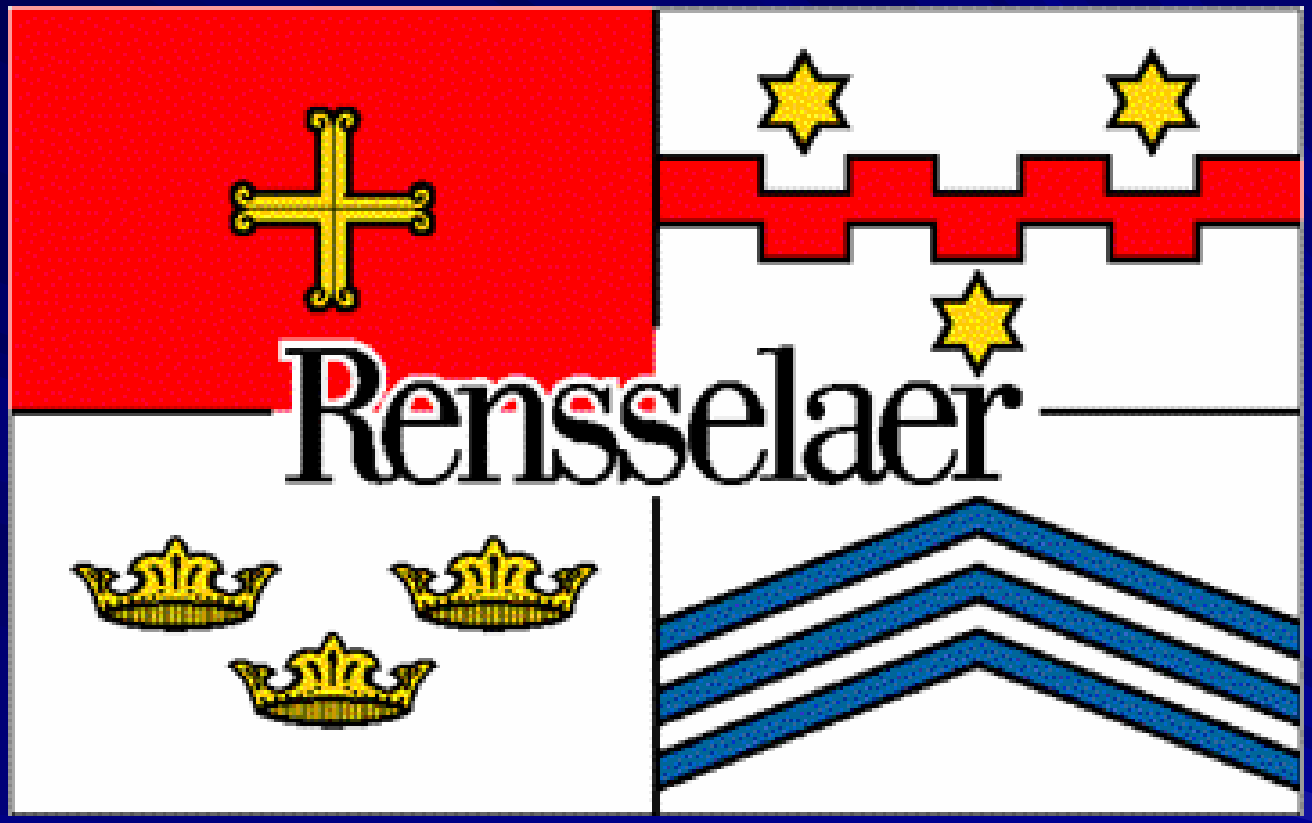

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Recent Advances in Multiphase Flow and Heat Transfer; Nuclear Engineering Perspective

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November 29, 2006

Presentation Outline

- Background
- Multiphase Flow Modeling Issues
- Illustrations of Recent Advances
- Summary

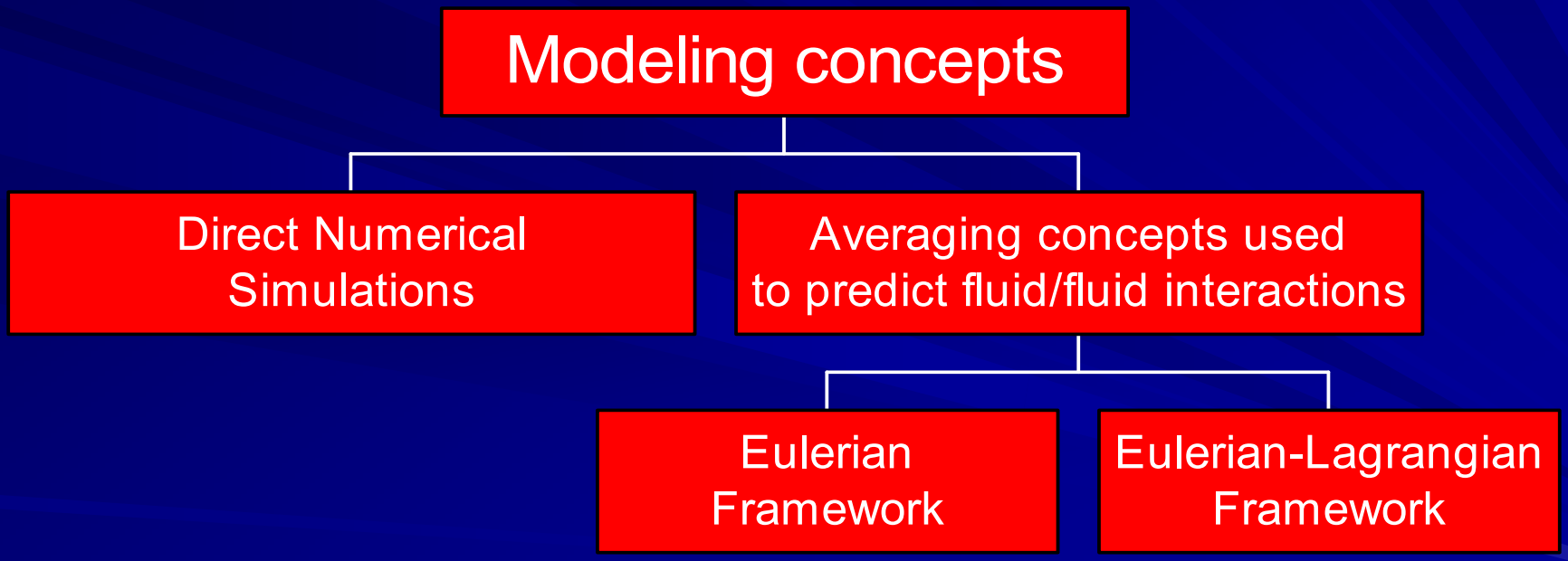
Background

Needs for advanced two-phase flow modeling methods and computational tools:

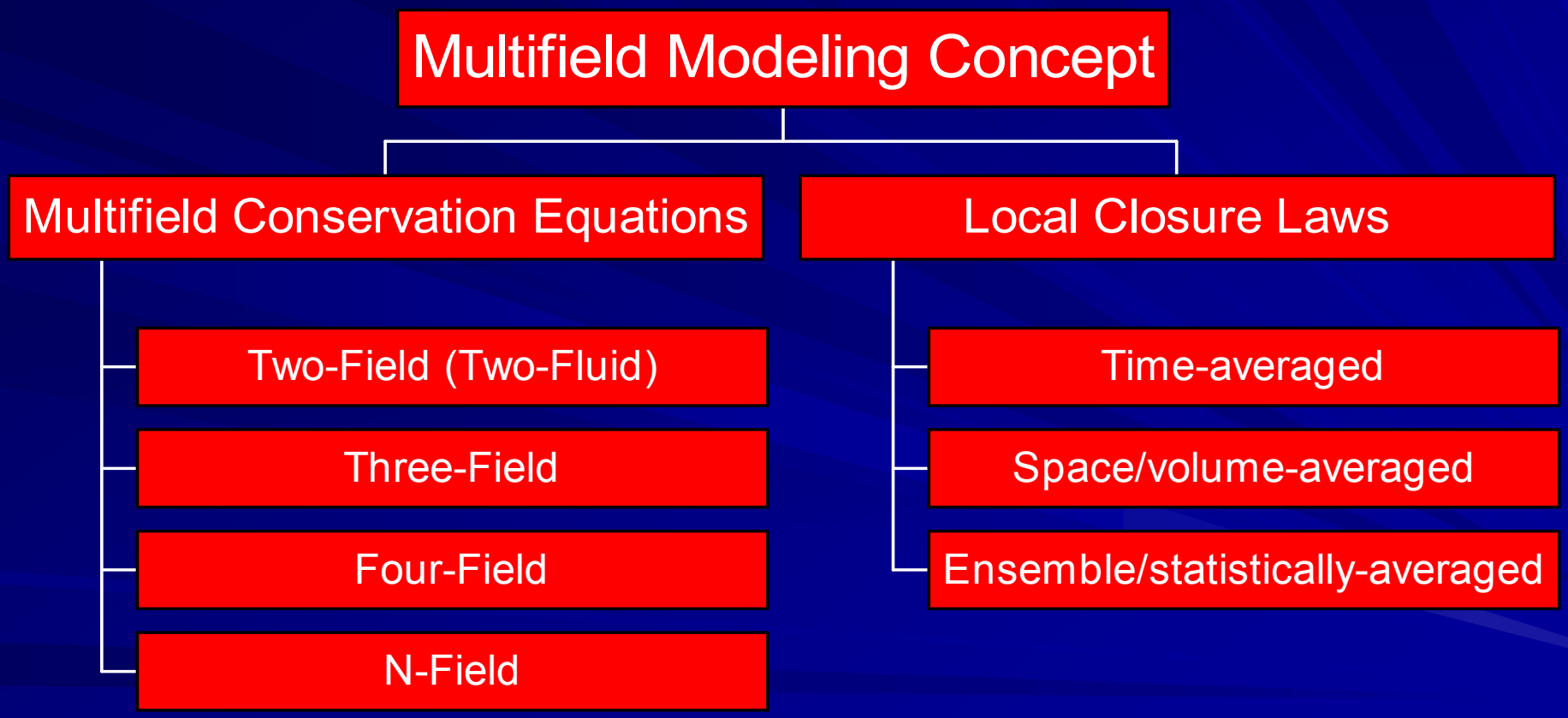
- Efficiency of power generation
- Development of next generation reactors
- Design and operation of chemical processing equipment
- Increasing safety requirements

Multiphase Flow Modeling Issues

Mechanistic Multidimensional Modeling of Multiphase Flow



Mechanistic Multidimensional Modeling of Multiphase Flow (*continued*)



Steps Toward Multiphase Model Development

Understand dominant physical phenomena

Deformable interface flow

Identify interface tracking method

First-principle "virtual" data base

Dispersed "particle" flow

Use appropriate averaging concept

Multifield Conservation Equations

- Mass

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \overline{\mathbf{v}}_k \right) = \Gamma_k$$

- Momentum

$$\frac{\partial \left(\alpha_k \rho_k \overline{\mathbf{v}}_k \right)}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \overline{\mathbf{v}}_k \overline{\mathbf{v}}_k \right) = -\alpha_k \nabla \overline{p}_k - \left(\overline{p}_k - \overline{p}_{ki} \right) \nabla \alpha_k$$
$$+ \nabla \cdot \alpha_k \left(\overline{\underline{\underline{\tau}}}_k + \underline{\underline{\tau}}_k^{Re} \right) + \alpha_k \rho_k \mathbf{g} + \mathbf{M}_k$$

- Energy

$$\frac{\partial \left(\alpha_k \rho_k \overline{e}_k \right)}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \overline{\mathbf{v}}_k \overline{e}_k \right) = -\nabla \cdot \left[\alpha_k \left(-\overline{p}_k \underline{\underline{\mathbf{I}}} + \overline{\underline{\underline{\tau}}}_k + \underline{\underline{\tau}}_k^{Re} \right) \cdot \overline{\mathbf{v}}_k \right]$$
$$-\nabla \cdot \left[\alpha_k \left(\overline{\mathbf{q}}_k'' + \mathbf{q}_k''^{Re} \right) \right] + \alpha_k \rho_k \mathbf{g} \cdot \overline{\mathbf{v}}_k$$

Major Interfacial Transfer Mechanisms

- Interfacial mass transfer:
  - bubble coalescence and breakup
  - droplet entrainment and deposition
  - particle/particle collisions
- Interfacial momentum transfer:
  - turbulence (particle-induced)
  - interfacial forces: drag, virtual mass, lift, turbulent dispersion (diffusion), wall-induced, “particle”-rotation-rotation
- Interfacial energy transfer:
  - (turbulent) heat convection
  - local phase change (evaporation/condensation)
  - inelastic collisions

Major Multiphase Flow Modeling Issues

- Consistency of formulation
  - Interpenetrating media vs. dispersed particle models
  - Force balance at equilibrium
  - Limitations of Eulerian/Eulerial frame of reference
- Flow regime-dependent closure laws
  - local vs. “particle”-size-scale models
  - flow-regime transition
  - coupling between flow topology and heat transfer modes (CHF)
- Multiscale phenomena
  - thin liquid film
  - gas/liquid/solid interactions
  - effect of surfactants and nanoparticles

Single-Phase Flow Modeling Issues

- Turbulence
  - Prandtl mixing length
  - High Re k-ε
  - Low Re k-ε
- Effect of variable fluid properties
  - Flow and heat transfer at supercritical pressure: ρ, μ, c_p, k, Pr
- Compressible flow
  - Critical flow
  - Wave propagation

Computational Issues

- Convergence and robustness of numerical solvers
  - residual tracking
  - consistency of numerical vs. physical limitations
- Multiple field modeling capabilities
  - maximum number of fields
- Accuracy and duration of simulations for transients and oscillatory flows
  - dual time-step convergence criteria
- Computational-grid-independence of results
- Ability to capture flow in complex geometries

NPHASE Code

- NPHASE is a pressure-based finite volume CMFD (Computational Multiphase Fluid Dynamics) code
- Development focused on improving robustness and convergence characteristics of multiphase flow simulations
- Built-in generic interfacial closure laws (on RHS of discretized equations
- Arbitrary (N) number of fields

Major features of NPHASE:

- choice of either segregated or coupled solvers
- primitive variables are: pressure, velocity, enthalpy, turbulent kinetic energy, and turbulence dissipation rate
- artificial dissipation used to control numerical pressure oscillations
- continuity satisfied through pressure correction equation, based on SIMPLEC

Recent Upgrades of NPHASE

- Implementation of efficient and accurate models of the properties of supecritical water and CO_2
- Encoding and coupling with NPHASE of a modified Level-Set Method
- Encoding and coupling with NPHASE of space-dependent model of reactor neutronics

Other CFD Codes Used in the Past by CMR Researchers

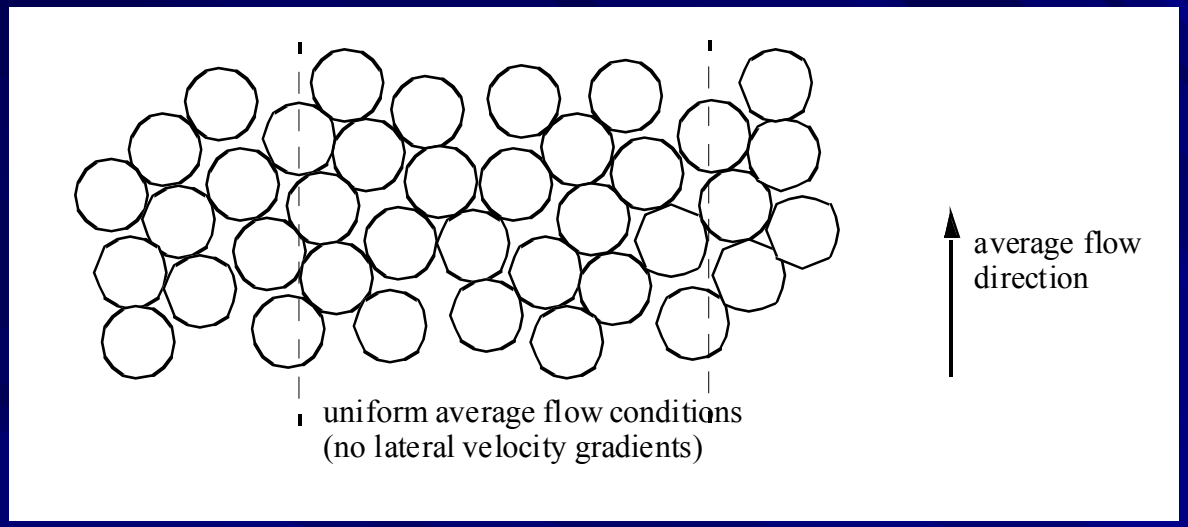
- PHOENICS
- FIDAP
- CFX
- FLUENT

Illustrations of Recent Advances*

(*) *details of recent research accomplishments at CMR can be found in the papers listed at the end of this presentation*

Consistency of Multifield Model Formulation for Dilute Dispersed Flows

Formulation of Fluid/Particle Model (Podowski, 2006)



Typical two-fluid formulation, applicable to packed particles

Particle motion (Lagrangean frame of reference)

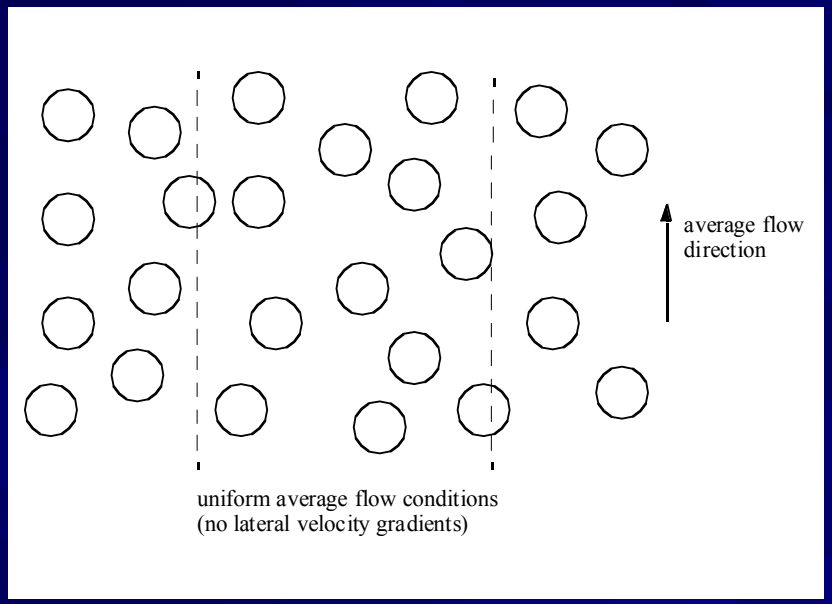
$$\rho_p \frac{d\mathbf{v}_p}{dt} = \rho_p V_p \mathbf{g} + \mathbf{F}_{p-p} - \mathbf{F}_{c-p}$$

