

Void Regions and Bubble Models in *FLOW-3D*

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Introduction

The purpose of this technical note is to describe to the reader general details of the treatment of void regions and their interaction with fluid in *FLOW-3D*¹ and to help better understand the program's capabilities and results, as well as its limitations.

In one-fluid problems in *FLOW-3D* the volume-of-fluid (VOF) function F defines the location of fluid #1 in the mesh. For example, $F(ijk)=1.0$ in a cell full of fluid. An open cell with no fluid is a *void* cell; $F(ijk)=0.0$ in such a cell.

Void cells represent regions of gas in which spatial variation of pressure and temperature, inertia and friction at the interface with fluid can be neglected. These assumptions are generally valid if

- the gas density is much smaller than that of the fluid,
- the gas speed is comparable with that of the fluid,
- the speed of sound in the gas is much greater than the speed of the mean flow.

All these conditions are present in many situations such as mold filling with liquid metal, water flow in rivers and ducts (with the exception of high winds, which could be accounted for with a special type of a free surface boundary condition in *FLOW-3D*), micro-fluidic devices and so on.

The one-fluid/void approach to modeling free surface is a powerful method that provides efficient and accurate solutions to general free surface flows [1]. Including the details of gas flow in such cases is usually computationally expensive and unnecessary.

The terms 'void' and 'bubble' in this article largely refer to the same computational objects. A slight distinction is that a void region may be called a 'bubble' when it is surrounded by fluid and its pressure and temperature vary dynamically – as in an actual bubble moving through liquid. In the context of the solver all such objects are referred to as 'void regions'.

Bubble models in *FLOW-3D* have many uses in complex flow situations involving non-equilibrium thermal and dynamic processes. Bubbles containing vapor can arise or disappear in a simulation because of phase change associated with cavitation or boiling. Gas bubbles can be

¹ *FLOW-3D* and TruVOF are registered trademarks in the USA and other countries.

affected or created by gas mass sources as well as through vents and valves connected to external pressure reservoirs. Turbulent liquid surfaces may entrain gas from bubbles and be bulked up by the added gas volume. All these possibilities as well as several basic techniques dealing with the identification and labeling of bubble regions are described in the remainder of this document.

Void Regions

A continuous region of void cells defines a void region, or a bubble. Each void region is characterized by uniform pressure and temperature, volume, surface area with fluid, energy and mass. Since void cells are assumed to contain no fluid, no flow equations are solved in them. Instead, an equation-of-state is solved for each void region, and the result is assigned to each cell of that void.

Pressure and volume are the primary characteristics of a void region. Void pressure is used as a boundary condition at the fluid free surface surrounding the void and is an important factor in obtaining accurate flow solutions.

Void temperatures are calculated and used only when the heat transfer model is activated.

Void regions can be of several types, depending on the physical models attached to them:

- constant pressure and temperature, IPHCHG=0 or 1 (0 is the default);
- adiabatic bubble, where its pressure is a function of the bubble volume, while its temperature is constant (i.e., user-defined), IPHCHG=3;
- thermal bubble, where a perfect gas equation-of-state is used to calculate the void pressure and temperature, IPHCHG=4;
- thermal bubble with phase change, where the bubble is assumed to contain the vapor of the surrounding liquid, IPHCHG=5.

Heat transfer with surrounding fluid and geometry components can be added to any of the listed void types. This is achieved simply by activating the heat transfer model and defining the respective heat transfer coefficients.

Free Surface Boundary Conditions

A void's pressure and temperature are used to define boundary conditions at free surfaces and walls that the void is in contact with. At a free surface, the adjacent void pressure defines the normal stress. Void pressures also contribute to the net force acting on components, including the General Moving Object (GMO) components, baffles, deforming walls and membranes.

Void temperatures are used to calculate linear and radiation heat fluxes at free surfaces and walls provided the heat transfer coefficients and emissivity are defined.

Void Volume, Pressure and Temperature

Tracking the evolution of a void region volume is important for an accurate calculation of its pressure and temperature. A bubble's volume changes because of the compression/expansion of the bubble, but may also do so for numerical reasons. For example, a fluid cell with $F(ijk) < 1.0$ may not be associated with a void region at $t=t^n$, but becomes such at $t=t^{n+1}$ if a surface or void cell becomes its neighbor. In that case, the bubble volume would increase on top of the legitimate change due to compression or expansion, resulting in a lower void pressure than would otherwise had been computed. This can happen when a void region is poorly resolved or when the free surface undergoes severe deformations.

