Modification of the upwind schemes for the computation of condensing two-phase flows

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Abstract: The eigenvalues and eigenvectors of the Jacobian matrix of the homogeneously condensing two-phase flow equations are derived. These are useful for all upwind schemes. Details of the implementation in the Roe scheme are described. Example calculations for condensing wet steam flow are provided, which compare well with the experimental results.

Keywords: two phase, wet steam, eigenvalues, eigenvectors, Jacobian matrix, upwind, the Roe scheme

1 INTRODUCTION

The upwind schemes [**1**–**3**] have become very popular for engineering calculations of compressible flow through passages of complex geometrical shapes. In this note, new equations are derived so as to make these established methods of computational fluid dynamics (CFD) to be applicable to the numerical solution of condensing two-phase flows. The developed numerical schemes can be used for both the Euler and Navier–Stokes equations.

The spatial discretization in the upwind schemes critically depends on the characteristics of the flow. An important component of the upwind schemes is, therefore, the eigenvalues and eigenvectors of the Jacobian matrix of the flow equations. The present work shows how the eigenvalues and eigenvectors alter when there are two phases present with homogeneous condensation (the governing equations for two-phase flow are different from their counterparts for single-phase flow). Specific details of the necessary changes are shown here for the Roe scheme, but the derived eigenvalues and eigenvectors are to be used with other upwind schemes as well.

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2 UPWIND SCHEMES FOR SINGLE-PHASE FLOW

The governing equations for a single-phase flow are the Euler or Navier–Stokes (NS) equations, which can be written in a two-dimensional conservative form as follows

$$\frac{\partial W}{\partial t} + \nabla \boldsymbol{F} = S \tag{1}$$

where

$$W = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, \quad \boldsymbol{F} = \begin{bmatrix} \rho u & \rho v \\ \rho u^2 + p & \rho uv \\ \rho uv & \rho v^2 + p \\ \rho uh & \rho vh \end{bmatrix}$$

S is the source term that distinguishes the NS from the Euler equations ($S = 0$ in Euler equations and $S =$ viscuous terms in NS equations).

Many methods have been developed for solving equation (1) in the past decades. In the upwind schemes, the value of a flux at any interface is constructed by combining the contributions from the left-side and right-side grid points, according to the characteristics of the flow equations. A piecewise constant (first-order accuracy) or a linear (second-order accuracy) distribution of variable W with the shock discontinuities occurring at each cell interface is used to obtain the Riemann solution. This idea has been extended and improved by various investigators including Roe [**1**].

2.1 The Roe scheme

Considering Roe's flux difference splitting, the flux vector $\boldsymbol{F}$ on an interface is approximated by

$$\boldsymbol{F}(W_{\mathrm{L}}, W_{\mathrm{R}}) = \frac{1}{2}[\boldsymbol{F}(W_{\mathrm{L}}) + \boldsymbol{F}(W_{\mathrm{R}}) - |\tilde{\mathbf{A}}(W_{\mathrm{L}}, W_{\mathrm{R}})| \times (W_{\mathrm{L}} - W_{\mathrm{R}})] \tag{2}$$

Here, $|\tilde{\mathbf{A}}(W_{\mathrm{L}}, W_{\mathrm{R}})|$ denotes the standard Roe matrix

$$\left|\tilde{\mathbf{A}}(W_{\mathrm{L}}, W_{\mathrm{R}})\right| = \tilde{\boldsymbol{E}} \cdot \left|\tilde{\Lambda}\right| \cdot \tilde{\boldsymbol{E}}^{-1}$$

where $\tilde{\Lambda}$ represents the eigenvalues of the Jacobian matrix and $\tilde{\boldsymbol{E}}$ is the corresponding eigenvectors.

