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A PHASE CHANGE MODEL FOR MULTIPHASE FLOWS

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ABSTRACT

In this paper we present a multiphase model which can be used to simulate phase change problems. The multiphase model resolves the interface between immiscible phases and belongs to the family of interface capturing methods. The resulting mathematical model was presented and was validated using the Stefan problem for which the exact solution exists. Qualitative tests on several simple one-and two-dimensional tests were also performed.

Keywords: Phase change model, volume of fluid, Stefan problem

1. INTRODUCTION

Multiphase flows with phase change are very common in everyday engineering practice. These flows are characterized with very intensive heat transfer and large mass transfer at locations where the phase-change takes place. Some interesting features of the flows with solid-liquid phase change are given in [1]. Here we consider flows where liquid evaporates at its boiling temperature. The phase-change process is in this case very rapid and the physical properties of the liquid and its vapor are very different, what makes numerical simulations of such flows a very challenging task.

2. MATHEMATICAL MODEL

The mathematical model which describes the flow of several immiscible fluids is made of the following conservation equations [2]:

• Momentum conservation

$$\frac{\partial}{\partial t} \int_{V} \rho_{m} v dV + \oint_{S} \rho_{m} v v \cdot dS = \oint_{S} T \cdot dS + \int_{V} f_{b} dV,$$

• Total mass conservation

$$\frac{\partial}{\partial t} \int_{V} \rho_{m} dV + \oint_{S} \rho_{m} v \cdot dS = 0,$$

Phase mass conservation

$$\frac{\partial}{\partial t} \int_{V} \rho_{i} \alpha_{i} dV + \oint_{S} \rho_{i} \alpha_{i} \boldsymbol{v} \cdot d\boldsymbol{S} = \int_{V} s_{\alpha_{i}} dV,$$

Energy conservation

$$\frac{\partial}{\partial t} \int_{V} \rho_{m} h dV + \oint_{S} \rho_{m} h v \cdot dS = \oint_{S} \mathbf{q} \cdot dS + \int_{V} s_{h} dV,$$

which are valid for an arbitrary solution domain of the volume V bounded by the surface S, with surface vector dS pointing outwards. Here, ρ_m is the mixture density, \boldsymbol{v} is velocity, \mathbf{T} is the Cauchy stress tensor, f_b is the momentum source, α_i is the volume fraction of phase i, h is the specific enthalpy, \boldsymbol{q} is the local heat flux and s_h is the energy source.

Boiling can take place only in the proximity of the liquid-vapor interface. The rate of evaporation/condensation is modeled as:

$$\dot{m} = K \cdot (T - T_{sat}),$$

where K is a scaling factor and T_{sat} is the saturation or boiling temperature. In our present model K is calculated as

$$K = \frac{mc_p}{h_{lv}\Delta \tau},$$

where m is mass of liquid in the case of evaporation or mass of vapor in the case of condensation present in the control volume, c_p is specific heat, h_{lv} is specific latent heat, and $\Delta \tau$ is timescale of the phase change. The rate of evaporation results in additional source terms in the energy and phase volume-fraction transport equations.

The mathematical model is solved using a cell-centered finite volume method as described in [3]. The method can be applied to numerical meshes made of polyhedral cells of an arbitrary shape. The transport equations are solved in a sequential manner using the SIMPLE algorithm.

3. RESULTS

The boiling model is validated using the Stefan problem [4], where we study 1D evaporation in a semi-infinity solution domain as shown in Fig.(1). Initially the liquid is at the saturation temperature. The heated wall is at the temperature ΔT above the saturation temperature. The liquid evaporates as it heats up and the newly created vapor pushes the liquid to the right and the vapor column grows displacing the liquid out of the domain. Both phases are incompressible.

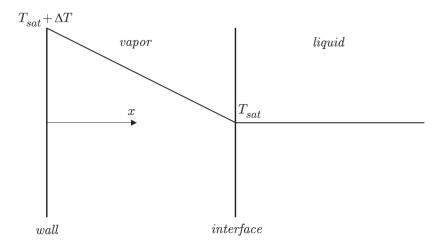


Figure 1: Stefan problem.