For coalescing void regions with different pressures the new void pressure is calculated as a volume-average of the pressure of the coalescing voids, consistent with Boyles Law [2].

Types of Void Regions

1. Constant pressure and temperature void regions (IPHCHG=0 or 1)

This is the default void model. A void's pressure and temperature can be defined by several means:

- a. Set the initial void pressure and temperature using PVOID and TVOID. These two variables define the default initial state of all void regions in the computational domain, including *new* voids that appear during the simulation.
- b. Use a *void pointer* by placing it inside the void at time $t=0.0$ and defining the pressure and temperature associated with it.

Note: Since version 11 of FLOW-3D both pressure and temperature defined by a void pointer can be time-dependent, in which case any void connected to that pointer at any time during the simulation will assume its current pressure and temperature.

- c. Define a mesh boundary condition of type *Fixed Pressure* and set fluid fraction at it to 0.0. In that case, all void regions connected to this boundary will assume its pressure and temperature which in turn can be time-dependent. Once a void region separates from such a boundary, it will maintain the values of pressure and temperature it had just prior to the separation.

The last two options allow users to give each void an initial state different from other voids.

2. Adiabatic bubbles (IPHCHG=3)

The term *adiabatic* in this model originates from a solution to the ideal case of a bubble with uniform pressure and temperature and no heat or mass transfer at its boundaries, where its pressure, p , is a simple function of the volume V :

$$p = p_0 \left(\frac{V_0}{V} \right)^\gamma, \quad (1)$$

The subscript '0' denotes the state of the bubble at a given time, and γ is the ratio of gas specific heats at constant volume and pressure, C_v and C_p .

In the solver, the new adiabatic bubble pressure, $PR(L)$, is calculated in PVORE as

$$PR(L) = PRN(L) \cdot \left(\frac{VOLN(LN)}{VOL(L)} \right)^\gamma \quad (2)$$

where L and LN are the new and old void region labels, and $PRN(L)$ is the void pressure at the previous time step.

3. Thermal bubbles (IPHCHG=4)

For thermal bubbles a polytropic or ideal gas equation of state is used to compute a new pressure

$$p = \rho RT \quad \text{or} \quad p = (\gamma - 1) \rho C_v T. \quad (3)$$

Here R is the universal gas constant, C_v is the gas specific heat at constant volume and ρ is the gas density.

It is also necessary to include the calculation of the total thermal energy of the gas in the bubble:

$$dE = q - pdV, \quad (4)$$

Where $E = \rho VC_v T$, q is the total amount of heat received by the bubble from surrounding fluid and geometry components in the time increment dt and pdV is the energy added or removed by the bubble's volume change by compression or expansion respectively.

4. Thermal bubbles with phase change (IPHCHG=5)

Evaporation of liquid may be used for cooling or for drying of materials. Coating processes often involve evaporation as an important factor. Evaporation (boiling) and condensation are also the primary flow-driving mechanisms in bubble jet printers.

A key concept involved in evaporation and condensation is that of the *saturation curve* that relates pressure and temperature values at which a vapor is at saturation conditions. That is, for a given temperature, a vapor at a pressure greater than its saturation pressure will undergo condensation to reduce its pressure, while if it is at a pressure lower than its saturation value there may be evaporation of liquid increasing the vapor pressure. The saturation state represents an equilibrium condition between the processes of evaporation and condensation.

Several options are available for defining the saturation curve. The simplest one is a Clapeyron equation giving p_{sat} as a function of temperature T is,

$$p_{sat} = PV1 \cdot \exp\left(\frac{-\left(\frac{1}{T} - \frac{1}{TV1}\right)}{TVEXP}\right). \quad (5)$$

In this equation $(PV1, TV1)$ is a point on the saturation curve. The quantity $TVEXP$ is an exponent that is often approximated by the expression

$$TVEXP = \frac{(\gamma - 1) \cdot c_v^{vap}}{CLHV1}, \quad (6)$$

where $CLHV1$ is the heat of transformation, or latent heat, of evaporation.