For the flux integration in the numerical implementation for two-dimensional flow, a simplification results if the velocity is expressed in terms of u_n and v_n, where they are, respectively, perpendicular and parallel to a face of control volume under consideration. Then, in determining $\partial \boldsymbol{F}/\partial W$, only the first column of F is relevant, as the second column does not contribute to the flux integration because the area perpendicular to v_n is zero. With this interpretation of the reference axes, the eigenvalues and eigenvectors are given by (without writing the subscript n for brevity)

$$\tilde{\Lambda} = \tilde{u} - \tilde{a},\ \tilde{u},\ \tilde{u},\ \tilde{u} + \tilde{a} \tag{3}$$

$$\tilde{\boldsymbol{E}} = \begin{bmatrix} 1 & 0 & 1 & 1 \\ \tilde{u} - \tilde{a} & 0 & \tilde{u} & \tilde{u} + \tilde{a} \\ \tilde{v} & \tilde{v} & \tilde{v} & \tilde{v} \\ \tilde{h} - \tilde{u}\tilde{a} & \tilde{v}^2 & \tilde{h} - \frac{\tilde{a}^2}{\gamma - 1} & \tilde{h} + \tilde{u}\tilde{a} \end{bmatrix} \tag{4}$$

The superscript $\sim$ above the variables indicates that they are Roe-averaged. The Roe-averaged value for a generic variable X can be calculated as

$$\tilde{X} = \frac{\sqrt{\rho_{\mathrm{L}}} X_{\mathrm{L}} + \sqrt{\rho_{\mathrm{R}}} X_{\mathrm{R}}}{\sqrt{\rho_{\mathrm{L}}} + \sqrt{\rho_{\mathrm{R}}}} \tag{5}$$

One uses equation (5) to calculate $\tilde{u}$, $\tilde{v}$, and $\tilde{h}$. $\tilde{a}$ is calculated from the relation $\tilde{a}^2 = (\gamma - 1)[\tilde{h} - (1/2)(\tilde{u}^2 + \tilde{v}^2)]$.

3 GOVERNING EQUATIONS FOR TWO-PHASE VAPOUR–DROPLET FLOW

A two-phase medium with homogeneous condensation (e.g. wet steam) consists of a very large number of very small liquid droplets dispersed within a vapour phase. In the absence of any velocity slip between the two phases, it can be shown [**4**, **5**] that the overall conservation equations for the vapour–droplet mixture can be expressed in the same form as the single-phase equations

$$\frac{\partial W}{\partial t} + \nabla \boldsymbol{F} = S \tag{6}$$

where

$$W = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, \quad \boldsymbol{F} = \begin{bmatrix} \rho u & \rho v \\ \rho u^2 + p & \rho uv \\ \rho uv & \rho v^2 + p \\ \rho uh & \rho vh \end{bmatrix}$$

However, the flow variables in equation (6) represent the mixture properties and the mixture may not be at thermodynamic equilibrium.

As the wetness fraction is small, and the density of the liquid phase is usually very much greater than that of the vapour phase, the volume occupied by the droplets can usually be neglected. The mixture density is then related to the vapour–phase density by the following equation

$$\rho = \frac{\rho_{\mathrm{g}}}{1 - w} \tag{7}$$

The mixture total enthalpy and total energy are calculated by combining the contributions from each phase

$$h = (1 - w)h_{\mathrm{g}} + wh_{\mathrm{l}} \tag{8}$$

$$e = (1 - w)e_{\mathrm{g}} + we_{\mathrm{l}} \tag{9}$$

The thermodynamic non-equilibrium is reflected in the fact that w in equations (8) and (9) is not the equilibrium value (for example, which can be obtained from the standard Mollier charts), but must be calculated from separate rate equations. Similarly, the enthalpy and energy terms in equations (8) and (9) have to be calculated at the respective phase temperatures (none of which may be equal to the saturation temperature, corresponding to the local pressure).

The number of the droplets can be calculated by integrating a suitable nucleation rate equation (e.g. the classical homogeneous nucleation rate equation). The sizes of the droplets, once nucleated, are governed by the droplet growth equation (one could use any suitable expression such as Gyarmathy's law; see, for example, reference [**6**] for details). Accounting for a large number of droplet groups in CFD application can be time-consuming. An effective method of maintaining a poly-dispersed droplet spectrum is given in reference [**4**]. A simpler approach is to consider only the first four moments of the droplet size distribution [**7**]. These moment equations are constructed according to the droplet

radius r raised to various powers. They describe the number, the radius, the surface area, and the mass of the droplets, and these correspond to r^n, $n = 0$, 1, 2, 3, respectively. The droplet moment equations can be written as

