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Modeling Phase Change and Homogeneous Bubbles

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<u>Overview</u>

For some time it has been possible using ***FLOW-3D***® to model the dynamics of flows containing large adiabatic bubbles. In this Technical Note we describe an extension of the adiabatic bubble model that adds non-adiabatic mass and energy changes. Solid-to-void heat transfer provides for heat exchange between the gas in a bubble and solid obstacles exposed to the bubble. Mass and energy exchanges resulting from phase changes at the bubble's surface can be included in cases where the bubble gas consists of liquid vapor.

The new model is referred to as the Homogeneous Bubble Model. The nomenclature is meant to emphasize the fact that the pressure and temperature of gas in a bubble are spatially uniform (i.e., homogeneous), but these values can vary with time. There can be many such bubbles in a calculation, each having its own temperature and pressure. Bubbles, by definition, must be larger than a computational grid cell.

Homogeneous bubbles have a simple formulation that is consistent with the liquid thermodynamic properties used in ***FLOW-3D***®. This was not true of the previous "Conservation Void" model. Because both the old and new models treat essentially the same physical processes, the Conservation Void model will eventually be removed from the program.

The Homogeneous Bubble model is available beginning with Version 8.0 of ***FLOW-3D***®.

<u>Description</u>

The equation-of-state for a bubble is the ideal gas equation,

$$p = (\gamma - 1)\,\rho c_v^{vap} T \qquad (1)$$

Here p is the bubble pressure, ρ it's gas density, c_v^{vap} is the specific heat at constant volume of the vapor, and T is the vapor temperature, which must be in an absolute scale. The quantity γ is the ratio of specific heats for the gas. Note that the gas constant for the bubble is equal to the product $(\gamma\text{-}1)c_v^{vap}$.

If there are no sources of mass or energy for a bubble it will behave as though it is adiabatic, changing pressure from some initial state (p_0,V_0) to a new state (p,V) according to,

$$p = p_0\left(\frac{V_0}{V}\right)^{\gamma} \qquad (2)$$

When phase changes occur it is necessary to have an analytical relation that expresses the saturation pressure of a vapor in terms of its temperature. In ***FLOW-3D***® the default for this relation is the Clapeyron equation that gives P_{sat} as a function of temperature T. A power law expression is also available,

$$
\begin{aligned}
P^{sat} &= pv1 * \left(\frac{T - tv0}{tv1 - tv0} \right)^{1/tv\exp} \qquad , \quad power-law \\
P^{sat} &= pv1 * \exp\left(-\left(\frac{1}{T + tv0} - \frac{1}{tv1 + tv0} \right) \Big/ tv\exp \right) \qquad , \quad Clapeyron \qquad (3)
\end{aligned}
$$

In these expressions (pv1,tv1) is a point on the saturation curve, tv0 may be used to make adjustments for different temperature units, and tvexp is an exponent constant. In the case of the Clapeyron equation the constant tvexp is given by tvexp=$(\gamma-1)c_v^{vap}$/clhv1, where clhv1 is the heat of transformation (latent heat) of evaporation.

The rate of phase change is typically modeled as proportional to something that measures the deviation from saturation conditions. A typical formulation [1] that is based on kinetic theory is,

$$
Net \quad mass \quad transfer = \sqrt{\frac{M}{2pR}} \left[c_{evap} \frac{P_l^{sat}}{\sqrt{T_l}} - c_{con} \frac{P_v}{\sqrt{T_v}} \right], \qquad (4a)
$$

where M is the molecular weight of the vapor, R the vapor gas constant, T is temperature, and subscripts l and v refer to liquid and vapor states. The superscript sat on P_l indicates the saturation pressure corresponding to liquid temperature T_l. Finally, the coefficients c_{evap} and c_{con} are the “accommodation coefficients” for evaporation and condensation, respectively.

The origin of this expression is that the mass flux, for example condensation on a liquid surface, must be proportional to the local vapor density and local velocity of the molecules at the surface. Assuming a Maxwellian velocity distribution the local velocity into the surface is [2],

$$
v_{in} = \sqrt{RT/2p}
$$

Combining this result with the vapor equation of state gives the second (condensation) term in the mass transfer expression Eq.4a. The evaporation term is arrived at in a similar way. The accommodation coefficient, say c_{con}, is the probability that vapor molecules striking the liquid surface are captured. With this interpretation, the accommodation coefficients should generally be less than or equal to unity.

Most often the evaporation and condensation accommodation coefficients are assumed to be equal, but there is no theoretical reason why this must be so. Furthermore, there are no theoretical predictions for these values. It is worth noting here that this expression is for the “net” mass transfer from liquid to vapor. It says nothing about the possibility of molecular exchanges between the liquid and vapor that transfer energy without a net mass exchange.

