

SHAN-CHEN MULTIPHASE MODEL

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MULTIPHASE VARIATIONS

The multiphase is a really broad term which includes quite different phenomena. For example one can distinguish the following phenomena belonging to multiphase phenomena:

- One-component different phases systems, i.e. water and water vapour.
- Many components one phase systems, i.e. oil and water.
- Many components many phases systems, i.e. oil, gas and water with water vapour.

In this lecture we will proceed with the one-component different phases systems.

MULTIPHASE MODELS

What does the multiphase model implies? Multiphase model implies certain things:

- The **equation of state** allowing the separation of phases. For example the famous van der Waals equation:

$$p(\rho) = \frac{\rho RT}{1 - b\rho} + a\rho^2$$

- The surface tension between phases acting along the interface. For example pressure buildup for the Laplace law is because of the surface tension. The surface tension acts along the curvature and can be represented through the following equation:

$$n_k(P_{ik}^{(1)} - P_{ik}^{(2)}) = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) n_i,$$

where P_{ik} is the **momentum flux** tensor in phases 1 and 2, n_i is the normal to the interface.

PHYSICAL UNDERSTANDING

How to deal with the equation of state - one can think about it as the attractive and repulsion force introduced on the microlevel. The surface tension acts along the interface and usually the reconstruction of the interface to determine a curvature is required.

Therefore, the one-component multiphase models can be described by two stages:

- The equation of state can be introduced to the momentum flux tensor $P_{\alpha\beta}$ or through the acting force (we will discuss it later).
- The surface tension inclusion which is a tricky part and usually is done through the interface reconstruction or through the acting force.

CFD MODELS

Basically the surface tension dictates as what the model will be used to simulate a multiphase system. A few approaches are incorporated in CFD:

- The front tracking technique, which impose additional tracking points on the interface and reconstructs interface with their help.
- Volume-of-Fluid (VOF) introduces the phase field which distinguish two phases. The transition between different phases is smooth. VOF reconstructs the interface and then impose boundary conditions.
- Diffuse interface models impose the smooth transition between phases and only integrally fulfill the boundary conditions on the interface.
- Level Set method introduces the distance function which implicitly gives the interface and its curvature.

The Shan-Chen model introduced here is the diffuse interface model which helps not to worry about boundary conditions. However, the interface is diffused over a few lattice units which are not physical (in nature, the interface occupies nm-mm scale).

DIFFUSE INTERFACE MODELS

For diffuse interface models (see review of Andersen) one needs to restore the following momentum flux tensor:

$$P_{\alpha\beta} = (p_0 - \frac{k}{2}(\nabla\rho)^2 - k\rho\Delta\rho)\delta_{\alpha\beta} + k\partial_\alpha\rho\partial_\beta\rho,$$

where p_0 is the bulk pressure responsible for different components, k is the surface tension coefficient which is involved in the surface tension calculation through the interface, as:

$$\sigma = k \int_{\text{interface}} \left(\frac{\partial\rho}{\partial n} \right)^2.$$

If the model satisfies these conditions then one has a one-component multiphase model.

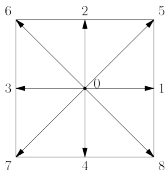
THE SHAN-CHEN FORCE. NAIVE ASSUMPTION

The Shan-Chen force accounts for the attraction force calculated over nearest neighbours of the pseudopotential function ψ :

$$F_\alpha(\mathbf{x}) = -G\psi(\mathbf{x}) \sum_i w_i \psi(\mathbf{x} + \mathbf{c}_i) \mathbf{c}_i,$$

where coefficient G controls the strength of the attraction. The function ψ is so-called pseudopotential $\psi = \psi(\rho)$, where ρ depends on time and location.

Therefore, we introduced a force to include the attraction. Let us analyze it through the Taylor expansion to see contributions to the equation of state and the surface tension.



TAYLOR EXPANSION

One can perform Taylor expansion of the force:

$$F_{\alpha}(\mathbf{x}) = -G\psi(\mathbf{x})\left(\frac{1}{3}\partial_{\alpha}\psi + \frac{1}{18}\partial_{\alpha}\Delta\psi\right) + O(\partial^5).$$

One can reconstruct the momentum flux tensor from the force by “reverse engineering”:

$$\begin{aligned}\partial_{\beta}P_{\alpha\beta} &= F_{\alpha} \\ P_{\alpha\beta} &= \left(\frac{\rho}{3} + \frac{G}{6}\psi^2 + \frac{G}{36}(\nabla\psi)^2 + \frac{G}{18}\psi\Delta\psi\right)\delta_{\alpha\beta} - \frac{G}{18}\partial_{\alpha}\psi\partial_{\beta}\psi\end{aligned}$$

Compare the momentum flux tensor with the diffuse interface method:

$$P_{\alpha\beta} = \left(p_0 - \frac{k}{2}(\nabla\rho)^2 - k\rho\Delta\rho\right)\delta_{\alpha\beta} + k\partial_{\alpha}\rho\partial_{\beta}\rho$$

They look identical if we assume relationships $\psi(\rho) = \rho$, $k = -G/18$, $p_0 = \frac{\rho}{3} + \frac{G}{6}\psi(\rho)^2$.