Averaged equations (Eulerian frame of reference)

$$\frac{\partial(\alpha_d \rho_d \overline{\mathbf{v}}_d)}{\partial t} + \nabla\cdot(\alpha_d \rho_d \overline{\mathbf{v}}_d \overline{\mathbf{v}}_d) = -\alpha_d \nabla \overline{p}_d - (\overline{p}_d - p_{di})\nabla\alpha_d + \alpha_d \nabla\cdot \underline{\underline{\tau}}_d^{tot} + \left(\underline{\underline{\tau}}_d^{tot} - \underline{\underline{\tau}}_d^{i}\right)\cdot\nabla\alpha_d + \alpha_d \rho_d \mathbf{g} + \mathbf{M}_d$$

$$\frac{\partial(\alpha_c \rho_c \overline{\mathbf{v}}_c)}{\partial t} + \nabla\cdot(\alpha_c \rho_c \overline{\mathbf{v}}_c \overline{\mathbf{v}}_c) = -\alpha_c \nabla \overline{p}_c - (\overline{p}_c - p_{ci})\nabla\alpha_c + \alpha_c \nabla\cdot \underline{\underline{\tau}}_c^{tot} + \left(\underline{\underline{\tau}}_c^{tot} - \underline{\underline{\tau}}_c^{i}\right)\cdot\nabla\alpha_c + \alpha_c \rho_c \mathbf{g} + \mathbf{M}_c$$

Dilute particles do not constitute a complete "field"



Force-balance on particles

Lagrangian form

$$\rho_p \frac{d\mathbf{v}_p}{dt} = \rho_p V_p \mathbf{g} - \mathbf{F}_{c-p}$$

Eulerian form

$$\frac{\partial(\alpha_d \rho_d \bar{\mathbf{v}}_d)}{\partial t} + \nabla \cdot (\alpha_d \rho_d \bar{\mathbf{v}}_d \bar{\mathbf{v}}_d) = -\alpha_d \rho_m \mathbf{g} + \alpha_d \rho_d \mathbf{g} + \mathbf{M}_d$$

Two-fluid form of dispersed-phase momentum equation

$$\frac{\partial(\alpha_d \rho_d \bar{\mathbf{v}}_d)}{\partial t} + \nabla \cdot (\alpha_d \rho_d \bar{\mathbf{v}}_d \bar{\mathbf{v}}_d) = -\alpha_d \nabla \bar{p}_d + \alpha_d \nabla \cdot \underline{\underline{\tau}}_d^{IS} + \alpha_d \rho_d \mathbf{g} + \mathbf{M}_d$$

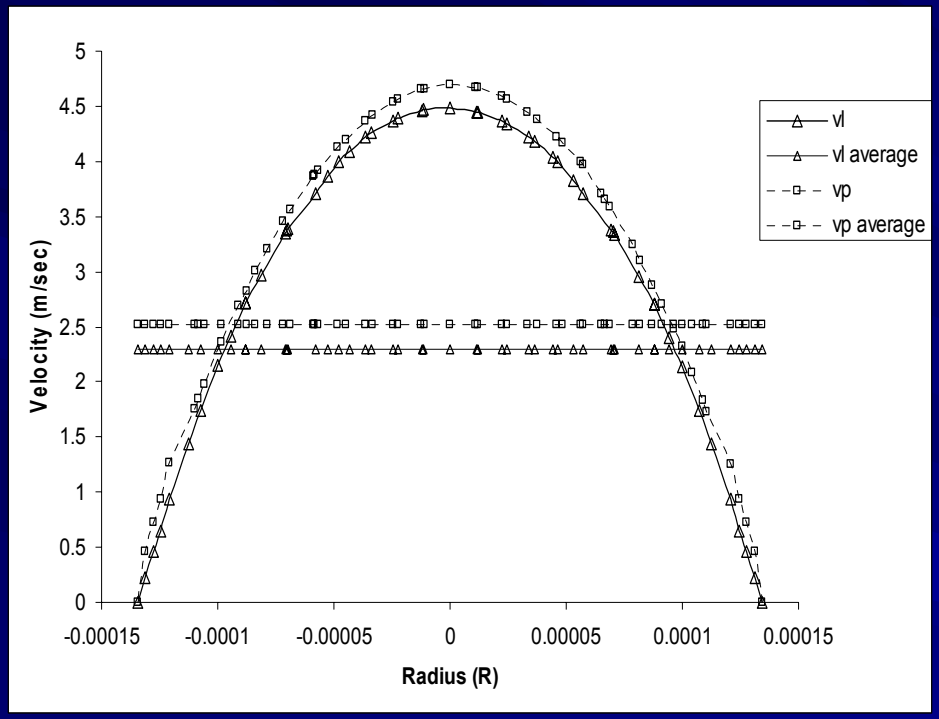
can be obtained if extra terms are defined as

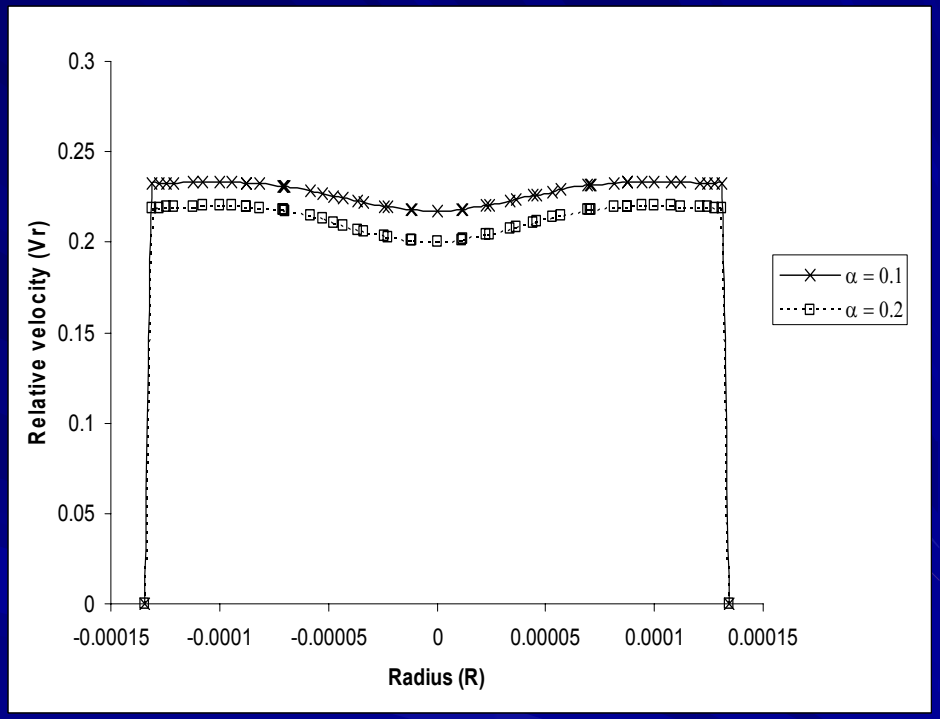
$$\underline{\underline{\tau}}_d^{IS} = \underline{\underline{\tau}}_d^{tot} = \underline{\underline{\tau}}_c^{tot}$$

$$\bar{p}_d = p_{di} = p_{ci} + \sigma K$$

Fully-Developed Dispersed Particle Flow (Tiwari et al., 2003)

(a) NPHASE result using standard Two-Field Model (with $\tau_d = 0$)





Radial velocity profiles: v_l , v_p

Relative velocity ($v_r = v_p - v_l$)

(b) NPHASE result with correct dispersed field model: $v_p = v_l$

Impact on 1-D Simulations (Podowski, 2004)

Example: RELAP5/MOD3.3 1-D model of gas/liquid vertical flow

Operating conditions:

G = 1000 kg/m^3-s, D = 2 cm,

$$\rho_f / \rho_g = 1000\ , \quad \alpha = 0.1\ , \quad \left(\frac{\partial p}{\partial z}\right)_{2\phi} \approx -900\ \mathrm{N/m^3}$$

RELAP wall-friction partitioning

$$\frac{\tau_f p_f}{A} = (1-\alpha)\left(\frac{\partial p}{\partial z}\right)_{2\phi} \frac{Z^2}{\alpha + (1-\alpha)Z^2}, \quad \frac{\tau_g p_g}{A} = \alpha\left(\frac{\partial p}{\partial z}\right)_{2\phi} \frac{1}{\alpha + (1-\alpha)Z^2}\ , \quad Z^2 = \frac{\lambda_f \rho_f \mathrm{v}_f^2}{\lambda_g \rho_g \mathrm{v}_g^2}$$

Predicted wall partitioning

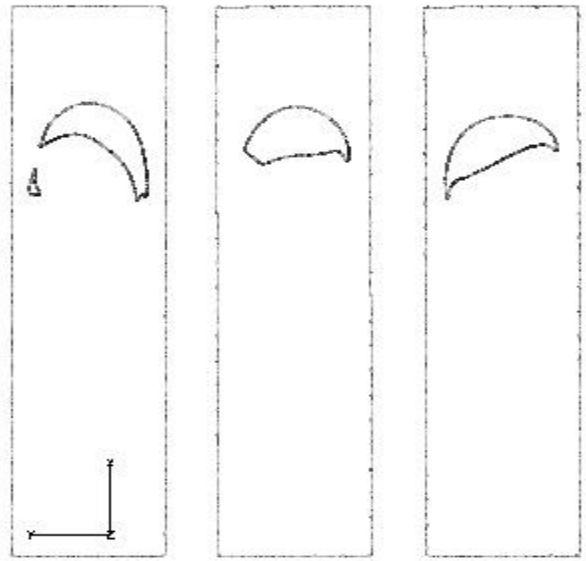
$$F^s_{f,RELAP} = -\frac{\tau_f p_f}{A} = -0.9998\left(\frac{\partial p}{\partial z}\right)_{2\phi} \approx -\left(\frac{\partial p}{\partial z}\right)_{2\phi}, \quad F^s_{g,RELAP} = -\frac{\tau_g p_g}{A} = -0.0002\left(\frac{\partial p}{\partial z}\right)_{2\phi} \approx 0$$

Correct wall shear partitioning

$$F^s_f = -\left(\frac{\partial p}{\partial z}\right)_{2\phi} \approx 800\ \mathrm{N/m^3}, \quad F^{Ind}_g = -\frac{\alpha}{1-\alpha}\left(\frac{\partial p}{\partial z}\right)_{2\phi} = 100\ \mathrm{N/m^3}$$

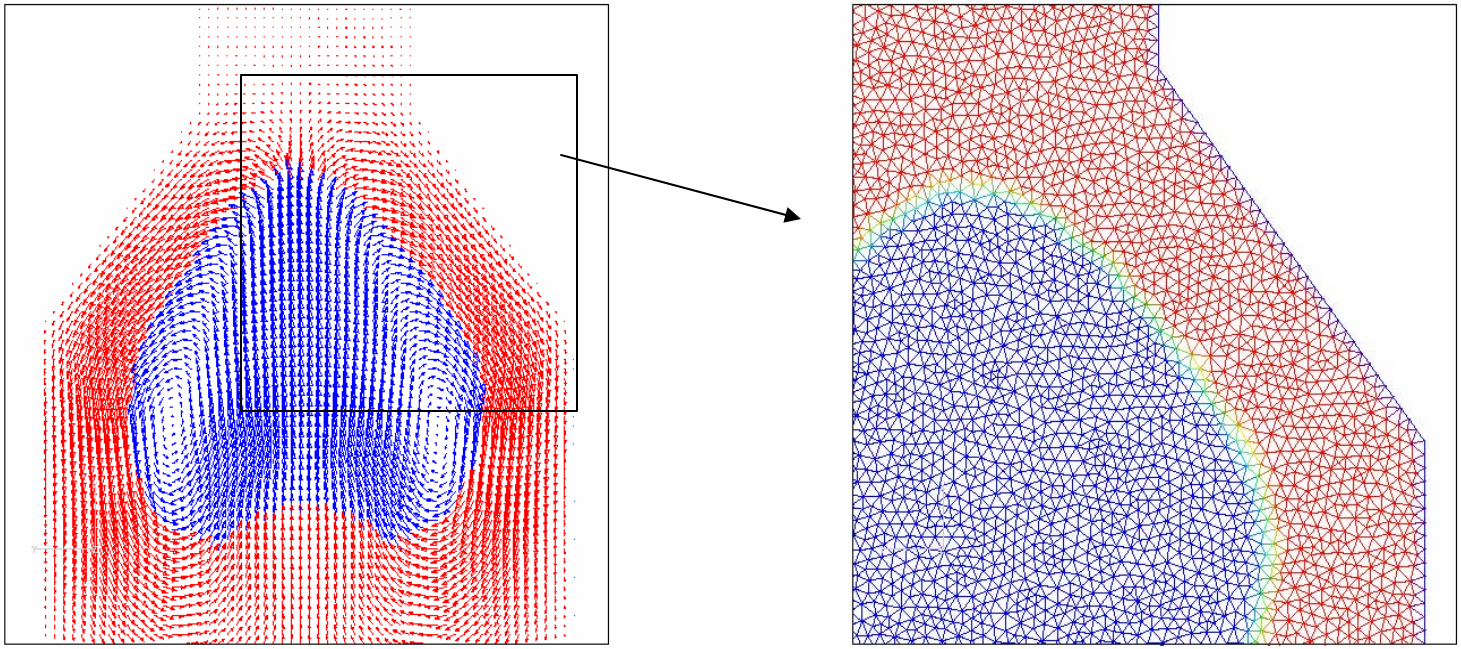
Modeling of Gas/Liquid/Solid Interfaces

Level-Set/NPHASE Simulation of Cap Bubbles in Air-Water Systems (Wierzbicki et al., 2006)



$t = 0.2s$ $t = 0.4s$ $t = 0.6s$

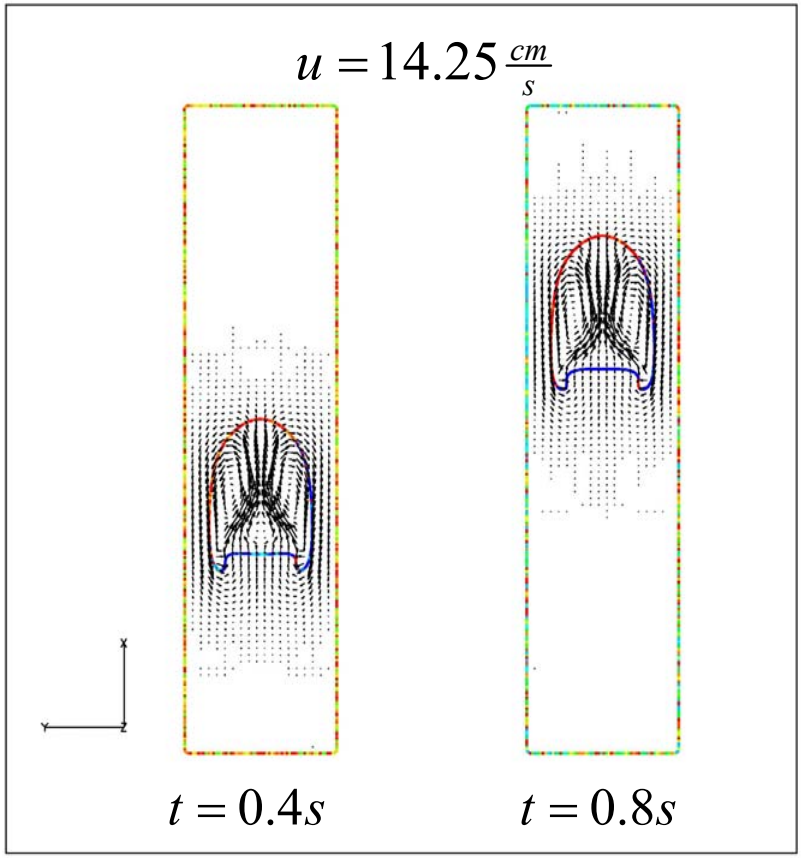
Bubble Rising in Converging Channel
(Wierzbicki et al., 2006)

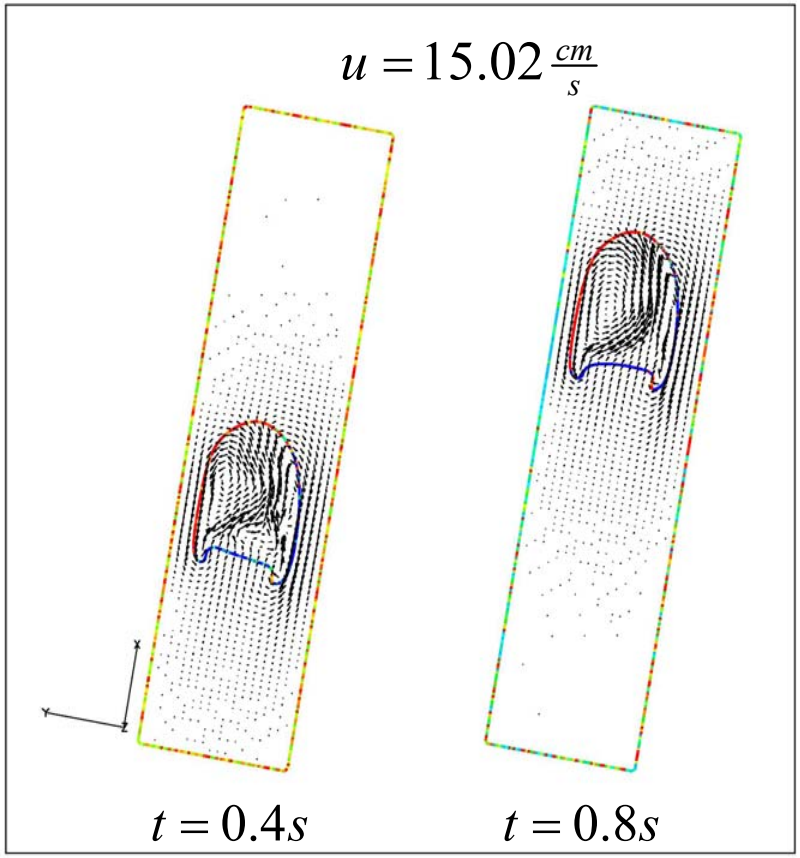


Velocity vectors and zero level set

Unstructured grid and transition region

Inclination Effect on Maximum Bubble Rise Velocity at Small Inclination Angle (Wierzbicki et al., 2006)

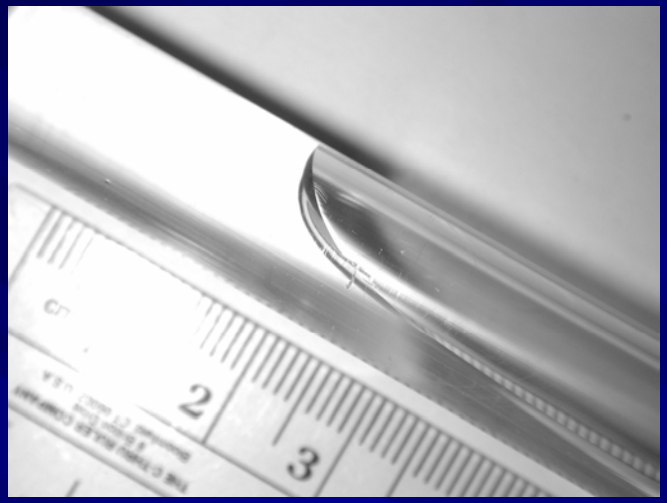




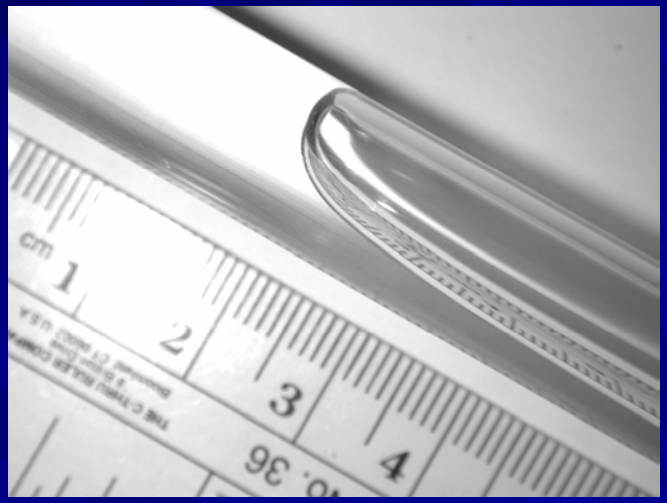
Importance of Understanding Dominant Physical Phenomena