$$\frac{\partial Q}{\partial t} + \nabla G = S^* \tag{10}$$

where

$$Q = \begin{bmatrix} \rho w \\ \rho Q_2 \\ \rho Q_1 \\ \rho Q_0 \end{bmatrix}, \quad G = \begin{bmatrix} \rho w u & \rho w v \\ \rho Q_2 u & \rho Q_2 v \\ \rho Q_1 u & \rho Q_1 v \\ \rho Q_0 u & \rho Q_0 v \end{bmatrix}, \quad S^* = \begin{bmatrix} S_1^* \\ S_2^* \\ S_3^* \\ S_4^* \end{bmatrix}$$

S^* is the source term of the liquid phase equations and can be written explicitly as

$$S_1^* = \frac{4}{3}\rho_l \pi r_c^3 J + 4\pi\rho_l \rho Q_2 \dot{r}$$
$$S_2^* = r_c^2 J + 2\rho Q_1 \dot{r}$$
$$S_3^* = r_c J + \rho Q_0 \dot{r}$$
$$S_4^* = J$$

Each of the source terms S^* contains two parts: the first term represents the new droplets generated by the nucleation process and the second term represents the contribution from the growth of existing droplets.

If it is assumed that the vapour phase behaves as an ideal gas, one can write the equation of state for the vapour phase as

$$p = \rho_g R_g T_g \tag{11}$$

Equation (6) is closed by an equation for the pressure, which can be derived by combining equations (7) to (9) and (11). The result is

$$p = (\gamma - 1)\frac{1 - w}{1 + w(\gamma - 1)}\left[e - \frac{1}{2}\rho(u^2 + v^2) + \rho w L\right] \tag{12}$$

Equation (12) reduces to the well-known result for a single-phase perfect gas when $w = 0$ is substituted in it (representing the absence of the liquid phase). L is the enthalpy of evaporation ($L = h_g - h_l$); for consistency, it should be calculated as a function of temperature. Equation (12) has been derived with an assumption that the liquid phase properties could be evaluated at the vapour temperature. This slight approximation simplifies the determination of the eigenvalues and the eigenvectors given later.

4 UPWIND SCHEMES FOR TWO-PHASE FLOW

For the numerical solution of a two-phase flow field, eight equations (given by equations (6) and (10)) have to be solved together. Of course, many more equations are required if the full poly-dispersed droplet spectrum is to be retained in the calculation [**4**].

For upwind two-phase schemes, the determination of the algebraic expressions for the eigenvalues and eigenvectors of the Jacobian matrix $\partial \boldsymbol{F}/\partial W$ is needed for the combined system of equations ((6) and (10)). A two-phase factor φ is introduced to simplify the mathematical calculations. Here, φ is defined as

$$\varphi = \sqrt{\frac{1 - w}{1 + w(\gamma - 1)}} \tag{13}$$

φ is a function of the wetness fraction and the specific heat ratio of the vapour phase. Equation (13) shows that $\varphi \to 1$ as $w \to 0$. The use of the factor φ in the pressure equation (equation (12)) simplifies the algebra considerably.

The eigenvalues and eigenvectors of the Jacobian matrix $\partial \boldsymbol{F}/\partial W$ can be determined by combining equations (6) and (10), with the help of equations (12) and (13). Algebra is involved, but with systematic elimination (and patience), the final results could be expressed in a neat form. Only the final results are quoted here.

The eigenvalues of the Jacobian matrix are

$$\Lambda = u - \varphi a,\ u,\ u,\ u,\ u + \varphi a,\ u,\ u,\ u \tag{14}$$

and the corresponding eigenvectors can be written as a 8×8 matrix

$$\boldsymbol{E} = \begin{bmatrix} 1 & 0 & 1 & 1 \\ u - \varphi a & 0 & u & u \\ v & v & v & v \\ h - u\varphi a & v^2 & h - \dfrac{a^2}{\gamma - 1} & h - (1 - w)L \\ w & 0 & w & 1 \\ Q_2 & 0 & 0 & 0 \\ Q_1 & 0 & 0 & 0 \\ Q_0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ u + \varphi a & 0 & 0 & 0 \\ v & 0 & 0 & 0 \\ h + u\varphi a & 0 & 0 & 0 \\ w & 0 & 0 & 0 \\ Q_2 & 1 & 0 & 0 \\ Q_1 & 0 & 1 & 0 \\ Q_0 & 0 & 0 & 1 \end{bmatrix} \tag{15}$$

u and v in equations (14) and (15) should be interpreted as perpendicular and parallel, respectively, to a face of control volume under consideration, as explained in the paragraph just before equation (3).