The temperature of the liquid phase is constant throughout the simulation, and equal to the initial saturation temperature T_{sat} , while the vapor temperature satisfies the following equation

$$\frac{\partial T}{\partial t} = \frac{k_v}{\rho_v c_{pv}} \frac{\partial^2 T}{\partial x^2}, \ \ for \ 0 \le x \le s(t).$$

 k_v , ρ_v and c_{pv} are thermal conductivity, density and specific heat of vapor. The position of the interface between the liquid and its vapor s(t) is a function of time. The boundary conditions for the portion of the solution domain occupied with vapor are

$$T(x = s,t) = T_{sat},$$

 $T(x = 0,t) = T_{sat} + \Delta T.$

The speed v_s at which the interface travels follows from the condition

$$\rho_v v_s h_{lv} = -k_v \frac{\partial T}{\partial x} \Big|_{x=s(t)}.$$

The position of the interface s(t) is given by the following expression [4]:

$$s(t) = 2\lambda \sqrt{\alpha t}$$

where α is the thermal diffusivity of the vapor:

$$\alpha = \frac{k_v}{\rho_v c_{pv}}.$$

Parameter λ is the solution of the transcendental equation

$$\lambda e^{\lambda^2} erf(\lambda) = \frac{c_{pv}\Delta T}{h_{lv}\sqrt{\pi}},$$
 where the error function is defined as

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

In our simulation ΔT is 25K, and material properties of vapor are $k_v = 0.0257$ W/(m·K), $c_{pv} = 1007$ $J/(kg \cdot K)$ and $h_{lv} = 2.2 \cdot 10^6 J/kg$.

The density ratio between liquid and its vapor has a significant impact on the stability of the solution procedure. Larger density ratios result in larger accelerations and velocities of the liquid. The liquid velocity is a function of the interface velocity v_s and the ratio of liquid and vapor densities:

$$v_l = \left(1 - \frac{\rho_v}{\rho_l}\right) v_{s.}$$

The problem is especially pronounced in the beginning of a simulation. Large liquid acceleration produces large pressure gradients. Vapor is all the time at rest, what results in large velocity gradients across the vapor-liquid interface.

Table 1: Different combinations of liquid and vapor density.

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$\rho_v\left(\frac{kg}{m^s}\right)$	$\rho_l\left(\frac{kg}{m^s}\right)$	$ ho_l : ho_v$
1	1000	1000
4	401	100
16	160	10
64	64	1

Four different combinations of liquid and vapor densities were tested, as shown in Table 1. The computational domain was 40 mm long. It was discretized with 100 control volumes. Grid with 200 points was tested and produced the same results, meaning that the solution obtained on the first grid was already grid independent.

It was assumed in the Stefan problem that the interface is all the time in thermodynamic equilibrium, what implies that the boiling timescale parameter $\Delta \tau$ is very small number. Very small values of Δτ could have a negative influence on the stability of the solution algorithm. Numerical experiments show that the value of $\Delta \tau$ does not have to be so small in order to get the right behavior of the system. The choice of the timescale parameter $\Delta \tau$ is to some extent arbitrary and the results do not depend on its value across a wide interval. In our example $\Delta \tau$ was set to 1 ms, what was also the size of the time step.

Figure 2 shows the liquid-vapor interface position as a function of time. Symbols show the numerical results and solid lines show the exact solution. One can see that the differences between numerical and analytical results are very small. Even when we had 1000 times larger density for liquid phase, the model worked well. The same numerical grid was used for all ratios of liquid and vapor densities. Other quantities like temperature and velocity also matched the exact values.

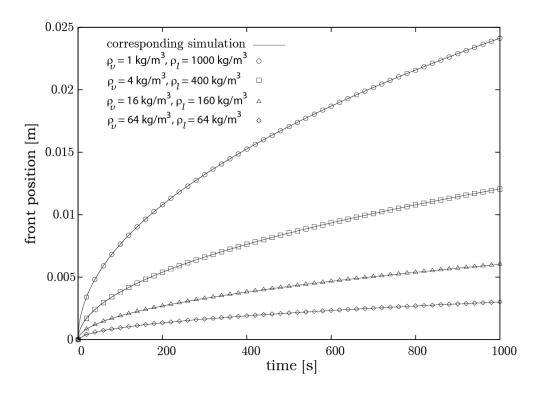


Figure 2: Position of the liquid-vapor interface as a function of time.

4. CONCLUSION

A multiphase mode capable of tracking interfaces between immiscible fluids was extended such that it can model boiling processes. In this case the model keeps the interface between liquid and vapor sharp. The model was successfully validated using the classical Stefan's problem, where we were able to reproduce the exact solution. At this stage, the model looks very promising and it will be applied to more complex flows with phase change.

5. REFERENCES

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