Alternatively, the user can define a saturation curve as a table by a set of data points of temperature vs. pressure. Finally, the saturation curve can be defined as

$$\log_{10}\left(\frac{p_{sat}}{p_{cr}}\right) = -\frac{7}{3}(1 + \omega)\left(\frac{T_{cr}}{T} - 1\right) \quad (7)$$

where w is the acentric factor and p_{cr} and T_{cr} are the pressure and temperature at the *critical* point, where liquid and vapor cease to be distinct phases. For example, for water this state occurs at $T=647$ K and $p=218$ atm.

The latent heat of vaporization, ΔH_{vap} , can also be defined in one of three ways: as a constant, $CLHV1$, a table of values vs. temperature, and as a polynomial fit to three user-defined points on the $\Delta H_{vap}(T)$ curve one of which must be the critical point, where $\Delta H_{vap} = 0$.

Void regions in this model are assumed to contain only the vapor of the liquid and their evolution is governed by the equation of state and the energy balance equation, Eqs. (3) and (4).

Phase change occurring at the void interface with liquid results in a net exchange of mass with the surrounding liquid. The phase change rate is proportional to the deviation from saturation

conditions, a typical non-equilibrium approximation. In the present case it is proportional to the difference in vapor pressure and what would be the saturation pressure if the vapor were in equilibrium with the liquid. The formulation for the mass flux \dot{m} at a location on the free surface, which is based on a kinetic theory model [3], is

$$\dot{m} = RSIZE \cdot (p_{sat} - p_{vap}) \cdot \sqrt{\frac{M}{2\pi RT_{liq}}} \quad (8)$$

Here M is the molecular weight of the vapor, R is the universal gas constant, T_{liq} is the liquid surface temperature, p_{sat} is the saturation pressure evaluated from the liquid temperature and p_{vap} is the vapor pressure. $RSIZE$ is a dimensionless ‘accommodation’ coefficient. Typically, a value on the order of 0.05 has worked well, but it could be as large as 1.0.

The computation of phase change is complicated by the fact that it is a highly non-linear process. To maintain stability at reasonable time-step sizes an implicit, iterative procedure is used to compute the mass and energy flux due to phase change.

The bubble dynamics is dependent on phase changes over the whole surface of the bubble, which may extend over many grid cells in several mesh blocks. Evaporation may be taking place on some portion of the surface, while condensation is occurring over the remainder (because of differences in liquid temperature at the interface). To account for such cases, phase change is first computed for all surface elements and the results are summed into the net mass transfer for each bubble. Then the bubble pressures are updated followed by a repeat computation of the phase change fluxes using the newly updated vapor pressures. This process generally converges in a few iterations. When updating bubble pressures a bubble temperature is needed. For this it is assumed to be equal to the average liquid surface temperature surrounding the bubble which in turn changes because of the phase change.

The issue of the bubble temperature definition is a difficult one because at first sight it would be thought that if we know the mass transfer taking place in a phase change then we would also have a good grip on associated energy transfer between liquid and vapor. Attempting to do this from a kinetic theory point of view does not work and tends to result in vapor temperatures that are either heading to zero or infinity. The reason for this is that considerable energy transfer can occur without a net mass transfer. The assumption of a bubble temperature equal to its average liquid surface temperature seems reasonable and has produced good results.

5. Constant pressure bubbles with vaporization (IPHCHG=1)

A simpler version of the *Thermal bubble phase change* model is also available, where only vaporization is accounted for and the mass transfer is not coupled to the bubble pressure and temperature. This approximation is suitable for simulating the drying of liquid to a large reservoir of gas, such as the drying of rain puddles to the atmosphere.

In this model the (constant) vapor content of the gas in the void regions is defined by the vapor partial pressure PV_0 , while $PVOID$ defines the total pressure in the void.

6. Cavitating voids (ICAV=1)

Cavitation can occur in fluid when the local pressure drops below a critical value, called *cavitation pressure*. Cavitation is often associated, for example, with hydraulic structures, flows in pipe lines and power plant intakes, around underwater torpedoes and boat propellers. The appearance of cavitation results in noise and may sometimes cause damage to structures.

