

ON THE GENERALIZED BOUSSINESQ APPROXIMATION FOR FLOWS OF REACTING MIXTURES

Christo Christov, Ivanka Zheleva

Христо Христов, Иванка Желева. **Обобщенное приближение Бусинеска для течений реагирующих смесей.** Для течений реагирующих смесей применяется классическое приближение Бусинеска и выводится система параболических в некотором смысле уравнений, которые очень удобные для численного решения. Уравнение непрерывности такое как и для несжимаемых жидкостей, но содержит источник, который обязан производной по времени от плотности. В модели учитываются процессы термодиффузии и диффузионный термоэффект. Обсуждаются условия, при которых предлагаемая система корректна.

Christo Christov, Ivanka Zheleva. **On the generalized Boussinesq approximation for flows of reacting mixtures.** The classical Boussinesq assumption is applied to the case of reacting liquid mixtures and a system of parabolic in a sense equations is derived that is much more tractable numerically than the original set. The equation of continuity is similar to that of incompressible liquid containing a source term due to the time derivative of density. The latter is crucial for employing the Boussinesq approximation to flows of reacting liquids. The effect of thermodiffusion and the diffusion thermoeffect are also accounted for in the model. The conditions for correctness of the proposed system are discussed.

INTRODUCTION

Recently, the methods of fluid dynamics has been increasingly employed in theoretical prediction of characteristics of chemical reactors with liquid or gaseous phases. A great deal of the available literature is connected chiefly with the influence of dynamics on chemical processes while the fluid is thought of as incompressible. Such an approach is called „forced-convection approximation” and proves efficient in a great diversity of chemical-reactor problems when solutions are dilute and / or the mixture is virtually incompressible.

The other extreme is to employ the full system of Navier—Stokes equations for viscous compressible heat-conducting fluid coupled with the equation of energy conservation, the equation of state and the diffusion equation for dissolved species with sources due to chemical reactions. Naturally, this approach takes a full account of the interaction between the dynamics and heat and mass transfer but in turn it requires highly intricated difference schemes and algorithms (see e.g. [1, 2]) when numerical solution to a specific problem is attempted. The worst enemy that imposes the most stringent limitations in difference schemes appears to be the acoustic waves. At the time the sound waves are in a sense „reversible” proceses

and contribute virtually nothing in the long term to reactor productivity. Therefore it seems attractive to filter out effects of acoustics without compromising the effects of heat and mass transfer.

The only way to switch off acoustics is to break in the model the link between the pressure and density, i.e. to assume that density is a function of temperature and concentrations of solutions. This assumption lies behind the reknown Boussinesq approximation (see for details [3, 4]). The latter appears to be an adequate model for natural thermal convection despite of its apparent inconsistency founded in the fact that the convective and time derivatives are neglected in continuity equation. This may be justified in natural thermal convection and even in solvent convection, but appears to be a serious shortcoming when chemical reactions with high or moderate rates are incorporated. In this case the time derivative of density is to be retained in continuity equation and some other oversimplifications of the classical Boussinesq approximation are to be abolished.

In the present paper are derived the governing equations for mixture flows with chemical reactions under the assumption that density is function of temperature and concentration only. The properties of the proposed system are discussed and a way of solution is outlined making use of Poisson equation for the pressure. A special attention is paid to the boundary conditions.

1. BASIC ASSUMPTIONS

Consider an inhomogeneous viscous liquid whose density is a function of the temperature T and the scalar parameter c only:

$$(1.1) \quad \rho = \rho(T, c),$$

where T is the absolute temperature. Such a liquid is an adequate model for homogeneous solutions with c bearing the meaning of concentration of the solute. For the sake of simplicity we consider here only two-component mixture. There are no principle obstacles to incorporate in the model more than one dissolved species, but it is not done here since the main purpose of the present work is to elucidate the means of obtaining a model for reacting flows that is more tractable numerically.

