Compressible Fluid Flow Modelling in COMSOL

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Abstract
A new compressible fluid flow Physics that takes into account the intrinsic compressibility of the fluid is implemented in COMSOL 6.2 using the Coefficient Form PDE in the Mathematics Interface. This Physics solves the standard Navier-Stokes equation along with a new continuity equation that relates the time dependent pressure inside a control volume to the divergence of the fluid flow in that volume. Results from the new Physics are compared with those from the incompressible fluid flow Physics in the standard COMSOL pre-built Laminar Flow CFD interface.
Keywords: Compressible fluid, incompressible fluid, Laminar Flow, speed of sound, Coefficient Form PDE.

Introduction
COMSOL offers three different fluid flow models in its single-phase Laminar Flow Physics interface. (1) Incompressible flow (2) Weakly compressible flow and (3) Compressible flow with low Mach numbers (<0.3). In the case of compressible flow, Navier-Stokes equation is solved together with the time-dependent continuity equation for density. The continuity equation allows only for the time-dependent density variations caused by external factors (e.g. temperature). However, in some applications, it is often required to know the pressure variations caused by the fluid compressibility. In this paper, we propose a modified continuity equation for the time-dependent pressure and solve the same with Navier Stokes equation using the coefficient form Partial Differential Equations in the Mathematics Interface.

Theory
The new continuity equation we propose for the pressure variations caused by fluid compressibility is as follows:

$$\frac{dP}{dt} + \rho c^2(\nabla.\boldsymbol{u}) = 0 \qquad \ldots(1)$$

where P, ρ and $\boldsymbol{u}$ are the pressure, density and velocity of the fluid, respectively, and c is the velocity of sound in the fluid. Eq. 1 relates the net flow of fluid into a control volume to the rate of change of pressure within that volume. Note that ρc^2 is simply the compressibility of the fluid. In this new compressible flow Physics, Eq. 1 is solved along with the Navier-Stokes equation given below [1].

$$\rho\frac{d\boldsymbol{u}}{dt} + \rho(\boldsymbol{u}.\nabla)\boldsymbol{u} = -\nabla P + \nabla.K \qquad \ldots(2a)$$

$$K = 2\mu S - \frac{2}{3}\mu(\nabla.\boldsymbol{u})I \qquad \ldots(2b)$$

$$S = \frac{1}{2}[\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T] \qquad \ldots(2c)$$

where K is stress tensor, μ is the fluid viscosity, S is the strain rate tensor, I is the unit matrix and the other symbols are as defined in eq. 1. A custom implementation of the solution of eqs.1 and 2 in COMSOL is achieved by casting the above two equations in the coefficient form Partial Differential Equation, as given below [2].

$$e_a\frac{d^2U}{dt^2} + d_a\frac{dU}{dt} + \nabla.(-c\nabla U - \alpha U + \gamma) + \beta.\nabla U + aU = f \qquad \ldots(3)$$

where U is the dependent variable solution vector, and the other symbols in the coefficients of the PDE will be identified in terms of the fluid properties, shortly. For our fluid flow problem, the dependent variable vector has four components, the three velocity components, u,v,w and the pressure, P.

$$U = [u\ v\ w\ P]^T$$

Thus, eq. 3 is a set of four equations, one for each component of U. However, it should be noted that there are only three independent variables, x, y and z. Furthermore, the dimensions of velocity and pressure are different, but the PDE expects the dimensions of all the dependent variables to be the same. Hence, all the dependent variables are normalized by choosing a suitable velocity norm v_0. The normalized dependent variable vector is given by

$$U^* = [u^*\ \ v^*\ \ w^*\ \ P^*]^T$$

where $u^*= u/v_0$, $v^*= v/v_0$, $w^* = w/v_0$ and $P^*=P/(\rho v_0^2)$.

