Impact of Recent Advancements in Multiphase Science on Nuclear Reactor Thermal-Hydraulics and Safety Studies

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Background

- Progress in multiphase science and technology has been driven to a large extent by nuclear reactor thermal-hydraulics
- However, needs for obtaining solutions to a variety of practical questions have had both pros and cons
  - Needs for solutions stimulate research stimulation
  - Urgency of producing results limits systematic investigations of the underlying physics
- Consequently, the maturity of this field has been questioned in the past, in particular as compared to the single-phase fluid mechanics and heat transfer

Presentation Overview

- State of knowledge and progress made in the issues
  - theoretical fundamentals of multiphase fluid mechanics and heat transfer
  - formulation and limitations of closure laws (models vs. correlations)
  - two-phase flow turbulence
  - boiling and condensation heat transfer
  - importance of understanding of the experimental and modeling uncertainties
  - validation vs. tuning
  - scaling principles and limitations
  - and challenges associated with next generation reactors
- Illustrations
  - from micro-scale phenomena, at or below the individual bubble level, to macroscale, such as the physico-chemistry of core meltdown phenomena

Fluid Mechanics of Multiphase Flow

- Typical modeling concepts
  - Eulerian (stationary) frame of reference
    - DNS/Interface-tracking method
    - RANS level methods
  - Eulerian/Lagrangian frame of reference
- Consistency of RANS-level modeling concept of gas/liquid flows
  - Formulation of RANS equations of motion
  - Use of ‘conservation’ principles

Formulation of RANS Equations of Motion

- Ensemble averaged (multifield) momentum equations become

continuous liquid

$$\frac{\partial[(1-\alpha)\rho_c\bar{\mathbf{v}}_c]}{\partial t}+\nabla\cdot[(1-\alpha)\rho_c\bar{\mathbf{v}}_c\bar{\mathbf{v}}_c]=-(1-\alpha)\nabla p_c+(p_c-p_c^i)\nabla\alpha$$
$$+(1-\alpha)\nabla\cdot\underline{\underline{\tau}}_c-(\tau_c-\underline{\underline{\tau}}_c^i)\cdot\nabla\alpha+(1-\alpha)\rho_c\mathbf{g}+\mathbf{F}_c^i-\Gamma\mathbf{v}_c^i$$

dispersed gas/vapor

$$\frac{\partial\left(\alpha\rho_{d,k}\bar{\mathbf{v}}_{d,k}\right)}{\partial t}+\nabla\cdot\left(\alpha\rho_{d,k}\bar{\mathbf{v}}_{d,k}\bar{\mathbf{v}}_{d,k}\right)=\alpha_k\rho_{d,k}\mathbf{g}-\alpha_k\rho_m\mathbf{g}+\mathbf{F}_{d,k}^i+\Gamma\mathbf{v}_{d,k}^i$$

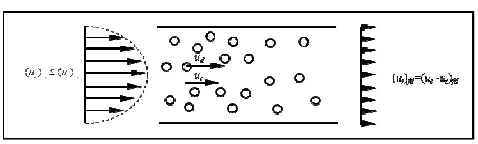
- Desired form of dispersed field equations used by CFD codes is

dispersed field-*k*

$$\frac{\partial\left(\alpha_k\rho_{d,k}\bar{\mathbf{v}}_{d,k}\right)}{\partial t}+\nabla\cdot\left(\alpha_k\rho_{d,k}\bar{\mathbf{v}}_{d,k}\bar{\mathbf{v}}_{d,k}\right)=-\alpha_k\nabla p_{d,k}-(p_{d,k}-p_{d.k}^i)\nabla\alpha_k$$
$$+\alpha_k\nabla\cdot\underline{\underline{\tau}}_{d,k}+(\underline{\underline{\tau}}_{d,k}-\underline{\underline{\tau}}_{d,k}^i)\cdot\nabla\alpha_k+\alpha_k\rho_{d.k}\mathbf{g}+\mathbf{F}_{d,k}^i+\Gamma_k\mathbf{v}_{d,k}^i$$

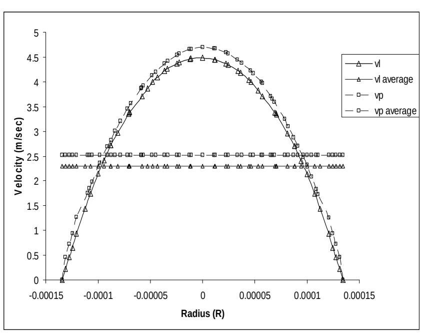
Implication of Misinterpretation of Dispersed Field Formulation

- Horizontal flow with gas field stress shear ignored (Tiwari et al.)