The main advantage offered by (1.1) is that the density is not a function of pressure p , i.e. the acoustics is switchen off and no Courant condition is imposed on the time increment when solving the respective equation numerically. Naturally, the pay for this radical simplification is certain approximation introduced which confinds the capability of the model proposed to moderate and slow rates of mass exchange when the pressure changes due to heat and mass transfer and/or chemical reactions are negligible. Fortunately it is the case in most chemical technologies that make use liquid mixtures. The same is true for gas phases when the temperature is not very high and combustion can-not take place.

Under the same assumption of moderate rates of heat and mass transfer one can use the linearized form of (1.1) which is the gist of the so-called Boussinesq approximation (see [3, 4]), namely:

$$(1.2) \quad \rho = \rho_0 \left(1 - \beta_1 \frac{T}{T_0} - \beta_2 \frac{c}{c_0} \right)$$

where $\beta_1 > 0$, i.e. the fluid grows lighter with increasing of temperature. The converse situation is rather exotic and has no meaning for virtually all technology

processes. Concerning the second coefficient it can be said that $(-\beta_2)$ is proportional to the differences between density of the solvent and that of the carrying liquid. For a great number of chemical systems β_1 and β_2 are indeed very small quantities which justifies the linearization (1.2). In the end it should be mentioned that approximation (1.2) is not crucial for the consideration that follows, but there are no known as a rule general formulae of type (1.1) for the different systems and thus (1.1) is not interesting from practical point of view.

If one is to consider mixtures the main uses is then the representation of mass flux j and heat flux q . We prefer to take into account the thermodiffusion and diffusion thermoeffect when posing the problem since they can trigger large-scale instabilities in reacting flows although being negligible in general in comparison with diffusion and heat conduction. So, following [3] we write:

$$(1.3) \quad j = -\rho D \nabla c - \alpha \rho D \nabla T$$

where D is the diffusion coefficient and α is called thermodiffusion coefficient, and for

$$(1.4) \quad q = -(\kappa + \alpha DN) \nabla T - DN \nabla c$$

where

$$(1.5) \quad N = \rho \left[\varphi - \left(\frac{\partial \varphi}{\partial T} \right)_{s,p} \cdot c + \alpha \left(\frac{\partial \varphi}{\partial T} \right)_{T,p} T \right]$$

In the last formula φ is the chemical potential

$$(1.6) \quad \varphi = \varphi_1 / m_1 - \varphi_2 / m_2$$

where m_i and φ_i are the molecular masses and chemical potentials of the respective species; $i=1$ refers to the lighter species.

In the end we specify the source of species due to the chemical reaction as usual

$$(1.7) \quad \psi = k_1 e^{-E/T}$$

where E is the energy of activation.

2. GOVERNING EQUATIONS

Having the physical laws specified in the previous section we are able now to derive a coupled system of equations for the mixture flows which we call henceforth generalized Boussinesq approximation.

The equation of continuity for a mixture coincides with that for a pure liquid:

$$(2.1) \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

provided that ρ is the density of the mixture and \mathbf{v} — the mean-mass velocity. The presence of the solvent is acknowledged through a separate balance equation (see

[5]), which is rewritten as follows keeping in mind the relations of the previous section, namely

$$(2.2) \quad \frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot \rho D(\nabla c + \alpha \nabla T) + k_1 e^{-E/T}$$

Respectively, the balance of total energy yields the generalized equation of heat conductivity

$$(2.3) \quad c_p \rho \cdot \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = \nabla \cdot [(\kappa + \alpha DN) \nabla T + DN \nabla c] + k_2 e^{-E/T}$$

where c_p is the specific heat for constant pressure.

We assume the liquid to be Newtonian viscous fluid governed by the Navier — Stokes equations:

$$(2.4) \quad \rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = - \nabla p + \mathbf{g} + \nabla (\mu \nabla \mathbf{v}) + \nabla (\lambda \nabla \cdot \mathbf{v})$$

where \mathbf{v} is the mean-mass velocity mentioned above, \mathbf{g} is the vector of external body forces (e.g. gravity), μ is the coefficient of shear viscosity and λ is the dilational coefficient (called sometimes "second viscosity coefficient"). The viscosity coefficients are functions of temperature and concentration:

$$(2.5) \quad \mu = \mu(T, c), \quad \lambda = \lambda(T, c)$$

which are thought of as known for the purposes of the present analysis. Usually, these relations are known in linearized form.

