

## A Study of the Phase Change in Three Phase Environment

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### Abstract

A two dimensional numerical study is done by developing an existing VOF solver of OpenFoam, a CFD open source software, to investigate the evaporation of droplets considering three phases, liquid, vapor and the surrounding gas. The mass transfer model is based on Fick's law and the mixing between the gas and the vapor is included. The velocities at the interface is considered different hence the volumetric change due to phase change effects is accounted. Validation, transport models, phase change model and mass transfer equation are described in details. The liquid and the vapor volumetric fractions as well as the temperature fields are described during falling of a single water droplet in a chamber, as an illustrative example. Furthermore, the streamline around the droplet is depicted and discussed. The solver, called interMixingHeatFoam to emphasizes the inclusion of energy effect in interMixingFoam, the OpenFOAM built-in solver.

### Introduction

Evaporation is the phenomena that happens in many natural and industrial applications like rain drops, cooling towers, fire fighting systems, HVAC systems, fuel injection system in diesel engines and gas turbines. Due to the importance of high efficiency in mechanical systems as well as the necessity of the reduction of fossil fuel consumption which is associated to the greenhouse gases production, the study of droplet evaporation has great value. In real conditions the droplet of a spray or the rain drop encounters air or fuel gas and if the ambient temperature is high enough it evaporates. So three phases are acting and also there is phase change between two of them causing mass transfer.

Since phase change is a multiphase problem, finding the accurate location of the interface is necessary. Most of the numerical studies including multiple phases can be categorized in two main methods; Lagrangian tracking and interface capturing. Renksizbulut's [14] moving mesh method and Gingold's [6] smoothed-particle hydrodynamic method are in Lagrangian category. On the other hand, there are two most popular methods for interface capturing; level set and VOF schemes. In the VOF method a color function, volume fraction of each phase, represents the phases and a sharp transition in the color function shows the interface. Similar to the VOF, in the level set method, the distance to the interface is the quantity which is transported. The problem with the level set method which is addressed by many authors is that the liquid mass conservation is not guaranteed [16]. To consider the break up, coalescence and complicated evaporation processes happening in sprays, the VOF is an appropriate approach which is used widely by researchers. Hardt et al [7] used a vaporization model, which was derived from an inhomogeneous Helmholtz equation. They applied the VOF and piecewise linear interface construction scheme in the Fluent to model two-phase problem of liquid and vapor. Kunkelmann and Peter Stephan [9] developed a code based on Hardt method [7] to simulate the phase change of liquid into the vapor. Nabil et al [11] and Samkhaniani and Ansari

[15] have also developed models for phase change heat transfer simulation. Kryukov et al [8] did a comparative study of hydrodynamic and kinetic methods for droplet vaporization into its vapor. Some other authors, on the other hand, trying to simulate a more real condition of spray evaporation by evaluating the effect of surrounding gas, e.g., air. Among those, Schlottke [16], AbouAl-Sood et al. [1], Strotos et al ([18],[17]), Fleckenstein and Bothe [5] and Ma and Bothe [10] have great attempts to develop models with the VOF.

In this study, the implementation of models developed by Fleckenstein and Bothe [5] and Ma and Bothe [10] for evaporation of liquid into surrounding gas stream in OpenFoam is described. The trajectory, heat and mass transfer and temperature of a single water droplet falling in an air channel is simulated by the solver called interMixingHeatFoam which emphasizes the inclusion of energy equation in the standard solver of OpenFOAM, interMixingFoam.

### Numerical Approach

We considered a three-phase problem, surrounding gas like air, the liquid of the droplet and the vapor. Therefore, by means of this method we can get better insight into the spray evaporation. The computational VOF method for numerical modeling is used. Based on the VOF the volumetric fraction of each phase in a cell is defined as following:

$$\alpha_i = \frac{\text{volume of the } i\text{th species in the cell}}{\text{total volume of species in the cell}} \quad (1)$$

and so,

$$\alpha_i = \begin{cases} 1 & \text{the cell is fully wet with species } i \\ 0 < \alpha_i < 1 & \text{the cell is partially filled with species } i \\ 0 & \text{the cell is empty of species } i \end{cases} \quad (2)$$

where  $i$  can be the surrounding gas, the liquid and the vapor and thus  $\alpha_l + \alpha_v + \alpha_g = 1$  in each cell. To satisfy the mass conservation equation, due to the evaporation, the transport equation for liquid species would be given by

$$\frac{\partial \alpha_l}{\partial t} + U^d \nabla \alpha_l = \frac{\dot{m}'''}{\rho_l} \quad (3)$$