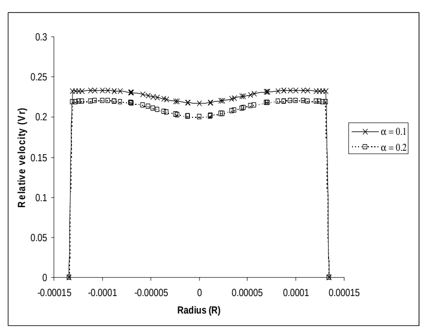


$(u_r)_{fd}\approx 0$

Actual relative velocity



Calculated gas and liquid velocities



Calculated relative gas-to-liquid relative velocity

Standard Two-Field Formulation of Dispersed Flow Models

- Phasic Momentum Conservation equations
  - Liquid $$\frac{\partial[(1-\alpha)\rho_l\mathbf{v}_l]}{\partial t}+\nabla\cdot[(1-\alpha)\rho_l\mathbf{v}_l\mathbf{v}_l]=-(1-\alpha)\nabla p+(1-\alpha)\nabla\cdot\boldsymbol{\tau}+(1-\alpha)\rho_l\mathbf{g}+\mathbf{F}^i_{v-l}$$
  - Gas $$\frac{\partial(\alpha\rho_v\mathbf{v}_v)}{\partial t}+\nabla\cdot(\alpha\rho_v\mathbf{v}_v\mathbf{v}_v)=-\alpha\nabla p+\alpha\nabla\cdot\boldsymbol{\tau}+\alpha\rho_v\mathbf{g}+\mathbf{F}^i_{l-v}$$
- Phasic Energy Conservation equations
  - Liquid $$\frac{\partial[(1-\alpha)\rho_l h_l]}{\partial t}+\nabla\cdot[(1-\alpha)\rho_l h_l\mathbf{v}_l]=-(1-\alpha)\nabla\cdot\mathbf{q}''+(1-\alpha)\frac{Dp}{Dt}+\Gamma_l h^i_l$$
  - Gas $$\frac{\partial(\alpha\rho_v h_v)}{\partial t}+\nabla\cdot(\alpha\rho_v h_v\mathbf{v}_v)=-\alpha\nabla\cdot\mathbf{q}''+\alpha\frac{Dp}{Dt}+\Gamma_v h^i_v$$
- Major modeling assumptions:
  - Local pressures of both phases are the same
  - For each phase, shear stress is proportional to local phase concentration
  - Interfacial forces add-up to zero

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Use of Conservation Principles

- Material conservation principles in Newtonian Fluid Mechanics are for
  - Mass
  - Momentum
  - Energy
- In the modeling of gas/liquid flows attempts have been made to introduce additional pseudo-conservation (or transport) equations for
  - Interfacial area concentration
  - Void fraction
- Ad-hoc additions of unphysical extra variables (e.g., pressure) have also been made for purely numerical reasons (solver convergence problems)
- Such artificial steps do not contribute to the 'maturity' of the field and may lead to serious misperception and prediction errors

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Interfacial Area Concentration (or Density)

- As measured quantity, interfacial area concentration represents very useful concept to improve the understanding of flow topology
- Interfacial area transport equation is given by

$$\frac{\partial A_i'''}{\partial t} + \nabla \cdot (\mathbf{v}_i A_i''') = \sum_j S_j$$

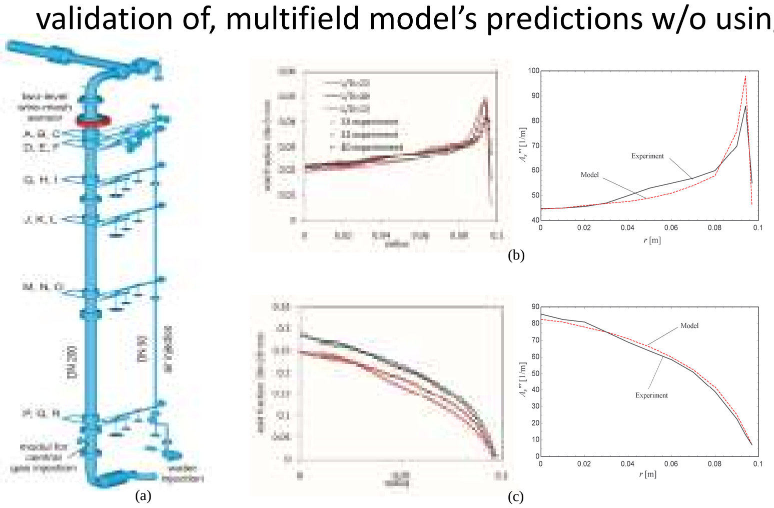
- Weak points

  The accuracy of predictions is based on the form of the RHS of the transport equation, given via several experimentally-tuned correlations