The coefficients in the PDE couple each dependent variable with every other dependent variable (including itself) and hence they are all (4x4) matrices. For example, c is a (4x4) matrix, each element of which is a (3x3) matrix, as given by the following equation fo $c\nabla U$:

$$c\nabla U = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \begin{bmatrix} \nabla u \\ \nabla v \\ \nabla w \\ \nabla P \end{bmatrix} \qquad \ldots(4a)$$

where

$$C_{11} = \begin{bmatrix} c_{1111} & c_{1112} & c_{1113} \\ c_{1121} & c_{1122} & c_{1123} \\ c_{1131} & c_{1132} & c_{1133} \end{bmatrix} \quad \ldots(4b)$$

and so on.
Similarly, α and β are (4x4) matrices whose elements are (3x1) vectors, e_a, d_a and a are (4x4) matrices whose elements are scalars, and f and γ are simply (4x1) vectors.
By writing down eq. 3 in component form (see Appendix) and expanding the individual terms, it can be own that c_{ijkl} is the coefficient of $\frac{\partial^2 U_j}{\partial k \partial l}$ in the component equation for U_i (i,j ={1,2,3,4} and k,l = {x,y,z}). Similarly, β_{ijk} is the coefficient of $\frac{\partial U_j}{\partial k}$ in the component equation for U_i. After writing down all the terms in eq. 3 explicitly, and comparing the corresponding terms in the PDE and the Navier Stokes / continuity equations, the following values of the coefficients can be established in terms of the kinematic viscosity $\nu=\mu/\rho$.

$$c_{11} = \begin{bmatrix} \frac{4}{3}\upsilon & 0 & 0 \\ 0 & \upsilon & 0 \\ 0 & 0 & \upsilon \end{bmatrix}; \; c_{12} = \begin{bmatrix} 0 & -{}^{2\upsilon}/_{3} & 0 \\ \upsilon & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$c_{13} = \begin{bmatrix} 0 & 0 & -{}^{2\upsilon}/_{3} \\ 0 & 0 & 0 \\ \upsilon & 0 & 0 \end{bmatrix}; \; c_{21} = \begin{bmatrix} 0 & \upsilon & 0 \\ -{}^{2\upsilon}/_{3} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$c_{22} = \begin{bmatrix} \upsilon & 0 & 0 \\ 0 & \frac{4}{3}\upsilon & 0 \\ 0 & 0 & \upsilon \end{bmatrix}; \; c_{23} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -{}^{2\upsilon}/_{3} \\ 0 & \upsilon & 0 \end{bmatrix}$$

$$c_{31} = \begin{bmatrix} 0 & 0 & \upsilon \\ 0 & 0 & 0 \\ -{}^{2\upsilon}/_{3} & 0 & 0 \end{bmatrix}; \; c_{32} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \upsilon \\ 0 & -{}^{2\upsilon}/_{3} & 0 \end{bmatrix}$$

$$c_{33} = \begin{bmatrix} \upsilon & 0 & 0 \\ 0 & \upsilon & 0 \\ 0 & 0 & \frac{4}{3}\upsilon \end{bmatrix}$$

All the other c coefficients are zero.

β_{ij} coefficients are as follows.

$$\beta_{11} = \beta_{22} = \beta_{33} = \begin{bmatrix} u^* v_0 \\ v^* v_0 \\ w^* v_0 \end{bmatrix}$$

$$\beta_{14} = \beta_{41} = \begin{bmatrix} v_0 \\ 0 \\ 0 \end{bmatrix}; \; \beta_{24} = \beta_{42} = \begin{bmatrix} 0 \\ v_0 \\ 0 \end{bmatrix}$$

$$\beta_{34} = \beta_{43} = \begin{bmatrix} 0 \\ 0 \\ v_0 \end{bmatrix}$$

Finally, d_a is given by the following diagonal matrix.

$$d_a = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \frac{v_0^2}{c_0^2} \end{bmatrix}$$

All the other coefficients in the PDE are zero.

In the case of two-dimensional flow, there are only two independent variables (x and y) and correspondingly only three dependent variables (u, v and P). In this case, c is a (3x3) matrix whose elements are 2x2 matrices, α and β are (3x3) matrices each element of which is a 2x1 vector, e_a, d_a and a are 3x3 matrices while γ and f are 3x1 vectors. The values of these coefficients can be easily deduced in a manner similar to the case of 3-dimensional flow.

