A new approach for three-phase flows

Jean-Marc Hérard

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Jean-Marc Hérard *

EDF-DRD, 78401 Chatou cedex, France

We present here a new model to describe three-field patterns or three-phase flows. The basic ideas rely on the counterpart of the two-fluid two-pressure model which has been introduced in the DDT framework, and more recently extended to water-vapour simulations. We show the system is hyperbolic without any constraining condition on the flow patterns. A detailed investigation of the structure of the Riemann problem is achieved. Regular solutions of the whole are in agreement with physical requirements on void fractions, densities and internal energies for a rather wide class of equations of state. Even more, this approach enables to perform computations of standard single pressure three-phase flow models, using relaxation techniques and coarse meshes. A few computational results confirm the stability of the whole approach.

I. Introduction

Some simulations in the framework of pressurized power reactors in the nuclear energy require using two-fluid models, and some others even ask for a three field description of the whole flow (see[1,2]). This may happen for instance when predicting the motion of liquid dispersed droplets inside a continuous gas phase, while some gas-liquid interface is moving in the core. Other applications involving a gaseous phase and two distinct liquids (for instance oil and water) also urge for the development of three field models.

Some models and tools have already been proposed, which basically rely on the two-fluid single-pressure formalism. These either assume that liquid droplets velocities and velocities in the surrounding gas phase are equal, or retain different velocities but assume in any case a local pressure equilibrium between the three components. A straightforward consequence is that these models suffer from the same deficiencies than standard two-fluid models. More clearly, the loss of hyperbolicity of the convective subset implies that computations on sufficiently fine grids rather easily enter "elliptic in time" regions ; as a consequence, even the most "stable" upwinding schemes lead to a blow up of the code when refining the mesh, though accounting for stabilizing drag effects (see[3] for instance for such a numerical experience).

An alternative way to deal with these flows consists in getting rid of the pressure equilibrium between phases. This was first introduced in the framework of the DDT (see,[4–15] among others), and more recently applied to water-vapour predictions (see[16–18]). One of the main advantages with the latter approach is that it inherits from the hyperbolic structure of Navier-Stokes equations -which seems quite reasonable- on the one hand; moreover, the overall entropy inequality provides some better understanding of various interfacial transfer terms. For all these reasons, it seems appealing to examine whether one might derive a similar framework to cope with three-phase or three-field flow structures. Such a trial is discussed in this paper. An underlying idea is that the interface between phases remains infinitely thin when submitted to pure convective patterns.

*Research Engineer, Département MFTT, 6 quai Watier, and Associate Research Director, CNRS, LATP, AIAA Member

We will first provide the main set of equations which includes source terms, viscous terms and convective effects. The main properties of the whole set will be examined, including a discussion on the solutions of the one dimensional Riemann problem. These properties enable to compute the whole set with help of rough schemes (Rusanov scheme) or more accurate approximate Riemann solvers such as the one introduced in.[19,20] A few computational results illustrate the whole, which issue from the computation of a Riemann problem.

II. Governing equations

The density, velocity, pressure, internal energy and total energy within phase k will be denoted ρ_k, U_k, P_k, $e_k = e_k(P_k, \rho_k)$ and $E_k = 0.5\rho_k U_k U_k + \rho_k e_k$ respectively. The volumetric fraction of phase labelled k is defined as α_k, and the three must comply with the constraint:

$$\alpha_1 = 1 - \alpha_2 - \alpha_3$$

The governing set of equations is:

$$(I + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = S(W) + \frac{\partial}{\partial x}(E(W)\frac{\partial W}{\partial x}) \tag{1}$$