“MAGIC” OF THE SHAN-CHEN FORCE

The magic of the Shan-Chen force is not only in the attraction force but in such a form of the attraction potential that it modifies not only the equation of state but also gives the surface tension through the higher order of Taylor expansion (term $\frac{G}{18}\psi\nabla\Delta\psi$).

THE CHOICE OF PSEUDOPOTENTIALS

However, the choice of $\psi = \rho(\mathbf{x}, t)$ is not the best in terms of stability. One can see that if we choose $\psi = \rho$, it becomes larger for larger ρ . Thus, the attractive potential contains a “disease” loop - the larger density ρ , the larger ψ given usually larger gradients which lead to instabilities. $\psi = \rho$ is good for small gas-liquid density ratios.

Therefore one wants to bound pseudopotential ψ for large ρ and have it proportional to ρ for smaller ρ . It can be achieved by the following choice of the pseudopotential (usual Shan-Chen pseudopotential):

$$\psi(\rho) = 1 - \exp(-\rho),$$

which is for small ρ equals to $\psi(\rho) = \rho$ and for large densities $\psi(\rho) = 1$. This choice of the pseudopotential allows larger separation for gas and liquid, usually no more than 60 – 70.

CRITICAL VALUES

We see that the form of the Shan-Chen force contributions resembles the momentum flux tensor of the diffuse interface method. **So what?**

The main question what kind of separation I can expect if the equation of state is modified through the force inclusion? Let us look to the equation of state:

$$p_0 = \frac{\rho}{3} + \frac{G}{6}(1 - \exp(-\rho))^2.$$

It is known from the thermodynamic theory that the critical values of pressure p_0 , density ρ_{crit} and temperature like parameter in the equation of state G_{crit} where the separation occurs can be obtained from these two equations:

$$\begin{aligned}\frac{dp_0}{d\rho} &= 0 \\ \frac{d^2p_0}{d\rho^2} &= 0,\end{aligned}$$

which becomes after algebraic manipulations as follows:

$$\begin{aligned}\frac{1}{3} + \frac{G_{crit}}{3} \exp(-\rho_{crit})(1 - \exp(-\rho_{crit})) &= 0 \\ -\frac{G_{crit}}{3} \exp(-\rho_{crit})(1 - \exp(-\rho_{crit})) + \frac{G_{crit}}{3} \exp(-2\rho_{crit}) &= 0.\end{aligned}$$

CRITICAL VALUES

One can solve the system for G_{crit} and ρ_{crit} to obtain in numbers:

$$G_{crit} = -4$$

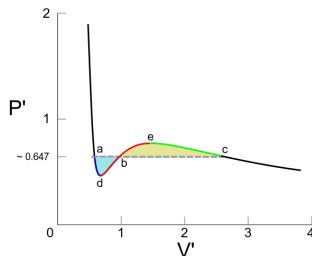
$$\rho_{crit} = \ln 2$$

That means if the system is initialized with the liquid density more than $\ln 2$ and the gas density less than $\ln 2$ and temperature-like parameter $G \leq -4$, then one will obtain the stable system with separated gas-liquid phases.

MAXWELL RECONSTRUCTION RULE

Still we don't know what will be values of ρ_{gas} and ρ_{liq} when one gives the value of G . To obtain these values one need to use the Maxwell reconstruction rule. The Maxwell reconstruction rule states that the integral around the transition pressure by the volume should equal to zero or in other words - the transition happens only for such pressures where the integral equals to zero which gives the equilibrium values of gas and liquid densities:

$$\int_{V_{liq}}^{V_{gas}} (P(V) - P) dV = \left(\int_{adb} + \int_{bec} \right) (P(V) - P) dV$$



Van der Waal Isotherm $T^* = 0.90$

MAXWELL RECONSTRUCTION RULE IN TERMS

As far as the equation of state uses density as the independent variable, one needs to translate the Maxwell reconstruction rule in terms of densities:

$$V \propto \frac{1}{\rho}$$
$$\int_{V_{liq}}^{V_{gas}} (P(V) - P) dV = \int_{\rho_{gas}}^{\rho_{liq}} \frac{(P(\rho) - P)}{\rho^2} d\rho = 0$$