For present purposes we have chosen to simplify the phase change rate to Eq.4b, where C is now a net "accommodation coefficient" and T_{bdy} in the denominator is the average liquid temperature along the surface of the bubble,

$$Net \quad mass \quad transfer = C\sqrt{\frac{M}{2pRT_{bdy}}}\left[P_l^{sat} - P_v\right], \qquad (4b)$$

In the next section we describe the way in which these elements are combined to make up the Homogeneous Bubble model.

Implementation

Bubbles in ***FLOW-3D®*** must be larger than a computational grid element so that a well-defined free surface exists to define the boundary of the bubble. Most often bubbles span regions that cover many grid elements. Any given calculation can have more then one bubble.

To describe the state of a homogeneous bubble we record its volume V, pressure P, and temperature T. Gas density in a bubble is computed from the equation-of-state (1). If a bubble intersects a mesh boundary that is specified as a fixed-pressure boundary, then the bubble state (P,T) is automatically set equal to that of the boundary (P_{bdy},T_{bdy}) and no phase change is computed. The assumption is that the boundary condition represents an infinite reservoir at the specified state.

Since homogeneous bubbles are an extension of adiabatic bubbles (i.e., the adiabatic condition is removed) it is necessary to input the ratio of specific heats γ that characterizes the gas in the bubbles. A non-zero value for γ is the flag that activates these models. In addition, when a non-zero specific heat at constant volume, C_v^{vap}, is specified for the gas this indicates the possibility for bubbles to exchange energy with their surroundings. That is, C_v^{vap} is needed to evaluate temperature when a bubble's internal energy changes.

The homogeneous bubble model will perform as an adiabatic bubble if there is no heat exchanged with the surroundings of the bubble. However, heat energy can be added to a homogeneous bubble by heat transfer from obstacle surfaces that lie inside the bubble. The heat-transfer coefficients are referred to obstacle-to-void heat-transfer coefficients. During a solution time cycle these thermal energies are computed and stored for each homogeneous bubble. Then at the end of a cycle the accumulated energy exchanges are used to update the final, homogeneous, bubble pressures.

Phase Changes

The effect of phase change on a bubble is complicated by the fact that there are typically many surface elements defining the boundary of a bubble. Each element has the capacity to undergo evaporation or condensation. In many cases, in fact, it is likely that both processes will be occurring simultaneously. For instance, a bubble intersecting a hot wall may be gaining vapor by evaporation at the liquid/vapor/solid contact line, while losing vapor by condensation along the bubble surface furthest from the wall.

Moreover, it's possible for evaporation or condensation from a single element to make a significant change in bubble pressure. This arises from the fact that even a small amount of liquid in a surface element may have a mass that is much larger than the mass of vapor in the bubble. This situation may be likened to a dog with a thousand large tails; unless the tails move in a coordinated way the dog will be unable to walk.

Our solution to this "stability" problem is to determine the bubble pressure implicitly. The idea is to find the bubble pressure, p_b, to use in the phase-change rate expression that produces a final bubble pressure equal to p_b. In other words, when all the phase-change contributions made to a bubble from the elements around its periphery are computed using p_b as the value of P_v in Eq.4, the resulting bubble pressure will be the same value, p_b.

That this approach must produce a stable result can be seen from the fact that a small value of p_b would lead to excessive vaporization and a large resulting bubble pressure. On the other hand, a large value of p_b produces excessive condensation and a small bubble pressure. The ideal is the p_b value that gives just the right amount of condensation/evaporation to produce a bubble having the same pressure, p_b. It is this value that insures the dog's tails are synchronized!

Unfortunately, finding the implicit pressure p_b is not an easy task when the phase-change rate is large. Even small changes in the bubble from one time step to the next can induce large changes in the net evaporation and/or condensation, which in turn induces large bubble pressure changes. The algorithm we have used for determining the implicit pressure employees a variety of strategies for limiting the search space and for accelerating the approach to a solution. In most cases only a few iterations (say 1 to 3) are necessary.

If a large accommodation coefficient is used, C in Eq.4, the number of iterations may increase because the initial guess each time step will be further from the converged value. To somewhat compensate for this the iteration procedure uses the saturation pressure corresponding to the average temperature of the liquid surface surrounding the bubble as a possible limiting value.

The convergence of the pressure iteration occurs when the implicit pressure p_b is found to change by less than 1% in successive iterations.

Energy Exchange with Phase Change

As mentioned earlier, there may be a problem with the energy exchange between liquid and vapor. For instance, suppose a bubble is undergoing a rapid volume expansion (say, a bubble in a superheated liquid). The expansion work cools the vapor in the bubble. From a kinetic theory point of view, we would expect that cold molecules of vapor would be more easily captured by the liquid and then replaced by hotter liquid molecules. In other words, we expect that there should be an energy transfer between the phases even though there is no net mass transfer.

