On Aggregated Regularized Equations for Homogeneous Binary Gas Mixture Flows with Viscous Compressible Components

Alexander Zlotnik (jointly with **Tatiana Elizarova**)

Department of Mathematics,
National Research University Higher School of Economics
Keldysh Institute of Applied Mathematics
Moscow, Russia

International Conference of Numerical Analysis and Applied Mathematics 2019
Greece, Rodos, September 23–28, 2019

There exist various models to describe compressible gas mixture flows, in particular, see monographs Nigmatulin (1990), Golovachev (1996), Giovangigli (1999) and Lebo & Tishkin (2006).

In Elizarova (2009) on the basis of the model kinetic equation, a regularized (quasi-gasdynamic, QGD) system of equations was constructed for the binary gas mixture flows in the absence of chemical reactions (the cold gas approximation).
For more information on QGD single-component gas models, see monographs: Chetverushkin (2008) and Elizarova (2009).
We also notice that their numerical implementation has recently (2018) been incorporated into the open source CFD software package OpenFOAM.

It was assumed that both components of the mixture have their own density, speed and temperature. The exchange terms in the mass balance equations were absent, but they were present in the momentum and total energy balance equations for both mixture components and described the interaction between the components. Their form was taken as in the kinetic equation under the assumption that the gases are monatomic.

This system of equations was applied for numerical simulation of 1D rarefied gas flows, the results were compared with those obtained by the Monte Carlo method, see Bird (1994), and were fairly accurate.

On the basis of these equations, a homogeneous model, where the velocities and temperatures of the both mixture components are the same, was also constructed in Elizarova (2009), in the particular case of equal adiabatic indices γ and Prandtl numbers α_{Pr} of the components. This model was also successfully applied to the numerical simulation of the same 1D flows.

Later in Elizarova, Zlotnik & Chetverushkin (2014), a generalization of the exchange terms in the full QGD system of equations for the binary gas mixture flows were given in the case of polyatomic gases, with arbitrary γ and α_{Pr} (its physical meaning was analyzed by Elizarova & Lengrand (2016)).

In addition, the QGD equations themselves were rewritten in another form like the compressible Navier-Stokes equations which is particularly convenient for discretization, and the mixture entropy balance equation with the non-negative entropy production was derived.

Application of the full QGD system of equations for numerical simulation of the mixture flows for sufficiently dense gases showed that as the number of intermolecular collisions increases, the exchange terms in the equations increase rapidly which leads to a rapid equalization of temperatures and velocities of the mixture components and, therefore, the possibility of transition to a homogeneous mixture model. Moreover, a computational instability arose, and thus a homogeneous model became more preferable from both physical and computational points of view.

In this study, a regularized system of equations is constructed for homogeneous binary mixture flows by aggregating equations from Elizarova, Zlotnik & Chetverushkin (2014). In the system, the mass balance equations for the both mixture components include diffusion flows for the components. For the solutions of the system, the mixture entropy balance equation with the non-negative entropy production is satisfied which confirms the physical correctness of the model. The model was tested by numerical simulating the problem of 2D Rayleigh-Taylor-type gravitational instability (concerning it, see the recent review Zhou (2017)).

The regularized (or QGD) system of equations for binary gas mixture flows

in the form of Elizarova, Zlotnik & Chetverushkin (2014) contains the mass, momentum and total energy balance equations for gases $\alpha = a, b$

$$\partial_t \rho_\alpha + \operatorname{div}\left[\rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha)\right] = 0, \tag{1}$$

$$\partial_t(\rho_\alpha \mathbf{u}_\alpha) + \operatorname{div}\left[\rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha)\otimes \mathbf{u}_\alpha\right] + \nabla p_\alpha$$
$$= \operatorname{div}\Pi_\alpha + \left[\rho_\alpha - \tau \operatorname{div}(\rho_\alpha \mathbf{u}_\alpha)\right]\mathbf{F}_\alpha + \mathbf{S}_{u,\alpha}, \tag{2}$$

$$\partial_t E_\alpha + \operatorname{div}\left[(E_\alpha + p_\alpha)(\mathbf{u}_\alpha - \mathbf{w}_\alpha)\right]$$
$$= \operatorname{div}(-\mathbf{q}_\alpha + \Pi_\alpha \mathbf{u}_\alpha) + \rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha)\cdot \mathbf{F}_\alpha + Q_\alpha + S_{E,\alpha}. \tag{3}$$

Here $\partial_t = \frac{\partial}{\partial t}$ and $\partial_i = \frac{\partial}{\partial x_i}$, the operators div and ∇ are taken with respect to spacial coordinates $x = (x_1, \ldots, x_n)$, $n = 1, 2, 3$.
The divergence of a tensor is taken with respect to its first index, and $\otimes$ and $\cdot$ are the signs of tensor and scalar products of vectors.
The main sought functions

$$\rho_\alpha > 0, \quad \mathbf{u}_\alpha = (u_{1\alpha}, \ldots, u_{n\alpha}), \quad \theta_\alpha > 0$$

are the density, velocity and absolute temperature of the gas α (depending on (x, t)).