Overall, once parameter G is given one needs to solve the following system of integral equations to obtain values of ρ_{gas} and ρ_{liq} :

$$\int_{\rho_{gas}}^{\rho_{liq}} \frac{p_0(\rho) - p}{\rho^2} d\rho = 0$$

$$p = p_0(\rho_{gas})$$

$$p = p_0(\rho_{liq})$$

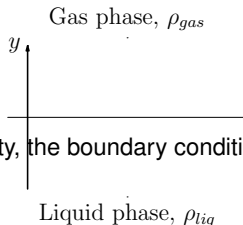
However, approaches presented before are only for the ideal case of the thermodynamics. The case of the diffuse interface is different - the transition happens because of the force and is diffused through a few lattice units. Overall, to see how the separation occurs for diffuse interface models one needs to eliminate the surface tension and solve the equation for the planar case.

The boundary conditions are as follows assuming that function $\rho = \rho(y)$:

$$\rho(\infty) = \rho_{gas}$$

$$\rho(-\infty) = \rho_{liq}$$

As far as the curvature of the interface is infinity, the boundary condition becomes $P_{yy} = const.$



THE SOLUTION FOR THE PLANAR CASE

For the one-dimensional case which we have here the momentum flux tensor is:

$$P_{yy}(\mathbf{x}) = p_0 = \frac{\rho}{3} + \frac{G}{6}\psi^2 - \frac{G}{18}\left(\frac{d\psi}{dy}\right)^2 + \frac{G}{18}\psi\frac{d^2\psi}{dy^2}$$

$$P_{yy}(\infty) = p_0 = \frac{\rho}{3} + \frac{G}{6}\psi^2(\rho_{gas})$$

$$P_{yy}(-\infty) = p_0 = \frac{\rho}{3} + \frac{G}{6}\psi^2(\rho_{liq})$$

The derivative of the pseudopotential by y can be expressed through the chain rules:

$$\frac{d\psi}{dy} = \frac{d\psi}{d\rho} \frac{d\rho}{dy} = \exp(-\rho)(1 - \exp(-\rho))\frac{d\rho}{dy}$$

In what follows we do notations $\dot{}$ standing for $\frac{d}{d\rho}$ and $'$ standing for $\frac{d}{dy}$. The equation you come up is:

$$p_0 = \frac{\rho}{3} + \frac{G}{6}\psi^2 - \frac{G}{36}(\dot{\psi}\rho')^2 + \frac{G}{18}\psi(\ddot{\psi}\rho'^2 + \dot{\psi}\rho'')$$

THE SOLUTION FOR THE PROFILE

The previous equation can be much simplified by the introduction of the new variable $z = \rho'^2$. Then the second order derivative becomes:

$$\rho'' = \frac{d}{dy} \sqrt{z} = \frac{1}{2\sqrt{z}} \frac{dz}{dy} = \frac{1}{2\sqrt{z}} \frac{dz}{d\rho} \frac{d\rho}{dy} = \frac{1}{2\sqrt{z}} \sqrt{z} \dot{z} = \frac{\dot{z}}{2}$$

Therefore one comes up with the the following first order differential equation for z :

$$\frac{G}{36} \psi \dot{\psi} \dot{z} + \frac{G}{36} (2\psi \ddot{\psi} - \dot{\psi}^2) z = p_0 - \frac{\rho}{3} - \frac{G}{6} \psi^2$$

The solution of the similar equation $y' + p(x)y = q(x)$ is known and equals to $y(x) = e^{-\int p(x)dx} \left(\int q(x) e^{\int p(x')dx'} dx + C \right)$. In our case the solution becomes:

$$z(\rho) = \frac{\psi}{\dot{\psi}^2} \frac{36}{G} \int_{\rho_{gas}}^{\rho} \left(p_0 - \frac{\rho}{3} - \frac{G}{6} \psi^2 \right) \frac{\dot{\psi}}{\psi^2} d\rho$$

$$\int_{\rho_{gas}}^{\rho_{liq}} \left(p_0 - \frac{\rho}{3} - \frac{G}{6} \psi^2 \right) \frac{\dot{\psi}}{\psi^2} d\rho = 0$$

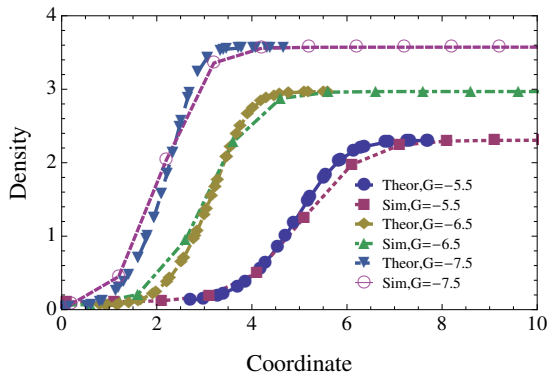
The latter equation is to satisfy boundary conditions.