where  $U^d$  is the velocity of the dispersed phase which is the liquid here and  $\dot{m}'''$  is the volumetric specific mass flux. In the same manner, the transport equation for the vapor phase would be

$$\frac{\partial \alpha_v}{\partial t} + U^c \nabla \alpha_v = -\frac{\dot{m}'''}{\rho_v} - \nabla \cdot (D_{vg} \nabla \alpha_v) \quad (4)$$

where  $U^c$  is the velocity of the continuous phase. It is assumed that the vapor phase has no relative motion to the surrounding gas so the velocity of the vapor and the surrounding gas are the same. In contrast, different velocities are summed for the dispersed and the continuous phases,  $U^d$  and  $U^c$ , for transport equations. Moreover, the tangential velocities are assumed to

be the same. By assuming no mixing between the liquid and the gas phase but between the gas and the vapor, there is no diffusion term in the liquid transport equation and  $D_{vg}$  is the diffusion coefficient of the vapor phase into the surrounding gas. The source term in transport equations can be calculated based on Fick's law of diffusion

$$\dot{m}''' = \frac{D_{vg}\rho_{gp}}{1-X_v}\nabla X_v \cdot \mathbf{n}_\Sigma |\nabla \alpha_l| \quad (5)$$

where  $X_v$  is the vapor mass fraction and can be expressed as

$$X_v = \frac{\rho_v}{\rho_{gp}} \quad (6)$$

and  $\rho_{gp}$  is the density for the whole gas phase including the vapor and is calculated from

$$\rho_{gp} = \frac{\rho_v \alpha_v + \rho_g \alpha_g}{\alpha_v + \alpha_g} \quad (7)$$

and  $\mathbf{n}_\Sigma$  is the surface normal vector of the interface and is defined as

$$\mathbf{n}_\Sigma = \frac{\nabla \alpha_l}{|\nabla \alpha_l|} \quad (8)$$

The mass transfer model that is used here is suitable for the cases where the liquid evaporates into the ambient gas and cannot be utilized for a pure liquid/vapor vaporization ([10]).

According to the VOF there are one field formulas for momentum and energy conservation equations. The resultant fields are the mass averaged values for the temperature and the velocity fields. Therefore, the momentum conservation equation is given by:

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \otimes \mathbf{U}) = -\nabla p + \rho \mathbf{g} + \nabla \cdot \mu [(\nabla \mathbf{U} + (\nabla \mathbf{U})^T)] + \mathbf{f}_\sigma \quad (9)$$

where  $p$  is the pressure,  $\rho \mathbf{g}$  is the force of gravity, the term  $\nabla \cdot \mu [(\nabla \mathbf{U} + (\nabla \mathbf{U})^T)]$  accounts for the viscous stress tensor. The term  $\mathbf{f}_\sigma$  is the surface tension force which is important in multi-phase problems and is evaluated based on the continuum surface force (CSF) model [3] for the dispersed phase volume fraction

$$\mathbf{f}_\sigma = \sigma \kappa \nabla \alpha_l \quad (10)$$

where  $\kappa$  is the mean curvature of the free surface of the liquid interface and is given by

$$\kappa = -\nabla \cdot \left( \frac{\nabla \alpha_l}{|\nabla \alpha_l|} \right) \quad (11)$$

Equation 11 is valid for the cases that the surface tension force is constant as considered here.

The energy equation in terms of specific enthalpy is used as following:

$$\frac{\partial (\rho C_p T)}{\partial t} + \nabla \cdot (\rho C_p T \mathbf{U}) = \nabla \cdot (k \nabla T) + \dot{m}''' h_{fg} \quad (12)$$

where  $h_{fg}$ ,  $C_p$  and  $k$  are the latent heat of evaporation, the specific heat in constant pressure and the thermal conductivity, respectively. All properties of the fluids including the density, viscosity, thermal conductivity, specific heat, latent heat and diffusivity assumed to be constant. According to the VOF, the local fluid properties are calculated based on the volume-averaged of the phases, i.e., for the density we have

$$\rho = \rho_l \alpha_l + \rho_v \alpha_v + \rho_g \alpha_g \quad (13)$$

With the same definition for the velocity we can have the volumetric velocity as

$$\mathbf{U}_v = \mathbf{U}^d \alpha_l + \mathbf{U}^c (1 - \alpha_l) \quad (14)$$

and so the mass averaged velocity would be

$$\mathbf{U}_m = \frac{\alpha_l \rho^d \mathbf{U}^d + (1 - \alpha_l) \rho^c \mathbf{U}^c}{\rho} \quad (15)$$