  Temporal changes of A_i''' (such as the evolution od interface velocity) cannot be measured

Use of Interfacial Area Concentration

- Interfacial area concentration can be deduced from, or used in the validation of, multifield model's predictions w/o using transport equation



Predicted and measured volumetric concentration and interfacial area density for bubbles of different sizes in TOPFLOW experiment (Prasser et al., 2007):

(a) experimental facility,

(b) 3 mm bubbles,

(c) (20 mm bubbles

Drift Flux Concept

- Very attractive computationally, since replaces a PD conservation equation with an algebraic relationship

$$\langle u_v\rangle = \langle j_v\rangle = \langle \alpha_v\rangle (C_o\langle j\rangle + V_{vj})$$

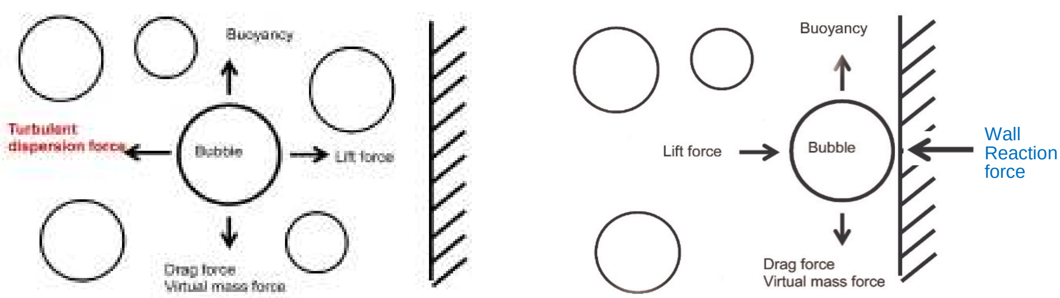
- Main application: to express average void fraction as a function of flow quality

$$\langle \alpha\rangle = \left[C_o\left(1+\frac{1-x}{x}\frac{\rho_v}{\rho_l}\right) + \frac{\rho_v V_{vj}}{Gx}\right]^{-1}$$

- Conceptual problem: two parameters, both varying with a change in either $\langle j_v\rangle$ or $\langle j\rangle$; thus, they cannot be determined independently from experiments
- Practical problem: for fixed $\langle j_v\rangle$, $\langle j\rangle$ and pressure, both C_o and V_{vj} vary dramatically with thermal conditions (adiabatic vs. heated channels)
- Restriction: applicable to one-dimensional models only
- Conclusion: DF concept is a high-uncertainty correlation not a physical model

Formulation and Limitations of Closure Laws

- Standard form of total interfacial force between continuous and dispersed fields is, $\mathbf{F}^i_{l-v} = -\mathbf{F}^i_{v-l} = \mathbf{F}^D_{l-v} + \mathbf{F}^{VM}_{l-v} + \mathbf{F}^L_{l-v} + \mathbf{F}^{TD}_{l-v} + \ldots$
- The concept is limited to the bulk of fluid away from solid walls



- Confusing question: how to account for the effect of the wall?

Formulation and Limitations of Closure Laws

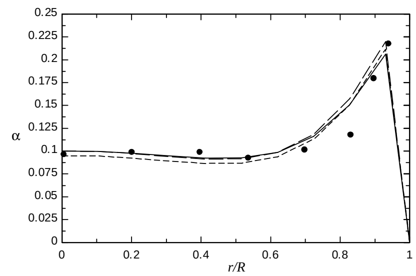
- In turbulent flows, lateral (or radial) void distribution can be evaluated based on th e balance between lift and turbulent dispersion forces

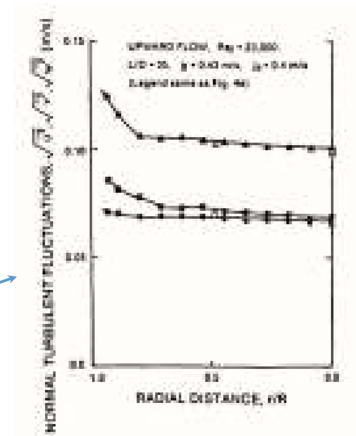
$$\mathbf{F}_{l-v}^{L} + \mathbf{F}_{l-v}^{TD} = 0$$

where

$$\vec{\mathbf{F}}_{l-v}^{L} = -C_L \alpha_v \rho_l \left(\overline{\mathbf{v}}_l - \overline{\mathbf{v}}_v\right) \times \left(\nabla \times \overline{\mathbf{v}}_l\right)$$

$$\mathbf{F}_{l-v}^{TD} = -C_{TD} \alpha_v \rho_l \kappa_l \nabla \alpha_v$$



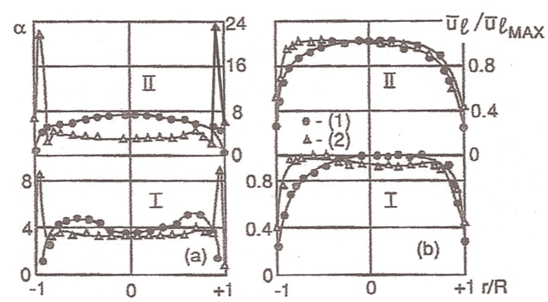


- Not fully-resolved issue: how to properly account for the nearly-constant radial component of kinetic energy?

