Numerical Fluid Mechanics II

Summer Semester 2018

DELIVERABLE TASK III:
Implimentation of Continious Species Transfer

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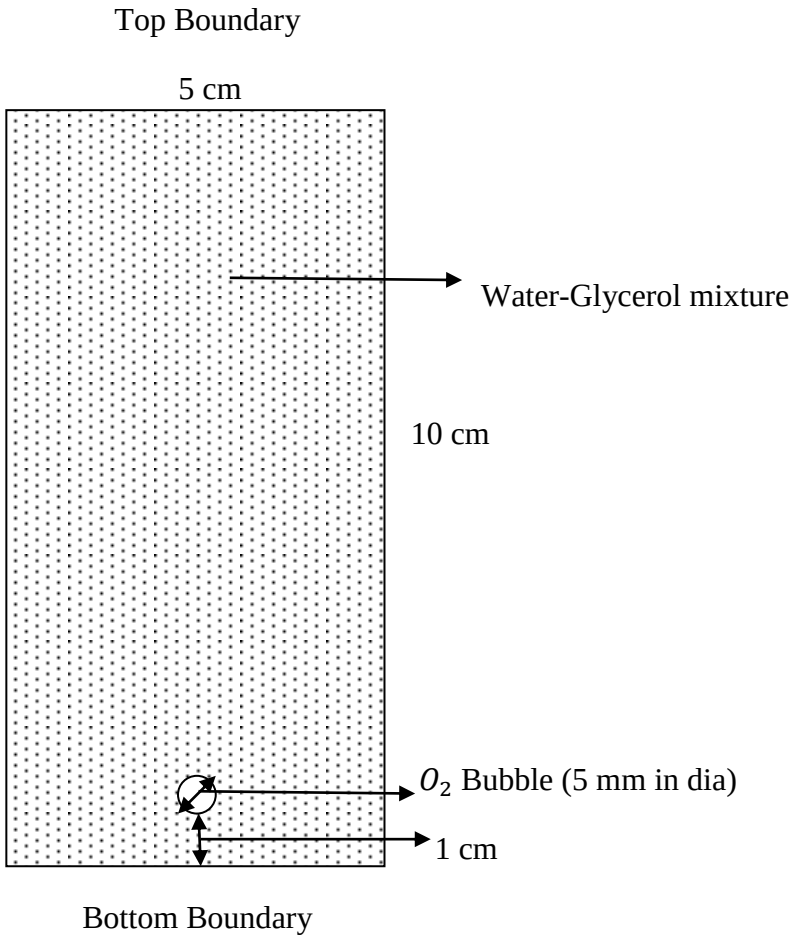
INTRODUCTION

In this deliverable task we have implemented the given continuous species transfer (CST) equation in the InterFoam solver. The task was to run the simulation showing the diffusion of oxygen from the bubble into a Water-glycerol mixture. The domain is of height h= 10cm, width=5cm and a bubble of diameter 5mm is inserted at 1cm above the bottom surface of the domain as shown in the figure below.



We took a mesh size of 200*400 (minimum 20 grid points per bubble diameter) and time step of 0.00001 second(such that CFL number is less than 0.05). We used SetFields file to define the volume scalar field for bubble of 5 mm dia and set the volume fraction to 0.And set the remaining domain to have volume fraction of 1.

InterFoam solver was used to solve the system because it can capture the interface using VOF (Volume of Fluid approach) for two incompressible isothermal immiscible fluids. Regular interFoam solves continuity, momentum and VOF equation (transport equation for volume fraction). In addition to solving regular flow fields we also modelled an additional equation for mass transfer in two phase flow and phase change (miscibility) of species at interface using CST equation.

The continuous species transfer equation reads as follows,

$$\frac{dC}{dx} + \nabla.(\mathrm{CU}) - \nabla.(< D >_a \ \nabla \mathrm{C}) - \nabla.\left[(D_1 - D_2)\alpha_1 \left(\frac{1}{\alpha_1 + \frac{1-\alpha_1}{H}} - 1\right)\nabla \mathrm{C}\right] - \nabla.\left[\frac{C}{\alpha_1 + \frac{1-\alpha_1}{H}}\left(\frac{1}{H}\frac{D_1 - D_2}{\alpha_1 + \frac{1-\alpha_1}{H}} - \left(D_1 - \frac{D_2}{H}\right)\right)\right] = 0$$

I: $\nabla.(\mathrm{CU})$ is the convective term of the equation which denotes the transport of one phase due to the velocity of another phase.

