Has the explicit or implicit volume fraction formulation an impact on mass transfer calculations?

Description

ANSYS Fluent offers two different approaches to describe the volume fraction (vof) transport equation for multiphase models: implicit and explicit. When considering mass transfer, is there a difference with respect to accuracy for these two formulations?

Solution

Yes, using default settings there can be a difference if the mass transfer depends on solution variables (e.g. concentration).

By default, Fluent solves the vof transport equation only once for a time step for the explicit formulation. For the implicit formulation vof is solved every iteration.

You can force that Fluent solves vof every iteration for the explicit formulation from the multiphase panel > expert. Then the results of both formulations should be identical, given a sufficiently small time step size and a well converged solution within each time step.

Background

The ANSYS Fluent Theory Guide [1] explains the mass transfer rate in chapter 17.7.2. Unidirectional Constant Rate Mass Transfer:

$$\boldsymbol{\dot{m}_{pq}} = \mathbf{max}[\mathbf{0}, \boldsymbol{\lambda_{pq}}] - \mathbf{max}[\mathbf{0}, -\boldsymbol{\lambda_{pg}}] \tag{1}$$

$$\boldsymbol{\lambda_{pg}} = \boldsymbol{\dot{r}\alpha_p\rho_p} \tag{2}$$

Where

$\dot{r}$	Constant rate in $1/s$
α_p	Volume fraction of phase p
ρ_p	Density of phase p
$\dot{m}_{pq}$	Mass transfer rate between phases p and q

This equation is solved and the result inserted into the vof transport equation.

The implicit formulation of the volume fraction transport equation uses the volume fraction of the current time step to calculate it. Therefore, the equation has to be solved iteratively within each time step.

The explicit formulation uses values from the previous time step. Hence it’s sufficient to solve it only once at the beginning of a time step.

Implicit formulation

$$\frac{\alpha_q^{n+1}\rho_q^{n+1} - \alpha_q^n \rho_q^n}{\Delta t} V + \sum_f \left(\rho_q^{n+1} U_f^{n+1} \alpha_{q,f}^{n+1}\right) = \left[S_{\alpha_q} + \sum_{p=1}^{q} \left(\dot{m}_{pq} - \dot{m}_{qp}\right)\right] V \tag{3}$$

Explicit formulation

$$\frac{\alpha_q^{n+1}\rho_q^{n+1} - \alpha_q^n \rho_q^n}{\Delta t} V + \sum_f \left(\rho_q^{n} U_f^{n} \alpha_{q,f}^{n}\right) = \left[S_{\alpha_q} + \sum_{p=1}^{q} \left(\dot{m}_{pq} - \dot{m}_{qp}\right)\right] V \tag{4}$$

Where

$n+1$	Index for current time step
n	Index for previous time step
α_q	Cell value of volume fraction of phase q
$\alpha_{q,f}$	Face value of the volume fraction of phase q
U_f	Volume flux through the face
V	Cell volume
$\dot{m}_{pq}$	Mass transfer from phase p to phase q
S_{α_q}	Volume fraction source term for phase q

Inserting the mass transfer equation into the two transport equations gives you a dependency on the volume fraction of the current time step for the implicit form but only a dependency on the volume fraction of the previous time step for the explicit form.

Let's consider a single cell filled completely with phase A: $\alpha_A^0 = 1$. A constant rate mass transfer is defined with $\dot{r} = 0.1/s$ from phase A to phase B. The density of both phases is equal to $\rho_A = \rho_B = 1\,kg/m^3$. When there is no convection and no additional source terms, the transport equation for the explicit case reduces to:

$$\frac{\alpha_A^{n+1}\rho_A^{n+1} - \alpha_A^n \rho_A^n}{\Delta t} = \dot{m}_{AB} - \dot{m}_{BA} \tag{5}$$

The mass transfer could be described with the volume fraction for the current (implicit) or the previous time step (explicit). For an explicit formulation and a time step size of $\Delta t = 1s$ the mass fraction of phase A reduces to 0.9 for the explicit formulation:

$$\dot{m}_{AB} = \dot{r}\alpha_A^n \rho_A = 0.1\,kg/m^3 s \tag{6}$$

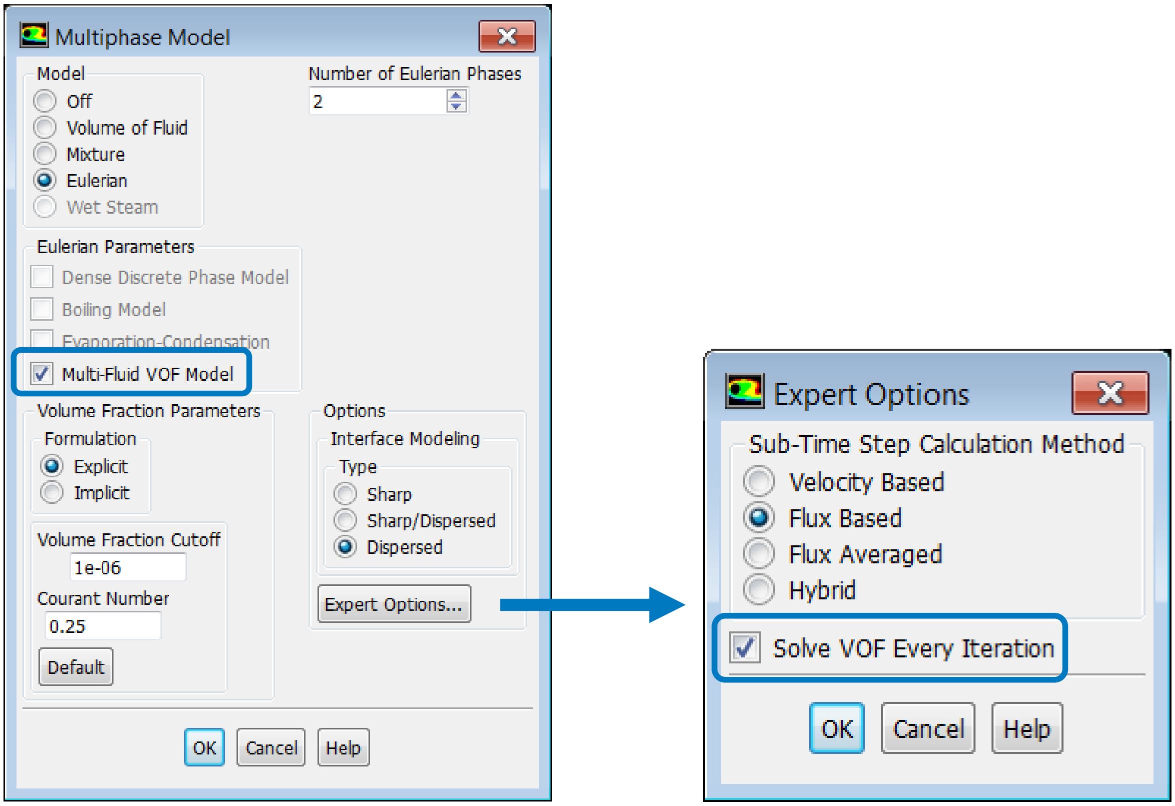
However, for the implicit formulation the mass transfer rate has to be calculated iteratively and Fluent ends up with a mass fraction of approximately 0.91 for phase A:

$$\dot{m}_{AB} = \dot{r}\alpha_A^{n+1} \rho_A = 0.091\,kg/m^3 s \tag{7}$$

Which result is more accurate?

The result for the explicit formulation as stated above in equation 6 is incorrect because the mass transfer rate is calculated based on the volume fraction of the previous time step. For the accurate result the mass transfer has to be based on the current time step as stated for the implicit formulation (equation 7). For most simulations this is not an issue because either the time step size is small enough that the change in the volume fraction is negligible or a mass transfer mechanism is used that doesn't depend on fast changing solution data.

In fact, Fluent uses the correct implementation (eq. 7) also for the explicit formulation. It just looks like it would use the incorrect formulation because the vof equation is solved only once for a time step. To resolve this issue you can solve vof every iteration like it is proposed in the documentation for moving mesh simulations where similar issues can occur (see ANSYS Fluent User's Guide [2], chapter 25.2.2.4 Expert Options and 25.3.7. Setting Time-Dependent Parameters for the Explicit Volume Fraction Formulation). In order to use this option for Eulerian simulations, you have to enable the Multi-Fluid VOF model.



Remember that for mass transfer you should always use the dispersed interface modeling type together with a diffusive interface scheme.

References

[1] ANSYS, Inc., "ANSYS Fluent Theory Guide, Release 17.1," ANSYS, Inc., 2016.

[2] ANSYS, Inc., "ANSYS Fluent User's Guide, Release 17.1," ANSYS, Inc., 2016.

Keywords: implicit; explicit; vof formulation; volume fraction parameters; Solve VOF Every Iteration; Euler; Eulerian; multiphase; mass transfer; difference; discrepancy; inaccuracy

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