Formulation and Limitations of Closure Laws

- In laminar flows, lateral (or radial) forces get practically reduced to a single component, i.e., the lift force, $\vec{\mathbf{F}}_{l-v}^{L}$
- If this is the case, no force equilibrium can be reached in the presence of lateral velocity gradient

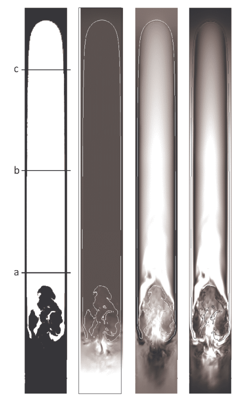
Predicted void fraction and liquid velocity for two values of Reynolds Number I: Re=990, II; Re=2280 [Valukina et al. 1979]



- Open questions:
  - Is laminar fully-developed flow possible?
  - Does bubble-induced turbulence result in turbulent-dispersion force?

Limitations of Multifield Modeling Concept

- Multidimensional ensemble-averaging concept is limited to dispersed flows, where the location of bubbles can be statistically considered to be a function of local flow conditions.
- Slug flows do not belong to such a category, since lateral phase distribution is predominantly determined by the shape of Taylor bubbles
- Nevertheless, good predictions have already been demonstrated of slug flows using 3-D multifield models
- Conclusion: model application has been stretched beyond conceptual limitations
- It is important to notice that a one-dimensional two-fluid model of slug flows is still conceptually consistent



DNS simulation od slug flow [Behafarid ant al., 2015]

Two-Phase Flow Turbulence

- All RANS models of turbulence are problematic, both single-phase and, in particular, two- or multiphase
- Highly tuned, fine-grid models are not applicable to gas/liquid flows, due to limitations imposed by bubble size
- Bubble-induced turbulence is normally determined using simple algebraic formula,
- Turbulence experts are mainly interested in velocity fluctuations. Thermal aspects of turbulence are still treated for both single- and two-phase flows via a 'magic' turbulent Prandtl number, $\mathrm{Pr}_t = 0.9$

Illustration of Generic Turbulence Modeling Issues

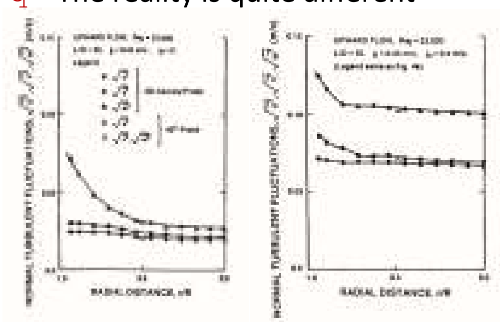
- Turbulent viscosity is normally given by

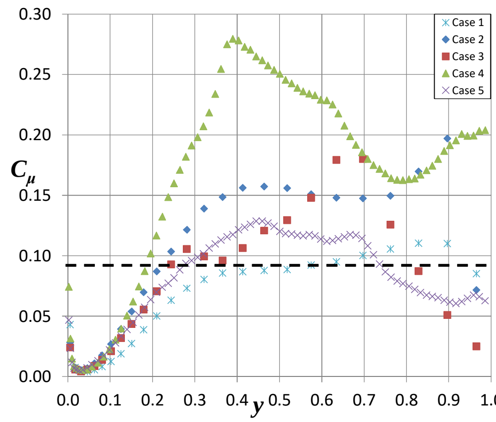
$$\nu_t = C_\mu \frac{k^2}{\varepsilon}$$