II: $\nabla.(< D >_a \ \nabla \mathrm{C})$ is the diffusive term which denotes the transport of one phase into another phase resulting from concentration gradients.

III: $\nabla.\left[(D_1 - D_2)\alpha_1 \left(\frac{1}{\alpha_1 + \frac{1-\alpha_1}{H}} - 1\right)\nabla \mathrm{C}\right] - \nabla.\left[\frac{C}{\alpha_1 + \frac{1-\alpha_1}{H}}\left(\frac{1}{H}\frac{D_1 - D_2}{\alpha_1 + \frac{1-\alpha_1}{H}} - \left(D_1 - \frac{D_2}{H}\right)\right)\right]$ is the term which denotes the cross interface transfer.

RESULTS AND CONCLUSION

a) Boundedness of the solution

Solving the VOF equation should guarantee the boundedness of α between 0 and 1. MULES (Multi dimensional Universal Limiter foe Explicit Solution) is implemented on openfoam which can solve this implicitly.

Mules solves hyperbolic equation for quantity β

$$\frac{\partial \beta}{\partial t} + \nabla . \bar{F} = \beta S_p + S_u$$

Where β is scalar field of interest, defined at center of cell

$\bar{F}$ is the flux of β

S_p is the implicit source term

S_u is the explicit source term

MULES can be called in OpenFOAM by taking argument:

MULES(β,∅, $\bar{F}$, S_p, S_u,1,0)

Where ∅ is the flux on faces used to determine the upwind direction for discretization of flux terms in MULES internal algorithm. By which α equation is solved in alphaEqn.H file.

Similarly we can also solve the concentration equation using MULES where the concentration is bounded by the limits 0 and 8. And concentration equation can be solved using MULES in CSTEqn.h

When considering computational domains entailing complex geometries, unstructured meshes of general topology are required. Then, depending on the mesh quality, discretization errors related to mesh skewness arise and cam severely deteriorate the numerical fidelity of the method resulting in loss of boundedness, accuracy and order of convergence.

The OpenFOAM uses the finite volume method (FVM) to solve the conservation equations which uses the integral notation of the equations. So representing the above CST equation in the integral form we get,

$$\int_{V_p} \frac{d(C)}{dt} dV + \int_{V_p} \nabla . (\mathrm{CU})\, dV - \int_{V_p} \nabla . (< D >_a \ \nabla \mathrm{C})\, dV - \int_{V_p} \mathrm{S(C)}\, dV = 0$$

Where, P is the centroid (computational node)of the cell and V_p is the cell volume.

The volume integrals are evaluated based on Gauss divergence theorem where the each integral terms are first converted into sum over the faces by using Gauss theorem. It is then approximated numerically as show below for each term,

Convection term:

$$\int_{V_p} \nabla.(\mathrm{CU})\, dV = \sum_f \boldsymbol{S}_f.(CU)_f$$

Where, the concentration(C) at the cell faces are approximated using the face interpolation scheme or differencing scheme. The choice of differencing schemes is a matter of boundedness and accuracy. The different differencing schemes used are stated as below,

Central differencing (CD) – Linear face interpolation :

The central differencing scheme is second order accurate but does not ensure the boundedness

Upwind Differencing (UD) – Flux dependent face interpolation: In this scheme the face value is determined from the cell value in the upstream flow direction. It ensures unconditional boundedness but at the cost of numerical diffusion.

There are some more sophisticated differencing schemes like Switching/blending schemes which attempt to preserve boundedness while maintaining a reasonable accuracy. This is accomplished by superposing CD and UD schemes.

$$\phi_{f=}\, \phi_{f(UD)} + \gamma\, (\phi_{f(CD)} - \phi_{f(UD)})$$

This will maintain the interface profile sharp as well as it preserves the boundedness of the transport quantity.

Diffusion term:

$$\int_{V_p} \nabla.(< D >_a \ \nabla \mathrm{C})\, dV = \sum_f \boldsymbol{S}_f.(< D >_a \ \nabla \mathrm{C})_f$$

Where, $< D >_a$ and $\boldsymbol{S}_f.\nabla \mathrm{C}$ both need to be evaluated at the cell faces. Highly orthogonal meshes give rises to unboundedness.