The cavitation model in **FLOW-3D** uses a constant cavitation pressure, $PCAV$, and is suitable for modeling cavitation occurring due to a localized reduction of pressure. Although a sufficient reduction in pressure can result in liquid vapor production, more typically a reduced pressure results in the release of dissolved gases, *e.g.*, air in water, out of solution. Every new void region that appears due to cavitation is assigned the cavitation pressure $PCAV$ which is maintained throughout the calculation unless it gets connected to a fixed-pressure mesh boundary with fluid fraction set to 0.0. A cavitation void pressure does not change with its volume, even if the adiabatic bubble model is turned on. The constant cavitating void pressure assumes that, compared to the time scale of the flow, the evolution of the gas happens much faster.

When a cavitation bubble moves into a region of pressure larger than the cavitation pressure, it is compressed by the surround fluid and may completely disappear. All the while the bubble remains at the specified cavitation pressure. A different type of cavitating bubble, based on phase change, is described below when non-equilibrium thermal processes are included in the model.

7. Thermal cavitation (boiling) model (ICAV=1, IPHCHG=5)

Cavitation can also occur when the heating of a liquid raises its saturation pressure above the local pressure in the liquid. This occurs, for example, during *boiling* of a liquid.

This model uses the saturation curve, *e.g.*, Eq. (5), to determine the local critical pressure as a function of the temperature. In this case, the gas coming out of the liquid is its *vapor*. The model is designed to describe cavitation upon heating, *i.e.*, boiling, as in bubble jet printers, but it can also handle the boiling effects due to a decrease in pressure.

The thermal cavitation model is coupled with the thermal bubble and phase change models described in the previous sections. At the end of each time cycle of a computation every grid cell containing liquid is tested to see if its pressure is less than the saturation pressure corresponding to the temperature in the cell. The saturation pressure is computed from the pressure-temperature saturation curve specified by the user (*e.g.*, the Clapeyron relation, Eq. (5)). If the cell pressure is less than its saturation pressure it is assumed that boiling begins. Just as in cavitation, the usual assumption is that there exist sufficient impurities or nucleation sites for this to happen.

Once the bubble grows to occupy at least one full grid cell it is recognized as a discrete thermal bubble. Its initial pressure and temperature are equal to the cell pressure and temperature just before it became empty, and continue to evolve as a function of the mass and heat fluxes as well the bubble size, Eqs. (3), (4) and (8).

Bubble nucleation rate

The rate of vapor bubble nucleation in the thermal cavitation model can be controlled in two ways. The *characteristic time for nucleation* parameter, CAVRT, defines the approximate time required for a bubble nucleation in a cell from the moment the local pressure in the liquid drops below the saturation point.

The second parameter controlling nucleation is the *superheat* temperature TV0. Nucleation of a vapor bubble can be delayed in highly purified liquids where nucleation sites are scarce. When liquid temperature becomes greater than the local saturation (or boiling) temperature – but less than TV0, - the nucleation rate is controlled by CAVRT. Nucleation can thus be delayed by defining a large value of CAVRT. Once the liquid temperature exceeds TV0, the local characteristic time for nucleation is reset to five time-step sizes, which effectively results in a fast, explosive boiling of the liquid. It is not uncommon for TV0 to exceed the boiling temperature by a two or three hundred degrees *K*.

The CAVRT-controlled nucleation is also overridden when nucleation occurs near a geometry component #N with a non-zero roughness, ROUGH(N), in which case it is assumed that nucleation sites are available and the nucleation time is reset to five time-step sizes, independent of TV0.

The current treatment of the coalescing vapor bubble dynamics in ***FLOW-3D*** is highly accurate and detailed, based on many years of experience with modeling flow in bubble-jet printer nozzles. Nevertheless, it is impossible to completely eliminate the sizeable influence of numerical parameters such as mesh resolution and the time step size on the solution. Therefore, it is always recommended to calibrate the model using the empirical parameters in it, such as CAVRT, RSIZE, TV0 and the heat transfer coefficients between liquid and the heater, liquid and void, and void and the heater².

Units

An important requirement for any bubble model that uses an equation-of-state, e.g., the adiabatic bubble model, is that pressures must be treated as absolute pressures - not gage pressures. Similarly, the absolute temperatures, in degrees *K* or *R*, are required when using the thermal bubble models.

² Newly formed thermal and vapor bubbles are designated as heat transfer voids of type #1.

Two-Fluid Liquid/Gas Model

If a more detailed solution for the gas dynamics within the bubbles is required, a two-fluid model consisting of incompressible liquid and compressible gas is also available, IPHCHG=2 [4].