To satisfy the mass continuity we must have

$$\nabla \cdot \mathbf{U}_v = \dot{m}''' \left( \frac{1}{\rho_l} - \frac{1}{\rho_{gp}} \right) \quad (16)$$

To consider the jump condition in the interface based on [10] the following relationship for the relative velocity is considered

$$\mathbf{U}_r = -\dot{m}'' \left( \frac{1}{\rho_l} - \frac{1}{\rho_{gp}} \right) \mathbf{n}_\Sigma = \mathbf{U}^d - \mathbf{U}^c \quad (17)$$

where  $\dot{m}''$  is the mass flux and equals to

$$\dot{m}'' = \frac{\dot{m}'''}{|\nabla \alpha_l|} \quad (18)$$

Therefore, the dispersed and the continuous phase velocities can be calculated. The mass averaged velocity can be calculated from the momentum equation and must be used in energy equation.

The velocity and the pressure are coupled via PISO loop with poisson's equation for the pressure. Equation 16 is used as source term in the pressure equation in order to include the effects of pressure changes due to the phase change:

$$\nabla \cdot \left( \frac{1}{\rho} \nabla p \right) = \nabla \cdot \mathbf{U}_m + \dot{m}''' \left( \frac{1}{\rho_l} - \frac{1}{\rho_{gp}} \right) \quad (19)$$

As the VOF is mass conservative but not volume conservative, without taking into account the equation 16 in the pressure-velocity coupling the volumetric change of the phase change is not calculated correctly.

The summary of the algorithm for calculating the Navier-Stokes, the mass transfer and the pressure equations is indicated in "Table 1".

### Illustrative Example

To investigate the interMixingHeatFoam code, a 2D case of a single water droplet with 1 mm radius falling in an air channel of size 20 mm × 200 mm is considered. The material properties are shown in "Table 2". The unsteady first order Eulerian method for time discretization is used and run-time modifiable time step is chosen based on the work of [4] to control the spurious currents. The droplet starts falling with no initial velocity in a chamber filled with air in atmospheric pressure and initial temperature of 363k, while the droplet temperature is 343k at initial time. No air flow is assumed in the channel and the droplet falls due to gravity. The droplet is resolved with 12 cells along the diameter at 0 time and leading to 3600 computational cells in the whole domain. The flow is assumed to be laminar. The lateral boundary conditions are assumed as walls and the top one has atmospheric condition. By using blockMesh utility of OpenFoam ([13]) to create meshes, then initializing the domain by setFields utility and next decomposing it to proceed with MPI parallel running of the interMixingHeatFoam, the case is run.

1. Initialize the simulation
2. While  $t < t_{end}$  do
  - a. Update  $\Delta t$  according to CFL condition
  - b. Do pressure-velocity coupling loop
    - i. Update the fluids properties
    - ii. Solve the momentum equation and update U
    - iii. PIMPLE algorithm
      - a. Solve Poisson's equation
      - b. Correct U
    - iv. Loop
    - v. Update turbulent properties
    - vi. Calculate the source terms
    - vii. Solve the transport equations, update volume fractions and update fluxes
    - viii. Solve the energy equation and update T
3. Loop

Table 1: interMixingHeatFoam solver algorithm

	$T_0$ [K]	$\rho$ [kg/m <sup>3</sup> ]	$h_{fg}$ [kJ/kg]	$\sigma$ [N/m]	$D_{vg}$ [m <sup>2</sup> /s]	$k$ [W/(m K)]	$c_p$ [J/(kg K)]	$\mu$ [pa.S]
Liquid Water	343	980	2260	0.0649		0.6673	4187	281.26E-06
Air	363	1			0.252E-4	0.03	1000	1.48E-05

Table 2: Material properties of water and air

More than 3.5 hours of 12 processors work was needed to solve 0.03 seconds of the simulations.

For the validation, the velocity and the displacement of the droplet in the timespan of 0 and 30 ms is considered. As the falling distance of the droplet in the simulation is too short, it did not reach the terminal velocity. So to calculate the falling speed of the droplet, the equations of motion are used resulting the values shown in "Table 3" for the vertical component of the velocity as well as the vertical distance. Comparing the calculated values with the average values of the simulation, demonstrate close agreement highlighting the correct implementation of the equations.

	Calculated	Simulation	Error %
Velocity(m/s)	0.2943	0.2912	1.05
Displacement(m)	0.004415	0.0041667	5.62

Table 3: Validation of the average velocity and the displacement

Another verification is done by looking at the streamlines of the flow at 20ms ("figure 1"). The colorful area represents the droplet. The presence of two vortices at the wake, identical to what is expected in similar laminar flows such as Strotose's work ([18]) is seen. Moreover, the liquid circulation areas are similar to the same work.