where $C_\mu = 0.09 \approx (0.3)^2 = constant$

is based on isotropic turbulence assumption

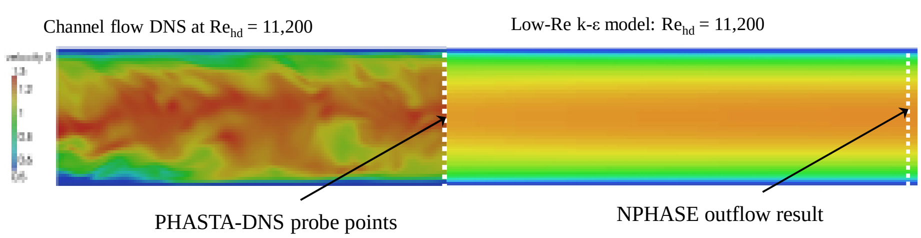
- The reality is quite different

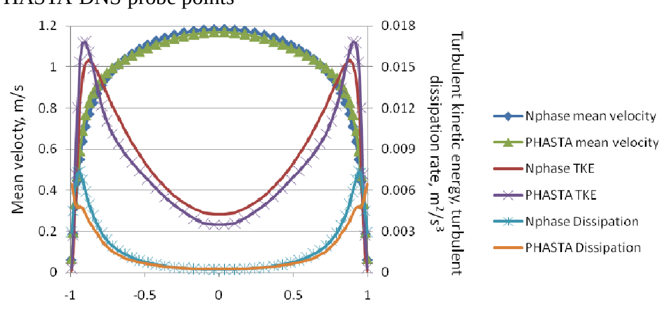




DNS-predicted lateral distribution of C_μ (Bolotnov & Podowski, 2012). Case-1 corresponds to single-phase flow, and Case-2 through Case-5 represent two-phase flows for different bubble sizes and gas/to-liquid density ratios

DND and RANS Predictions for Turbulent Pipe Flow [Bolotnov et al., 2012]





Boiling and Condensation Heat Transfer

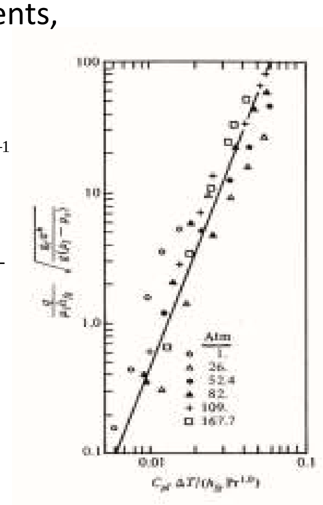
- Traditional approach to surface boiling
  - Correlations with varying numbers of adjustable coefficients, preferably applicable to a wide range of conditions
  - Example: Roshenow correlation for pool boiling

$$\frac{q''}{\mu_l h_{fg}}\sqrt{\frac{\sigma}{g(\rho_l-\rho_v)}} = B(\varphi\Delta T)^{m+1}$$

$$\varphi^{m+1} = \frac{k_l^{0.5}\rho_l^{17/8}c_{p,l}^{19/8}h_{fg}^{(m-23/8)}\rho_g^{(m-15/8)}}{\mu_l\rho_{fg}^{9/8}\sigma^{(m-11/8)}T_{sat}^{(m-15/8)}}$$

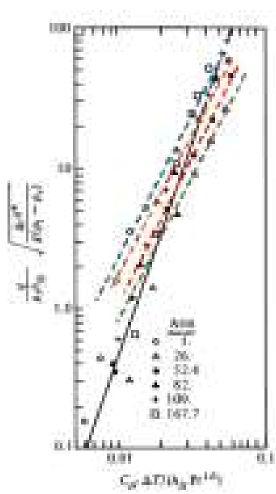
$$B = \frac{\sqrt{2}}{\pi}\frac{C_1C_2^{5/3}C_3^{12}\rho_g^{(m-15/8)}}{g^{9/8}T_{sat}^{(m-15/8)}} f(r_c)$$

- Drawbacks
  - Large uncertainties
  - Limited information about underlying physics



Boiling and Condensation Heat Transfer

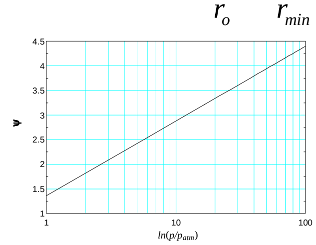
- Step toward mechanistic modeling (Podowski)
  - Based on bubble nucleation principles
  - Explicit effect of pressure
  - Single adjustable coefficient (surface property-dependent)
- Advantages
  - Improved accuracy
  - Partially mechanistic
- Next step
  - Complete model of bubble ebullition cycle