Long air bubble flowing in distilled water along inclined tube

Experiment

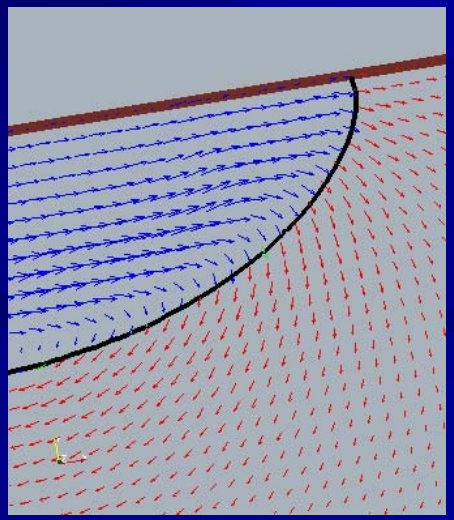


Clean inner tube surface (u_B=10 cm/s)

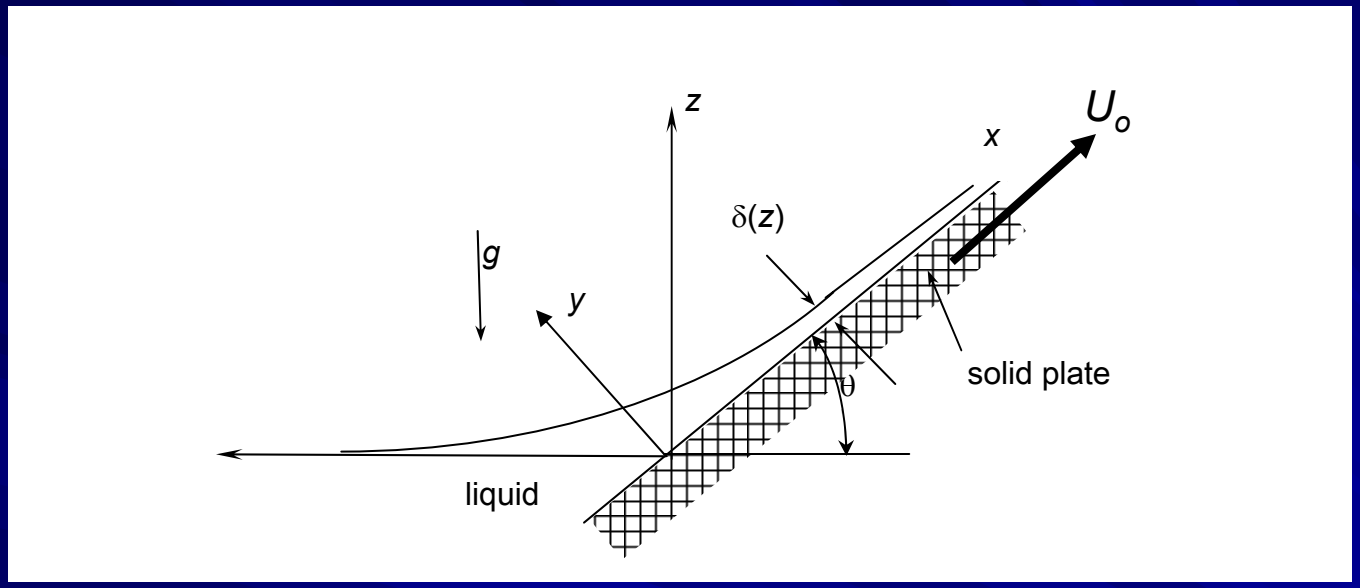


Nano-particle coated surface (u_B=8 cm/s)

Level-Set/NPHASE Simulation



Super-Thin Liquid Film on Inclined Wall (Podowski & Kumbaro, 2004)



- Film momentum equation is

$$\frac{\partial \tau_{yx}}{\partial y} = -\frac{\partial(\sigma K + \Phi)}{\partial x} + \rho g_x$$

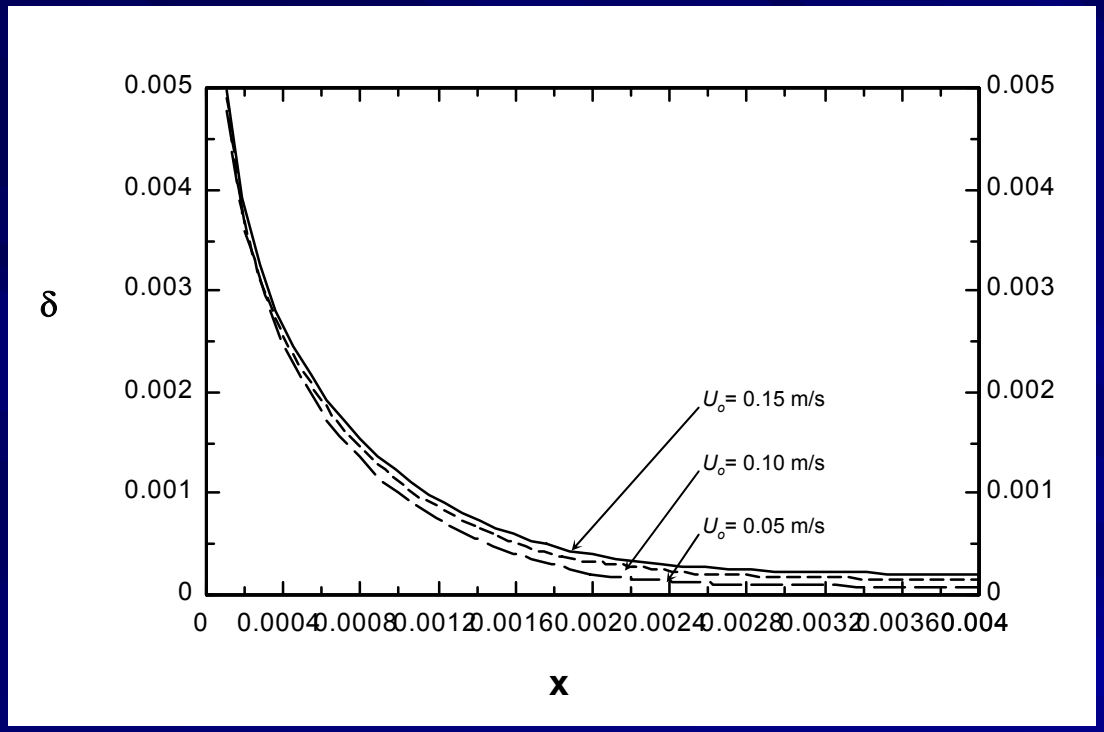
where:

$$K = \frac{\delta''}{(1+\delta'^2)^{3/2}}$$

$$\Phi = \frac{B}{\delta^n}$$

Hamaker constant

Effect of Wall Velocity on Thickness of Moving Film (Podowski & Kumbaro, 2004)



Liquid film profile

$$\Delta = \beta (Ca)^{\omega}$$

where

$$Ca = \frac{\mu U_0}{\sigma}$$

$$\Delta = \frac{\delta_\infty}{a} = \delta_\infty \sqrt{\frac{\rho g}{\sigma}}$$

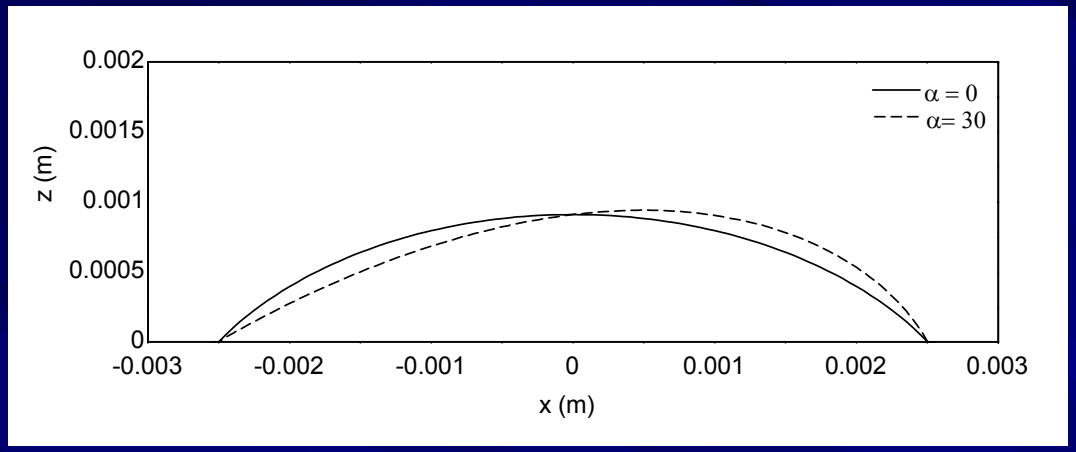
Simplified model (Probstein, 1994):

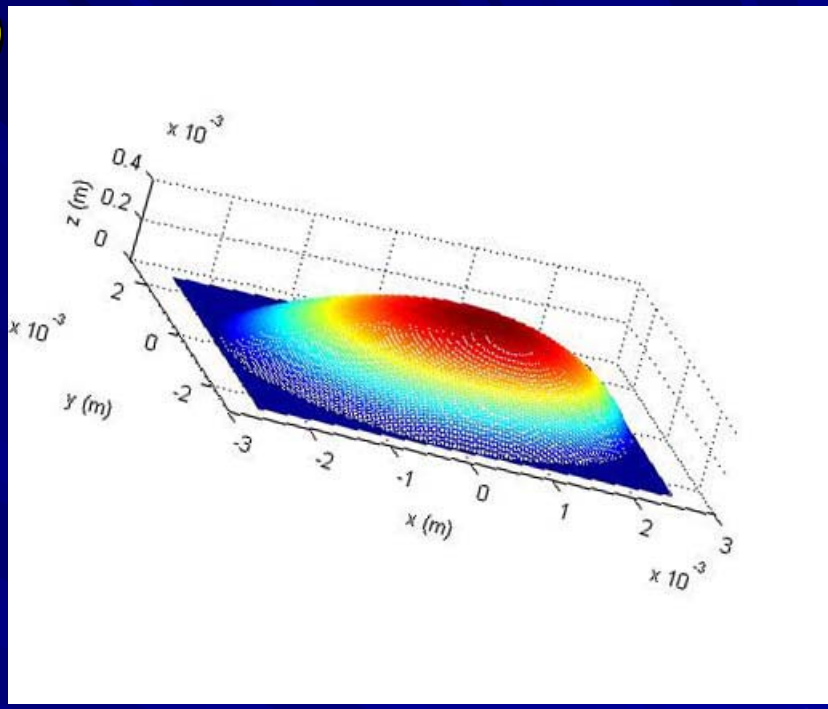
$$\Delta = 0.946 (Ca)^{0.667}$$

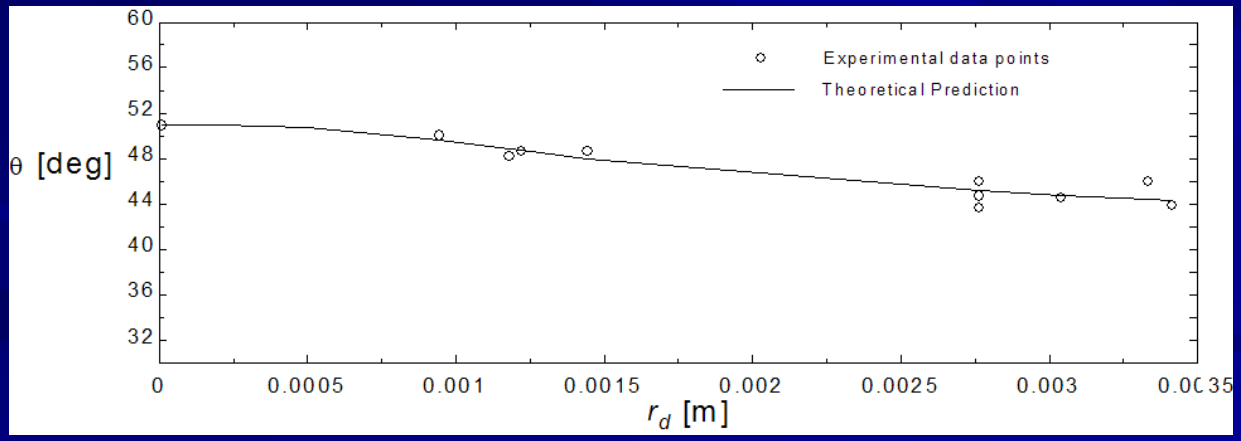
Complete flow model (Podowski & Kumbaro, 2004):

$$\Delta = 0.834 (Ca)^{0.542}$$

Theoretical Predictions of Droplet Shape
(Vafaei & Podowski, 2004; 2005)







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Multidimensional Modeling of Particulate Flows in Complex Geometries

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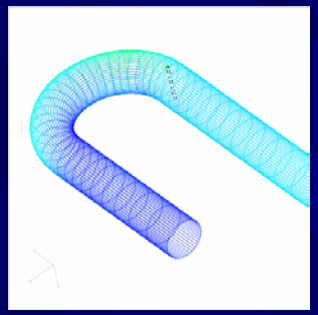
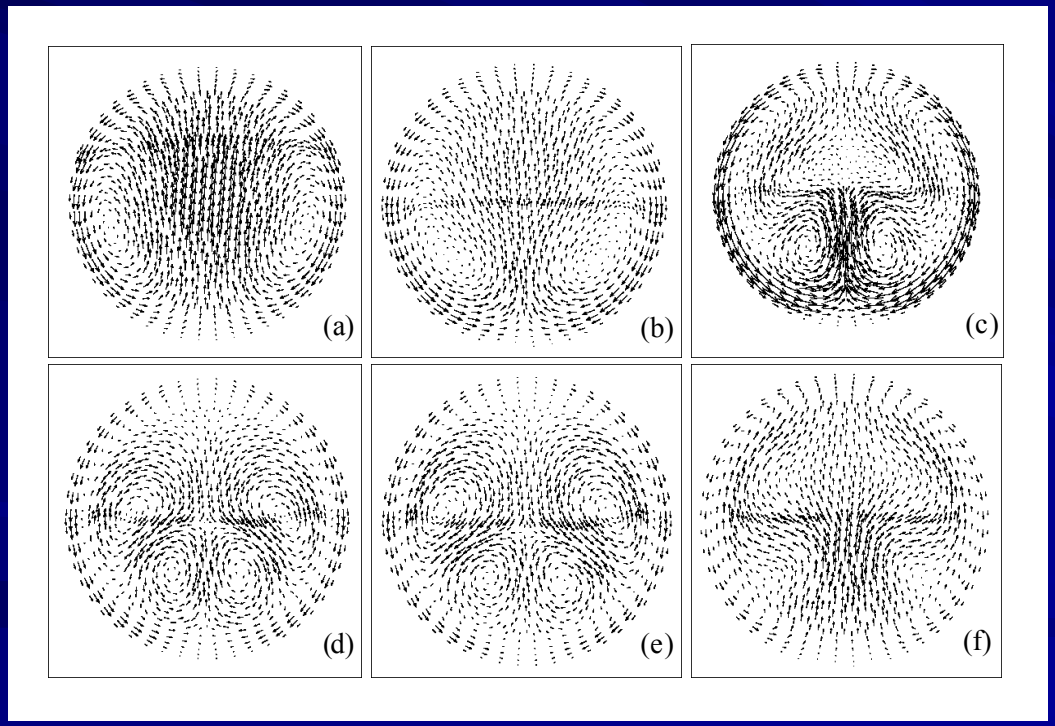
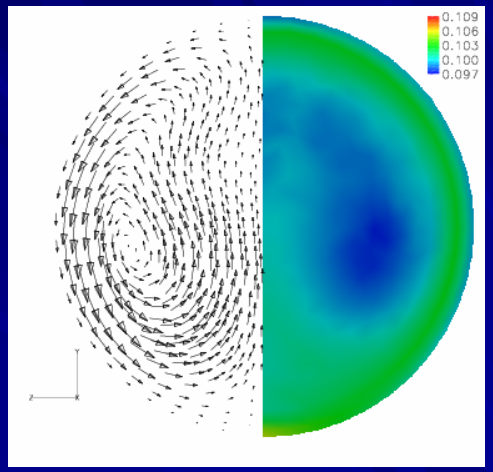
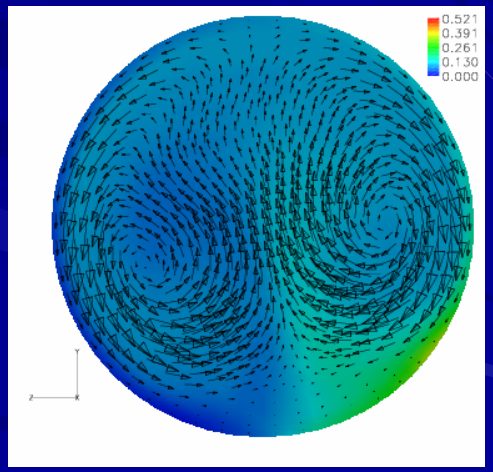
NPHASE Predictions of Velocity Field and Particle Concentration in U-Bend (Tiwari et al., 2004)





