Constant-Temperature Flow of Two Miscible Fluids Inside a Cylinder

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In this paper numerical results concerning the flow patterns for the classical and a new compressible approach will be presented. The numerical method is an extension (to include the effects of unsteadiness and compressibility) of the control volume method. To achieve this purpose the problem to solve was chosen in such a way that the classical approach does not require to take into account any convective terms.

The model problem and physical consideration. The flow and the concentration distribution of mixture inside a closed cylinder will be investigated. The mixture consists of water and glycerin, which are miscible in any proportion and whose density obeys the ”simple-mixture” formula

$\rho(\Phi) = \rho_W \Phi + \rho_G (1 - \Phi)$ (1) whitin 1% error for the whole range ($\Phi \in [0, 1]$) of the water-volume fraction (the glycerin is supposed to fill the lower half of the cylinder).

It is supposed the cylinder is entirely filled at the initial time and will remain completely filled during the process, allowing to avoid the problem of a free-surface boundary condition on the top of the mixture. Instead, a simple wall-boundary condition for the top of the cylinder can be enforced.

Because the diffusion process is a very slow one and the temperature in the laboratory is practically constant it follows, from a thermodynamically point of view, that the cylinder must be considered an open system and the whole process as an isotermic one.

Obviously, an iterative free-surface boundary condition is not too difficult to implement into a numerical method. On the other hand, any other algebraic relation giving the mixture density as a function of components density will give the opportunity to close the problem formulation without using an energy as long as the diffusion is slow enough that the hypothesis of an isothermal process holds (and usually that is the case for the diffusion of two liquids).

The mathematical model. Because the assumption $divu = 0$ could be false in certain condition it was clear that an unsteady and compressible Navier-Stokes model is necessary in order to solve the problem.

Due to the symmetry with respect to OX-axis , this problem can be treated as an axisymmetric one.

The equation involved are :

-continuity, $\frac{\partial \rho}{\partial t} + div(\rho \mathbf{u}) = 0$ (2)

-momentum $\frac{\partial \Phi}{\partial t} + div(\Phi \mathbf{u}) = div \left(\frac{D}{1 - \zeta \Phi} grad\ u \right)^T$ (3)

-"simple mixture" assumption (Eq. (1)).

Here the tensor $D = 1/2 \left[grad\mathbf{u} + (grad\mathbf{u})^T \right]$ (4) is the stress deviator, $\Pi = p + 2/3\mu div\mathbf{u}$ and $\zeta = \frac{\rho_G - \rho W}{\rho_G}$. After some algebra, we obtain:

$\frac{\partial \Phi}{\partial t} + div(\Phi \mathbf{u}) = div \left[D_W (\Phi)\ grad\ \Phi \right]$ (5)

and $div\left(\mathbf{q}_W + \mathbf{q}_G\right) = 0$. ($\mathbf{q}_W$ is the flux of water across boundary ∂V of the control volume).

In order to have a compressible conservative law, Eq. (3) requires another small change to:

$\frac{\partial (\rho\phi)}{\partial t} + div\left(\rho\phi\mathbf{u}\right) = D\ div\ \left[(1 - \zeta\rho\phi)\ grad\ \phi \right]$ (3')

where a change of the dependent variable to $\phi = \Phi/\rho$ was necessary and the nondimensional density ρ is defined as $\rho = (1 - \zeta\Phi)\,\rho_G = \frac{1}{1 + \zeta\phi}\,\rho_G$ (6)

The initial condition for the problem could be:

$u(\mathbf{x}, 0) = 0,\ \forall \mathbf{x} \in \Omega = (0, L) \times (0, R)$

$\Phi\left(\mathbf{x}, 0\right) = \Phi_0(\mathbf{x}) = 1 - \delta\left(1 - \frac{L}{2}\mathbf{i}\right) = \begin{cases} 1, \forall \mathbf{x} \in (0, L/2) \\ 0, \forall \mathbf{x} \in (L/2, L) \end{cases}$, but any initial distribution $\Phi_0(x)$ of the concentration can be used.

The boundary conditions for the velocity require no slip conditions at the walls $\mathbf{u}(x,t)\left|_{x\in\partial\Omega\backslash centerline}\right. = 0$ and at the centerline ($r = 0$), the normal derivative of the axial velocity $\mathbf{u}$ (along Ox axis) and the radial velocity v (along *or* axis) must vanish $\partial\mathbf{u}(\mathbf{x}, t)/\partial n\left|_{centerline}\right. = v(\mathbf{x}, t)\left|_{centerline}\right. = 0$. For the concentration the boundary condition is $\partial\phi/\partial n\left|_{\partial\Omega}\right. = 0$.