The system of governing equations is coupled with the equation of state (1.1) (or its linear version (1.2)).

3. TYPE OF THE SYSTEM

The most important feature of the system proposed in the previous section is that (2.1) is not an evolution equation for evaluating function ρ . The latter is defined from (1.1), provided that T and c are thought of as known functions, i.e. (2.1) has the form

$$(3.1) \quad \text{div } \mathbf{v} = \Phi(r, t) \equiv \frac{d\rho}{dt} = \frac{\partial \rho}{\partial c} \cdot \frac{dc}{dt} + \frac{\partial \rho}{\partial T} \cdot \frac{dT}{dt}$$

where the full derivatives of c and T are taken from (2.2) and (2.3) respectively. Thus, the problem under consideration is akin mathematically to that of flow of viscous liquid with prescribed density at each point with c and T playing the role of functional parameters. The cited problem is known to be correct [6] for sufficiently large values of viscosity μ . If $\Phi \neq 0$ then the only condition for correctness appears to be

$$\int_{\Omega} \Phi(r, t) d\tau = \oint_{\Gamma} v_n ds$$

where Ω is the region occupied by the flow and Γ is its boundary. Resorting to the linear equation of state (1.2) and being reminded of definition (3.1) of Φ the last equality is recast as follows:

$$(3.2) \quad \left(-\frac{\beta_1 k_2}{T_0 \varrho c_p} - \frac{\bar{\beta}_2 k_1}{c_0} \right) \int_{\Omega} e^{-E/T} d\tau - \left[\frac{\kappa + \alpha DN}{\varrho c_p T_0} \bar{\beta}_1 + \frac{\varrho \alpha D}{c_0} \bar{\beta}_2 \right] \oint_{\Gamma} \frac{\partial T}{\partial n} ds \\ - \left(\frac{DN}{\varrho c_p T_0} \bar{\beta}_1 + \frac{\varrho D}{c_0} \bar{\beta}_2 \right) \oint_{\Gamma} \frac{\partial c}{\partial n} ds = \oint_{\Gamma} v_n ds$$

where the dependence of ϱ , κ , D on spatial coordinates is neglected since it introduces only effects of second-order. Equality (2.2) requires that the total flux through the region be equal to the internal fluxes due to chemical reaction added to the fluxes due to the temperature and concentration gradients at the boundary.

It is important now to check the correctness of the initial-boundary problem for pair of coupled equations (2.2), (2.3). The crucial point here is to show that they form a parabolic system for the vector unknown (T, c) . Since the boundary conditions are standard and so do the Laplace operators, the only cause of breaking the ellipticity of the right-hand side operators is the interaction between the different Laplace operators. The condition for ellipticity is

$$D^2(\varrho \alpha + N)^2 - 4\varrho D(\kappa + \alpha DN) < 0$$

or which is the same

$$(3.3) \quad \left(\alpha - \frac{N}{\varrho} \right)^2 < \frac{4\kappa}{\varrho D}$$

The last equality expresses the condition to be satisfied from the members α and N in order to have a correct elliptic boundary-value problem for the pair (T, c) . Then thinking of the velocity v and ϱ as known functions they are solved by means of a standard numerical method for elliptic equations.

4. CONCLUDING REMARKS

Employing the classical Boussinesq assumption that the density ϱ is not a function of pressure p we derive a system of equations that are significantly more tractable in numerical treatment with Courant condition relaxed. The essential development ahead from the classical Boussinesq theory is that the time derivative of density is not neglected arriving to a source term in the continuity equation. The latter is crucial for modelling reacting flows where the mass exchange results in significant temporal changes of temperature and concentration and hence — of density. We name the model derived "generalized Boussinesq approximation" and show the conditions under which the respective mathematical problem is correct.

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