Diffuse interface approach to CFD-based simulation of gas-liquid systems

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Diffuse Interface Approach to CFD-Based Simulation of Gas-Liquid Systems

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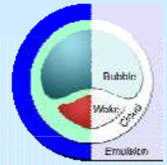
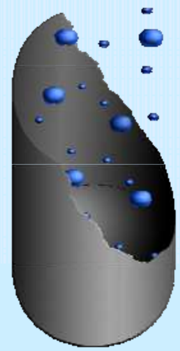
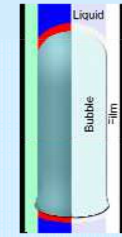
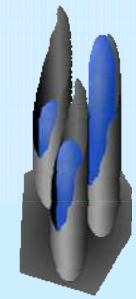
Miniaturization and Multi-phase CFD





- Process intensification and miniaturization has led to alternative technologies for multi-phase contacting (i.e. monoliths)
- The modular nature of this technology is better suited to CFD-based optimization, where the process dynamics remain consistent during industrial scale-up.
- Simulation of interfacial phenomena in small-scale geometries is complicated by a change in the predominant forces acting on the fluids.

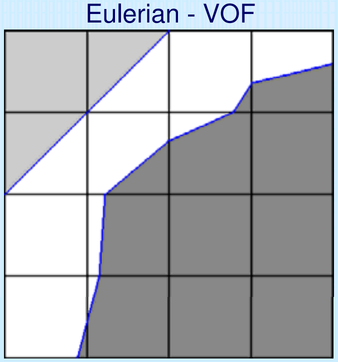




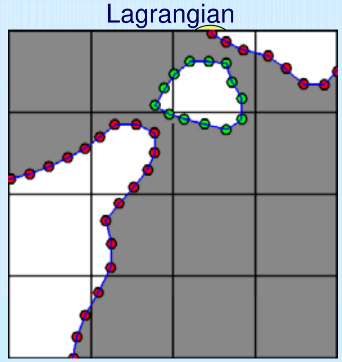
Multi-Phase CFD: Sharp Interface

Sharp interface tracking methods describe the transition between phases as a discontinuity, from which topology is reconstructed to evaluate property transitions and surface forces.

Eulerian - VOF

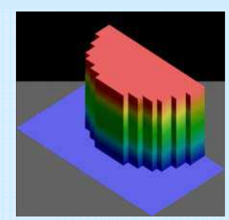


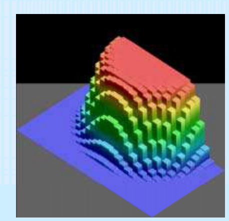
Lagrangian



Diffuse Interface Approach

- The interface between phases is described as a region of finite width, across which physical properties transition smoothly
- Phase interactions are described by resolving thermodynamic relationships within the artificially thickened interface.
- Surface forces are evaluated as a function of free energy variation, eliminating the need to reconstruct the interface geometry.
- Topological changes are handled implicitly



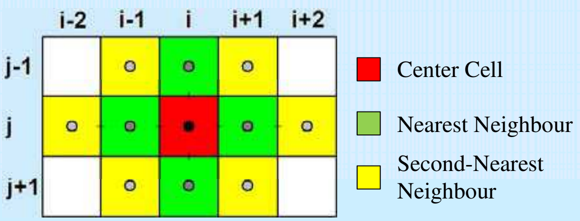


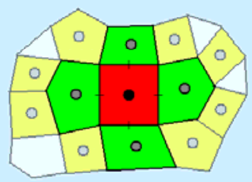
DI Approach: Current Limitations

Spontaneous Drop Shrinkage and Continuity Loss:

When the DI approach is used as an interface tracking technique, the contour $\phi = 0.5$ is frequently used to delineate between phases. While ϕ is conserved, the area within the contour is not.

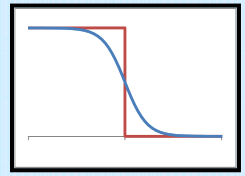
Application To Non-Uniform Meshes and Surface Force Approximations

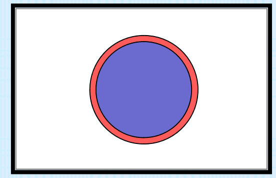




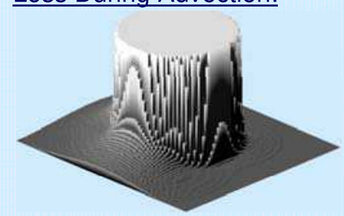
Continuity Loss: Sources and Effects

Initial Conditioning:





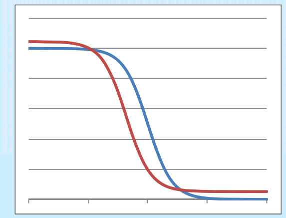
Loss During Advection:



Spontaneous Drop Shrinkage:

$$H(\phi) = \int_V Surface\ Energy + Bulk\ Free\ Energy$$

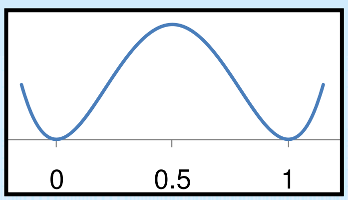
Assume:	Negligable Volume, Near Zero	Infinite Volume, Dominant energy
Reality:	Concentration of Free Energy on Interface	Finite Volume, Near Zero



Conventional Approach: Double-Well Function

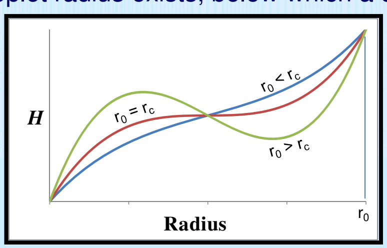
Simplified Energy Density Function:

$$f_{Double-Well}(\phi) = 0.25\phi^2(1-\phi)^2$$



Spontaneous Drop Shrinkage: Critical Radius 2-D

For a set interface width and computational domain volume, a critical droplet radius exists, below which a droplet will eventually disappear.



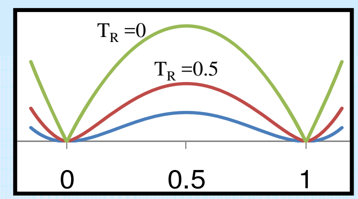
$$r_C \approx \left(\frac{\sqrt{6}}{8\pi} V\varepsilon\right)^{1/3}$$

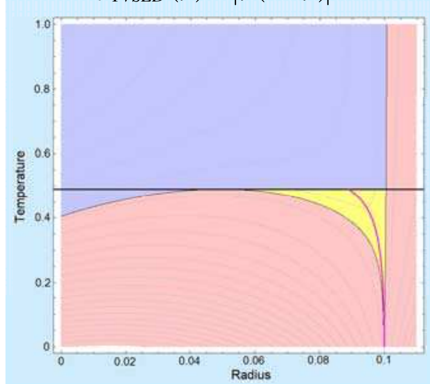
Yue et al., J. Comp. Phys., 223 (2007)

Proposed Approach: TVSED Function

Temperature Variant SEDFunction:

$$f_{TVSED}(\phi) = |\phi(1-\phi)|^{1+T_R}$$





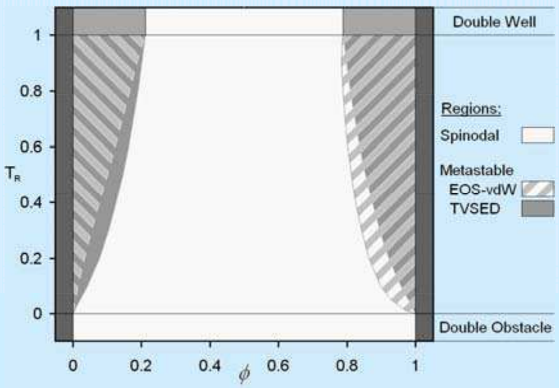
Critical Radius – 2D

$$r_c = \left[\frac{\sqrt{1+2T_R}}{\sqrt{2}(T_R+1)}\left(\frac{1+2T_R}{4T_R}\frac{V}{\pi}\right)^{T_R} \ldots \ldots \varepsilon\ {}_2F_1\left[\frac{1}{2}, -\frac{(1+T_R)}{2}; \frac{3}{2}; 1\right]\right]^{\frac{1}{2T_R+1}}$$

Continuity Loss During Advection

Continuity loss during advection occurs due to the formation of meta-stable mixtures in the bulk phases, caused by poor separation dynamics.