In conclusion the mathematical formulation of the problem is:

"Solve eqs. (2), (4), and (3') subjected to the constraint (6), with above-mentioned two initial conditions as well as three boundary conditions".

If the velocity field $\mathbf{u}$ is not solenoidal any more, it can be easily proved the existence of another solenoidal field.

There is nothing special in the non dimensional form of the equations involved into the compressible model by using: $S = T_0/(U_0 L)$ (Strouhal number), $Pe = U_0 L/D$ (Peclet number), $\mathrm{Re} = \rho_G U_0 L/\mu_G$ (Reynolds number) and $F = U_0^2/(gL)$ (Froude number)

If the length (height of cylinder), diffusion coefficient (diffusion coefficient of the mixture), density (glycerin density), viscosity (glycerin viscosity) and acceleration (acceleration of gravity) the scale are obvious, not the same can be stated about the scale of time and velocity.

Results and discussion. As the main purpose of this work is to look for differences between classical (pure diffusion) and a new (compressible Navier-Stokes) approaches to the problem of mixing water and glycerin it was very important to check the convergence of the numerical procedure.

Three problem have been considered to be solved:

(i) the first problem is a quasi 1D problem. It consists of a 2D problem, but with periodical boundary conditions for velocity along the vertical boundaries (which are perpendicular) to the discontinuity in concentration), i.e. $\partial \mathbf{u}/\partial \mathbf{x}\left|_{\{x=0,x=1\}}\right. = \partial \mathbf{v}/\partial \mathbf{x}\left|_{\{x=0,x=1\}}\right. = 0$.

(ii) The second problem was a pure 2D problem. For this problem the boundary conditions along the right ($x = 1$), for the velocity is $\mathbf{u}\left|_{\{x=1\}}\right. = \mathbf{v}\left|_{\{,x=1\}}\right. = 0$. Along the line $\mathbf{x} = 0$ the boundary condition of problem (i) is applied, so that the actual domain for the computation is twice as wide.

(iii) The third problem is the one of interest (a pseudo 3D problem, with axis-symmetric flow).

The second one was considered in order to minimize the changes due to the introduction of a wall. The third problem is what is actually wanted to be solved.

As the problem is unsteady, it was also necessary to preserve the same Courant number $CN = c\triangle t/\triangle x$ when the dimension of the grid is halved.

Several problems appear during the computation of the solution for these problems.

The conservation of mass is of great importance in these problems. Usually a control volume approach has very good properties in this respect. But for these problems the conservation of mass is hard to achieve.

In order to understand the effect of the sharp gradients on the wrong sign of the velocity near the top and bottom boundaries some other initial conditions for the distribution of the concentration had been taken into account.

The aspect ration of the control volume should be kept as close to unity as possible. Actually, using aspect ration larger than 5 can increase dramatically the number of iterations.

The diffusion coefficient $D = 10^{-6}$ m^2/s which gives an acceptable time of about 92.6 days to reach the steady state within 0.1%.

Some results have been obtained for the flow inside the cylinder, using a numerical simulation of the unsteady compressible Navier-Stokes equations. For $\triangle t = 10^{-4}s$ and $\triangle x_{\min} = 1.5 \times 10^{-3}m$ (in the mesh, near the interface between glycerin and water) a maximum velocity of $U_{\max} = 1.5 \times 10^{-3}m/s$ was found. To keep a balance between the unsteady terms $\partial \cdot /\partial t$ and the convective terms Strouhal number $S = L_0/(U_0 T_0)$ must be close to 1, giving $L_0 = 1.5 \times 10^{-6}\mathrm{m}$. This shows that for the equations we solved (Navier-Stokes and diffusion) the convective term is about 1000 times smaller and can be neglected.

Since the contribution of the convective terms is less than 1% this explain why there is no difference between $1D$ and $2D$ solution.

Conclusion. From obtained numerical results it is shown that there is no difference between classical result (using the pure diffusion equation) and the new approach (using an unsteady compressible Navier-Stokes model).

Even if there is a flow driven by an external pressure gradient, that can make the convective term significant, one can expect no difference between the classical approach (using a convective unsteady diffusion equation) when compared to the new approach.

So the conclusion is that using the unsteady compressible Navier-Stokes equation is useless (and only time consuming) in the study of such phenomena.