It requires an initial condition $W(x, 0) = W_0(x)$ and suitable boundary conditions. The state variable W, the fluxes $F(W)$, $G(W)$ and the source terms $S(W)$ lie in $\mathbb{R}^{11}$. We set:

$$W^t = (\alpha_2, \alpha_3, \alpha_1\rho_1, \alpha_2\rho_2, \alpha_3\rho_3, \alpha_1\rho_1U_1, \alpha_2\rho_2U_2, \alpha_3\rho_3U_3, \alpha_1E_1, \alpha_2E_2, \alpha_3E_3)$$

and, noting $m_k = \alpha_k\rho_k$:

$$F(W)^t = (0, 0, m_1U_1, m_2U_2, m_3U_3, \alpha_1(\rho_1U_1^2 + P_1), \alpha_2(\rho_2U_2^2 + P_2), \alpha_3(\rho_3U_3^2 + P_3),$$
$$\alpha_1U_1(E_1 + P_1), \alpha_2U_2(E_2 + P_2), \alpha_3U_3(E_3 + P_3))$$

Second rank tensors $C(W), D(W), E(W)$ lie in $\mathbb{R}^{11\times11}$. The non-conservative convective terms are :

$$\begin{cases} D(W)\dfrac{\partial W}{\partial t} = (0,0,0,0,0,0,0,0,-P_2\dfrac{\partial \alpha_2}{\partial t} - P_3\dfrac{\partial \alpha_3}{\partial t}, P_2\dfrac{\partial \alpha_2}{\partial t}, P_3\dfrac{\partial \alpha_3}{\partial t}) \\ C(W)\dfrac{\partial G(W)}{\partial x} = (U_1\dfrac{\partial \alpha_2}{\partial x}, U_1\dfrac{\partial \alpha_3}{\partial x}, 0,0,0, P_2\dfrac{\partial \alpha_2}{\partial x} + P_3\dfrac{\partial \alpha_3}{\partial x}, -P_2\dfrac{\partial \alpha_2}{\partial x}, -P_3\dfrac{\partial \alpha_3}{\partial x}, 0,0,0) \end{cases} \tag{2}$$

Viscous terms should at least account for the following contributions (thermal fluxes might be included):

$$E(W)\frac{\partial W}{\partial x} = (0,0,0,0,0, \alpha_1\mu_1\frac{\partial U_1}{\partial x}, \alpha_2\mu_2\frac{\partial U_2}{\partial x}, \alpha_3\mu_3\frac{\partial U_3}{\partial x}, \alpha_1\mu_1U_1\frac{\partial U_1}{\partial x}, \alpha_2\mu_2U_2\frac{\partial U_2}{\partial x}, \alpha_3\mu_3U_3\frac{\partial U_3}{\partial x}) \tag{3}$$

Source terms $S(W)$ account for mass transfer terms, drag effects, energy loss, and other contributions. To simplify our presentation, we only retain here the effect of pressure relaxation and drag effects. Thus:

$$S(W) = (\phi_2, \phi_3, 0, 0, 0, S_{U_1}, S_{U_2}, S_{U_3}, U_1S_{U_1}, U_1S_{U_2}, U_1S_{U_3}) \tag{4}$$

We also set $\phi_1 = -\phi_2 - \phi_3$ and we recall that the momentum interfacial transfer terms must comply with:

$$S_{U_1}(W) + S_{U_2}(W) + S_{U_3}(W) = 0$$

III. Main properties

We focus first on the homogeneous problem associated with the left hand side of (1). We define as usual specific entropies s_k and speeds c_k in terms of the density ρ_k and the internal energy e_k:

$$(c_k)^2 = \frac{\gamma_k P_k}{\rho_k} = (\frac{P_k}{(\rho_k)^2} - \frac{\partial e_k(P_k, \rho_k)}{\partial \rho_k})(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k})^{-1}$$
$$\gamma_k P_k \frac{\partial s_k(P_k, \rho_k)}{\partial P_k} + \rho_k \frac{\partial s_k(P_k, \rho_k)}{\partial \rho_k} = 0$$

Property 1 :
1.1 The homogeneous system associated with the left hand side of (1) has eigenvalues:
$\lambda_{1,2,3} = U_1$, $\lambda_4 = U_2$, $\lambda_5 = U_3$, $\lambda_6 = U_1 - c_1$, $\lambda_7 = U_1 + c_1$, $\lambda_8 = U_2 - c_2$, $\lambda_9 = U_2 + c_2$, $\lambda_{10} = U_3 - c_3$,$\lambda_{11} = U_3 + c_3$. Associated right eigenvectors span the whole space $\mathbb{R}^{11}$ unless $U_1 = U_k + c_k$ or $U_1 = U_k - c_k$, for $k = 2, 3$.

