j g)_{i+\frac{1}{2}} - (K_{jS})_{i+\frac{1}{2}} v_{j,i+\frac{1}{2}} - [K_{GL} (v_k - v_j)]_{i+\frac{1}{2}} \end{aligned} \quad (4)$$

Here the  $K_{jS}$  are the coefficients of structure drag while  $K_{GL}$  represents the interphase drag. These formulae are along the lines of KFIX [2] or SIMMER [3] and no particular remarks need be made about them. They are supplemented by the gas equation of state:

$$p = p(\rho_G, e_G) \quad (5)$$

Expressions are also supplied for the drag coefficients. Lockhart-Martinelli correlations are used for the structure drag while for the liquid-gas drag the expression used in KFIX [2] is employed with a fixed droplet radius  $r_D$ .

### 3. Time Discretisation and Solution Procedure

SRIGHT is very flexible in the degree of implicitness of its time discretisation. The equations (2), (4) and the energy equations analogous to (2) are all of the form

$$\frac{\partial}{\partial t} Q_\lambda = R_\lambda; \quad \lambda - \text{general cell index} \quad (6)$$

where  $Q_\lambda$  is a volume concentration of mass, momentum or internal energy and the  $R_\lambda$  are the

rates of change of such quantities. If superscript  $n$  indicates current values and superscript  $n+1$  those at the end of a timestep of duration  $\Delta t$  then (6) is discretised in general as

$$Q_{\lambda}^{n+1} - Q_{\lambda}^n = \Delta t(\theta R_{\lambda}^{n+1} + (1-\theta)R_{\lambda}^n) \quad (7)$$

where the coefficient  $\theta$  allows for all possible degrees of implicitness, e.g.  $\theta=0$  fully explicit,  $\theta=1$  fully implicit. There are different  $\theta$  for the different terms appearing in the discretised conservation equations, the values of which can be specified by the user. For stability reasons the  $p dV$  work term in the gas energy equation and the pressure and drag terms in the momentum equations are treated purely implicitly.

The conservation equations discretised after (7) together with (5) and the drag laws form a non-linear algebraic system in the "new" variables  $V_j, e_j, p$  and  $\alpha_G$  which must be solved for all  $N$  cells. The method of solution adopted in SRIGHT is the Newton-Raphson iteration technique. Each of the conservation equations may be written in the form:

$$f_j(\underline{X}_{i-1}, \underline{X}_i, \underline{X}_{i+1}) = (S_j)_i \quad (8)$$

where  $\underline{X}$  is the vector of new variables and the subscripts  $i, i+1$  refer to cell  $i$  and its nearest neighbours. The  $S_j$  are source terms arising from "old" values of the variables and any physical sources or sinks. To solve the equations (8) given  $\underline{X}_i^{(k)}$  as the values at the  $k^{\text{th}}$  iteration we seek a vector of increments  $\delta \underline{X}_i$  such that the  $\underline{X}_i^{(k+1)}$  defined by

$$\underline{X}_i^{(k+1)} = \underline{X}_i^{(k)} + \delta \underline{X}_i \quad (9)$$

satisfy the equations (8) exactly. Expanding  $f_j$  in Taylor series one finds that Newton-Raphson approximations to the increments satisfy

$$\frac{\partial f_j}{\partial \underline{X}_{i-1}} \delta \underline{X}_{i-1} + \frac{\partial f_j}{\partial \underline{X}_i} \delta \underline{X}_i + \frac{\partial f_j}{\partial \underline{X}_{i+1}} \delta \underline{X}_{i+1} + f_j(\underline{X}_{i-1}^{(k)}, \underline{X}_i^{(k)}, \underline{X}_{i+1}^{(k)}) - (S_j)_i = 0 \quad (10)$$

The functions  $f_j$  arising from the momentum equations contain the vectors  $\underline{X}$  for next nearest neighbours also. For numerical convenience the increments of these are not included explicitly in the iteration but the latest iterate values are included in the  $S_j$ . This might affect the rate of convergence of the iteration in some instances but should not change the  $\{\underline{X}_i\}$  to which the iteration converges. When this procedure is followed then with a suitable ordering of the variables (9) takes the form

$$\underline{A}\{\delta \underline{X}_i\} = \underline{B} \quad (11)$$

where  $\{\delta \underline{X}_i\}$  is a column vector containing the increments for all  $N$  cells and  $A$  is a  $6N \times 6N$  block tridiagonal matrix. The system (11) may be solved directly for the increments  $\delta \underline{X}_i$ . The  $\underline{X}$  values at the  $k+1^{\text{th}}$  iteration are calculated from (9) and the process repeated until convergence.