Numerical Implementation in COMSOL

A simple rectangular geometry and a cylindrical geometry were chosen, respectively, to test the implementation of the new Physics interface in 2D and 3D. Fig. 1 is a partial screen shot view of the COMSOL model for a 3D cylinder showing the equations and some of the coefficients in the Coefficient Form PDE.

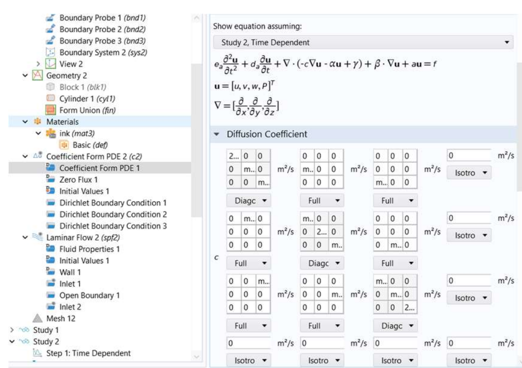

Figure 1. A partial screen shot of the COMSOL model showing the equations and some coefficients for the Coefficient Form PDE implementation of the new compressible fluid flow physics.

The following Dirichlet boundary conditions were used. At the inlet, a pressure step was applied at t=0. The time-dependent response of the fluid was studied by monitoring the average fluid velocity at the outlet. The Dirichlet boundary condition P=0 was applied to the outlet. At the walls of the cylinder no slip boundary condition was applied by setting all the velocity components to zero. For comparison, another study was done on the same geometry using the standard COMSOL incompressible Laminar Flow Physics Interface.

Simulation Results

The velocity surface plots for the 2D rectangular geometry at an arbitrary intermediate time for both the incompressible Laminar Flow Physics model and the new Compressible Fluid model are shown in Fig.2. For the case of incompressible fluid, a constant velocity along the flow direction is seen, as expected. On the other hand, the compressible flow shows a velocity variation along the flow direction. Quantitative 1D plots of the velocity along the centerline of the rectangle for the Laminar Flow model and the compressible flow model are shown in Fig. 3.

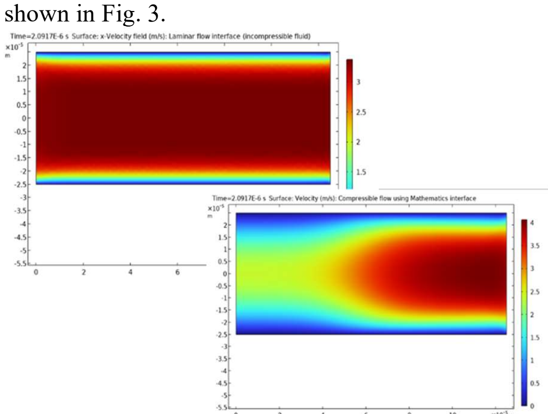

Figure 2. Velocity surface plots for the incompressible Laminar flow interface and the compressible flow interface using Mathematics interface.

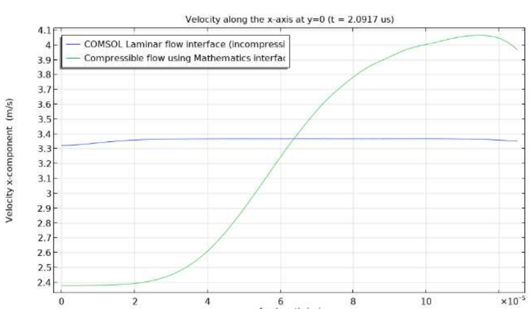

Figure 3. Velocity along the centerline for the incompressible and the compressible flow models. Notice the (nearly) constant velocity for the incompressible flow vs. variable velocity along the flow direction for the compressible flow.

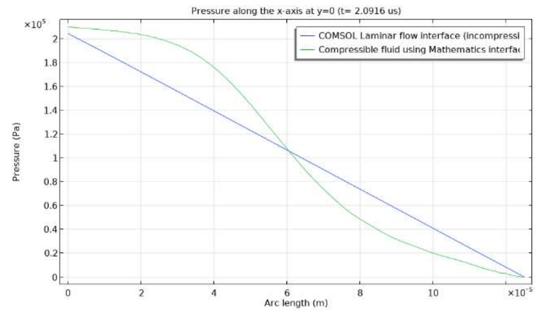

Figure 4. Pressure along the centerline of the rectangle for the incompressible and the compressible flow models. Notice the linear distribution of pressure for the incompressible flow vs. non-linear pressure distribution for the compressible flow.