1.2 Fields associated with eigenvalues λ_k with k in $(1, 2, 3, 4, 5)$ are Linearly Degenerate ; other fields are Genuinely Non Linear.

The list of Riemann invariants through LD fields associated with $k = 4, 5$ and GNL fields may be computed quite easily using variable: $Z^t = (\alpha_2, \alpha_3, s_1, s_2, s_3, U_1, U_2, U_3, P_1, P_2, P_3)$ (see appendices A,B,C in[21]).

Property 2 :
2.1 The latter system admits the following Riemann invariants through the $1-2-3$ LD wave:

$$I_1^{1-2-3}(W) = m_2(U_2 - U_1) \qquad I_2^{1-2-3}(W) = m_3(U_3 - U_1)$$
$$I_3^{1-2-3}(W) = s_2 \qquad I_4^{1-2-3}(W) = s_3 \qquad I_5^{1-2-3}(W) = U_1$$
$$I_6^{1-2-3}(W) = \alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3 + m_2(U_1 - U_2)^2 + m_3(U_1 - U_3)^2$$
$$I_7^{1-2-3}(W) = 2e_2 + 2\frac{P_2}{\rho_2} + (U_1 - U_2)^2 \qquad I_8^{1-2-3}(W) = 2e_3 + 2\frac{P_3}{\rho_3} + (U_1 - U_3)^2$$

2.2 We note $\Delta(\psi) = \psi_r - \psi_l$. Apart from the $1-2-3$ LD wave, the following exact jump conditions hold for $k = 1, 2, 3$, through any discontinuity separating states l, r moving with speed σ:

$$\Delta(\alpha_k) = 0$$
$$\Delta(m_k(U_k - \sigma)) = 0$$
$$\Delta(m_k U_k(U_k - \sigma) + \alpha_k P_k) = 0$$
$$\Delta(\alpha_k E_k(U_k - \sigma) + \alpha_k P_k U_k) = 0$$

We need to define:

$$a_k = (s_k)^{-1}(\frac{\partial s_k(P_k, \rho_k)}{\partial P_k})(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k})^{-1} \tag{5}$$

and: $\eta_k = Log(s_k)$, but also the pair (η, F_η) such that : $\eta = -m_1\eta_1 - m_2\eta_2 - m_3\eta_3$, and: $F_\eta = -m_1\eta_1 U_1 - m_2\eta_2 U_2 - m_3\eta_3 U_3$. Drag terms $S_{U_k}(W)$ and source terms $\phi_k(W)$ in (1) comply with:

$$0 \leq a_2(U_1 - U_2)S_{U_2}(W) + a_3(U_1 - U_3)S_{U_3}(W) \tag{6}$$

$$0 \leq a_1(\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3) \tag{7}$$

Condition (7) reads:

$$\phi_2(P_1 - P_2) + \phi_3(P_1 - P_3) \leq 0$$

since $\phi_1 + \phi_2 + \phi_3 = 0$ and $a_1 > 0$ for standard EOS.

Property 3 :
Closures in agreement with the above mentionned constraints (6),(7) ensure that the following entropy inequality holds for regular solutions of (1):

$$\frac{\partial \eta}{\partial t} + \frac{\partial F_\eta}{\partial x} \leq 0 \tag{8}$$

We from now will assume that the conditions (6) , (7) are fulfilled. For conveniency we will choose here :

$$\phi_2 = f_{1-2}(W)\alpha_1\alpha_2(P_2 - P_1)/(P_1 + P_2 + P_3) \tag{9}$$
$$\phi_3 = f_{1-3}(W)\alpha_1\alpha_3(P_3 - P_1)/(P_1 + P_2 + P_3) \tag{10}$$

where positive scalar functions $f_{k-l}(W)$ denote bounded frequencies. It is easy to check that:

$$\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3 > 0$$

Even more, the governing equation of $\pi = \alpha_1\alpha_2\alpha_3$ guarantees that regular solutions $\alpha_k(x,t)$ remain in the admissible range $[0,1]$. We will rely on standard closures of the form (see[2] for instance):

$$S_{U_2}(W) = \psi_2(W)(U_1 - U_2) \tag{11}$$
$$S_{U_3}(W) = \psi_3(W)(U_1 - U_3) \tag{12}$$

where the scalar functions $\psi_2(W)$, $\psi_3(W)$ should remain positive. Hence (6) and (7) hold.