Also the total energy together with the pressure and specific internal energy for the perfect polytropic gas α are as follows

$$E_\alpha = \frac{1}{2}\,\rho_\alpha|\mathbf{u}_\alpha|^2 + \rho_\alpha\varepsilon_\alpha,\ \ p_\alpha = R_\alpha\rho_\alpha\theta_\alpha = (\gamma_\alpha - 1)\rho_\alpha\varepsilon_\alpha,\ \ \varepsilon_\alpha = c_{V\alpha}\theta_\alpha,$$

where $R_\alpha > 0$ is the gas constant, $\gamma_\alpha = \frac{c_{p\alpha}}{c_{V\alpha}} = \frac{R_\alpha}{c_{V\alpha}} + 1$ is the adiabatic index as well as $c_{V\alpha} > 0$ and $c_{p\alpha} > 0$ are the specific heat capacities at constant volume and pressure.
In these equations, $\Pi_\alpha = \Pi_\alpha^{NS} + \Pi_\alpha^\tau$ and $\mathbf{q}_\alpha = -\varkappa_\alpha\nabla\theta_\alpha + \mathbf{q}_\alpha^\tau$ are the viscous stress tensor and heat flux.
Here Π_α^{NS} is the classic Navier-Stokes viscosity stress tensor

$$\Pi_\alpha^{NS} \equiv \Pi_\alpha^{NS}(\mathbf{u}_\alpha) = \mu_\alpha\big[2\mathbb{D}(\mathbf{u}_\alpha) - \tfrac{2}{3}\,(\operatorname{div}\mathbf{u}_\alpha)\mathbb{I}\big] + \lambda_\alpha(\operatorname{div}\mathbf{u}_\alpha)\mathbb{I},$$
$$\mathbb{D}_{ij}(\mathbf{u}_\alpha) = \tfrac{1}{2}\big[\nabla\mathbf{u}_\alpha + (\nabla\mathbf{u}_\alpha)^T\big],\ \ \nabla\mathbf{u}_\alpha = \{\partial_i u_{j\alpha}\}_{i,j=1}^n,$$

where $\mu_\alpha = \mu_\alpha(\rho_\alpha,\theta_\alpha) > 0$, $\lambda_\alpha = \lambda_\alpha(\rho_\alpha,\theta_\alpha) \geqslant 0$ and $\varkappa_\alpha = \varkappa_\alpha(\rho_\alpha,\theta_\alpha) > 0$ are the coefficients of dynamic and bulk viscosity and thermal conductivity as well as $\mathbb{I}$ is the unit tensor.
In practice, both physical and artificial viscosity and thermal conductivity coefficients are used as well as their sums, see Elizarova (2009).

The regularizing tensor Π_α^τ, velocities $\mathbf{w}_\alpha$ and $\widehat{\mathbf{w}}_\alpha$ and heat flux $\mathbf{q}_\alpha^\tau$ are given by the formulas

$$\Pi_\alpha^\tau = \rho_\alpha \mathbf{u}_\alpha \otimes \widehat{\mathbf{w}}_\alpha + \tau\big[\mathbf{u}_\alpha \cdot \nabla p_\alpha + c_{s\alpha}^2 \rho_\alpha \operatorname{div} \mathbf{u}_\alpha - (\gamma_\alpha - 1) Q_\alpha\big]\mathbb{I},$$

$$\mathbf{w}_\alpha = \frac{\tau}{\rho_\alpha}\big[\operatorname{div}(\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha) + \nabla p_\alpha - \rho_\alpha \mathbf{F}_\alpha\big],$$

$$\widehat{\mathbf{w}}_\alpha = \frac{\tau}{\rho_\alpha}\big[\rho_\alpha (\mathbf{u}_\alpha \cdot \nabla)\mathbf{u}_\alpha + \nabla p_\alpha - \rho_\alpha \mathbf{F}_\alpha\big],$$

$$-\mathbf{q}_\alpha^\tau = \tau\big[\mathbf{u}_\alpha \cdot (c_{V\alpha} \rho_\alpha \nabla \theta_\alpha - R_\alpha \theta_\alpha \nabla \rho_\alpha) - Q_\alpha\big]\mathbf{u}_\alpha, \qquad (4)$$

where $\tau = \tau(\rho_a, \mathbf{u}_a, \theta_a, \rho_b, \mathbf{u}_b, \theta_b) > 0$ is the relaxation parameter and $c_{s\alpha} = \sqrt{\gamma_\alpha(\gamma_\alpha - 1)\varepsilon_\alpha}$ is the sound speed of the gas α.