Appropriate convergence criteria appear to be problem-dependent; currently SRIGHT uses the simple test

$$\max_i |\delta p_i| / |p_i| < \epsilon \quad (12)$$

It was chosen in SRIGHT to determine the derivatives appearing in (10) analytically. The unwinding formulae of type (1), (3) give rise to jumps in the derivatives when the local velocity changes direction but experience to date suggests that this does not give rise to convergence difficulties.

#### 4. Comparison with a Semi-Implicit Technique

It is instructive to compare the solution procedure set out in the previous section with that employed in a semi-implicit code, for example SIMMER. The space discretisation is performed in the same way while the time discretisation combines explicit, implicit and multi-step features. The liquid continuity equation (2) is first solved explicitly to provide the new values of  $\alpha_L, \alpha_G$  since  $\rho_L$  is assumed constant. The new liquid internal energy is also evaluated explicitly.

The momentum equations (4) are then treated semi-implicitly with the pressure and drag terms using new values and the convection terms using old values of the variables. The value of the velocity-dependent drag coefficient  $K_{GL}$  is obtained by a two-step method explained below. The gas energy is first estimated to provide values for the calculation of the new pressures and then recalculated once the end of step velocities are known. The equation of state (5) is used to express  $\{V_{G,L}, \rho_G, e_G\}$  in terms of the pressure field alone and an ICE-type iteration based on the departure from local mass conservation of the gas is followed to determine this field [5]. The new velocities are finally determined from the new pressures and the calculation is ready for another cycle. The interphase drag coefficient  $K_{GL}$  depends on  $V_{GL} \equiv V_G - V_L$ , the new value of which is estimated from a combination of the momentum equations with the neglect of certain terms in which the estimated pressure gradient  $\partial p / \partial x$  is taken to be the average of the absolute values of  $\partial p / \partial x$  in adjacent cells. This equation is solved for  $V_{GL}$  and hence  $K_{GL}$  which is used in the discretised momentum equations (4). The resulting value of the interphase drag is only an estimate but it is not recalculated on the basis of the final velocity values at the end of the step. This can affect the accuracy of the procedure as will be seen in the next section.

#### 5. Application to Two Test Problems

To validate SRIGHT and to gain some experience with it the code has been applied to two situations where other solutions are available for comparison. The first is a simple single phase shock tube problem while the second is the same problem using a mixture of gas and particles. In the calculations reported all  $\theta$  values were set to 0.5, i.e. time-centered. For the single-phase shock tube analytical results are available. The initial conditions were as indicated in Fig. 1 with a space step of 0.9144 m and a timestep of 0.5 ms. A pressure convergence tolerance of  $\epsilon = 10^{-4}$  was imposed and was achieved after 3 iterations each timestep. The computed velocity distribution at 1.5 ms after rupture of the diaphragm is shown in Fig. 1. Typically for a dissipative scheme the shock front and rarefaction are somewhat smeared but their positions are well predicted.

The second problem, a "dusty shock", employed the same geometry with an initial 5:1 pressure ratio and with the high-pressure absolute temperature 35% greater than that in the

low-temperature region. A uniform initial volume fraction of the second (dust) phase was imposed with  $\alpha_L = 0.142\%$ , the fixed particle radius being 1 mm. The physical sequence of events is similar to that in the single-phase shock, with a zone behind the shock front in which the dust particles accelerate to the local gas velocity. In this problem it was possible to compare the SRIGHT predictions with those of SIMMER, a comparison of SIMMER calculations and analytical and other results having been performed in Jones and Jones [7]. Fig. 2 shows the gas velocity at 250 ms as calculated by the two codes with the same data as an example of the results. The discrepancy is striking. After some investigation the root cause of this and other discrepancies was identified as the much higher interphase slip calculated by SIMMER. As was outlined in Section 4 there is no iteration in the code to ensure self-consistency of the interphase drag coefficient  $K_{GL}$ . A check on the consistency achieved can be made by comparing the estimated and final end of step slip values, which is done in Fig. 3. Curves A refer to a timestep of 1 ms, curves B to the same calculation with a timestep of 0.1 ms. In the region just behind the shock where slip values are changing most rapidly differences between estimate and final value of up to 60% may be seen in calculation A, which an order of magnitude reduction in timestep reduces to 26%. SRIGHT by iterating over each timestep ensures that a self-consistent slip velocity is employed and one may expect the SIMMER slip to converge to it in the limit of small timesteps. This behaviour is in fact observed as may be seen in Fig. 3.

Apart from ensuring better calculation of the interphase slip and drag than semi-implicit techniques the implicit version of SRIGHT has other advantages as were revealed by further calculations. For instance it was found that the calculated results were relatively insensitive to the timestep. Raising the step from 0.1 ms to 1 ms altered the calculated gas velocity by 1-2%, while the number of iterations required to achieve convergence in the relative pressure to a tolerance of  $\epsilon = 10^{-4}$  rose from 2 to 4. Energy conservation is also markedly improved in the calculations performed here. With a timestep of 0.1 ms after 250 ms there was a final total energy deficit of 12.5% of the kinetic energy, which was only doubled on raising the timestep by an order of magnitude. These results are significantly better than the authors' experience with energy conservation in semi-implicit codes.