Thermodynamic Regions



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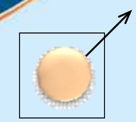
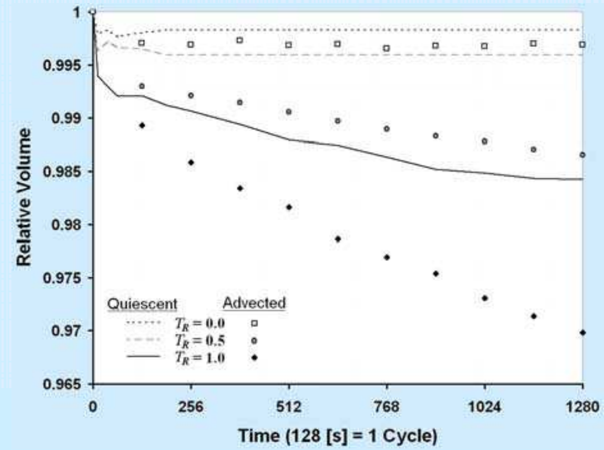
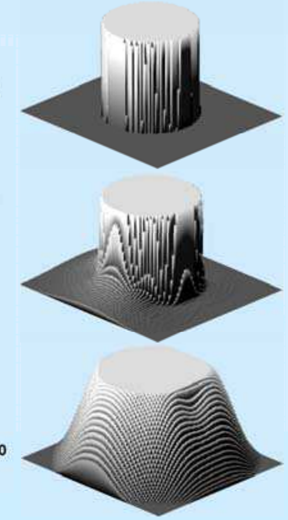
Diagonal Advection Simulations







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Two-Phase Flow: Momentum Transfer

Navier-Stokes for Laminar Flow:

$$\rho\left[\frac{\partial U}{\partial t} + \nabla\cdot(UU)\right] = -\nabla\cdot \mathrm{P} + \nabla\cdot\left[\mu\left(\nabla U + \nabla U^{T}\right)\right] - \rho\vec{g}$$

Surface forces accounted for in the pressure tensor.

Continuity:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho U) = 0$$

Note: As per Ding et al. (2007), the volume averaged velocity is used to obtain a solenoidal velocity field, thereby simplifying the PISO algorithm used for determining the pressure field.

Ding, H., Spelt, P.D.M., Shu, C., Diffuse interface model for incompressible two-phase flows with large density ratios, J. of Comp. Phys., 226 (2007), 2078-2095.

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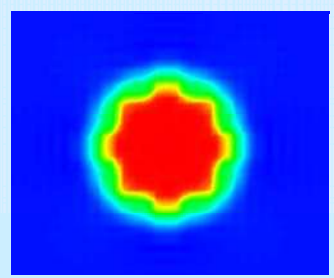
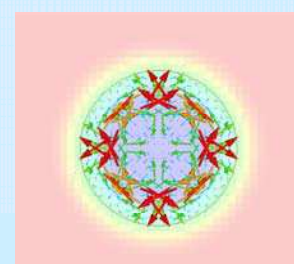
Pressure Tensor: Surface Force Est.

The pressure tensor for diffuse interface simulations is commonly based on the Korteweg tensor, with isotropic terms incorporated into the isotropic pressure, p.

$$\nabla\cdot P = \nabla p - \lambda\left(\nabla\left(\left|\nabla\phi\right|^{2}\right) - \nabla\cdot\left(\nabla\phi\otimes\nabla\phi\right)\right)$$



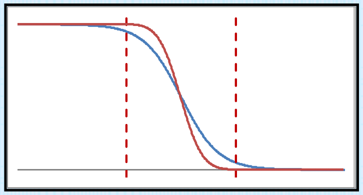


Surface Force and Gamma Filtering

By applying a filter to ϕ, variations in the pressure tensor can be localized to the center of the interface where ϕ is more linear, minimizing the error introduced by low-order estimates of $\nabla\phi$

$$\phi^* = 0.5 + 0.5\sin(\theta)$$

$$\theta = \left[\min(\max(\phi,\varphi), 1-\varphi) - 0.5\right]\frac{\pi}{1-2\varphi}$$



$$\nabla \cdot P = \nabla p - \lambda^*\left[\nabla\left(\left|\nabla\phi^*\right|^2\right) - \nabla\cdot\left(\nabla\phi^*\otimes\nabla\phi^*\right)\right]$$

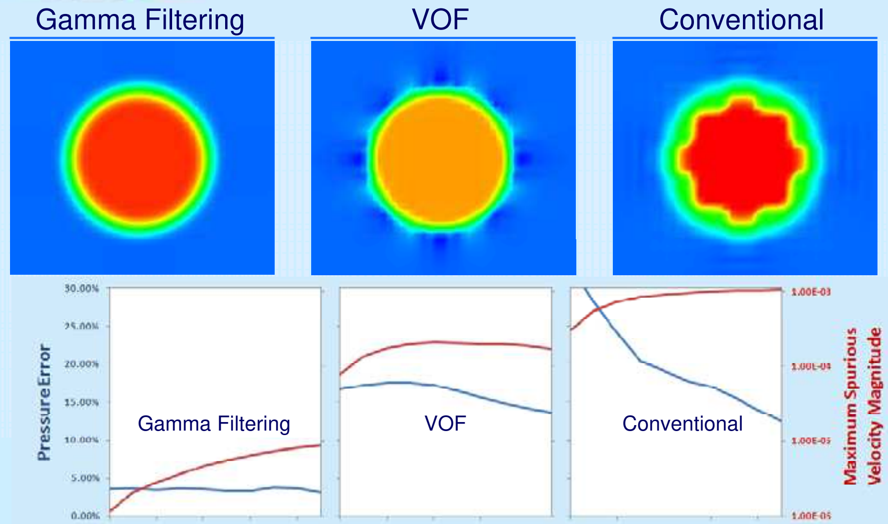
$$\beta = \left(\frac{\pi}{2(1-2\varphi)}\right)^2$$