To see more capability of the code the volumetric fraction of the liquid and the vapor along with the temperature fields at 0s, 15ms and 30ms are shown in "figures 2,3 and 4". Although the change of the liquid fraction due to small changes can not be seen easily the increasing amount of the vapor during the time is noticeable. Due to the high value of the latent heat of the evaporation of water, when the droplet evaporates the temperature

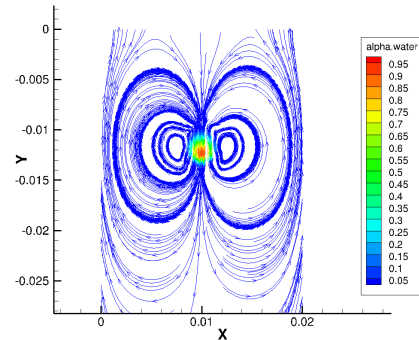


Figure 1: Streamlines at 20 ms

field drops dramatically around it and the cool area increases during the time which is shown in the "figure 4".

## Conclusions

The interMixingHeatFoam enables the simulation of liquids into ambient gas to study the phase change phenomena by means of the VOF considering heat transfer. It has the ability to do three dimensional simulation, use OpenFOAM turbulent models and post-processing utilities and for the OpenFOAM-users can be easily adapted for the evaporation investigation. The strength of the code is considering the effect of volume changes due to the phase change that makes a more accurate simulation. Additionally, the gas phase includes two phases of the gas and the vapor that empowers the users to visualize the presence of vapor separately, in contrast to the codes that just account one phase for the whole gas phase. By knowledge of the authors this is the first code implemented in OpenFOAM with the aforementioned capability. One limitation of the interMixingHeatFoam is that the fluid properties are assumed to be

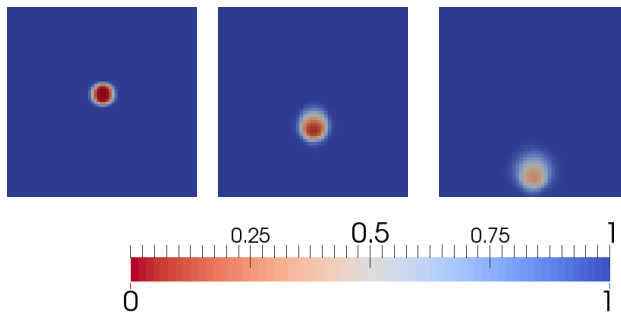


Figure 2: Contours of liquid volumetric fraction at  $t=0$ , 15 ms and 30 ms from the left

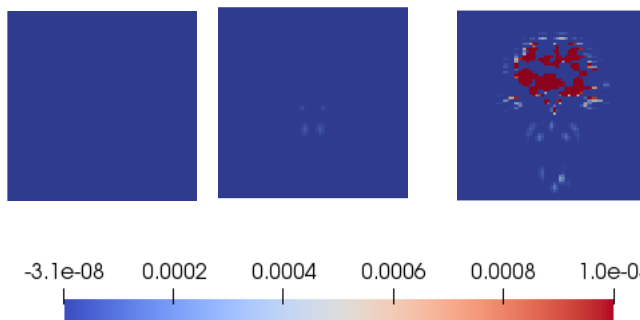


Figure 3: Contours of vapor volumetric fraction at  $t=0$ , 15 ms and 30 ms

constant. Although, it can be adapted to calculate the properties as a function of temperature or pressure for each specified fluids. Besides, it does not benefit of the moving mesh utility which leads to more computational time for fine meshes. It also would be more beneficial if the condensation was included.

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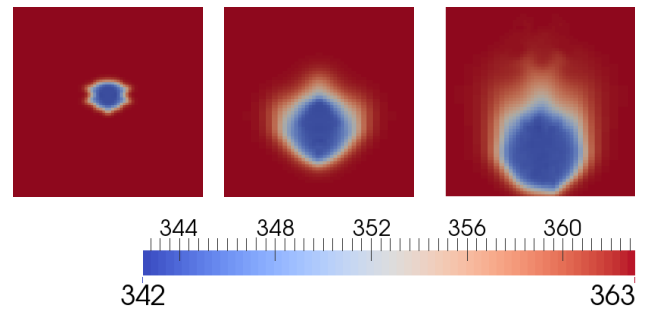


Figure 4: Contours of temperature (k) at  $t=0$ , 15 ms and 30 ms

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