## 6. Conclusions

The fully implicit numerical solution procedure embodied in SRIGHT is found to be superior for one-dimensional problems to the semi-implicit procedures to be found in the literature as regards accuracy and consistency. It is also able to accommodate additions to the model employed, e.g. the inclusion of added mass terms, without major alterations. The examination of the effect of certain extensions to the basic model of [2,4,5] is now underway at Ispra using SRIGHT.

## References

- [1] SPALDING, D.B., "Computer Simulation of Loss of Coolant Accidents in Pressurised Water Reactor Nuclear Plants", Num. Methods for Transient and Coupled Problems, 3-35 (ed. Lewis, R.W.; Pineridge Press 1984).
- [2] RIVARD, W.C., TORREY, M.D., "K-FIX: A Computer Program for Transient Two-dimensional Two-fluid Flow", LA-NUREG-6623, NRC-4 (1977).

- [3] SMITH, L.L., "SIMMER-II: A Computer Program for LMFBR Disrupted Core Analysis", NUREG/CR-0453, LA-7515-M (1980).
- [4] EdF-CEA-Framatome (equipe mixte), "Code CATHARE-1 Dossier descriptif D213-1, D214-1, Modèle d'écoulement diphasique monodimensionnel en régime transitoire", Note TT/EM/11 (January 1984).
- [5] HARLOW, F.H., AMSDEN, A.A., "Numerical Calculation of Multiphase Fluid Flow", J. Comp. Phys. 17, 19 (1975).
- [6] CLOUTMAN, L.D., HIRT, C.W., ROMERO, N.C., "SOLA-ICE, A Numerical Solution Procedure for Transient Compressible Fluid Flow", LA-6236 (July 1976).
- [7] JONES, I.P., JONES, A.V., "The Numerical Solution of Simple One-dimensional Multiphase Flows in Shock Tubes", Numerical Methods in Laminar and Turbulent Flow (ed. Taylor, C.) 863-876 (Pineridge Press, Swansea 1981).

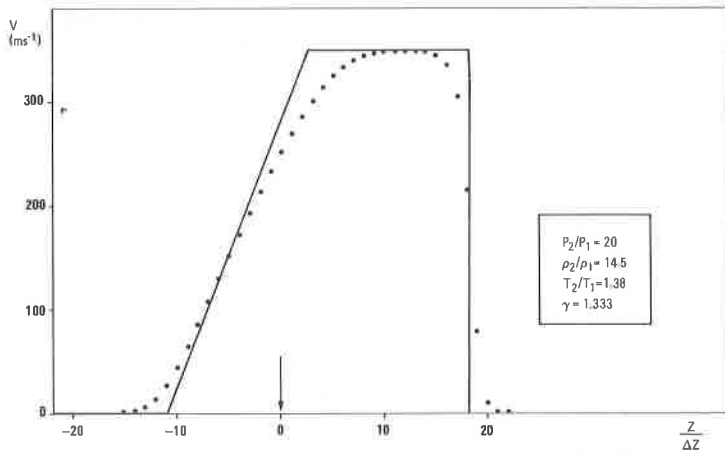


Fig. 1 - SRIGHT velocity profile in a single-phase shock tube problem

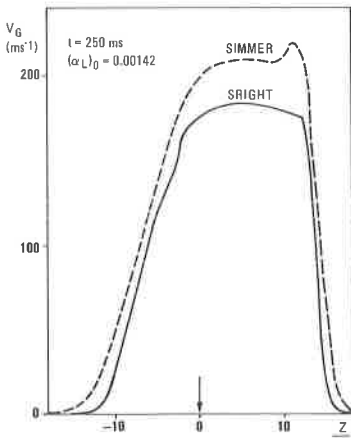


Fig. 2 - Gas velocity in a dusty shock. Comparison of SRIGHT and SIMMER

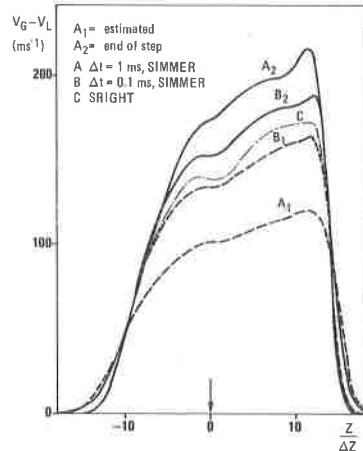


Fig. 3 - Relative velocity. SIMMER estimated and end of step values and SRIGHT results