$$\Delta T_w^* = C_{pb}\left(q''^*\right)^{0.5}$$

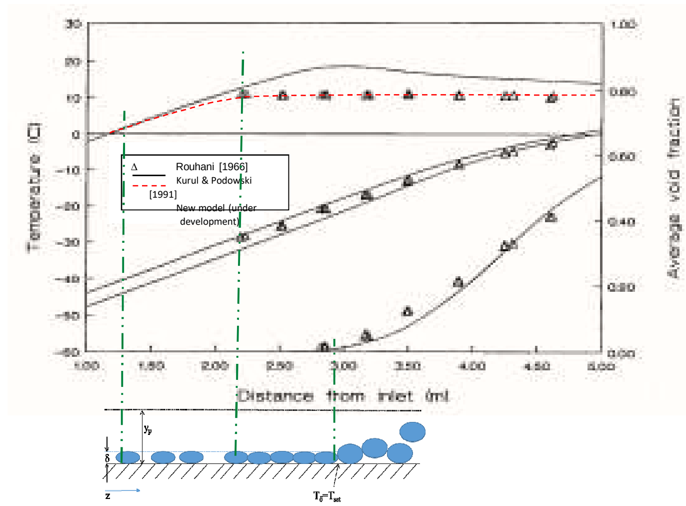
$$C_{pb} = 2\Psi\frac{c_p}{h_{fg}Pr}\sqrt{\frac{2\mu_l v_{fg}T_{sat}}{k_l}\sqrt{\sigma g(\rho_l-\rho_v)}}$$

$$\Psi+\sqrt{\Psi^2-1} = \frac{r_{max}}{r_o} = \frac{r_o}{r_{min}}$$



Forced-Convection Boiling

- Closure laws for CFD models (Podowski)
- Approach
  - Superposition on fluid flow equations
- Example of progress
  - Model of subcooled boiling
- Existing model
  - Limited to subcooled liquid flow
- Next step
  - Better physics
  - Generalized
  - Higher accuracy



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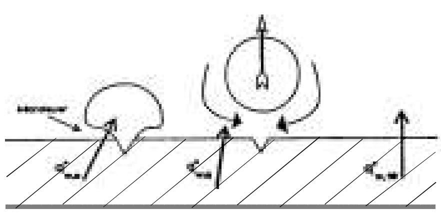
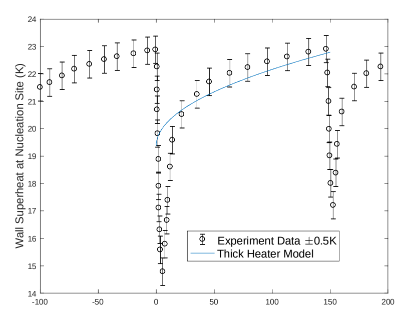
Analytical Model of Bubble Ebullition Cycle

- Major step forward
- Tested/validated for low heat-flux pool boiling
- Model for high heat fluxes still under devopment





Predictions of temperature variations in pool boiling [Wang & Podowski, 2017]

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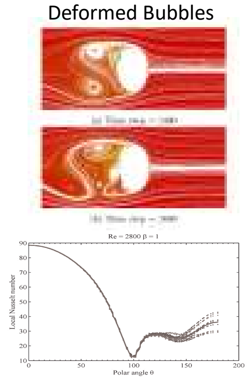
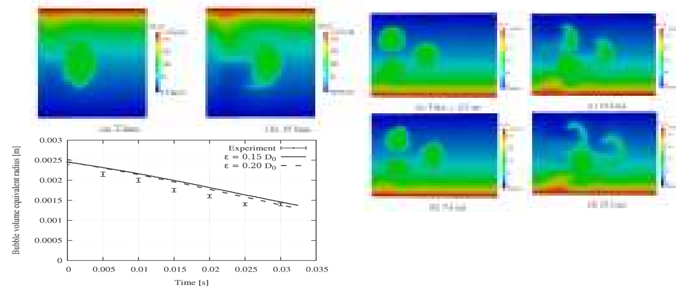
Multiscale-Based-Approach to New Closure Laws for Interfacial Heat Transfer with Phase Change (Jiao & Podowski)

- DNS-level simulations used as virtual experiments
- Mechanistic approach to simultaneous evaporation and condensation

Local heat Transfer around Deformed Bubbles



Bubble Condensation/Evaporation along heated Wall

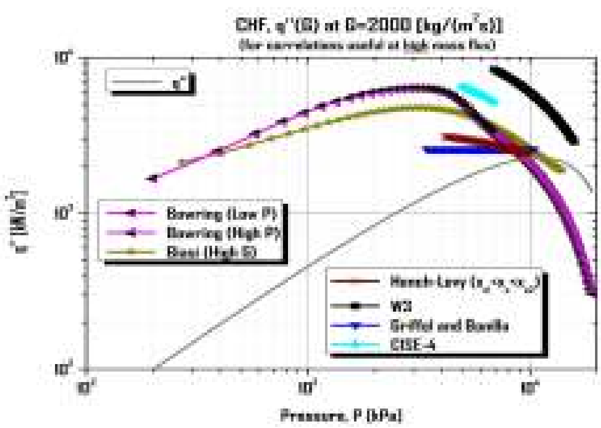


New Closure Law for Nonspherical Bubbles

$$Nu_{av}(Re,Pr,\beta) = (2+0.188Re^{0.577})Pr^{0.4}(1.979-5.237\cdot 19.16^{-\beta})$$