- Source term:

$$\int_{V_p} \mathrm{S}(\mathrm{C})\, dV$$

All terms that cannot be considered as convection, diffusion or temporal terms in the generic transport equation are to be loosely classified as source and sink terms. In order to promote both stability and boundedness, typically linearization with respect to C is performed before the actual discretization is applied to the source term $\mathrm{S}(\mathrm{C})$.

From the simulation we can notice that, the concentration will never increase more than the maximum value (8 molm^{-3}), at the initial time whole mass of oxygen is concentrated in the bubble. As the time passes by the oxygen gets dissipated into the mixture.

b) Contour of the concentration field at the final time:

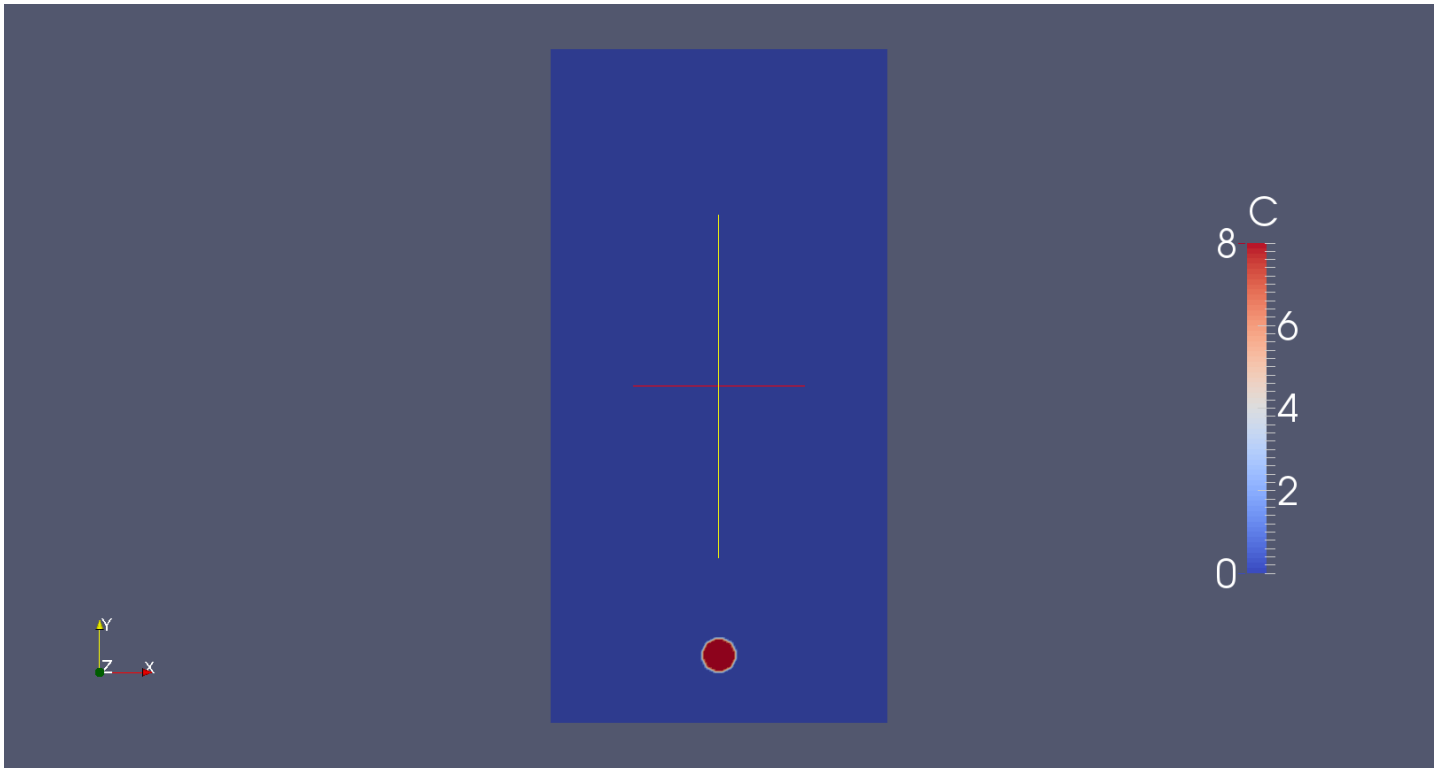


Fig. Contour of the concentration(C in molm^{-3}) field at t= 0 seconds