The quantities $\mathbf{S}_{u,\alpha}$ and $S_{E,\alpha}$ are the exchange terms depending on all the sought functions and interconnecting the equations for the gases a and b, see them in Elizarova, Zlotnik & Chetverushkin (2014) (with the physical motivation in Elizarova & Lengrand (2016)).

Below the explicit form of $\mathbf{S}_{u,\alpha}$ and $S_{E,\alpha}$ is not required, and only the equalities $\mathbf{S}_{u,a} + \mathbf{S}_{u,b} = 0$ and $S_{E,a} + S_{E,b} = 0$ are essential.

$\mathbf{F}_\alpha$ and $Q_\alpha \geqslant 0$ are the given body force density and heat source intensity.

The above system of regularized equations for binary mixture flows is quite complex and contains $2(n+2)$ scalar sought functions ρ_α, $\mathbf{u}_\alpha = (u_{1\alpha}, \ldots, u_{n\alpha})$ and θ_α, $\alpha = a, b$. Therefore simplified models for binary mixture flows are of high practical interest.

For the homogeneous binary mixture, it is assumed that $\mathbf{u}_a = \mathbf{u}_b = \mathbf{u}$ and $\theta_a = \theta_b = \theta$ (Nigmatulllin, 1987). Let also $\mathbf{F}_a = \mathbf{F}_b = \mathbf{F}$. To derive the equations for such a mixture flows, we perform an aggregation of the above written equations. Namely, we preserve the mass balance equations for the components (1), sum up the momentum and total energy balance equations (2) in $\alpha = a, b$ and take in all the equations $\mathbf{u}_a = \mathbf{u}_b = \mathbf{u}$ and $\theta_a = \theta_b = \theta$. As a result, we obtain the following system of equations

$$\partial_t \rho_\alpha + \operatorname{div}\left[\rho_\alpha(\mathbf{u} - \mathbf{w}^{(\alpha)})\right] = 0, \quad \alpha = a, b, \tag{5}$$

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}\left[\rho(\mathbf{u} - \mathbf{w}) \otimes \mathbf{u}\right] + \nabla p = \operatorname{div}\Pi + \left[\rho - \tau \operatorname{div}(\rho\mathbf{u})\right]\mathbf{F}, \tag{6}$$

$$\partial_t E + \operatorname{div}\left[\tfrac{1}{2}\rho|\mathbf{u}|^2(\mathbf{u} - \mathbf{w}) + c_{pa}\rho_a\theta(\mathbf{u} - \mathbf{w}^{(a)}) + c_{pb}\rho_b\theta(\mathbf{u} - \mathbf{w}^{(b)})\right]$$
$$= \operatorname{div}(-\mathbf{q} + \Pi\mathbf{u}) + \rho(\mathbf{u} - \mathbf{w}) \cdot \mathbf{F} + Q. \tag{7}$$

They contain the aggregated density and pressure

$$\rho = \rho_a + \rho_b, \quad p := p_a + p_b = (R_a\rho_a + R_b\rho_b)\theta,$$

together with the aggregated total and specific internal energies

$$E = \tfrac{1}{2}\rho|\mathbf{u}|^2 + \rho\varepsilon, \quad \varepsilon := \tfrac{\rho_a}{\rho}\varepsilon_a + \tfrac{\rho_b}{\rho}\varepsilon_b = c_V\theta.$$

The summands of the viscous stress tensor $\Pi = \Pi^{NS} + \Pi^{\tau}$ are

$$\Pi^{NS} := \Pi_a^{NS}(\mathbf{u}) + \Pi_b^{NS}(\mathbf{u}) = \mu\big[2\mathbb{D}(\mathbf{u}) - \tfrac{2}{3}\,(\operatorname{div}\mathbf{u})\mathbb{I}\big] + \lambda(\operatorname{div}\mathbf{u})\mathbb{I},$$

$$\Pi^{\tau} := \Pi_a^{\tau} + \Pi_b^{\tau} = \rho\mathbf{u}\otimes\widehat{\mathbf{w}} + \tau\big[\mathbf{u}\cdot\nabla p + c_s^2\rho\operatorname{div}\mathbf{u} - (\gamma_a Q_a + \gamma_b Q_b) + Q\big]\mathbb{I},$$