Property 4 :
We assume perfect gas state law within each phase ($k = 1,2,3$). We consider a single wave associated with λ_m, separating states l, r. If the initial conditions satisfy: $(\alpha_k)_{L,R}(1-\alpha_k)_{L,R} \neq 0$, for $k = 1,2,3$ the connection of states through this wave ensures that all states are in agreement with: $0 \leq \alpha_k$, $0 \leq m_k$, $0 \leq P_k$.

Actually, the proof is almost obvious when focusing on a single field connected with eigenvalue λ_k where $k = 4$ to 11. Turning then to the $1,2,3$-field, the main guidelines (see appendix E in[21]) are the same as in.[17] Details on some suitable forms of mass and energy transfer terms can be found in appendix F in.[21]

IV. Numerical approach

The whole enables to introduce a fractional step approach in agreement with the overall entropy inequality, which is again the counterpart of the one described in.[17] We thus simply compute approximations of the convective subset :

$$(I + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = 0 \tag{13}$$

and then account for source terms and viscous terms updating values through the step:

$$(I + D(W))\frac{\partial W}{\partial t} = S(W) + \frac{\partial}{\partial x}(E(W)\frac{\partial W}{\partial x}) \tag{14}$$

This fractional step method is in agreement with the whole entropy inequality. When neglecting viscous contributions, the second one turns to an ordinary differential system .

Our basic approach to compute convective terms relies on the Godunov approach.[22,23] More precisely here, we use the schemes introduced in[17] to compute approximations of the system (13). This is achieved with help of either the Rusanov scheme or the approximate Godunov scheme VFRoe-ncv.[19] In order to cope with the standard step (13) which requires discretizing convective effects, a rather efficient way consists in using the approximate Godunov scheme introduced in[19] with the specific variable:

$$Z^t = (\alpha_2, \alpha_3, s_1, s_2, s_3, U_1, U_2, U_3, P_1, P_2, P_3) \tag{15}$$

(see[20] which details the main advantages of such a choice). Computations below have been obtained with the former scheme, while fulfilling standard CFL conditions.

One must be careful when providing approximations of system (14). Otherwise, the stability of locally equal-pressure regions may be violated. The connection with the scheme introduced in[24] is obvious.

This approach has another advantage, since it also enables to cope with the instantaneous pressure equilibrium assumption. This is useful to compute models such as those described in[2] for instance. Owing to the entropy structure (see appendix D in[21]), one may actually introduce the pressure relaxation step involved in (14) as a tool to compute the single pressure models detailed in.[2] This is the counterpart of what has been achieved in the two-phase framework (see[25, 26] or[3] for instance).

V. A few computations of the shock tube apparatus

We restrict here to some simple computations of the shock tube apparatus. We use a uniform mesh with 10000 cells and set $CFL = 0.49$ in order to avoid the interaction of waves within the cells. In these computations, all source terms and viscous terms have been neglected, in order to assess the stability of the whole convective subset.