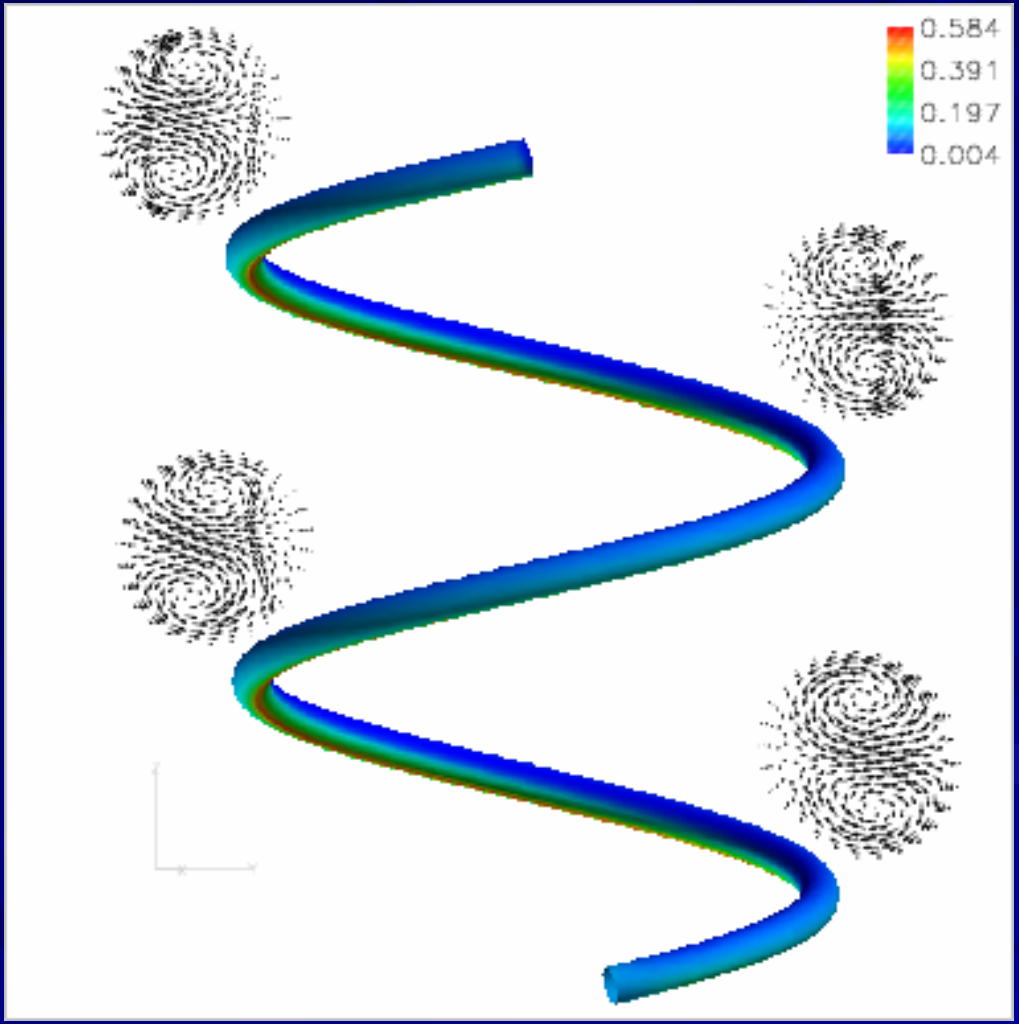


without gravity



with gravity

3-D Simulation of Particle Flow in Helical Micro-Tube (Tiwari et al., 2006)



Multidimensional Modeling of Flow and Heat Transfer in Supercritical Fluids

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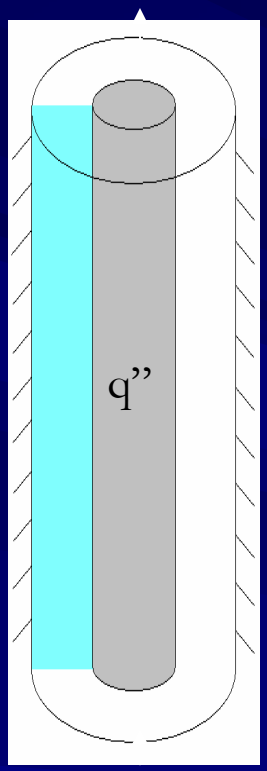
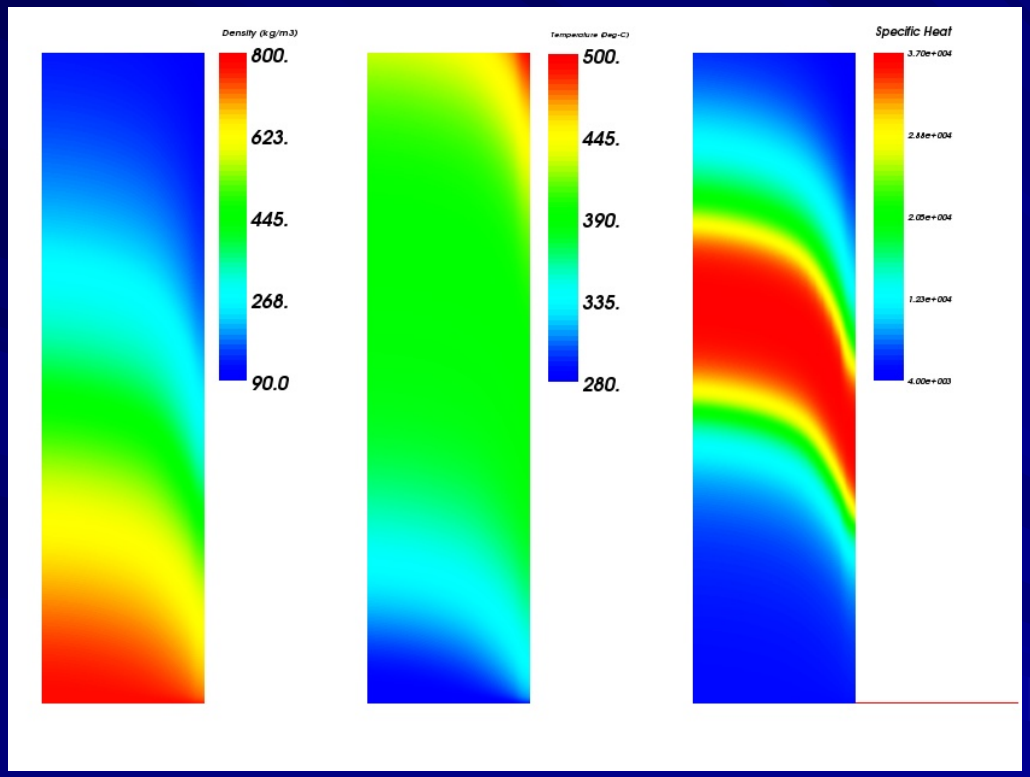
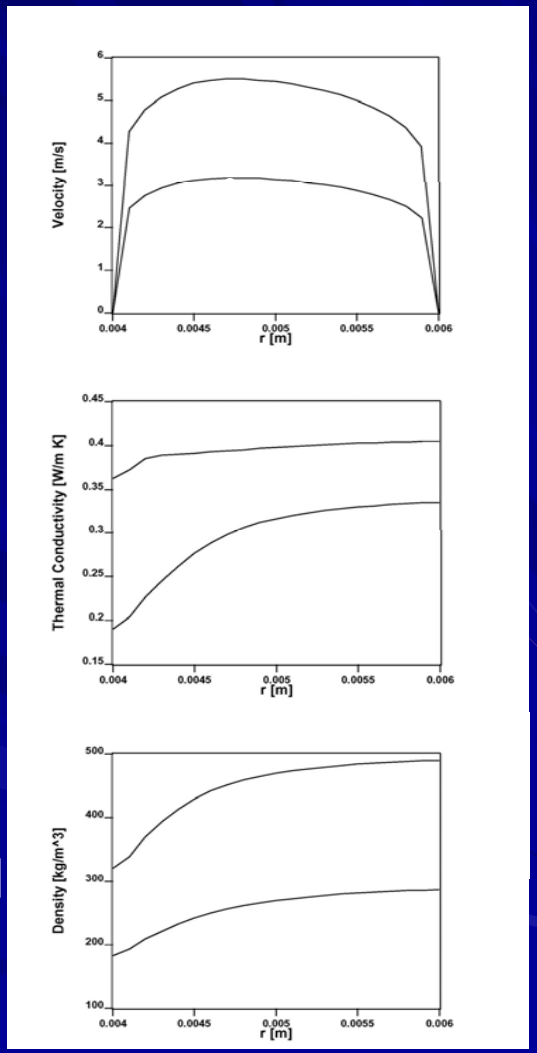
Typical Property Variation in a Heated Channel with Supercritical Water (Gallaway et al., 2006)



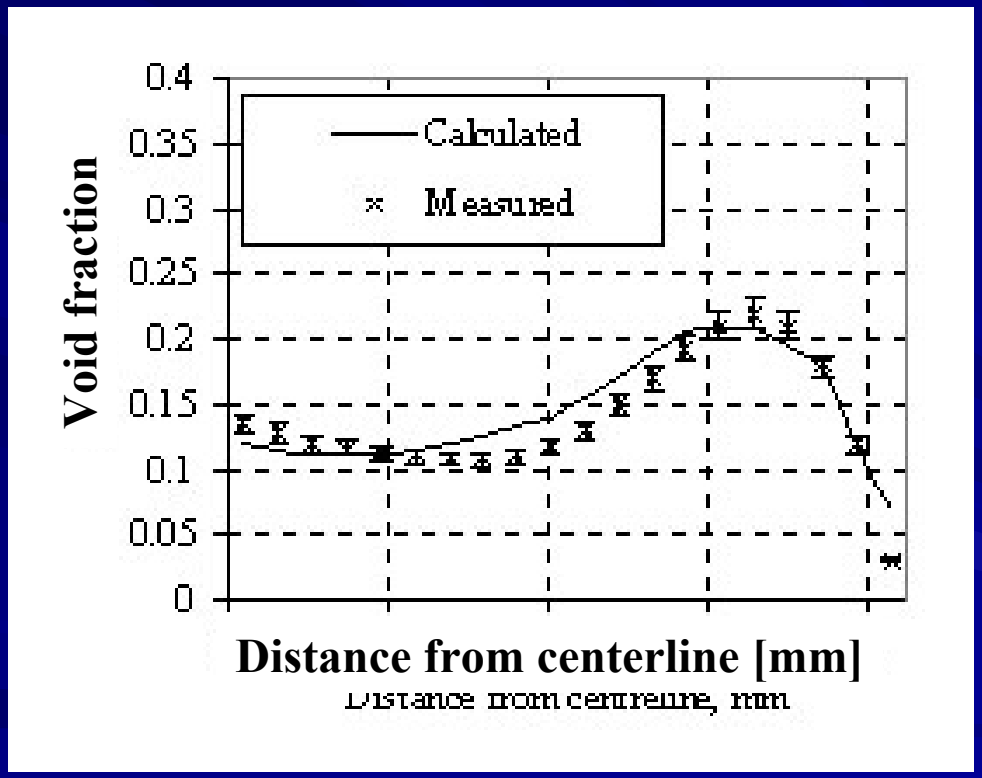


Density [kg/m^3] Temperature [^{o}C] Specific heat [J/kg-^{o}C]

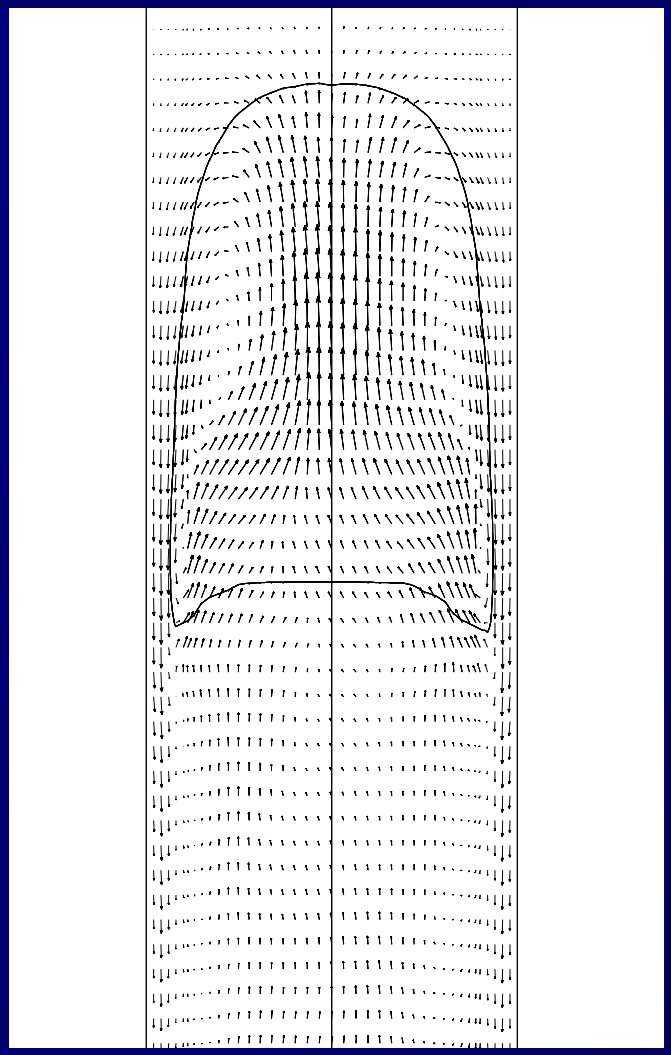


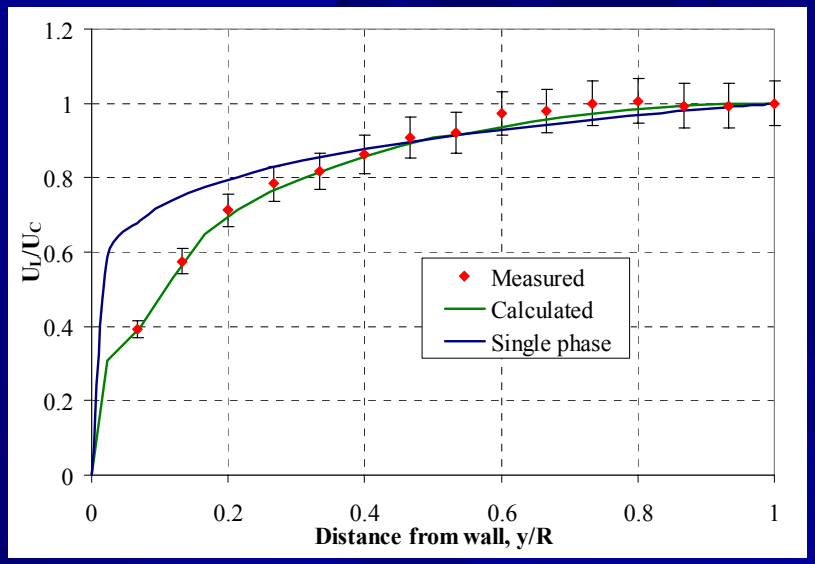
Multidimensional Modeling of Various Flow Regimes

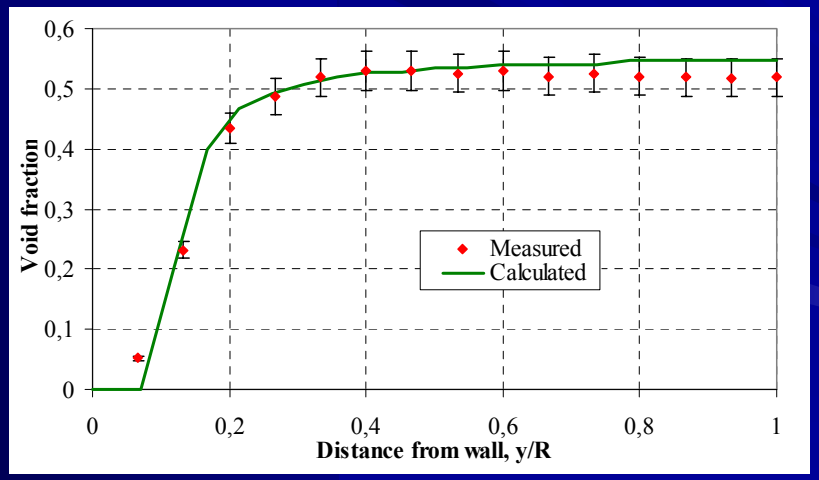
Predictions of Void Distribution in Adiabatic Bubbly Flow
(Anglart & Podowski, 1999)



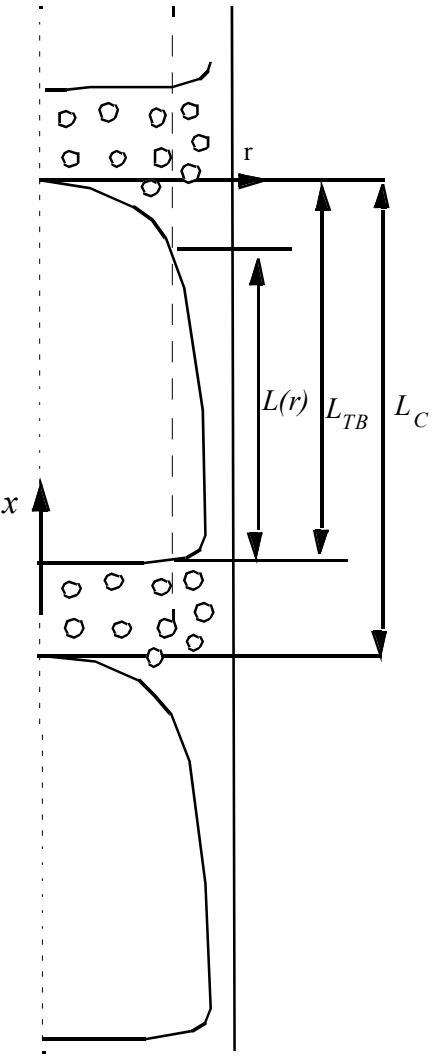
3-D VOF Predictions of Slug Flow (Anglart & Podowski, 2001)







Three-Field Model of Slug Flow (Podowski at al., 2004)



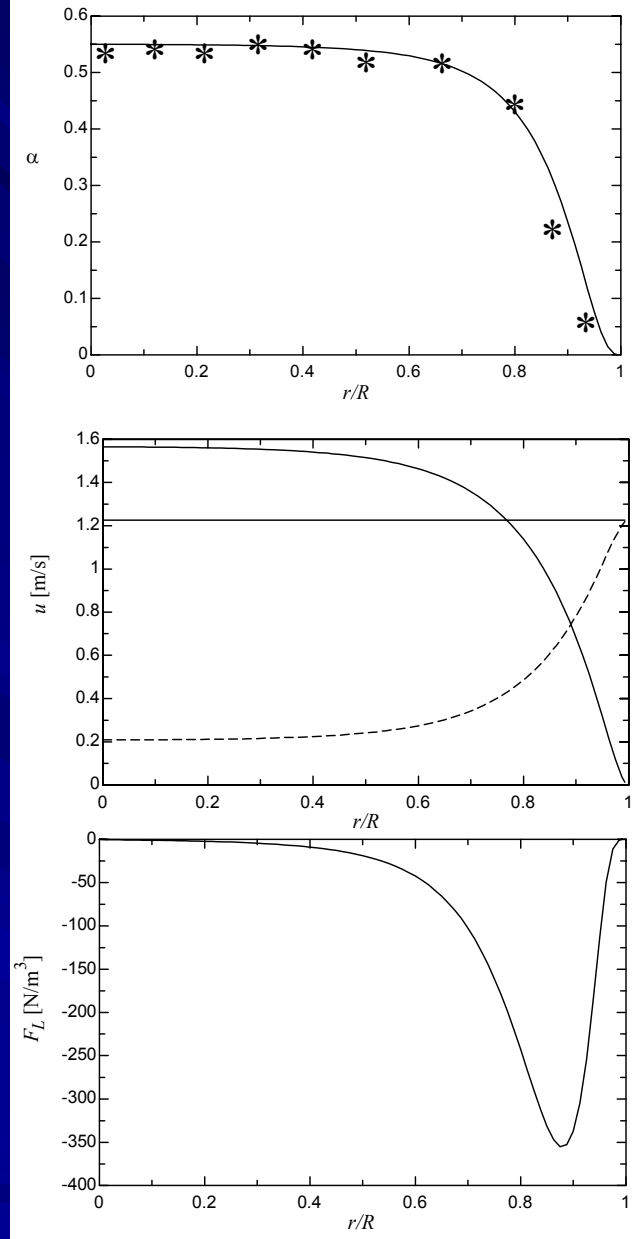
Taylor-bubble/liquid force

$$\mathbf{M}_k = \mathbf{M}_k^D + \mathbf{M}_k^L + \mathbf{M}_k^{BID} + \mathbf{M}_k^{excess}$$