5 SIMPLIFIED IMPLEMENTATION OF UPWIND SCHEMES FOR TWO-PHASE FLOW

The 8×8 matrix given in section 4 is accurate, but a computational scheme based on it might be time-consuming and, in this section, it is shown how a simpler approach is possible.

It is noticed that the wetness fraction w plays an important role both in the phase-transition equations (equation (10)) and in the dynamic equations (Euler/NS given by equation (6)). Equations (6) and (10) are fully coupled through the variable w. The three other variables, i.e. Q_0, Q_1, and Q_2, do not directly appear in equation (6) and influence it only implicitly through their effect on w. In the present work, the authors, therefore, have taken the pragmatic approach of solving equation (6) simultaneously with the equation that specifies the evolution of the wetness fraction w. The three other supplementary equations for the liquid phase (giving Q_0, Q_1, and Q_2 in equation (10)) are solved separately. In the example calculations given in section 6, the authors refer to this approach as '5–5 Roe scheme'.

The new form of the 5-element governing equations (either Euler or NS) for the two-phase flow is

$$\frac{\partial W}{\partial t} + \nabla \boldsymbol{F} = S \tag{16}$$

$$W = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho w \end{bmatrix}, \quad \boldsymbol{F} = \begin{bmatrix} \rho u & \rho v \\ \rho u^2 + p & \rho uv \\ \rho uv & \rho v^2 + p \\ \rho uh & \rho vh \\ \rho uw & \rho vw \end{bmatrix}$$

The same procedure, as described in section 4, is applied for the algebraic determination of the eigenvalues and eigenvectors for the 5×5 equation system.

The eigenvalues of the resulting Jacobian matrix are

$$\Lambda = u - \varphi a,\ u,\ u,\ u,\ u + \varphi a \tag{17}$$

and the corresponding eigenvectors are

$$\boldsymbol{E} = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 \\ u - \varphi a & 0 & u & u & u + \varphi a \\ v & v & v & v & v \\ h - u\varphi a & v^2 & h - \dfrac{a^2}{\gamma - 1} & h - (1 - w)L & h + u\varphi a \\ w & 0 & w & 1 & w \end{bmatrix} \tag{18}$$

Equations (17) and (18) are general and can be used with any upwind scheme. In the two-phase Roe scheme, each variable in equations (17) and (18) has to be interpreted as Roe-averaged quantities. In addition to $\tilde{u}$, $\tilde{v}$, and $\tilde{h}$, as shown in section 2, $\tilde{w}$ is also calculated using equation (5). However, the enthalpy h applies to the mixture. Thus, although a in equations (17) and (18) is still the speed of sound in vapour alone (i.e. $a = \sqrt{\gamma p/\rho_g}$), the Roe-averaged value of a, for the two-phase flow, is calculated from $\tilde{a}^2 = (\gamma - 1)[\tilde{h} - (1/2)(\tilde{u}^2 + \tilde{v}^2) + \tilde{w}L]$.

Equations (17) and (18) can be compared with equations (3) and (4). The two-phase equations contain 5 and 5×5 elements when compared with 4 and 4×4 elements in the single-phase equations. The single-phase terms are recovered when $w = 0$. The characteristic speeds are different, as the speed of sound in a vapour–droplet mixture differs from that in the vapour alone.

Guha [**5**, **6**] describes the various speeds of sound in two-phase mixtures. Depending on the various assumptions of mass, momentum, and energy transfers between the two phases, four limiting speeds of sound have been identified from the fully frozen speed a_f to the fully equilibrium speed a_{e3}. An intermediate speed a_{e2} has been established in these references, which corresponds to the equilibration of droplet temperature and velocity slip but frozen vapour thermal relaxation.