We assume that the perfect gas law holds within each phase: $\rho_k e_k = (\gamma_k - 1)P_k$, setting $\gamma_1 = 7/5$, $\gamma_2 = 1.05$ and $\gamma_3 = 1.01$. Initial conditions are : $(\alpha_2)_L = 0.4$, $(\alpha_3)_L = 0.5$, $(\alpha_2)_R = 0.5$, $(\alpha_3)_R = 0.4$, $(U_1)_L = 100$, $(\tau_1)_L = 1$, $(P_1)_L = 10^5$, $(U_1)_R = 100$, $(\tau_1)_R = 8$, $(P_1)_R = 10^5$, $(U_2)_L = 100$, $(\tau_2)_L = 1$, $(P_2)_L = 10^5$, $(U_2)_R = 100$, $(\tau_2)_R = 8$, $(P_2)_R = 10^5$, $(U_3)_L = 100$, $(\tau_3)_L = 1$, $(P_3)_L = 10^5$, $(U_3)_R = 100$, $(\tau_3)_R = 8$, $(P_3)_R = 10^5$, for the first case (fig. (1-3)), and: $(\alpha_2)_L = 0.4$, $(\alpha_3)_L = 0.5$, $(\alpha_2)_R = 0.5$, $(\alpha_3)_R = 0.4$, $(U_1)_L = 0$, $(\tau_1)_L = 1$, $(P_1)_L = 10^5$, $(U_1)_R = 0$, $(\tau_1)_R = 8$, $(P_1)_R = 10^4$, $(U_2)_L = 0$, $(\tau_2)_L = 1$, $(P_2)_L = 10^5$, $(U_2)_R = 0$, $(\tau_2)_R = 8$, $(P_2)_R = 10^4$, $(U_3)_L = 0$, $(\tau_3)_L = 1$, $(P_3)_L = 10^5$, $(U_3)_R = 0$, $(\tau_3)_R = 8$, $(P_3)_R = 10^4$, for the second test.

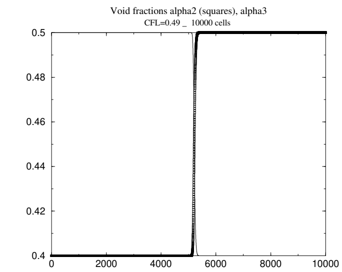

Figure 1. Void fractions α_2, α_3

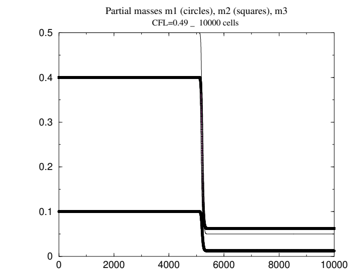

Figure 2. Partial masses m_1, m_2, m_3

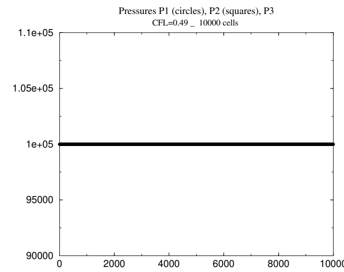

Figure 3. Pressures P_1, P_2, P_3

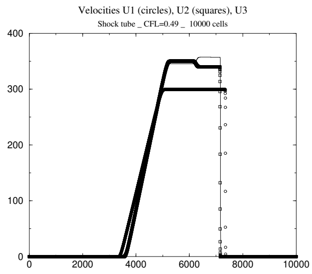

Figure 4. Velocities U_1, U_2, U_3

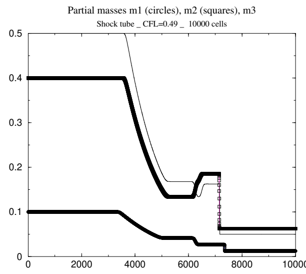

Figure 5. Partial masses m_1, m_2, m_3

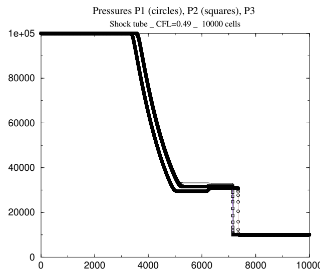

Figure 6. Pressures P_1, P_2, P_3

VI. Conclusion

This new model benefits from important properties. From a physical point of view, an interesting point is that it preserves the positivity of (expected) positive quantities : void fractions, mass fractions and internal energies, at least when restricting to sufficiently simple EOS. Its mathematical properties enable us to construct nonlinear stable numerical methods, and thus to explore highly unsteady flow patterns. Conditions to obtain a existence and uniqueness of the exact solution of the one dimensional Riemann problem cannot be obtained easily. A specific difficulty is linked with the possible occurence of the resonance phenomena. Another point, which seems worth being noted, is that the counterpart of the average "candidate" interface velocity $V_I = (m_1U_1 + m_2U_2)/(m_1 + m_2)$ no longer arises in the three-field framework.