The gas in this case can consist of both vapor and a non-condensable gas such as air or helium, forming a two-component gas mixture. Phase change for two-fluid bubbles is similar to that for thermal bubbles, Eq. (8), and also uses a saturation pressure curve, Eqs. (6) and (7), or a table lookup. Gas bubbles are initiated in same way as in the thermal bubble model, but, of course, they would not contain the non-condensable gas - only vapor. The non-condensable gas can be introduced into bubbles through the initial and mesh block boundary conditions, as well as at mass sources.

Two-fluid bubbles offer great generality but they do so at the expense of a more intense computational effort. When the limitations of the simpler bubble models are not satisfied, however, then this more detailed and fully dynamic model offers a way forward.

Bubble Model Interaction with Other Models

The void/bubble models can be combined and interact with several other modeling options in **FLOW-3D**. Most of these involve the use of sources or sinks of gas. Several of these possibilities are described here.

1. Air entrainment

The air entrainment model in **FLOW-3D** describes the entrainment of air by turbulent free surface flow such as water flow in rivers and canals, at spillways and sluice gates [5]. The entrained air is described with a volume concentration of gas in the fluid.

If the adiabatic bubble model is activated, then the volume of entrained air affects the pressure in the bubble, according to Eq. (1). This model is useful when, for example, modeling syphon spillways where a large volume of air is trapped in the upper section of a spillway, which is then gradually entrained and carried downstream by the flow. The reduction in the pressure in the trapped gas region is an important factor in the proper functioning of the spillway.

Similarly, air released at a free surface back into a void region by drift (*i.e.*, by a two-phase relative drift velocity) is added to the bubble. No phase change is present for this type of mass exchange between bubbles and liquid.

2. Two-phase drift flux model

The two-phase drift-flux model in **FLOW-3D** describes the flow of a particulate phase inside a continuous fluid phase, such as crude oil droplets in water, argon gas bubbles in liquid metal or dust particles in air [6].

When the particulate phase represents gas, a special option exists to allow these bubbles to escape at free surface into the surrounding void. If the adiabatic bubble model is activated, the escaped gas contributes to the volume and pressure of the adjacent void region per Eq. (1).

The drift-flux model can be combined with the air entrainment model to add the buoyancy and bulking effects as well as the escape of air back into the atmosphere.

3. Valves

Valves (or vents) are useful simple tools for modeling the venting of gas to external gas reservoirs without the inclusion of the details of the actual venting channels. A typical use for vents is to remove air from the die cavity during filling with liquid metal in casting or with sand in sand core making.

The adiabatic bubble model must be activated for the valve model to work.

There is no modeling distinction between the terms *vent* and *valve*. Each is defined as a point location in the computational grid. If the grid cell containing a valve is less than half full of liquid, $F(ijk) < 0.5$, then it is assumed that the valve is uncovered by the liquid and can transfer gas between the void region adjacent to the cell and the external gas region. If the cell is more than half filled with liquid the valve is shut off.

A valve is characterized by its location, the external pressure, p_{ref} , and the flow loss coefficient, $VALC$. The coefficient is a construct of its flow area A_{val} , a loss coefficient C_{val} , compressibility factor Y and a representative gas density ρ_{val} ,

$$Flowrate = VALC \sqrt{|p - p_{ref}|}, \quad VALC = \frac{A_{val} C_{val} Y}{\sqrt{\rho_{val}}} \quad (9)$$

Gas can either enter or leave through a valve depending on whether the reference pressure is larger or smaller, respectively, than the pressure of the bubble containing the valve.

4. Permeable mold

A geometry component of type *Permeable mold* is permeable to gas but not liquid. In terms of the *FAVOR*TM representation, it is a non-porous, solid, component. Similar to valves, such objects are useful when modeling the escape of air through a sand mold during the filling with liquid metal. Unlike the valves, however, a permeable mold allows the gas to escape though the whole *unwetted* part of its cavity surface.

A permeable model is characterized by porosity, average sand grain size, average mold thickness and the external pressure. These are converted to the gas volume flux at each surface element of

the mold cavity exposed to a void, based on the difference between the void pressure in the cell and the external pressure. The net gas flow then contributes to the volumes and pressures of the void regions adjacent to the mold, per Eq. (1).