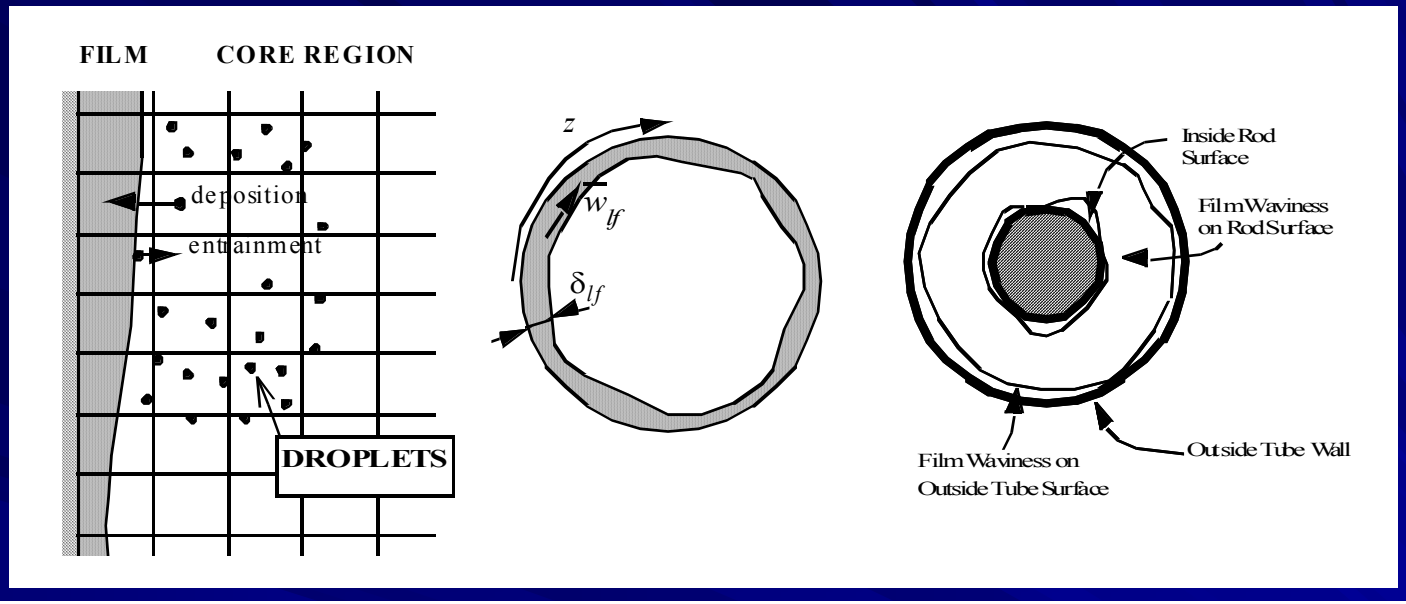
Bubble-induced turbulence

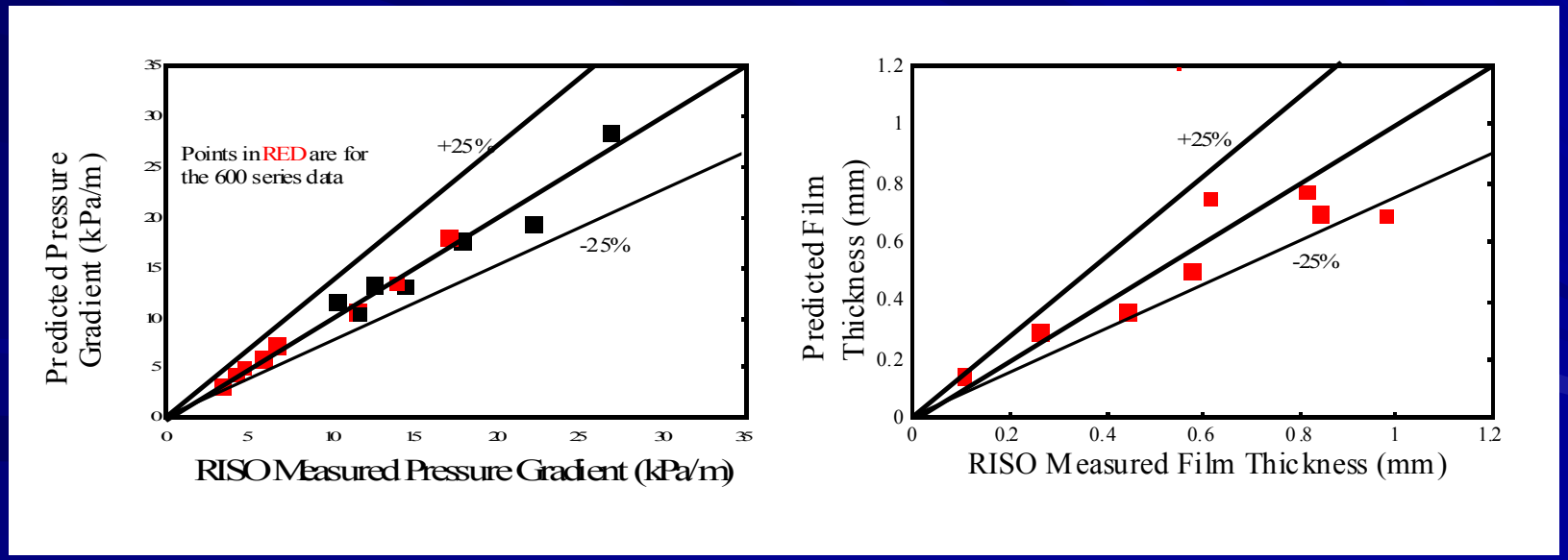
$$\mu_{BI}^t = \rho_l l^2 \left| \frac{\partial \overline{u}}{\partial y} \right|$$

$$\frac{l}{R} = 0.142 \langle \alpha \rangle \left[\frac{y}{R} + 1.8 \left(\frac{y}{R} \right)^2 + 25 \left(\frac{y}{R} \right)^2 \right]$$

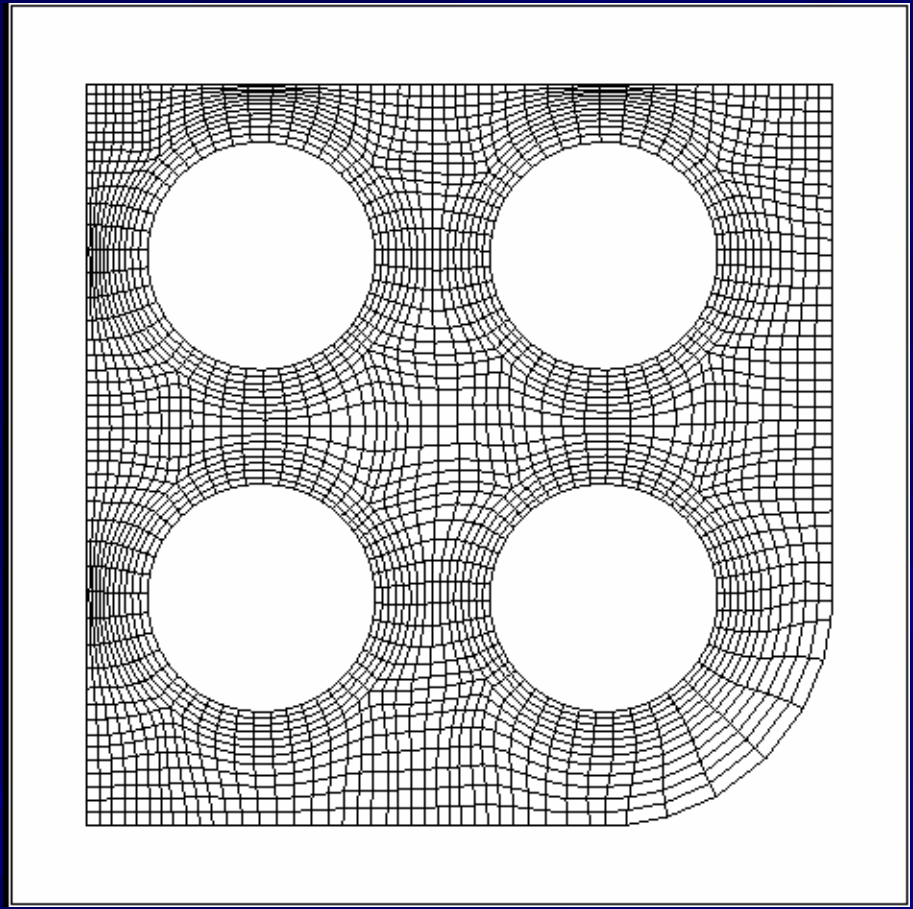


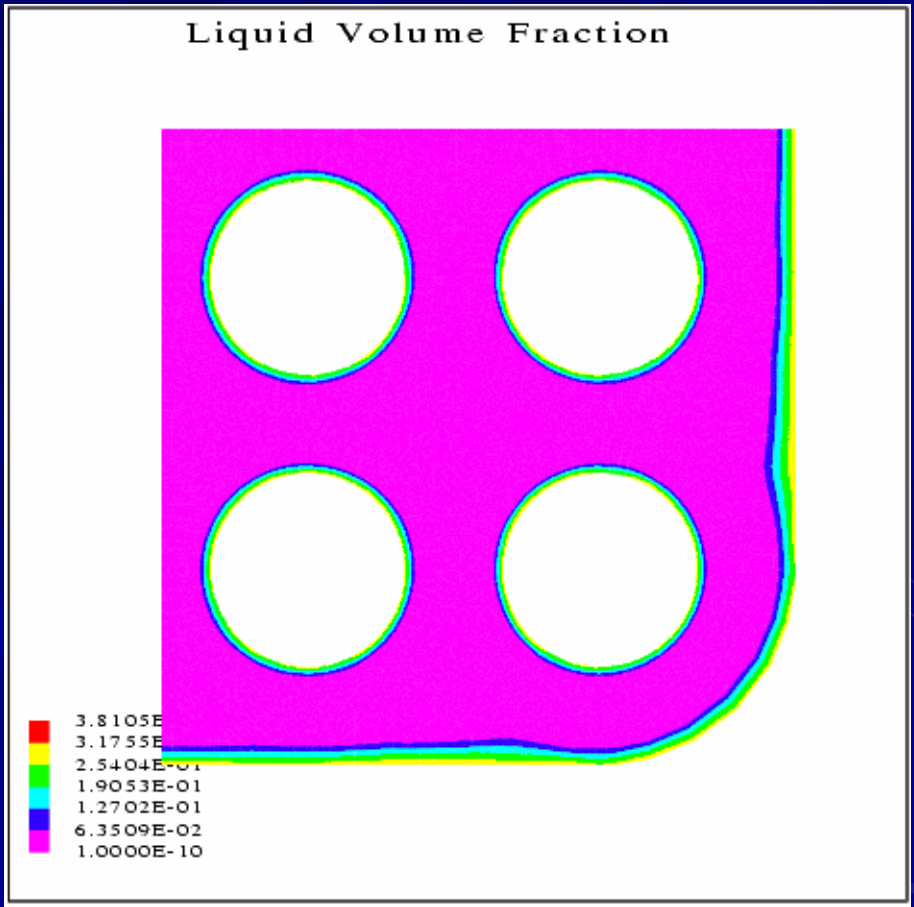
Annular Flow in Annulus (Antal et al., 2001)





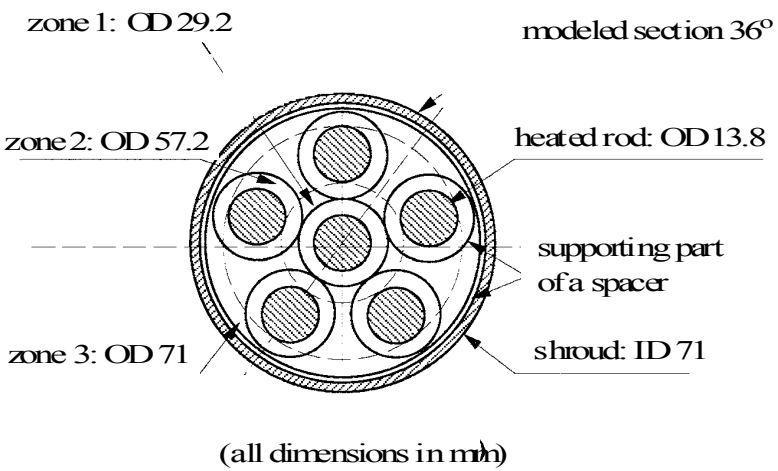
Annular Flow in BWR Fuel Assembly (Antal & Podowski, 1999)

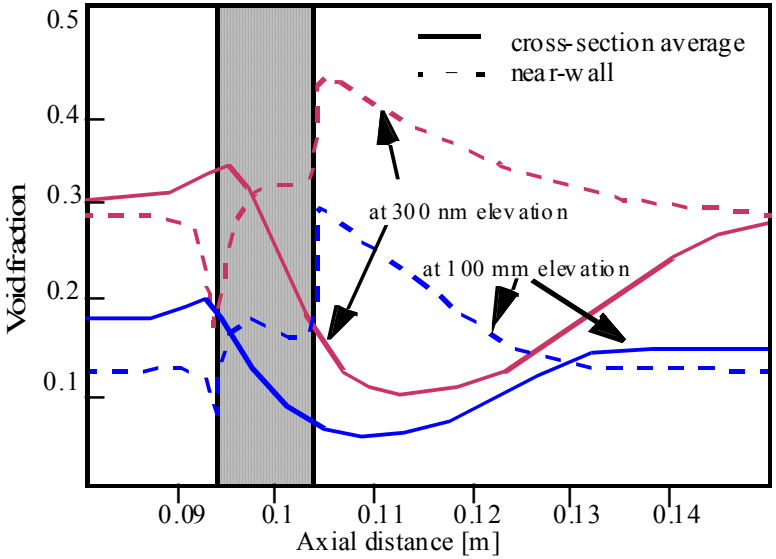


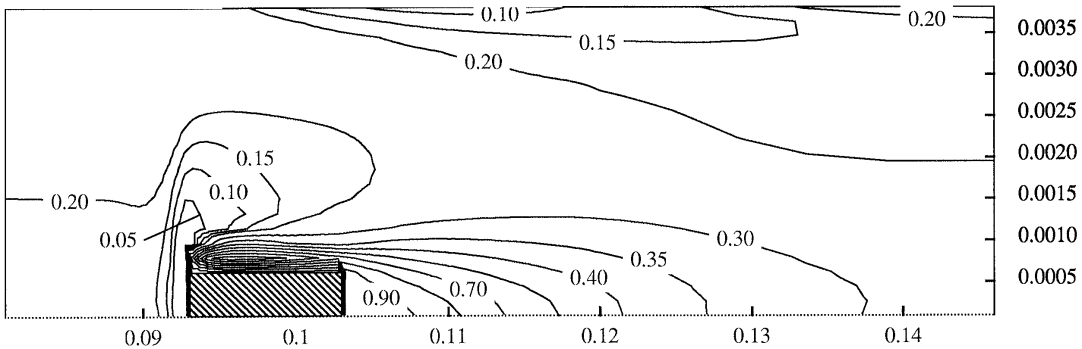


Effect of Local Flow Obstacles

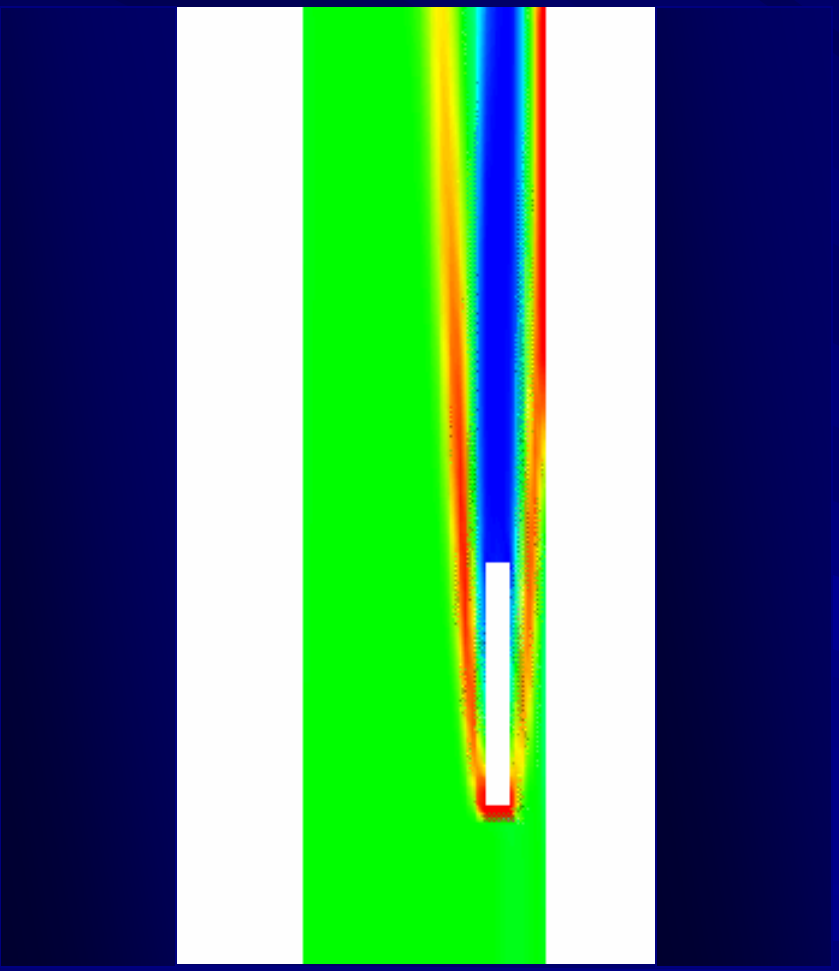
Two-Phase Bubbly Flow around Spacers in Rod Bundles (Anglart et al., 1997)