PROFILES

Overall the profiles $\rho(y)$ can be restored by reversing the following equation:

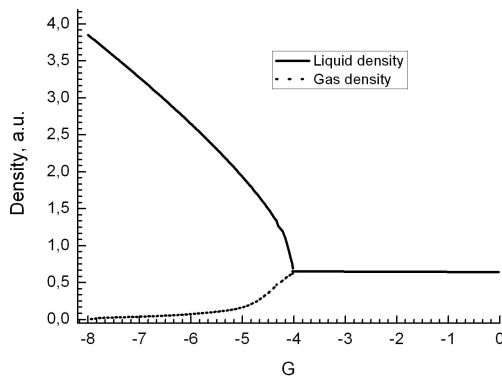
$$z = \rho'^2; \quad y = \int_{\rho_{gas}}^{\rho} \frac{d\rho'}{\sqrt{z(\rho')}}}$$

The simulation and theoretical profiles for different temperature-like parameter G are presented in the figure below.



GAS AND LIQUID BRANCHES

One can solve the system of equations to obtain not only profiles but also gas and liquid densities depending on temperature-like parameter G :



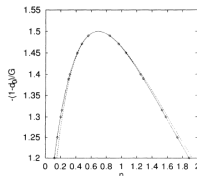
THERMODYNAMIC INCONSISTENCY

Notice that the Maxwell reconstruction rule is quite different in the case of the real Shan-Chen force:

$$\int_{\rho_{gas}}^{\rho_{liq}} \left(p_0 - \frac{\rho}{3} - \frac{G}{6} \psi^2 \right) \frac{\dot{\psi}}{\psi^2} d\rho = 0$$

Usual Maxwell reconstruction rule is as follows:

$$\frac{\dot{\psi}}{\psi^2} \frac{36}{G} \int_{\rho_{gas}}^{\rho_{liq}} \left(p_0 - \frac{\rho}{3} - \frac{G}{6} \psi^2 \right) \frac{d\rho}{\rho^2} = 0$$



It is so-called a thermodynamic inconsistency which leads to different values of gas and liquid densities in comparison with the Maxwell reconstruction. One can see the difference in the figure below (courtesy of Shan and Chen). y axis is the temperature like parameter G , x axis is the density. One can see that two curves (maxwellian and shan-chen) are different.

BOUNDARY CONDITIONS

As far as the Shan-Chen model is one-component model all the boundaries conditions for one phase stay (pressure, velocity, BB conditions). However, for the wall boundary conditions one needs to do something with the Shan-Chen force which accounts for all neighbours densities. There are two approaches as to handle the solid boundaries:

- The first one is a logical choice. As far as the Shan-Chen force accounts for densities of nearest neighbours, i.e. $\mathbf{F} = -G\psi(\mathbf{x}) \sum_i w_i \psi(\mathbf{x} + \mathbf{c}_i) \mathbf{c}_i$. In this case if one wants a function ψ defined on walls, one needs to specify density ρ_{wall} . From simulations one can see that ρ_{wall} controls the contact angle.
- Another approach is to specify (not widely used) another parameter G_{ads} , which transforms a force:

$$\begin{aligned}\mathbf{F} &= -G\psi(\mathbf{x}) \sum_i w_i \psi(\mathbf{x} + \mathbf{c}_i) \mathbf{c}_i \\ &= -G\psi(\mathbf{x}) \sum_{fluid} w_i \psi(\mathbf{x} + \mathbf{c}_i) \mathbf{c}_i - G_{ads} \psi(\mathbf{x}) \sum_{wall} \mathbf{c}_i\end{aligned}$$

BE AWARE

There are a few different things which you need to know before starting working with the Shan-Chen model:

- Limited stability, basically for dynamic problems you don't want to simulate systems with smaller $G \leq -7$. Usually spurious currents coming from discretization destroy stability.
- Additional condensation and evaporation occurring in the systems
- Problems with the initialization and stabilization
- While the liquid densities are predicted correctly one needs to be aware about the vapour branch densities. Because of the discrete effects the vapour density is not predicted correctly and one needs to be accurate with the gas liquid density ratio prediction.
- The original force implementation is due to shift of velocity $\rho \mathbf{u}^{eq} = \rho \mathbf{u} + F\tau$, absolutely inconsistent choice. Gives the dependency of the surface tension on τ
- The surface tension is not specified explicitly and needs to be calculated through the Laplace law.

BUT..

But there is always something good:

- Really fast to implement and see first results
- Good for problems involving macroscopic phenomena, bulk pressures.
Not so good for interface shapes.
- Good for the simulation of liquids.
- Be always in a stable regime. Match your non-dimensional parameters.

The next lecture is about binary liquid model which avoids condensation.