

Temperature for VOF

The temperature equation could be modified as follow to account for the variable CP due to VOF (with Cp in each phase constant). The Cp effective is not working because it's mainly for variable Cp du to temperature.

The average Cp could be written as follow using the color function  $\Phi$ .

$$Cp = \frac{Cp_L * \rho_L * \Phi + Cp_G * \rho_G * (1 - \Phi)}{\rho} = Cp_G + \frac{\rho_L}{\rho} (Cp_L - Cp_G) * \Phi \quad (1)$$

The energy equation is:

$$\rho Cp \frac{\partial T}{\partial t} + \rho Cp V \nabla T = \nabla \cdot (\lambda \nabla T) \quad (2)$$

The energy equation will become:

$$\rho Cp_G \frac{\partial T}{\partial t} + \rho Cp_G V \nabla T = \nabla \cdot (\lambda \nabla T) - \rho_L (Cp_L - Cp_G) * \Phi \frac{\partial T}{\partial t} - \rho_L (Cp_L - Cp_G) * \Phi V \nabla T$$

$$\rho Cp_G \frac{\partial T}{\partial t} + \rho Cp_G V \nabla T = \nabla \cdot (\lambda \nabla T) - \rho_L * (Cp_L - Cp_G) * \Phi \left[ \frac{\partial T}{\partial t} + V \nabla T \right] \quad (3)$$

In gxsurf, I have computed the source for temperature equation corresponding to the following term:

$$-\rho_L * (Cp_L - Cp_G) * \Phi \left[ \frac{\partial T}{\partial t} + V \nabla T \right]$$

We still need to add the term (which is easier, but I didn't now how to deal with it in group 13 in gxsurf) (unless we create a separate gxtempvof.):

The source corresponds to the following term:

$$-(Cp_L - Cp_G) * \Phi * \rho_L * \frac{\partial T}{\partial t}$$

Which when discretized is:

$$-(Cp_L - Cp_G) * \Phi * \rho_L \left[ \frac{T^{n+1} - T^n}{\Delta t} \right]$$

*which can be written as:*

$$\frac{(Cp_L - Cp_G) * \Phi * \rho_L}{\Delta t} [T^n - T^{n+1}]$$

This gives us a source with:

$$CO = \frac{(Cp_L - Cp_G) * \Phi * \rho_L}{\Delta t}$$

And

$$VAL = T^n$$

The other source is:

$$-\rho_L * (Cp_L - Cp_G) * \Phi * VVT$$

The  $VVT$  term is computed in gxsurf through the SEM approach.

The  $\Phi$  in the above formulas should be taken at time n+1 so it should be SURN.

**NB: These sources should not be computed in solids and in solids the Cp should keep it's value of Cp solid.**

In the subroutine gxsurprp.for, we need to modify the computation of CP to have CP=CP of light phase only. So this should be activated only for VOF and SEM. Could be extended to HOL if subroutine of HOL is modified.

The average temperature should be computed using:

$$T_{average} = \frac{\sum_1^{NX*NY*NZ} Cp * T * VOL}{\sum_1^{NX*NY*NZ} Cp * VOL}$$

Where Cp is computed using equation 1, ie:

$$Cp = \frac{Cp_L * \rho_L * \Phi + Cp_G * \rho_G * (1 - \Phi)}{\rho} = Cp_G + \frac{\rho_L}{\rho} (Cp_L - Cp_G) * \Phi$$