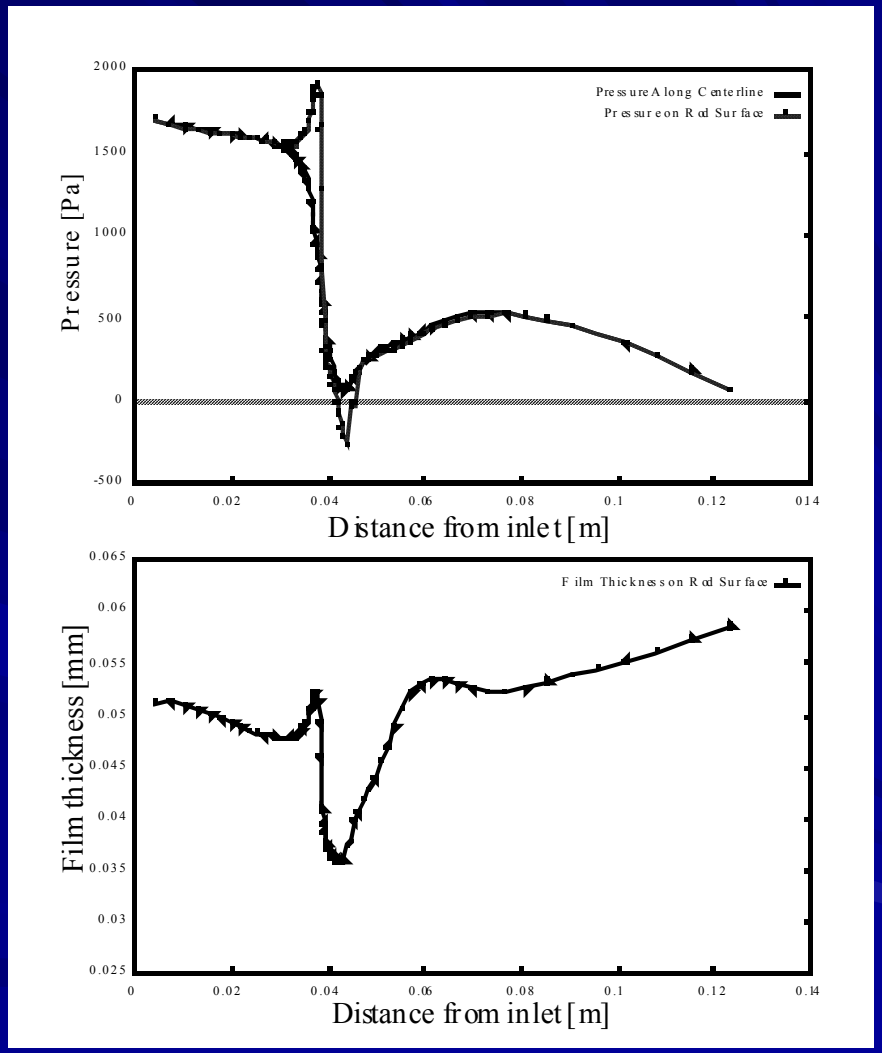




Annular Two-Phase Flow Around Spacer (Antal et al., 2001)

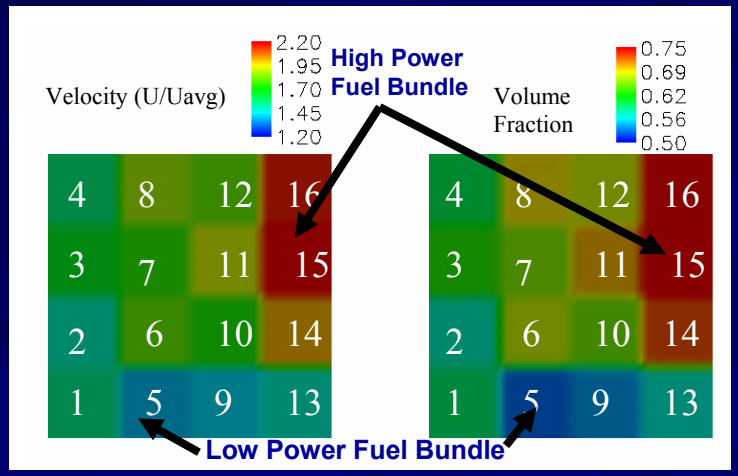


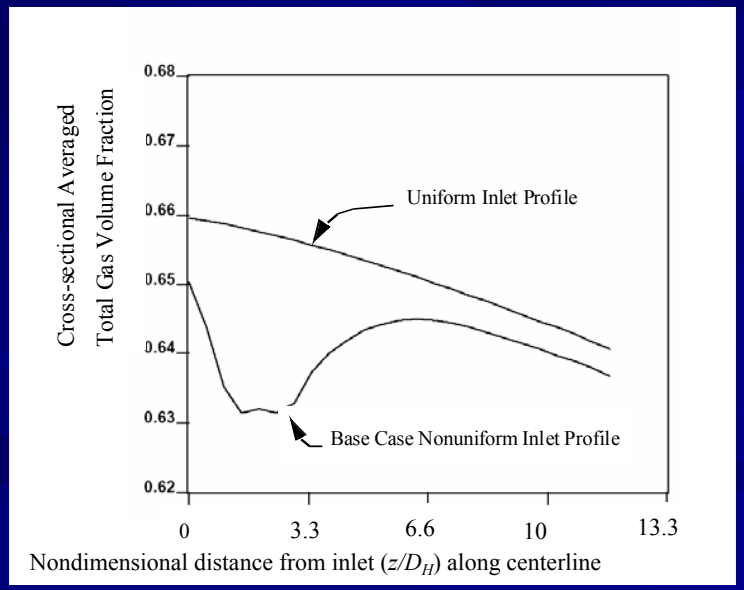
Droplet concentration

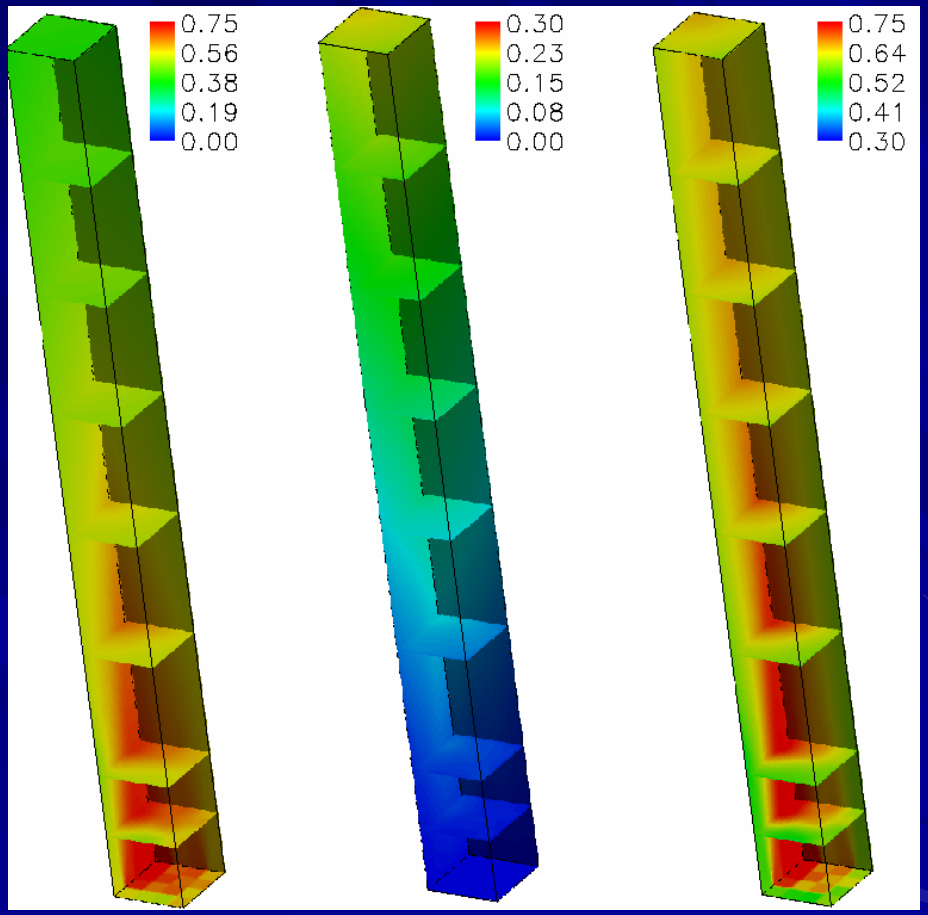


Bubbly-to-Churn-Turbulent Flow Regime Transition

NPHASE Simulation of Two-Phase Flow in Adiabatic Chimney of Advanced BWR (Antal et al., 2005)







Small Bubble Field | Large Bubble Field | Total Gas Fraction

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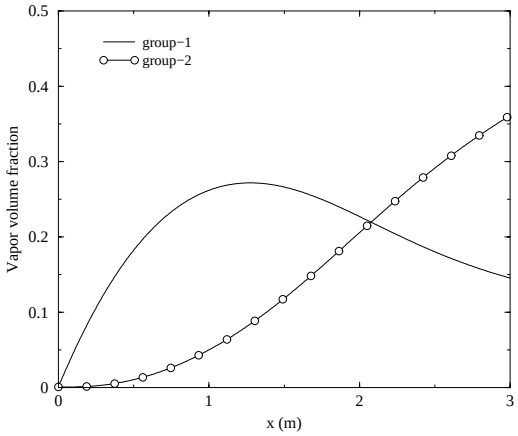
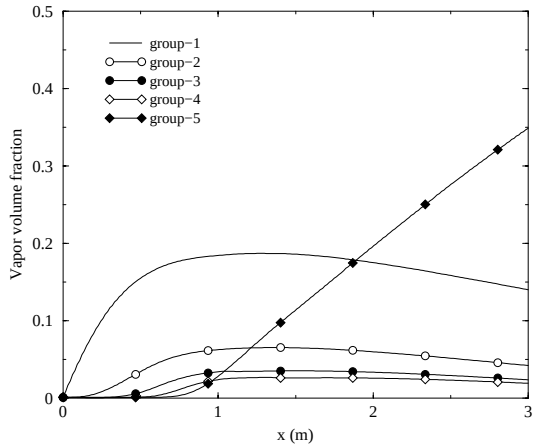
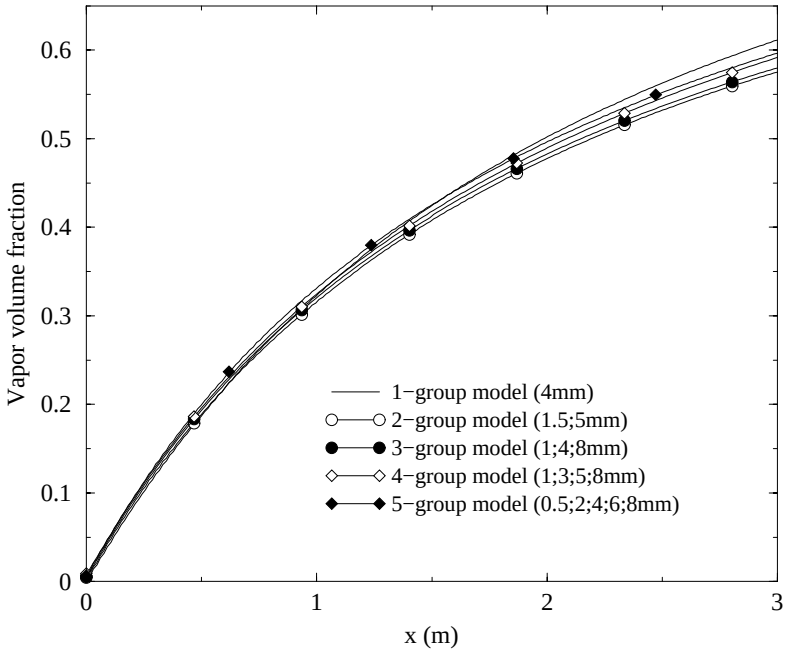
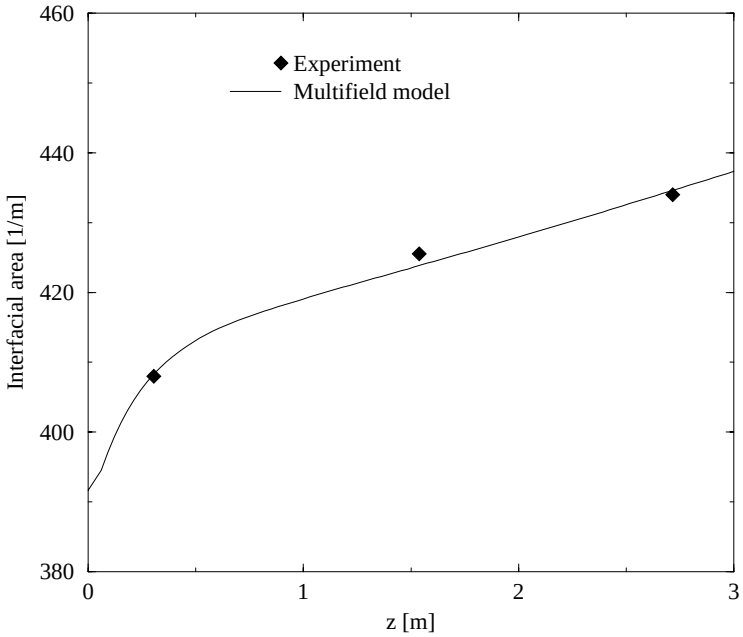
Multiple-Size-Group Model of Boiling Channel
(Kumbaro & Podowski, 2006)





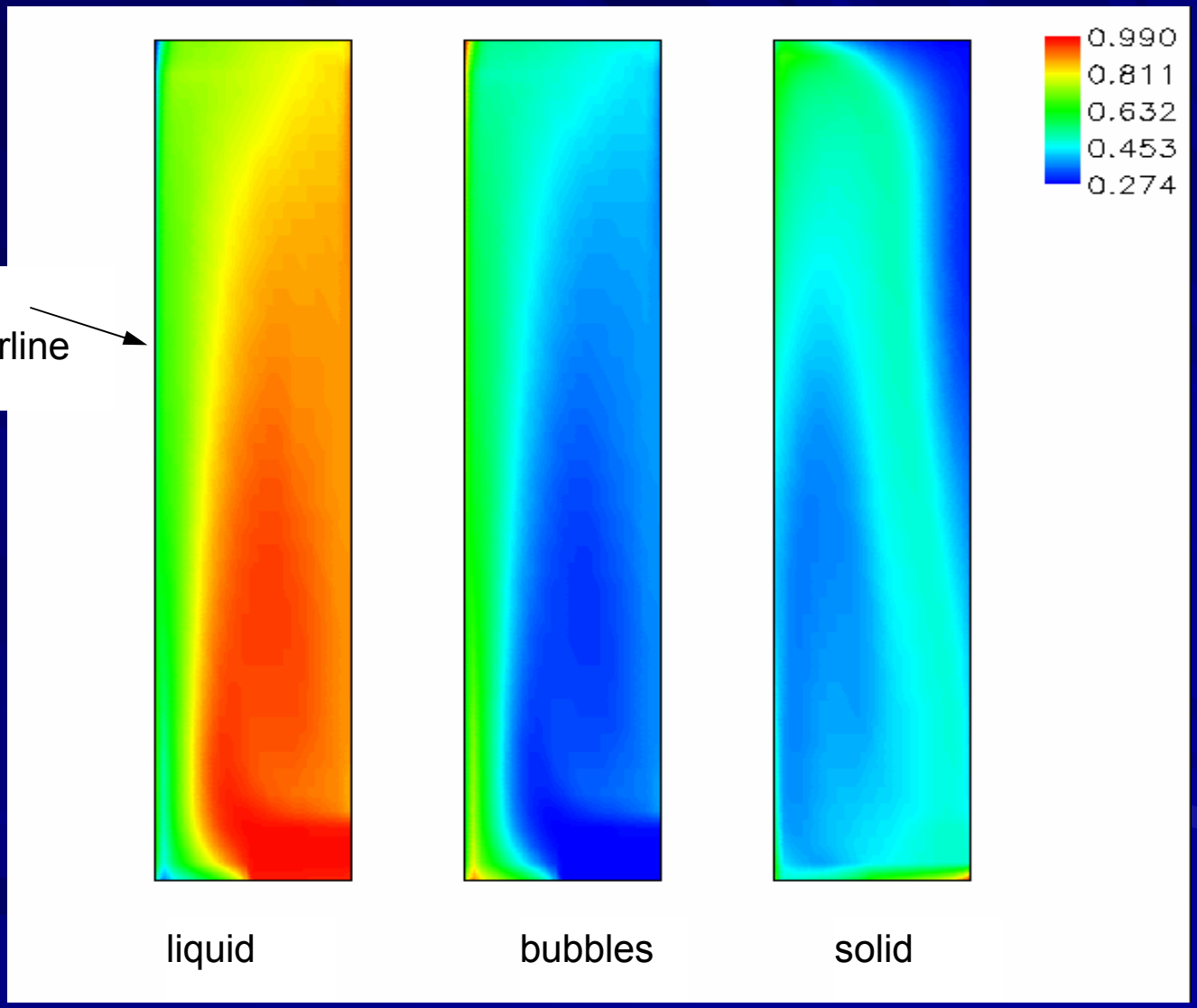




Effect of number of bubble sizes on void fraction

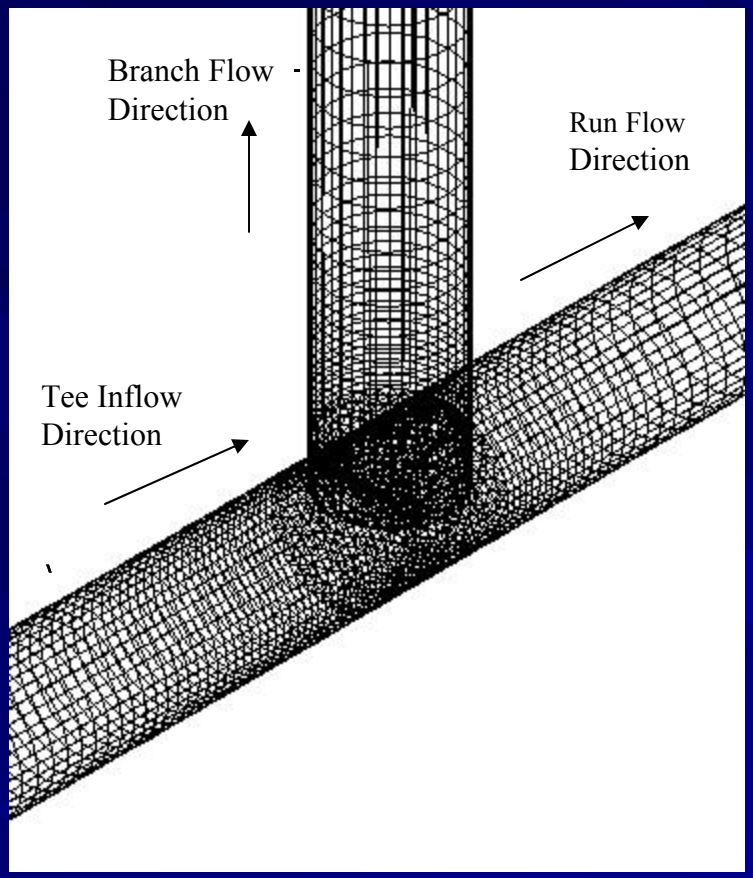
Three Component Flow (Gas/Liquid/Solid)