Critical Heat Flux

- Illustration of current predictive capabilities

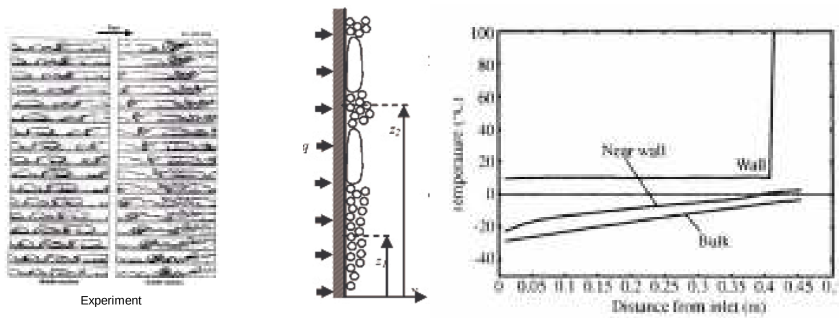


CHF calculated using different models/correlations [Piela, 2014]

- Observation: good predictions of CFD simulations not always reflect better underst anding of underlying physics

Critical Heat Flux

- Some progress has already been made to ward mechanistic modeling principle



Critical heat flux using a mechanistic model of low-quality CHF (Alajbegovic et al, 1997; Podowski .& Antal, 2002)

Table 1: Predicted critical heat fluxes.

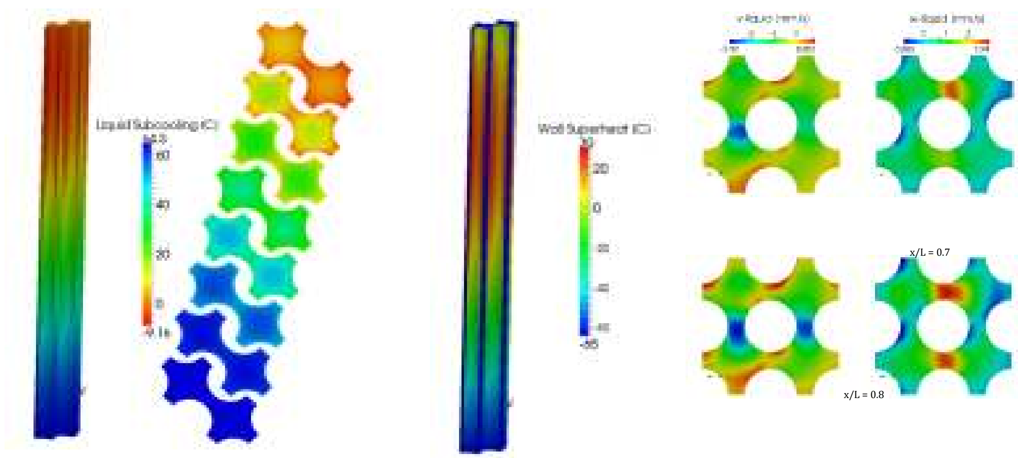
ΔT_{sub} (K)	Measured (6) (kW/m^2)	Predicted (kW/m^2)	Relative error
[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]

Table 2: Predicted critical heat fluxes.

ΔT_{sub} (K)	Measured (6) (kW/m^2)	Predicted (kW/m^2)	Relative error
[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]

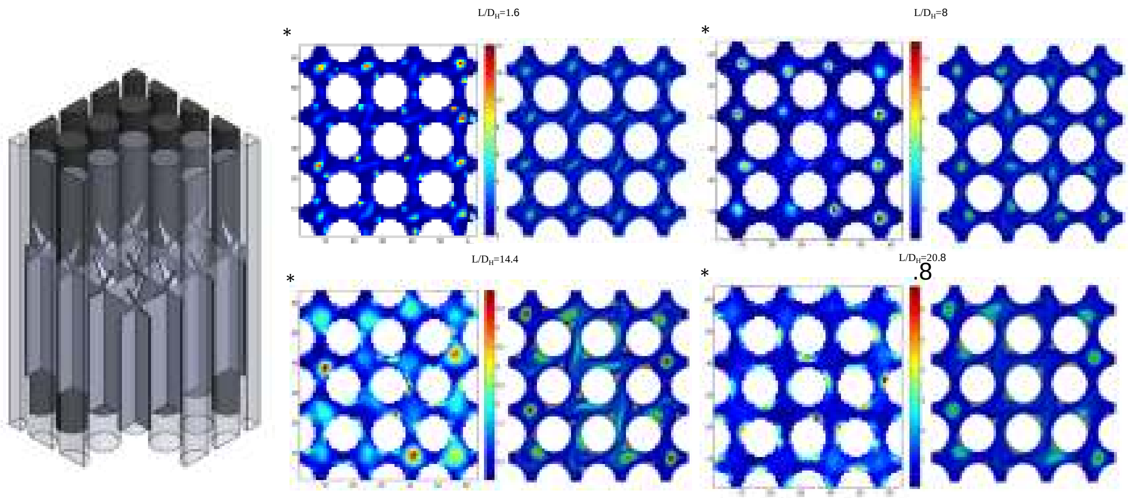
- Better treatment of near-wall bubble behavior is still needed
- Work is underway on the development of new model