$$\lambda^*\nabla\left(\left|\nabla\phi^*\right|^2\right) = \lambda^* 2\beta\left|\cos(\theta)\nabla\phi\right|\left\{\cos(\theta)\nabla\left|\nabla\phi\right| - \delta_\phi 2\sqrt{\beta}\left|\nabla\phi\right|\sin(\theta)\nabla\phi\right\}$$

$$\delta_\phi = \begin{matrix} 1 & \varphi < \phi < 1-\varphi \\ 0 & \phi \geq 1-\varphi, \phi \leq \varphi \end{matrix}$$

$$\lambda^*\nabla\cdot\left(\nabla\phi^*\otimes\nabla\phi^*\right) = \lambda^*\beta\left\{\cos^2(\theta)\left[(\nabla^2\phi)(\nabla\phi) + (\nabla\phi)\cdot\nabla(\nabla\phi)\right] - 2\sqrt{\beta}\sin(2\theta)(\nabla\phi\otimes\nabla\phi)\cdot\nabla\phi\right\}$$

Surface Force Results



Summary

- While the diffuse interface approach to interface tracking has advantages over the sharp interface approach for modeling small-scale flows, it's application has been limited due to continuity losses and the need for highly structured grids.
- The current practice of adopting the double-well function is partially responsible for the observed loss in continuity. By using an energy density for immiscible fluids, overall phase continuity is improved.
- Estimates for pressure can be improved through the use of a filtering parameter, limiting pressure variations to the central region of the interface where the equilibrium profile is linear.
- These improvements enable the use of the diffuse interface technique on unstructured grids, a requirement for most practical applications where it may be of use.

Questions?

Scalar Transport Equations:

Convective Cahn-Hilliard Equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi U) + \nabla \cdot (\Gamma J) = 0$$

Diffusive Flux, J, maintains the interface profile through chemical potential gradients, $\nabla \eta$:

$$J = -\nabla \eta = \frac{\lambda}{\varepsilon^2}\left(\varepsilon^2 \nabla(\nabla^2 \phi) - f''(\phi)\nabla \phi\right)$$

ε - Capillary Width

λ - Mixing Energy Density

f - Free energy density governing interfacial dynamics and the equilibrium profile of ϕ

Multi-Phase CFD: Approach Limitations

The ability of each method to resolve complex multi-phase flow is often limited by shortcomings inherent to the numerical approach.

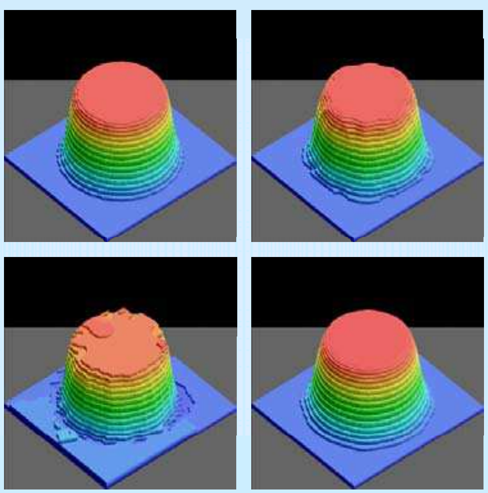
Lagrangian	Eulerian	
Front Tracking	Sharp Interface (VOF)	Diffuse Interface (PF)
• Book keeping • Complex Topology • Coalescence & Breakup • CSF model	• CSF model • Coal. & Breakup • Interface smearing and reconstruction	• Larger grid needed to resolve interface • 4th order derivative → High order schemes • Spontaneous drop shrinkage

While a number of these limitations have been addressed, the associated increase in complexity often results in a method which is too cumbersome for general application to multi-phase flow problems.

Pressure Profiles: Method Comparison

Phase Field

Grad Gamma



VOF

CSF-Kim