As with the valve model, the adiabatic bubble model is required for the permeable mold model to work.

5. Sources and sinks

Geometry components have a general capability for being sources and sinks of fluid. The volume or mass flow rate (positive for sources and negative for sinks) can be defined as a tabular function of time and is uniformly distributed over the entire open surface of the source component. Gas can be added or subtracted from bubbles and void regions in this way.

If there is no gas in a cell containing the source component, then no gas can be removed. The converse is not true, for if gas is injected into a cell that is filled with liquid then liquid is forced out of the cell. If that gas region eventually uncovers a full grid cell then it becomes a discrete bubble with the initial pressure equal to the cell pressure just before liquid was completely expelled from it and temperature equal to the specified source temperature value.

6. Mesh boundaries

Mesh boundaries of type *pressure*, *velocity* or *flow rate* can also control the adjacent void pressures and temperatures if the boundary fluid fraction value is set at 0.0.

As mentioned earlier, a void connected to a pressure boundary immediately assumes the boundary pressure and temperature irrespective of the type of the void.

A specified velocity or flow rate boundary acts as a source or sink, depending on the direction of the flow, of gas for any void connected to it, similar to the sources or sinks defined with geometry components described in the previous section.

Explicit/Implicit Void Pressure Solver

Two options exist in *FLOW-3D* for the calculation of void pressure that depends on its volume: explicit and implicit.

The simpler explicit solver calculates the void pressure at the end of each time step based on the change in volume for each void region, using Eq. (1). This procedure may be stable for large and relatively ‘soft’ bubbles. However, for smaller and ‘stiffer’ bubbles the explicit solution typically becomes unstable.

The origin of the instability is easy to understand if we draw an analogy between a compressing/expanding bubble and a spring – in both cases the counter force increases during

compression and decreases upon expansion [7]. If the time step size is too large, then a bubble expansion in one time step will result in an over-compression in the next one with the feedback between pressure and volume continuing to increase the amplitude of the volume change in subsequent time steps. The result is an oscillation in the bubble volume and pressure with exponentially growing amplitude which is clearly unphysical. A time-step size stability limit could be evaluated for simple bubble shapes based on the analogy with springs, but it is not possible to accurately do so in general 3D flows, where there may be multiple bubbles of complex shapes.

The (default) implicit solver *estimates* what a bubble’s pressure would be at the end of a time step. The estimated values are then used to adjust fluid pressures and velocities at the beginning of the time step. Finally, the actual void pressures are computed from the position of the free surface at the end of the time step. The estimate calculations are based on the velocities of fluid normal to the free surface and are coupled with the iterative fluid pressure solver. Free surface is *not* actually moved during the fluid and bubble pressure-velocity iteration.

The incorporation of the bubble pressure change estimate into the fluid pressure solver augments fluid pressures and velocities in anticipation of the bubble’s counteraction to fluid motion. For example, if a bubble is being compressed, an anticipated increase in its pressure will result in smaller velocities at the end of the pressure iteration. The bubble will then compress less than if no estimate of its pressure change was done as is in the explicit solver, thus eliminating the overshoot and making the solution stable.

‘Stiff’ bubbles

Even when using the implicit bubble solver, solution around small – the size of a few computational cells - ‘stiff’ bubbles may be noisy if not unstable [8]. By *stiff* we mean a bubble for which a small change in volume results in a large change in its pressure. From Eq. (1) we can derive

$$\frac{dp}{dV} = -\gamma \frac{p}{V}, \quad (10)$$

which is the sensitivity of the bubble pressure to its volume. From Eq. (10) it can be seen that smaller bubbles (small V in the denominator) are more likely to be ‘stiff’. Small numerical errors in tracking void volumes that are always present in any calculation, may become relatively more significant for smaller bubbles, translating into pressure noise in the bubble and in the surround fluid. These numerical errors associated with any small bubble are also the reason why the implicit bubble model cannot always stabilize a solution.

Equation (10) also suggests that using a smaller initial void pressure, *i.e.*, assuming a partial vacuum, reduces the bubble pressure sensitivity. This, obviously, may change the problem being simulated, but it could be an acceptable compromise producing faster and more stable solutions.

Summary

In this technical note we give a general outline of the physical models for void and bubble regions currently available in **FLOW-3D**.

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