The pressure along the centerline for the incompressible flow and the compressible flow are shown in Fig. 4. For the incompressible flow, a linear distribution of pressure is seen, as expected. On the other hand, for the compressible flow, a non-linear distribution is seen. The applied pressure step to the inlet and the response of the fluid velocity at the outlet are shown in Fig. 5. The oscillations of the fluid velocity (due to the fluid compressibility) are clearly seen superimposed over the gradual exponential rise of the average velocity from zero to its final steady sate value.

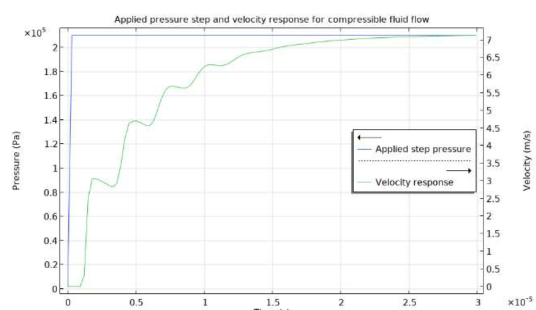

Figure 5. Applied step pressure and velocity response for the compressible flow. Notice the oscillations in the velocity (due to the fluid compressibility) as the average velocity ramps up from zero to its steady state value.

Velocity slice plot for the compressible flow in a 3D cylinder is shown in Fig. 6. The expected variation of the velocity along the axis of the cylinder is clearly seen. Comparison of exit velocities in a 3-D cylindrical geometry between the incompressible Laminar flow and the compressible flow is shown in Figure 7.

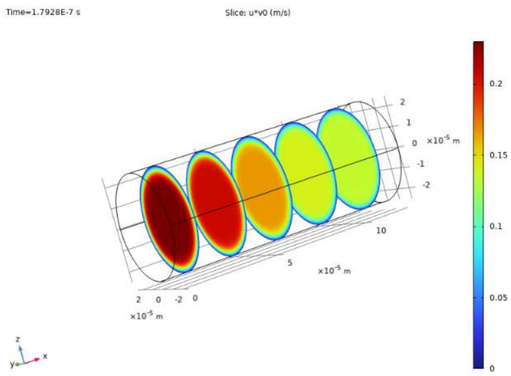

Figure 6. Velocity slice plot for the compressible flow in a 3D cylindrical geometry.

Once again, the compressible flow shows the oscillations, which are absent in the incompressible flow. Even though the oscillations are small in this 3D cylindrical geometry, the agreement between the two models (other than the oscillations) is remarkable, considering that the two results come from completely different Physics interfaces. This validates the correctness of the implementation of the new compressible flow equations using the PDE formulation.

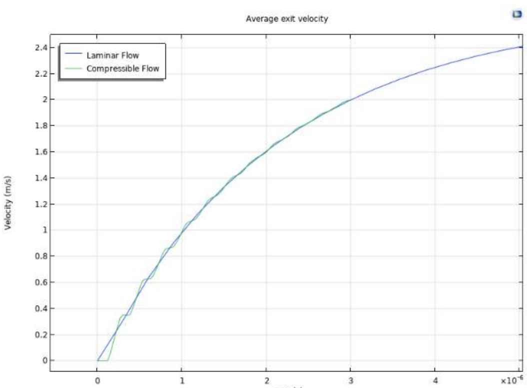

Figure 7. Comparison of exit velocities in a 3D cylinder for the incompressible Laminar flow and the compressible flow.

Conclusions

A new compressible flow Physics that takes into account the intrinsic fluid compressibility is implemented in COMSOL using the Coefficient Form PDE in the Mathematics Interface. The results from the new Physics are compared with those from the incompressible Laminar Flow Physics interface available in the Standard COMSOL implementation. Excellent agreement between the results from the two Physics interfaces (Custom compressible flow Physics vs. Standard incompressible flow Physics) is demonstrated when the compressibility effects are small.