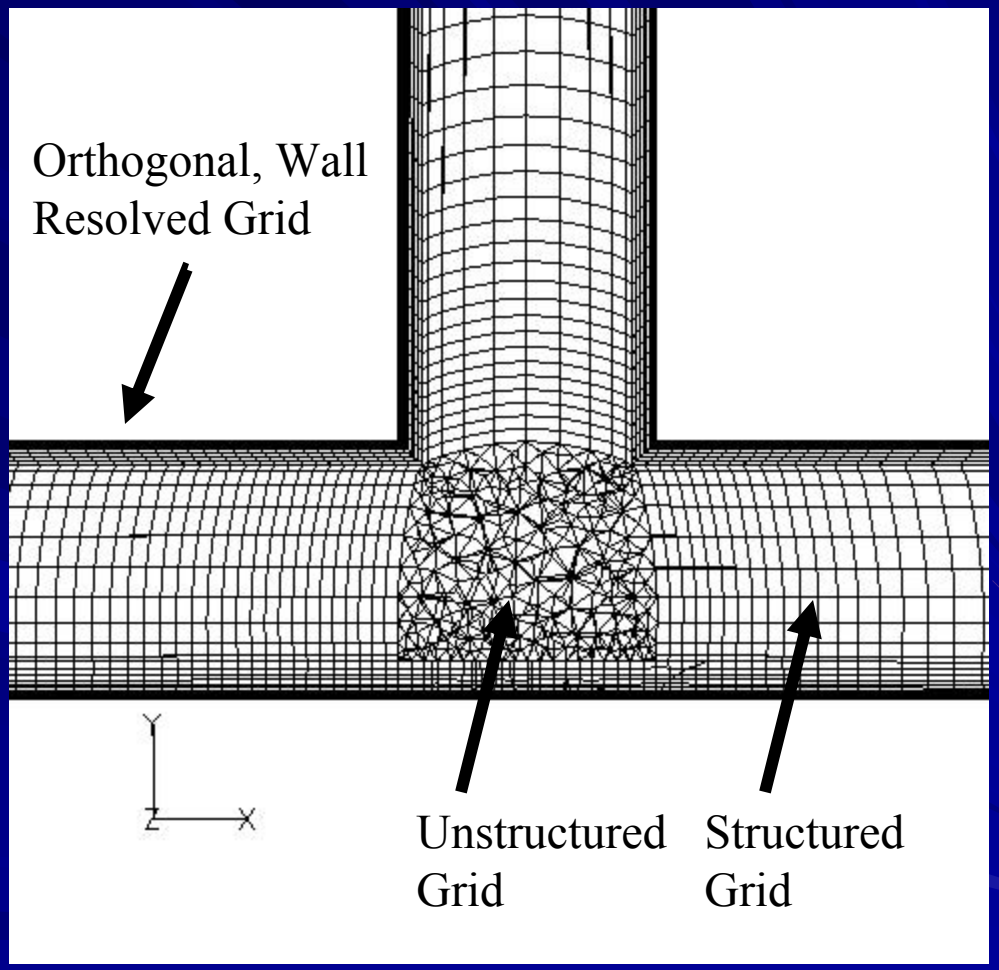
NPHASE Prediction of Volume Fractions in Bubble Column (Antal et al., 2000)



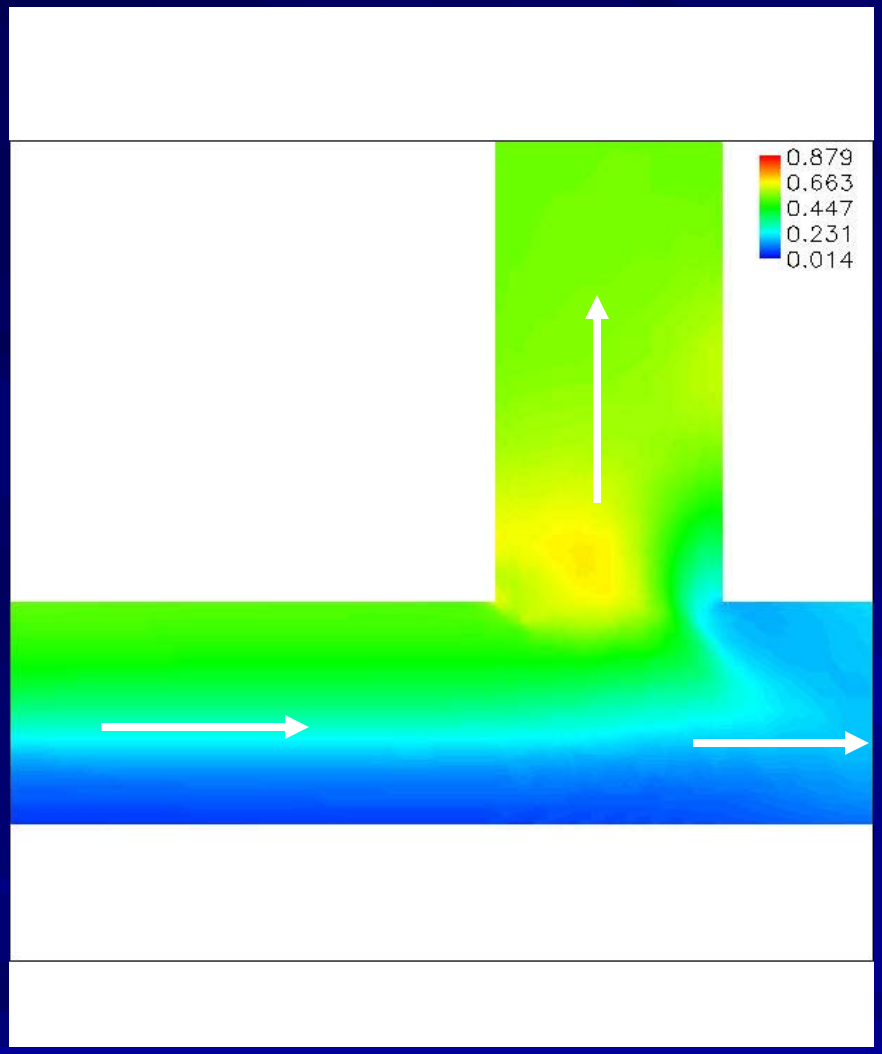
Flow in Branching Conduits

Gridgen Grid of 3D Equal Diameter Tee (Antal & Podowski, 2001)

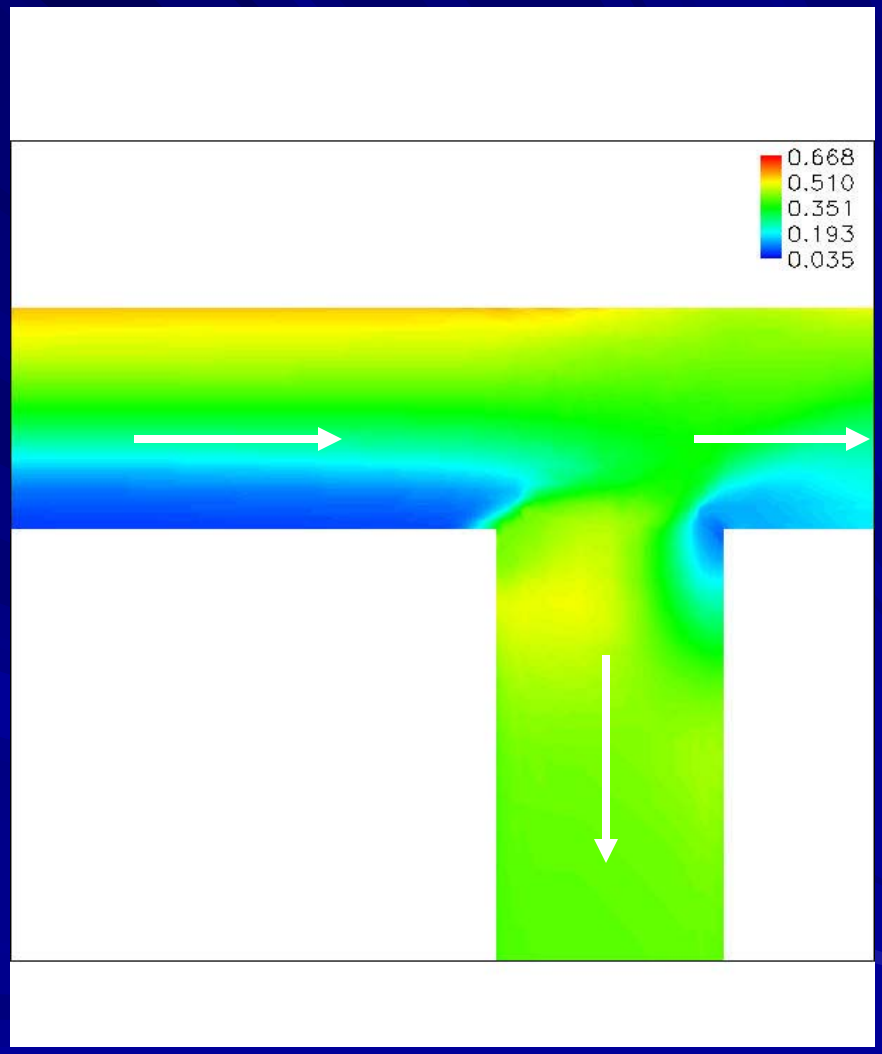




3D Simulation of Flow in 90° Tee
(Antal & Podowski, 2001)



Branch facing upward



Branch facing downward

Modeling of Forced-Convection Low-Quality Boiling

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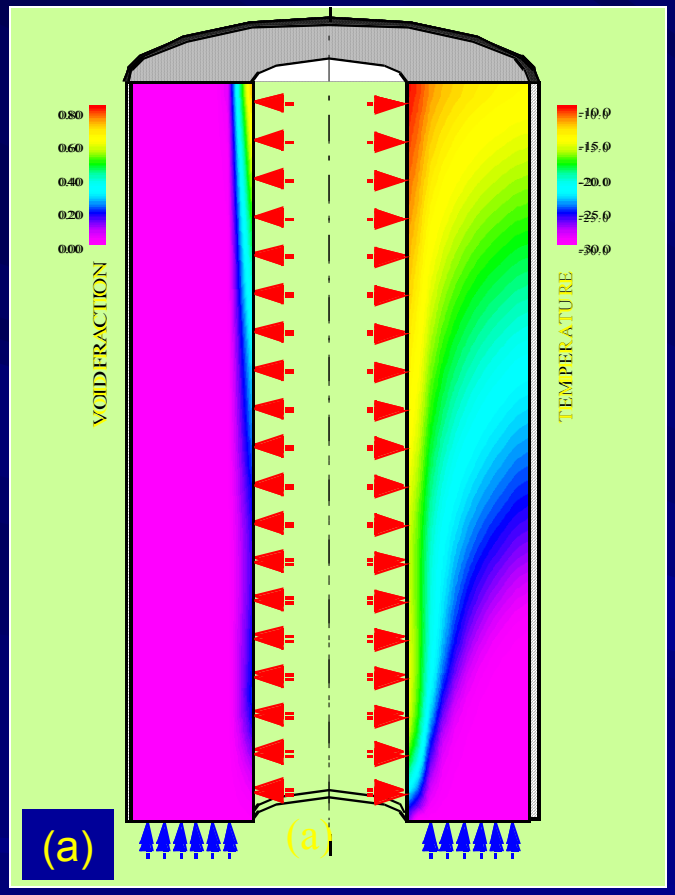
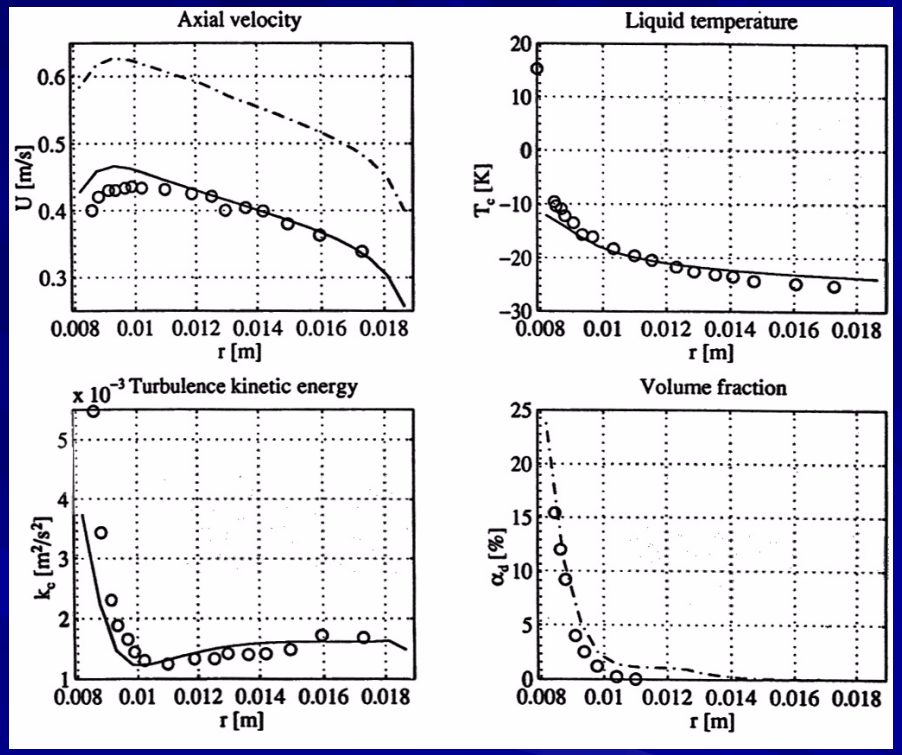
Predicted and Measured Local Hydrodynamic and Thermal Parameters for Subcooled Boiling in Annular Channel Heated from Inside

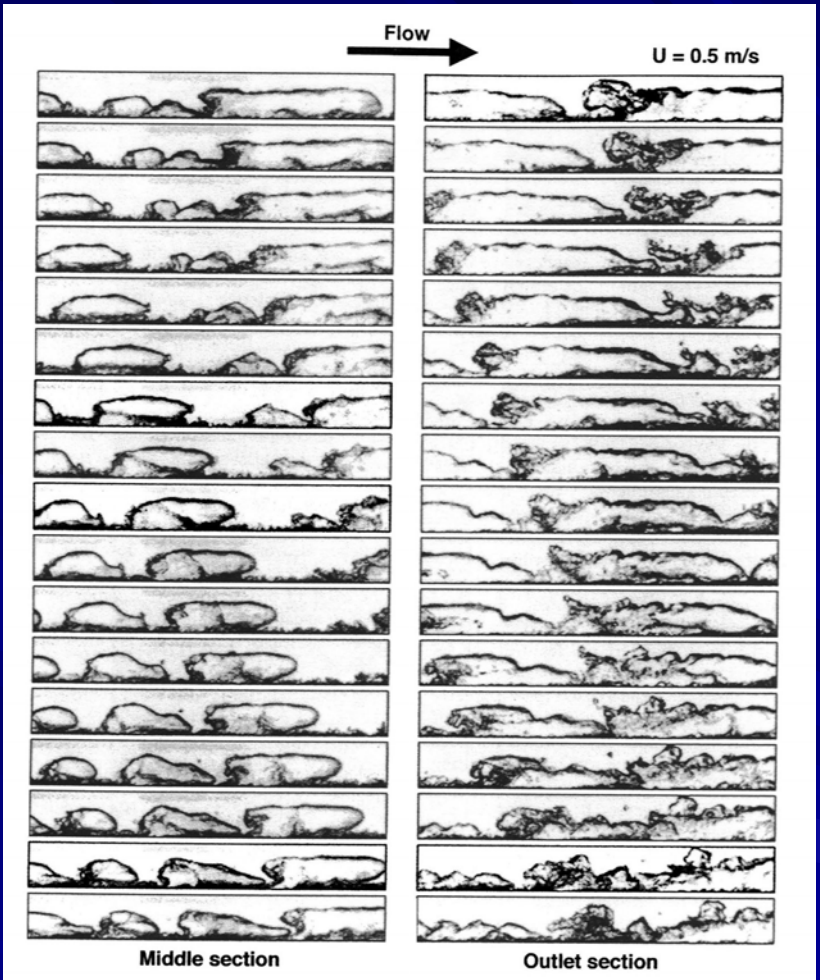




(b)

(a) local void and temperature distributions along the channel (Kurul et al., 1996),
(b) comparison between calculations and data for radial distributions of major parameters at channel exit (Alajbegovic et al., 1996)

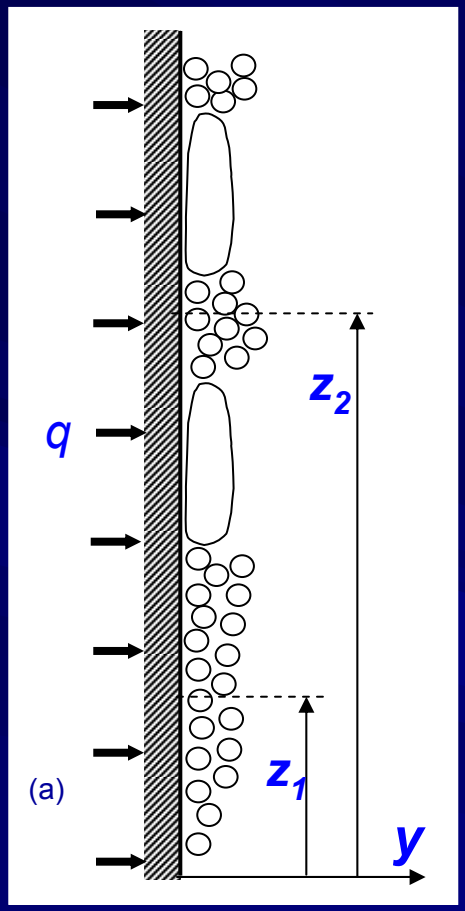
CHF in Subcooled Boiling

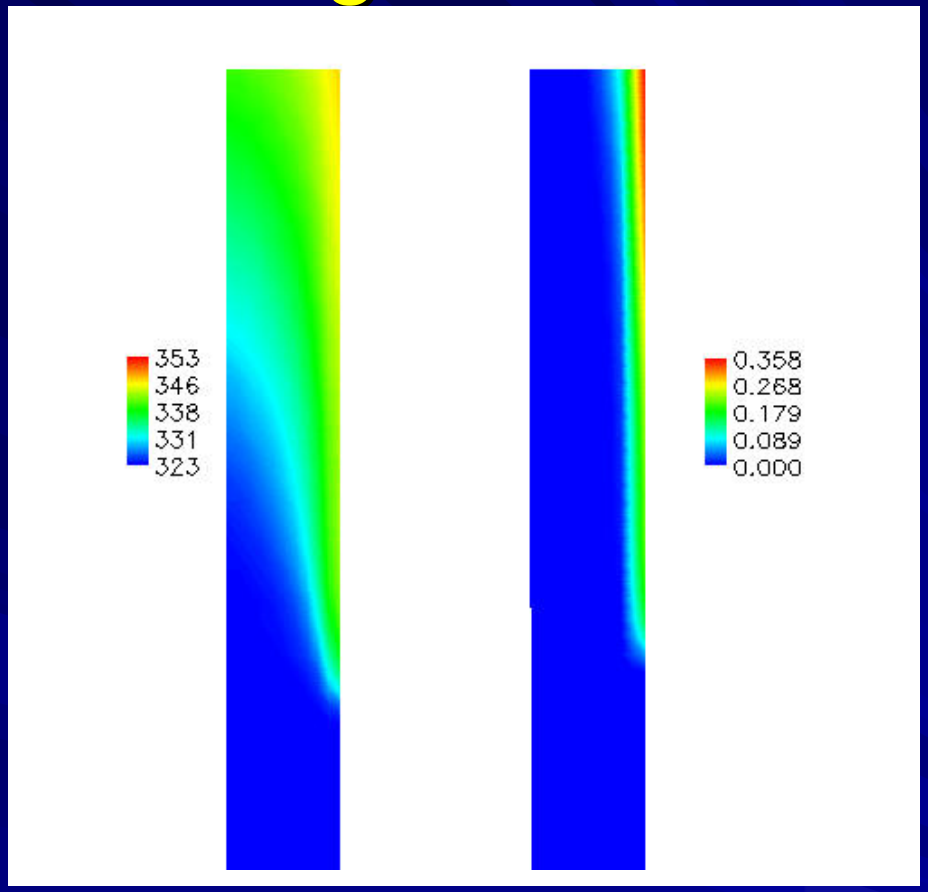


Flow visualization near heated (Moudawar et al., 2002)