with $\mu := \mu_a + \mu_b$, $\lambda := \lambda_a + \lambda_b$ and $Q := Q_a + Q_b$,
and the regularizing velocities are

$$\mathbf{w} := \frac{\rho_a}{\rho}\mathbf{w}^{(a)} + \frac{\rho_b}{\rho}\mathbf{w}^{(b)} = \frac{\tau}{\rho}\big[\operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p - \rho\mathbf{F}\big],$$

$$\widehat{\mathbf{w}} = \frac{\tau}{\rho}\big[\rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \rho\mathbf{F}\big].$$

The aggregated heat flux and its regularizing summand are expressed by the formulas $-\mathbf{q} := -\mathbf{q}_a - \mathbf{q}_b = (\varkappa_a + \varkappa_b)\nabla\theta - \mathbf{q}^\tau$ and

$$-\mathbf{q}^\tau := -\mathbf{q}_a^\tau - \mathbf{q}_b^\tau = \tau\Big\{\mathbf{u}\cdot\big[c_V\rho\nabla\theta - \theta(R_a\nabla\rho_a + R_b\nabla\rho_b)\big] - Q\Big\}\mathbf{u}.$$

The following aggregated squared sound speed and physical coefficients of the mixture are introduced:

$$c_s^2 := \frac{\rho_a}{\rho}c_{sa}^2 + \frac{\rho_b}{\rho}c_{sb}^2,\ c_V := \frac{\rho_a}{\rho}c_{Va} + \frac{\rho_b}{\rho}c_{Vb},\ c_p := \frac{\rho_a}{\rho}c_{pa} + \frac{\rho_b}{\rho}c_{pb},\ R := c_p - c_V$$

and $\gamma := \frac{c_p}{c_V} = \frac{R}{c_V} + 1$. With the help of them, other important natural formulas for the mixture pressure are valid: $p = R\rho\theta = (\gamma-1)\rho\varepsilon$.
But, for mixtures, c_V, c_p, R and γ are functions of the component concentrations $\frac{\rho_a}{\rho}$ and $\frac{\rho_b}{\rho} = 1 - \frac{\rho_a}{\rho}$ rather than constants.
Notice that when aggregating is performed, some quantities are taken additively, i.e., we just sum up them (as ρ_α, p_α, etc.), while others are taken as linear combinations with the weights-concentrations $\frac{\rho_\alpha}{\rho}$ (as ε_α, $\mathbf{w}^{(\alpha)}$, etc.). Additivity of ρ, $\rho\varepsilon$, $c_V\rho$, $\rho\mathbf{w}$, $\rho\widehat{\mathbf{w}}$, etc., is taken into account. When summing, the exchange terms in Eqs. (6) and (7) have been reduced.

The derived system of regularized equations for homogeneous binary mixtures is much simpler than the original one (1)–(3) and contains only $n+3$ sought scalar functions ρ_a, ρ_b, $\mathbf{u}=(u_1,\ldots,u_n)$ and θ.
In the simplest case of gases with the same $c_{V\alpha}$ and $c_{p\alpha}$, the total energy balance equation and the expression for $\mathbf{q}^\tau$ take the standard for a single-component gas form of type (3) and (4) (in Π and $\mathbf{q}$, the aggregated viscosity and thermal conductivity coefficients have to stand).

Next, for $\tau=0$, the resulting system of equations (5)–(7) goes into the Navier-Stokes type system of equations for compressible binary mixtures

$$\partial_t\rho_\alpha+\operatorname{div}(\rho_\alpha\mathbf{u})=0,\quad \alpha=a,b,$$

$$\partial_t(\rho\mathbf{u})+\operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u})+\nabla p=\operatorname{div}\Pi^{NS}+\rho\mathbf{F},$$

$$\partial_t E+\operatorname{div}\left[(E+p)\mathbf{u}\right]=\operatorname{div}(-\mathbf{q}+\Pi^{NS}\mathbf{u})+\rho\mathbf{u}\cdot\mathbf{F}+Q$$

with the above introduced p, Π^{NS}, Q and $-\mathbf{q}=(\varkappa_a+\varkappa_b)\nabla\theta$.

If also $\mu_\alpha=\lambda_\alpha=\varkappa_\alpha=0$, then we obtain a system of equations of the Euler type for compressible binary mixtures with $\Pi^{NS}=0$ and $\mathbf{q}=0$.