References

[1] COMSOL Multiphysics Reference Manual: CFD Module: Theory for the Single Phase Flow Interfaces.

[2] COMSOL Multiphysics Reference Manual: Equation Based Modeling: Modeling with PDEs: The Coefficient Form PDE.

Acknowledgements

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Appendix

In the component form eq. 3 may be written as follows:

$$e_{ai}\frac{d^2U_i}{dt^2} + d_{ai}\frac{dU_i}{dt} + \frac{\partial}{dk}\sum_{k=1}^{3}\sum_{j=1}^{4}\sum_{l=1}^{3} c_{ijkl}\frac{\partial^2 U_j}{\partial k \partial l} + \sum_{j=1}^{4}\sum_{k=1}^{3}\beta_{ijk}\frac{\partial U_j}{\partial k} + \sum_{j=1}^{4} a_{ij}\,U_j = f_i\,,\quad i=\{1,2,3,4\}. \qquad \ldots\text{(A1)}$$

In eq. A1, the coefficients α and γ are assumed to be zero for simplicity, as they are in the present case. (Note: k, $l = \{1,2,3\}$ corresponds to $\{x, y, z\}$.)

Returning to the Navier-Stokes equation, the strain-rate tensor (eq. 2C) is given by

$$S = \begin{bmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{xy} & S_{yy} & S_{yz} \\ S_{xz} & S_{yz} & S_{zz} \end{bmatrix}$$

$$S_{xx} = {\partial u}/{\partial x}\;; S_{yy} = {\partial v}/{\partial y}\;;\; S_{zz} = {\partial w}/{\partial z}\;;$$

$$S_{xy} = \frac{1}{2}\left({\partial u}/{\partial y} + {\partial v}/{\partial x}\right);$$

$$S_{xz} = \frac{1}{2}\left({\partial u}/{\partial z} + {\partial w}/{\partial x}\right);$$

$$S_{yz} = \frac{1}{2}\left({\partial v}/{\partial z} + {\partial w}/{\partial y}\right);$$

Hence $\nabla . S$ is given by the following vector:

$$\begin{bmatrix} \dfrac{\partial^2 u}{\partial x^2} + \dfrac{1}{2}\left(\dfrac{\partial^2 u}{\partial y^2} + \dfrac{\partial^2 v}{\partial y \partial x}\right) + \dfrac{1}{2}\left(\dfrac{\partial^2 u}{\partial z^2} + \dfrac{\partial^2 w}{\partial z \partial x}\right) \\ \dfrac{1}{2}\left(\dfrac{\partial^2 u}{\partial x \partial y} + \dfrac{\partial^2 v}{\partial x^2}\right) + \dfrac{\partial^2 v}{\partial y^2} + \dfrac{1}{2}\left(\dfrac{\partial^2 v}{\partial z^2} + \dfrac{\partial^2 w}{\partial z \partial y}\right) \\ \dfrac{1}{2}\left(\dfrac{\partial^2 u}{\partial x \partial z} + \dfrac{\partial^2 w}{\partial x^2}\right) + \dfrac{1}{2}\left(\dfrac{\partial^2 v}{\partial y \partial z} + \dfrac{\partial^2 w}{\partial y^2}\right) + \dfrac{\partial^2 w}{\partial z^2} \end{bmatrix}$$

$$\nabla.(\nabla.\boldsymbol{u})I = \begin{bmatrix} \dfrac{\partial}{dx}\left(\dfrac{\partial u}{\partial x} + \dfrac{\partial v}{\partial y} + \dfrac{\partial w}{\partial z}\right) \\ \dfrac{\partial}{dy}\left(\dfrac{\partial u}{\partial x} + \dfrac{\partial v}{\partial y} + \dfrac{\partial w}{\partial z}\right) \\ \dfrac{\partial}{dz}\left(\dfrac{\partial u}{\partial x} + \dfrac{\partial v}{\partial y} + \dfrac{\partial w}{\partial z}\right) \end{bmatrix}$$

Substituting the above expressions in eq. 2a and comparing the corresponding terms in the expanded Navier Stokes equation together with the continuity equation with the PDE (eq. A1) given above, the values of the PDE coefficients can be easily derived.