Another part of our current work concerns the comparison with standard single pressure three-field models, when restricting to coarse meshes. This is achieved using relaxation techniques, following ideas from.[3, 24–30]

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Appendix

We examine in this appendix the structure of the convective set of equations. Restricting to regular solutions, we rewrite the convective system issuing from (1), that is:

$$(Id + D(W))\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = 0$$

in the form:

$$\frac{\partial Z}{\partial t} + A(Z)\frac{\partial Z}{\partial x} = 0$$

using the specific variable:

$$Z^t = (\alpha_2, \alpha_3, s_1, s_2, s_3, U_1, U_2, U_3, P_1, P_2, P_3)$$

This provides a system in reduced form. The occurence of terms proportional to $\dfrac{\partial \alpha_2}{\partial x}, \dfrac{\partial \alpha_3}{\partial x}$ inhibits the fully symmetrized form, unless pressure-velocity equilibrium is reached. The matrix of convective terms is:

$$A(Z) = \begin{pmatrix} U_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & U_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & U_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & U_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ (P_2 - P_1)/m_1 & (P_3 - P_1)/m_1 & 0 & 0 & 0 & U_1 & 0 & 0 & \tau_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & U_2 & 0 & 0 & \tau_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & U_3 & 0 & 0 & \tau_3 \\ 0 & 0 & 0 & 0 & 0 & \gamma_1 P_1 & 0 & 0 & U_1 & 0 & 0 \\ \gamma_2 (U_2 - U_1) P_2/\alpha_2 & 0 & 0 & 0 & 0 & 0 & \gamma_2 P_2 & 0 & 0 & U_2 & 0 \\ 0 & \gamma_3 (U_3 - U_1) P_3/\alpha_3 & 0 & 0 & 0 & 0 & 0 & \gamma_3 P_3 & 0 & 0 & U_3 \end{pmatrix}.$$

It admits the following right eigenvectors:

$$\begin{aligned} r_1^t &= (1, 0, 0, 0, 0, 0, a_7, 0, (P_1 - P_2)/\alpha_1, a_{10}, 0) \\ r_2^t &= (0, 1, 0, 0, 0, 0, 0, a_8, (P_1 - P_3)/\alpha_1, 0, a_{11}) \\ r_3^t &= (0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0) \\ r_4^t &= (0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0) \\ r_5^t &= (0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0) \\ r_6^t &= (0, 0, 0, 0, 0, \tau_1, 0, 0, -c_1, 0, 0) \\ r_7^t &= (0, 0, 0, 0, 0, \tau_1, 0, 0, c_1, 0, 0) \\ r_8^t &= (0, 0, 0, 0, 0, 0, \tau_2, 0, 0, -c_2, 0) \\ r_9^t &= (0, 0, 0, 0, 0, 0, \tau_2, 0, 0, c_2, 0) \\ r_{10}^t &= (0, 0, 0, 0, 0, 0, 0, \tau_3, 0, 0, -c_3) \\ r_{11}^t &= (0, 0, 0, 0, 0, 0, 0, \tau_3, 0, 0, c_3) \end{aligned}$$

noting:

$$a_7 = \gamma_2 P_2 \tau_2 (U_2 - U_1)/(\alpha_2 \delta_2) \qquad a_{10} = -\gamma_2 P_2 (U_2 - U_1)^2/(\alpha_2 \delta_2)$$
$$a_8 = \gamma_3 P_3 \tau_3 (U_3 - U_1)/(\alpha_3 \delta_3) \qquad a_{11} = -\gamma_3 P_3 (U_3 - U_1)^2/(\alpha_3 \delta_3)$$
$$\delta_k = (U_k - U_1)^2 - (c_k)^2$$

for $k = 2, 3$. Recall that $c_k = (\gamma_k P_k \tau_k)^{1/2}$. Obviously, this set of eigenvectors no longer spans the whole space when either δ_2 or δ_3 is null.