Promising Applications of Multifield Model in Reactor TH: Example-1



Three-dimensional distributions of temperature, void fraction and liquid velocity along and between fuel elements in a four-channel section of reactor fuel assembly [Shaver et al., 2015]

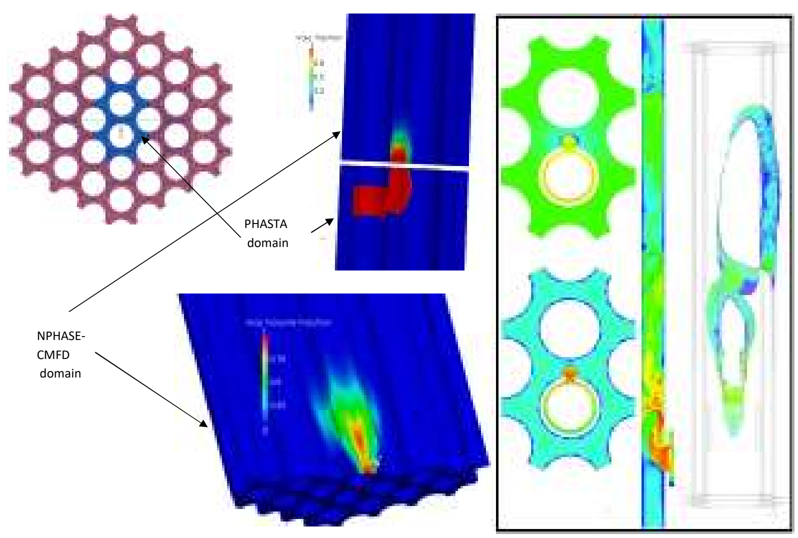
Promising Applications of Multifield Model in Reactor TH: Example-2



- Local void fraction distribution at different axial locations along a parallel-rod assembly upstream of a spacer grid (Waite & Podowski, 2017).

Promising (but rarely uesd) Approach: Multiscale Simulations

- Coupled DNS and RANS level simulations of fission product gas release from failed fuel elements of a Gen,IV liquid metal reactor following a loss-of-flow accident (Bolotnov et al, 2011).
- Color contours on the RHS include the top-views of PHASTA-calculated pressure and velocity fields, followed by a side view of the velocity field and a 3D shape of the interface colored by velocity.



Summary of Selected Multiphase Modeling Issues

- Multifield models of multiphase flow: importance of consistency of model formulation
- Model complexity should be consistent with our understanding of underlying physic (both qualitatively and quantitatively)
- In the case of varying geometry and boundary conditions (such as in the case of severe accident simulations), level of model complexity should decrease with increasing uncertainties (e.g., core meltdown progression)
- Major unresolved issue: two- and multiphase flow turbulence
- Assessment, verification and validation of component models in both stand-alone and coupled fashion, are of critical importance
- Assessment of experimental uncertainties is vital (e.g., effect of spacers, CHF)
- Results should be (nearly) independent of numerical solution schemes

Indicators of Progress (Examples)

- Improved understanding of the effect of bubble size on phase distribution in dispersed flows
- Extensive verification of closure laws of multiphase fluid mechanics, including gas/liquids and gas/liquid/solid flows
- Development and experimental validation of multiple-scale models of interfacial heat transfer with phase change (condensation and/or evaporation)
- Evidence on the ability of the multifield model to properly capture major characteristics of two-phase and heat transfer in complex geometries of reactor coolant channels
- The formulation of theoretical mechanistic models of bubble ebullition cycle

Loose Ends (Examples)

- Modeling of unstructured flow regimes, including the effect of bubble deformation on interfacial forces
- Understanding the mechanisms behind flow regime transition
- Predictive capabilities of developing flows
- Mechanistic modeling of boiling heat transfer at high heat fluxes, up to temperature excursion and CHF
- RANS-level modeling of turbulence (both singe-phase and two-phase)
- Understanding the limits of scalability of low-pressure experiments as a vehicle to formulate data base for prototypical high pressure reactor conditions
- Insufficient attention given to the importance of understanding the effect of physical (experimental) uncertainties on proper model validation and ranking of importance of selected modeling details

Thank you for your attention!