The present analysis shows that for the upwind numerical schemes of two-phase flow, the characteristics are altered and that the sonic speed in pure vapour is modified by a factor φ. As in the present analysis also velocity equilibration between the two phases has been assumed, the magnitude of $\varphi\ a$ is close to a_{e2}. However, $\varphi\ a$ and a_{e2} are not exactly equal because a slightly simplified droplet temperature equilibration is used here. As explained after equation (12), this slight simplification was necessary so that explicit equations for the corresponding eigenvectors could be determined.

The Roe scheme also needs the inverse of the matrix given in equation (18). This can be determined numerically (e.g. by the Gauss–Jordan method) at each interface of the control volumes at each time step, but it would take significant

computational time for doing so. Therefore, the algebraic elements of the inverse matrix were also determined, which reduce the computational time. The algebraic components are, however, too lengthy to reproduce here.

6 EXAMPLE CALCULATIONS

In section 5, the authors showed how to construct the 5–5 Roe scheme for homogeneously condensing two-phase flow. Some example calculations using this scheme are shown in Figs 1 to 3. For this purpose, a two-dimensional time-marching computer program has been developed that works with unstructured grids. All calculations are performed on Barschdorff's nozzle [**8**].

Figure 1 shows the convergence history of the developed 5–5 Roe two-phase scheme. In the same figure, only for the purpose of comparison, the convergence history of another scheme – the '4–4 Roe scheme' – has also been included. A separate time-marching computer program had to be written for this. The philosophy of the 4–4 Roe scheme may be explained as follows. As equation (6) is similar in form to equation (1), which is extensively used for single-phase calculations, it could be thought that the eight equations for the two-phase flow could be solved by a decoupled two-stage process. In the first stage, equation (6) would be solved with assumed liquid phase properties, and in the second stage, this solution would be updated by the solution of equation (10). One could then make straightforward adaptation of the upwind schemes from single-phase CFD for the solution of equation (6). This approach is referred here as the '4–4 Roe scheme'.

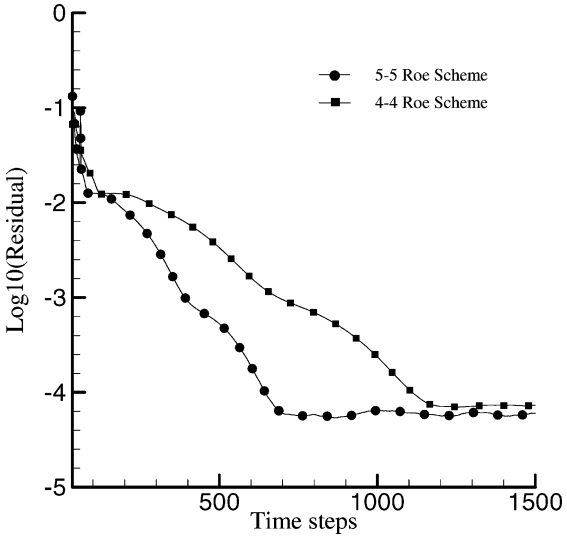

Fig. 1 Comparison of the convergence history of 5–5 Roe scheme with 4–4 Roe scheme for wet steam flow (inlet $p_0 = 78390$ Pa and $T_0 = 380.5$ K)

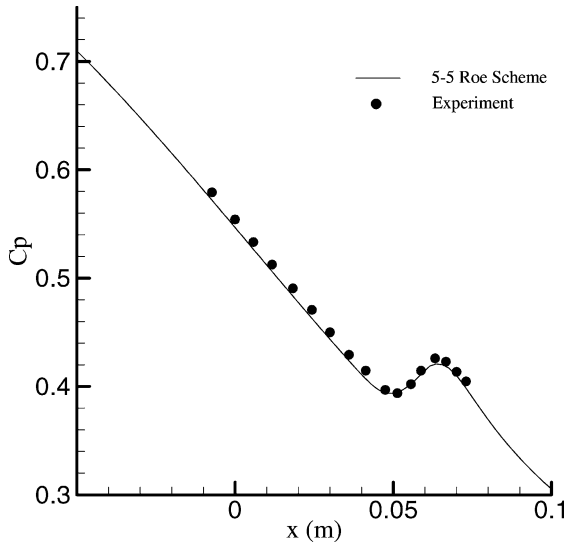

Fig. 2 Computed and measured static pressure distributions along the axis of the Barschdorff nozzle showing 'condensation shock' (inlet $p_0 = 78390$ Pa and $T_0 = 380.5$ K)