The regularized equations for homogeneous binary mixtures (5)–(7) imply the aggregated density, kinetic energy and specific internal energy balance equations

$$\partial_t\rho + \operatorname{div}\big[\rho(\mathbf{u}-\mathbf{w})\big] = 0,$$

$$\partial_t\big(\tfrac{1}{2}\rho|\mathbf{u}|^2\big) + \operatorname{div}\big[\tfrac{1}{2}\rho|\mathbf{u}|^2(\mathbf{u}-\mathbf{w})\big] + \nabla p\cdot\mathbf{u}$$
$$= \operatorname{div}\Pi\cdot\mathbf{u} + \big(\rho - \tau\operatorname{div}(\rho\mathbf{u})\big)\mathbf{F}\cdot\mathbf{u},$$

$$\partial_t(\rho\varepsilon) + \operatorname{div}\big[\rho\varepsilon\mathbf{u} - \big(\rho_a\varepsilon_a\mathbf{w}^{(a)} + \rho_b\varepsilon_b\mathbf{w}^{(b)}\big)\big] + p\operatorname{div}\mathbf{u}$$
$$-\operatorname{div}\big(p_a\mathbf{w}^{(a)} + p_b\mathbf{w}^{(b)}\big) = -\operatorname{div}\mathbf{q} + \Pi : \nabla\mathbf{u} - \rho\widehat{\mathbf{w}}\cdot\mathbf{F} + Q,$$

where : denotes the scalar product of tensors.
Now we define also the entropies of the component α and the mixture

$$s_\alpha = S_{0\alpha} - R_\alpha\ln\rho_\alpha + c_{V\alpha}\ln\varepsilon_\alpha,\quad S_{0\alpha} = \mathrm{const},\quad \alpha = a, b,$$

$$s = \frac{\rho_a}{\rho}s_a + \frac{\rho_b}{\rho}s_b.$$

Theorem

The following homogeneous binary mixture entropy balance equation holds

$$\partial_t(\rho s) + \operatorname{div}\left[\rho s\mathbf{u} - \left(\rho_a s_a \mathbf{w}^{(a)} + \rho_b s_b \mathbf{w}^{(b)}\right)\right] + \operatorname{div}\left(\frac{\mathbf{q}}{\theta}\right)$$
$$= \mathcal{P}^{NS} + \mathcal{P}_a^\tau + \mathcal{P}_b^\tau,$$

with the entropy production $\mathcal{P}^{NS} + \mathcal{P}_a^\tau + \mathcal{P}_b^\tau$*, where*

$$\mathcal{P}^{NS} = 2\frac{\mu}{\theta}\mathbb{D}(\mathbf{u}) : \mathbb{D}(\mathbf{u}) + \left(\lambda - \frac{2}{3}(\mu)\right)\frac{1}{\theta}(\operatorname{div}\mathbf{u})^2 + \frac{\varkappa_a + \varkappa_b}{\theta^2}|\nabla\theta|^2 \geqslant 0,$$

$$\mathcal{P}_\alpha^\tau = \tau\frac{\rho_\alpha}{\theta}\left|\frac{\widehat{\mathbf{w}}^{(\alpha)}}{\tau}\right|^2 + \tau\frac{R_\alpha}{\rho_\alpha}\left[\operatorname{div}(\rho_\alpha\mathbf{u})\right]^2 + \tau c_{V\alpha}\rho_\alpha\Big[(\gamma_\alpha - 1)\operatorname{div}\mathbf{u}$$
$$+\mathbf{u}\cdot\nabla\ln\theta - \frac{(\gamma_\alpha - 1)Q_\alpha}{2p_\alpha}\Big]^2 + \frac{Q_\alpha}{\theta}\left(1 - \frac{\tau(\gamma_\alpha - 1)Q_\alpha}{4p_\alpha}\right),$$

moreover, $\mathcal{P}_\alpha^\tau \geqslant 0$ *under the known condition* $\tau(\gamma_\alpha - 1)Q_\alpha \leqslant 4p_\alpha$*,*
$\alpha = a, b$.

The proof exploits the aggregated density and specific internal energy balance equations and mainly follows Zlotnik & Gavrilin (2011) and Chetverushkin & Zlotnik (2017).
The result is crucial in view of the physical correctness of the model.

See more details and related numerical results on the 2D Rayleigh-Taylor type gravitational instability on mixing layers of heavy and light gases in:

T.G. Elizarova, A.A. Zlotnik and E.V. Shilnikov, Regularized equations for numerical simulation of flows of homogeneous binary mixtures of viscous compressible gases, *Computational Mathematics and Mathematical Physics*, Vol. 59, No. 11 (2019).

Note that the constructed model can be generalized to a larger number of the mixture components.