The problem is how to model this process? A quick literature search of bubbles with phase change revealed that every model reported uses some "arbitrary" assumption to set the temperature (energy) of the bubble. Some, for example, assume that the vapor density remain constant [1], others that the pressure of the bubble is the saturation (equilibrium) value corresponding to the average liquid-interface temperature [2].

In our model we want to maintain the possibility for non-equilibrium conditions. At the same time we want to insure that certain limiting situations are correctly modeled. To this end we have used the following approach. At the end of a cycle of time advancement, by amount δt, the phase-change and heat-transfer models have computed how much mass and energy in each bubble is to be exchanged with the bubble's surroundings. We must then compute a new bubble pressure to complete the computational cycle. To do this, the key assumption is that the internal energy of the new bubble, before the bubble volume is changed, is computed in terms of the average temperature of the surrounding liquid surface. This average, T_{bdy}, is computed as a surface-area average,

$$T_{bdy} = \frac{\int T_l dA_{sur}}{\int dA_{sur}} \quad . \tag{5}$$

This T_{bdy} is used for the average temperature in the phase-change expression Eq.4b.

If there is heat exchange from solid surfaces in the bubble, or compression/expansion work because of volume changes, then these are added separately. In this way, a vapor bubble stays close to the average boundary temperature, but still exhibits non-equilibrium effects.

This model has the advantage of preserving the limiting cases of adiabatic behavior when there is no energy exchange, and simple heat exchange in the absence of phase changes.

Energy changes in the liquid are somewhat easier to deal with. If Δm is the mass exchange between liquid and vapor in an element, the corresponding change in the liquid energy in the element is,

$$\begin{aligned} \Delta E &= \Delta m\left(H_{lv} + e_l\right), \qquad && if \quad \Delta m \geq 0 \\ &= \Delta m\left(H_{lv} + c_v^{vap} T_v\right), && if \quad \Delta m \leq 0. \end{aligned} \tag{6}$$

Here H_{lv} denotes the latent heat for vaporization and e_l is the specific energy of the liquid at temperature T_l.

Model Testing

Three simple test cases have been used to verify that the homogeneous bubble model does satisfy expected limiting situations. These cases used the simplest computational model consisting of two grid cells. The bubble occupied at least one cell and a portion of the other.

Adiabatic Compression

No phase change or heat-transfer was allowed in the first test. Liquid was entering one boundary at a constant rate causing the bubble volume to be compressed. After a 5% decrease in bubble volume the computation was stopped and the bubble pressure and temperature were compared with theoretical values for an adiabatic compression. The agreement was within 0.6% in pressure and 0.07% in temperature.

Heat Exchange with a Solid

In the second test, an obstacle was places at one end of the two-cell domain with a specified heat flux. After a given time the bubble pressure and temperature were compared with the theoretical values for a vapor of fixed volume subjected to a specified energy increase. Agreement was nearly exact.

Phase Equilibrium

In the third test one grid cell contained some liquid while the remainder of the space was a vapor bubble. The bubble pressure and temperature were values corresponding to a sudden expansion in volume of 10%. This corresponds to a pressure 13.7% below the saturation value with respect to the liquid temperature. Even with an accommodation coefficient of C=0.1 only one cycle of computation was necessary to bring the vapor to within 0.6% of its equilibrium value. With time the pressure asymptotically approaches its equilibrium value, while the temperature remains at the same value as the liquid surface.

Input Data for ***FLOW-3D***®

To use this model in ***FLOW-3D***® the following equivalencies between input data and model parameters should be observed:

Input for bubbles:

gamma = γ, ratio of specific heats for vapor

cvvap = c_v^{vap}, specific heat at constant volume for vapor

Input for phase change:

rsize = C, accommodation coefficient

clhv1=H_{lv}, latent heat for vaporization

Input for pressure-temperature saturation curve:

pv1=pv1, point on saturation curve corresponding to tv1

tv1=tv1, point on saturation curve corresponding to pv1

tv0=tv0, input parameter for possible temperature scaling

tvexp=tvexp, exponent in saturation relation

Sample Bubble Jet Problem

A better demonstration of the capabilities of the new homogeneous bubble model is shown by an example of a vapor-bubble generated ink jet. An axisymmetric nozzle of diameter 56μm is filled with generic ink. To model the application of a sudden heat source at the bottom of the nozzle a small hemispherical bubble of diameter 20μm was initialized with a pressure of 10 bars and a corresponding saturation temperature of 452°K. Surrounding the bubble a spherical region of fluid having diameter 40μm was initialize to have the same hot temperature 452°K. The remainder of the ink was at room temperature, 293.2°K and atmospheric pressure of 1 bar.