Figure 1 shows that the convergence history of the coupled two-phase solver (the 5–5 Roe scheme) is better than that of the decoupled two-phase solver (the 4–4 Roe scheme). Figure 2 shows the comparison of the numerical prediction of the pressure distribution calculated by the 5–5 Roe scheme with experimental results. Figure 3 shows the two-dimensional contour plot of the frozen Mach number in the nozzle, again calculated by the 5–5 Roe scheme for the two-phase flow.

7 CONCLUSIONS

The eigenvalues and eigenvectors of the Jacobian matrix of the homogeneously condensing two-phase flow equations are derived. The eigenvalues are essential for all upwind schemes. The

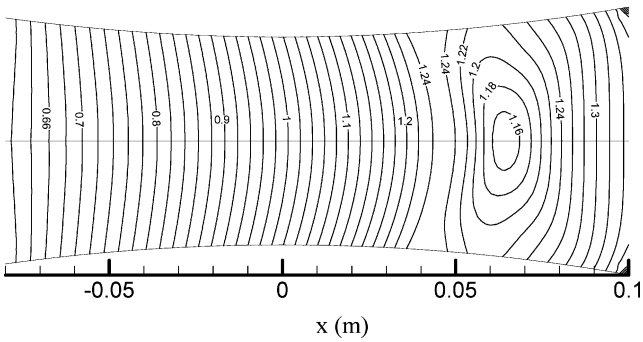

Fig. 3 Mach number contour for wet steam computation in the Barschdorff nozzle (inlet $p_0 = 78390$ Pa and $T_0 = 380.5$ K)

eigenvectors are necessary for all flux-difference upwind schemes (Roe and Osher) in the flux integration. The eigenvectors are also to be used in flux vector splitting methods (van Leer, AUSM [**9**]) when implicit time integration [**10**] is used.

A two-dimensional time-marching computer program, based on the 5–5 Roe scheme developed here, has been written for homogeneously condensing two-phase flows. The program works with unstructured grids. A few example calculations for wet steam are provided. The numerical predictions compare well with the experimental results.

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APPENDIX

Notation

a	speed of sound in the vapour phase $a = \sqrt{\gamma p/\rho_g}$
$\mathbf{A}$	Jacobian matrix of the flow equations
c_p	specific heat at constant pressure
C_p	pressure coefficient (defined as p/p_0)
e	total energy per unit volume
$\boldsymbol{E}$	eigenvectors
h	total enthalpy per unit mass
J	nucleation rate
L	enthalpy of evaporation ($L = h_g - h_l$)
n_i	number of droplets in group i (per unit mass)
p	static pressure
p_0	total pressure
Q_0	sum of the number of droplets per unit mass ($Q_0 = \Sigma n_i$)
Q_1	sum of the radii of droplets per unit mass ($Q_1 = \Sigma n_i\, r_i$)
Q_2	sum of the surface area of droplets per unit mass ($Q_2 = 4\pi\Sigma n_i\, r_i^2$)
r	average radius of droplet ($r = \sqrt{Q_2/(4\pi Q_0)}$)
$\dot{r}$	droplet growth rate ($\dot{r} = \mathrm{d}r/\mathrm{d}t$)
r_i	droplet radius in group i
r_c	critical radius
R_g	specific gas constant
t	time
T_0	total temperature
u	x-component of velocity
v	y-component of velocity
w	wetness fraction
x	distance along nozzle axis
γ	specific heat ratio of the vapour
Λ	eigenvalues
φ	two-phase factor
ρ	density

Subscripts

L	variables on the left
R	variables on the right
g	vapour phase
l	liquid phase

Superscript

$\sim$	Roe-averaged