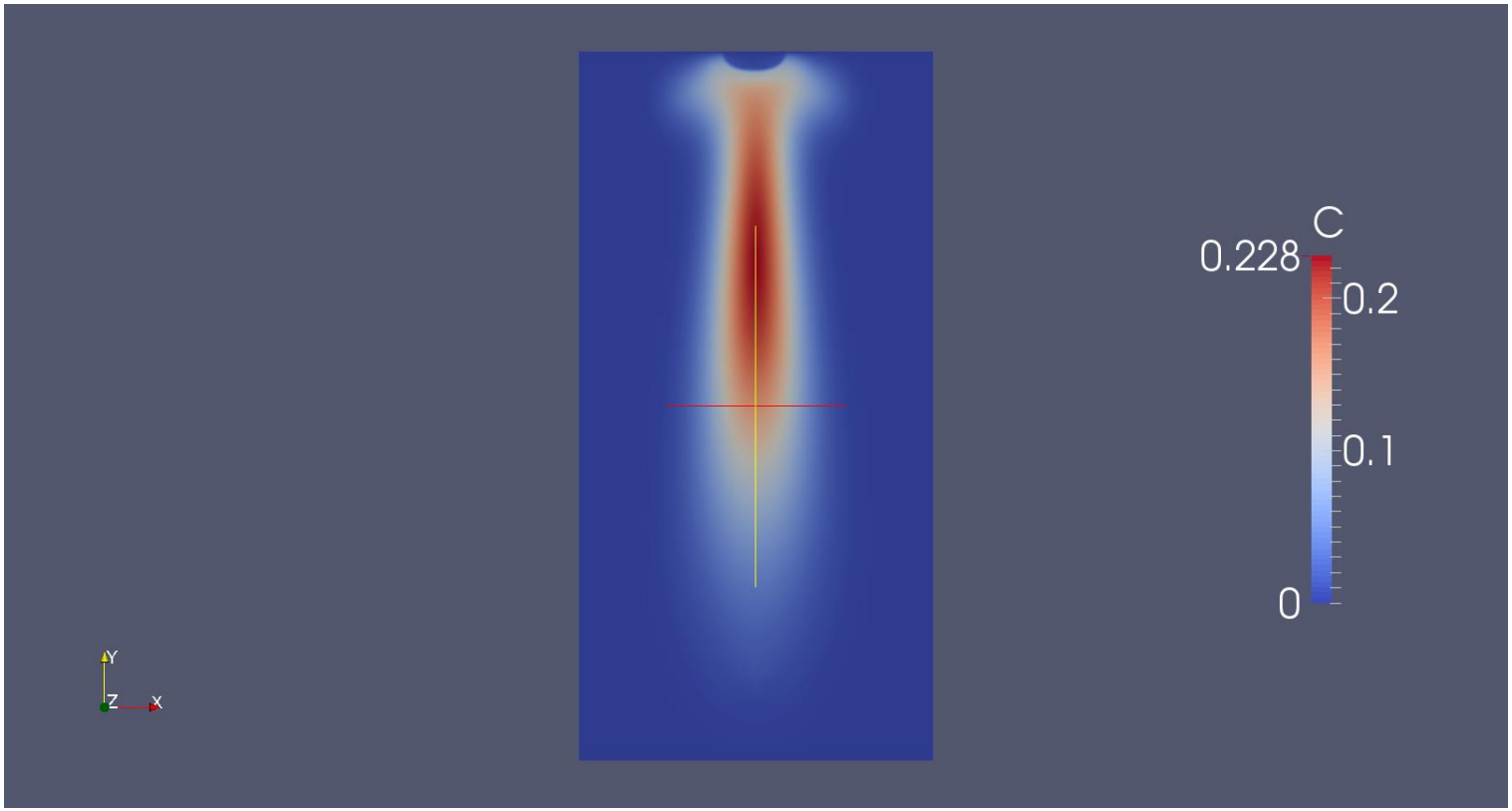


Fig. Contour of concentration(C in molm^{-3}) field at the final time

- At the initial stage, the concentration of oxygen in bubble is maximum i.e. 8 molm^{-3}
- The oxygen molecules rises from bottom of the surface to the top due to the low density of the bubble i.e. Convection(advection) transfer of species from bubble to liquid take place
- Due to the concentration gradient the oxygen in the bubble diffuses into the water-glycerol mixture i.e. mass transfer of the oxygen from the bubble.

- Also CST equation also take care of the cross interface flow of component through the boundary.
- At the end of simulation all the oxygen species get transferred to the water glycerol mixture and concentration of oxygen in bubble is almost empty. All the gets dissipated into the water glycerol mixture on its motion to top surface.