The accommodation coefficient was somewhat arbitrarily chosen to be 0.1. Most fluid properties were those of water, except for the surface tension value that was only about 0.68 times that of water. A simple power-law expression, known to be good for water, was used to model the relation between saturation pressure and temperature.

Figure 1 shows four snapshots of the computed results. The first plot is the initial configuration. Plot 2 shows the flow after a time of 10μs when the bubble has reached its maximum expansion and is beginning to collapse. The third plot, at time 15μs, is immediately after the bubble has completely collapsed. Finally, the last plot of the simulation, at t=50μs, shows a detached ink jet leaving the nozzle.

This problem required 52s of CPU time on a 450MHz Pentium III, PC computer.

Summary

These sample cases demonstrate that the homogeneous bubble model can successfully treat the three limiting cases of adiabatic conditions, simple heat addition, and equilibrium producing phase change. The last example also offers a dynamic demonstration of the new modeling capabilities provided by the homogeneous bubble model.

More complicated test cases having experimental data for making comparisons are difficult to find. This is partly due to the fact that the accommodation coefficient is an adjustable parameter so that choosing its value to match experiments may cover up many sins.

It is hoped that this model will prove itself to be useful in that it does account for the exchange of energy between a liquid and its vapor. Whether or not the rate is exactly correct may be of secondary importance.

References

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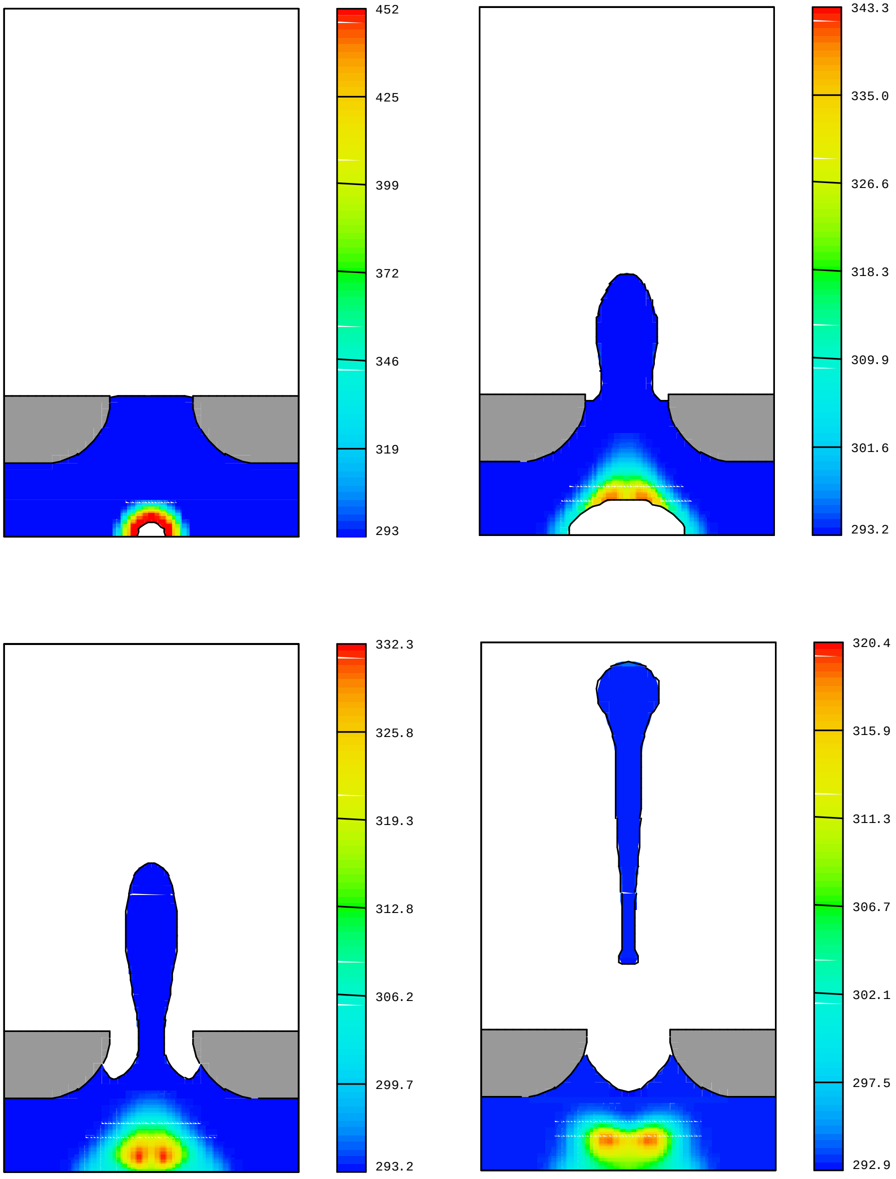

Figure 1. Example of bubble-driven ink jet. The problem is initialized with a small bubble surrounded by a layer of hot liquid.