Predictions using Three-Field Model

(Podowski & Antal, 2002)



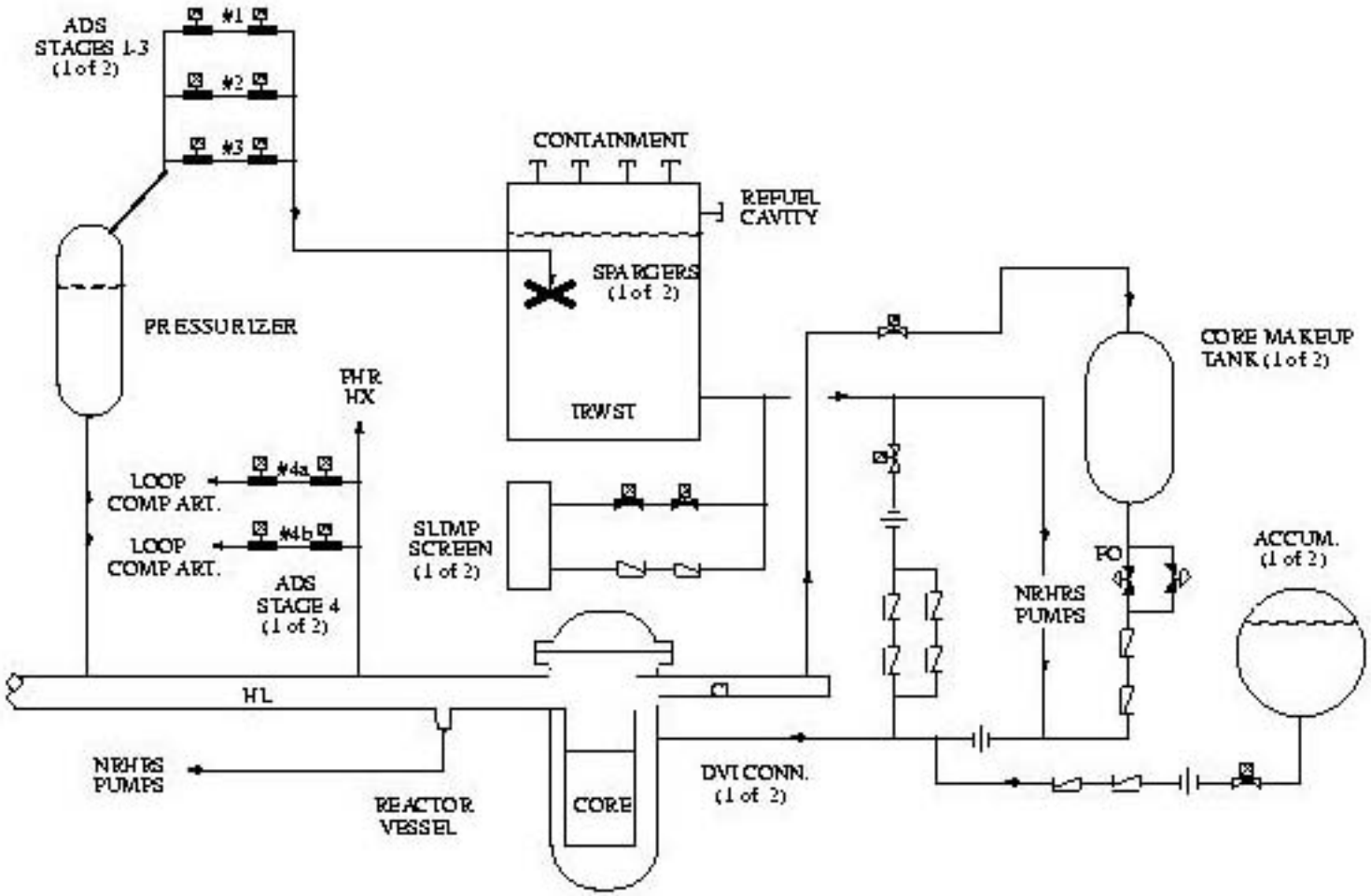


Temperature [K] and void fraction contours

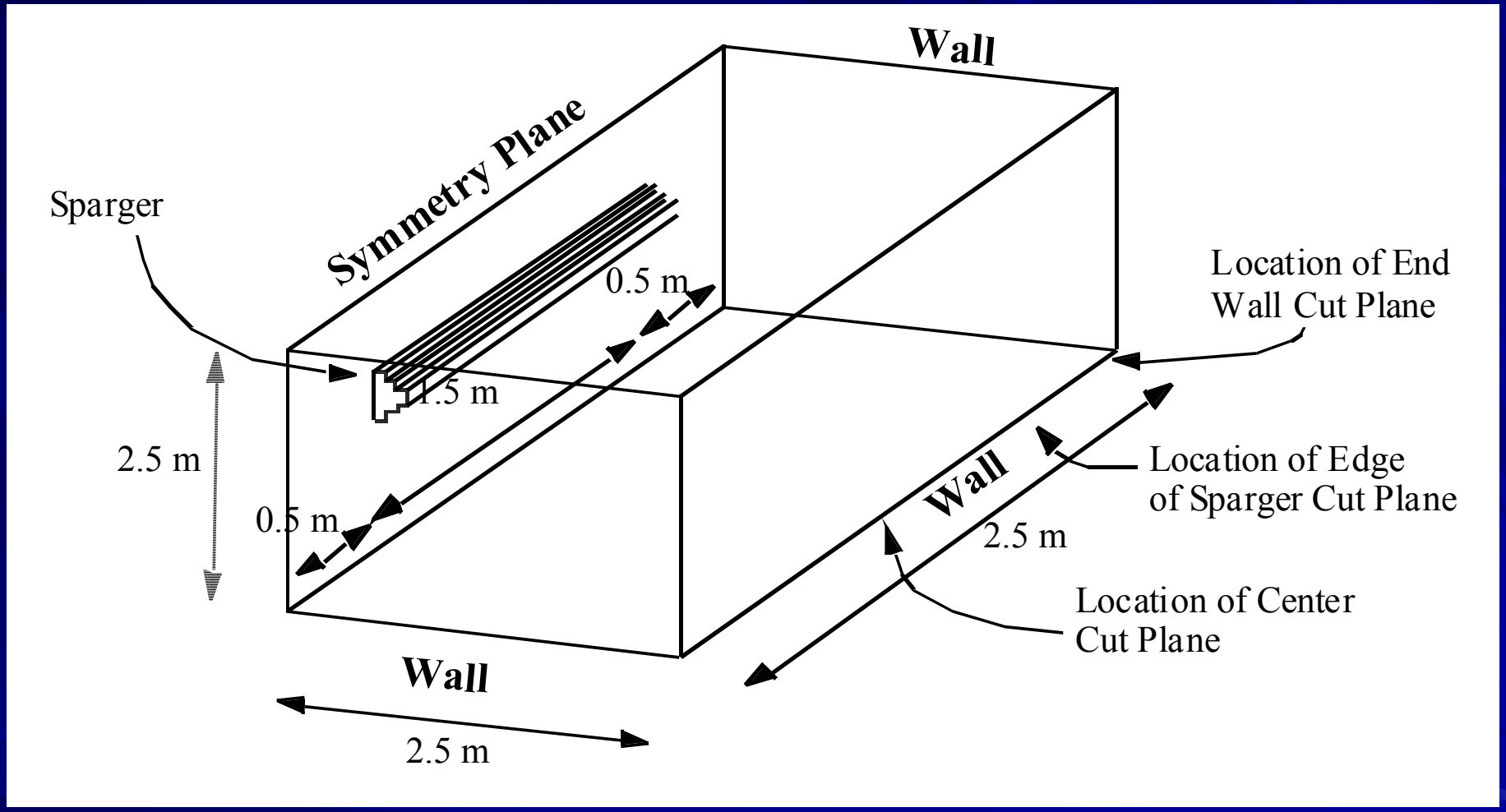
Mass Flux [kg/m^{2}s]	Liquid Subcooling [K]	Predicted CHF [kW]	Measured CHF [kW]	Error [%]
512	30	241	241	2
512	20	172	211	16
1236	30	305	332	8

Steam/Water Mixture Injection into Large Liquid Pool

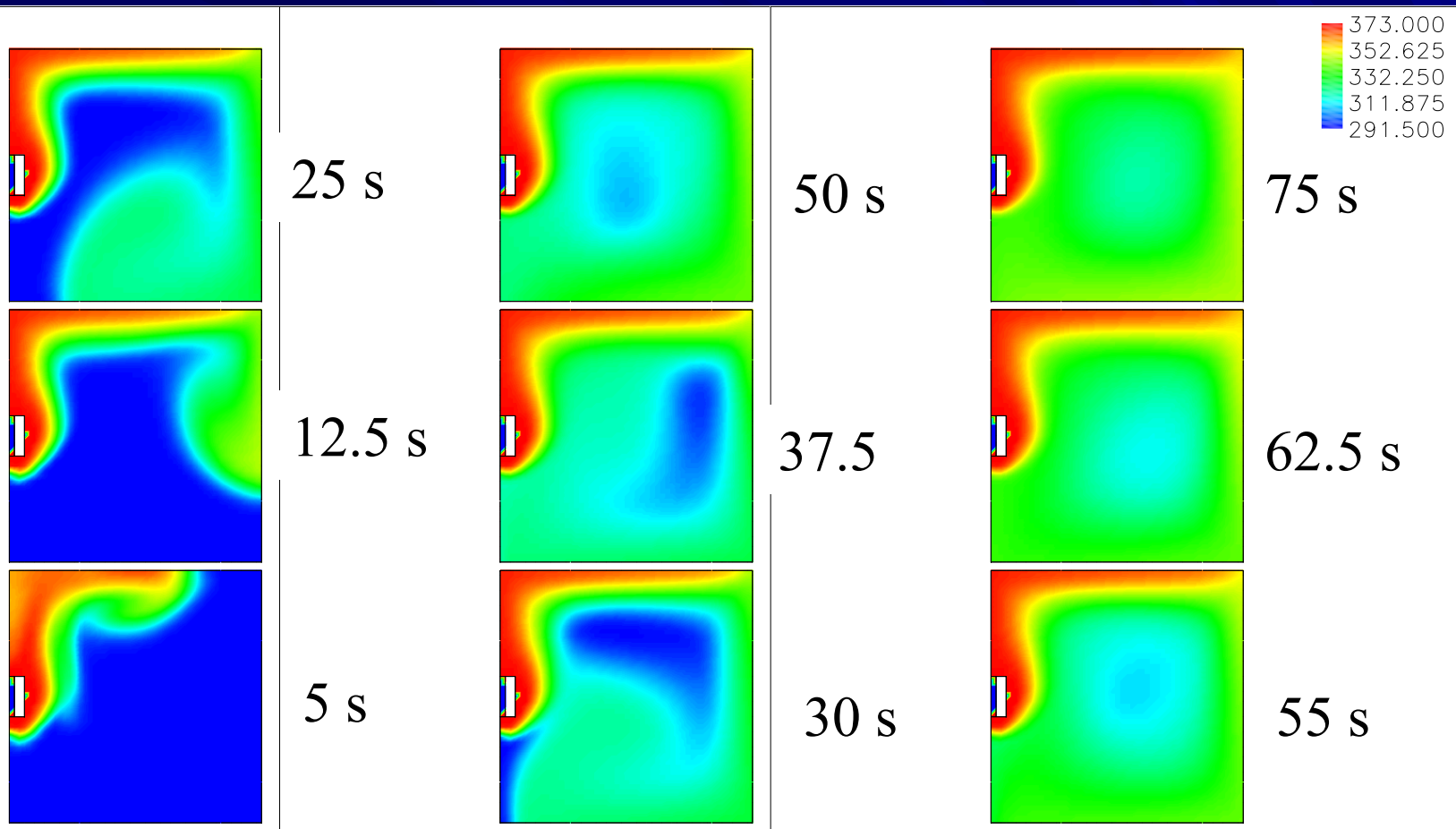
AP-600 Reactor System



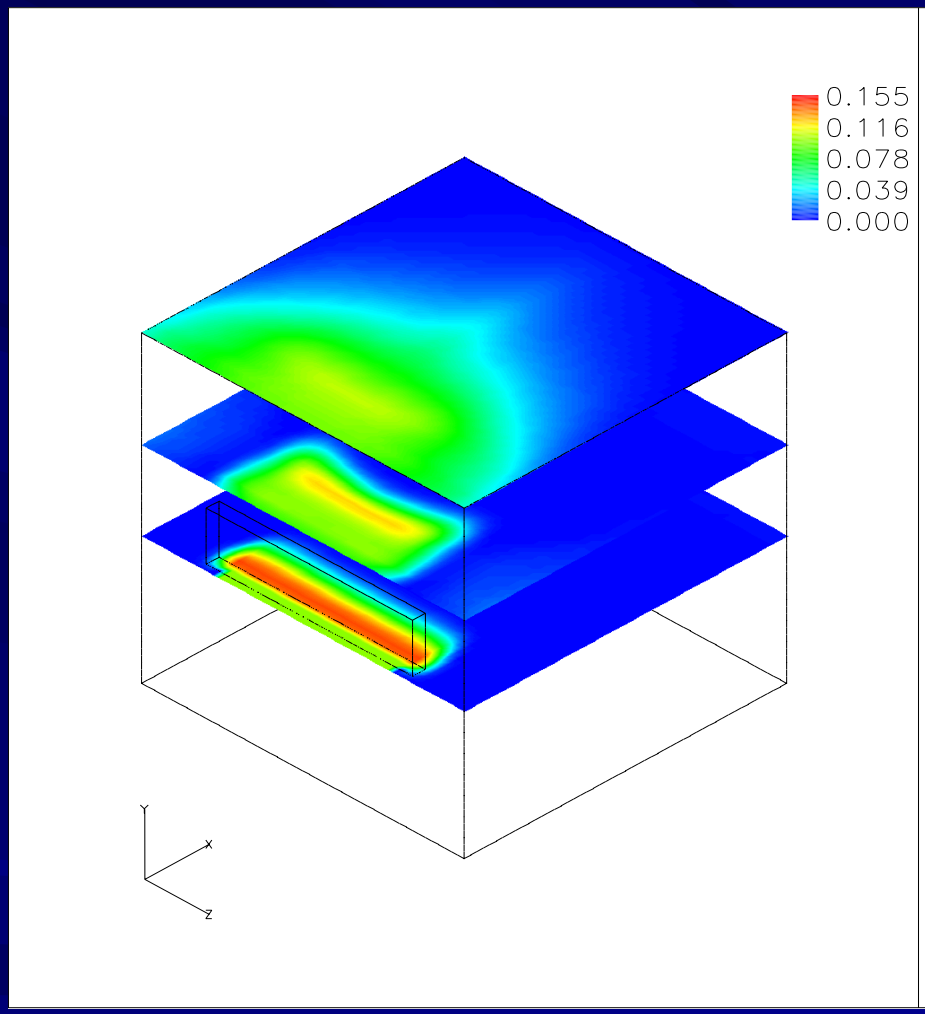
3-D Model of IRWST Pool



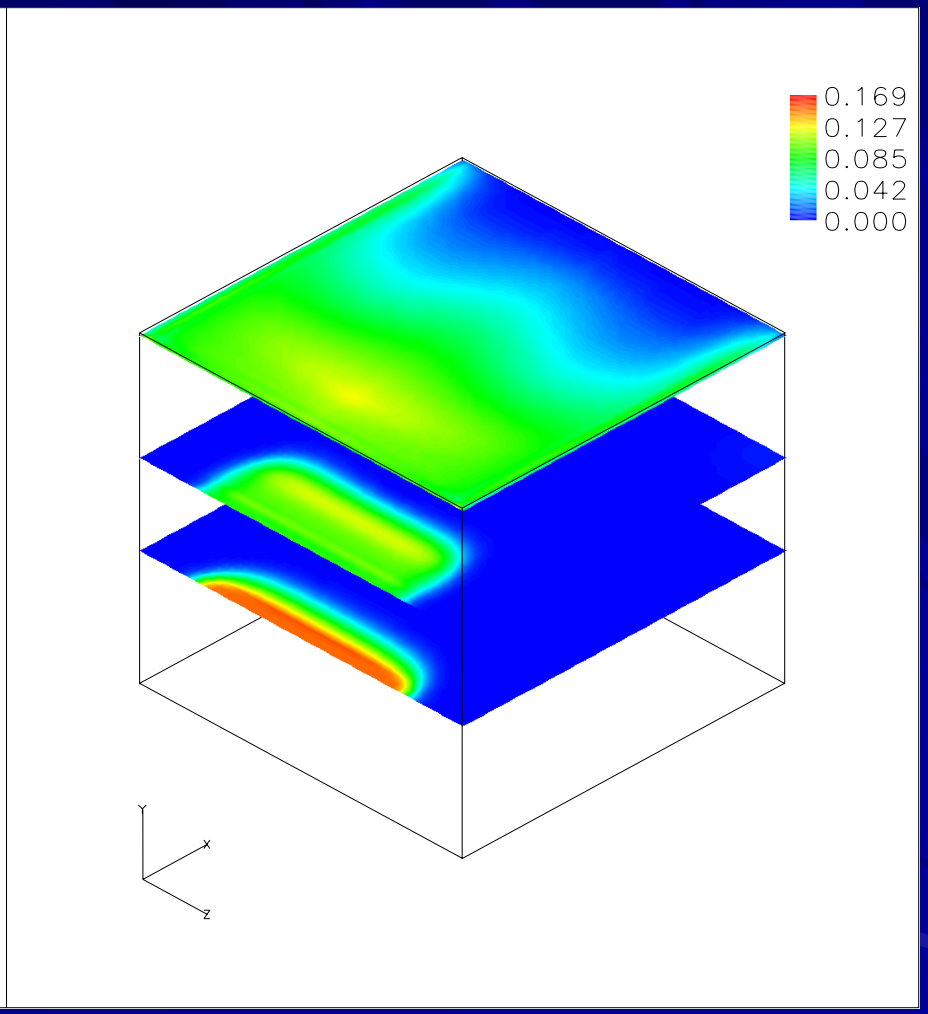
Prediction of Pool Temperature in IRWST Following Steam/Water Injection through Sparger (Antal et al., 2000)



3-D Void Profiles in IRWST (Antal et al., 2001)

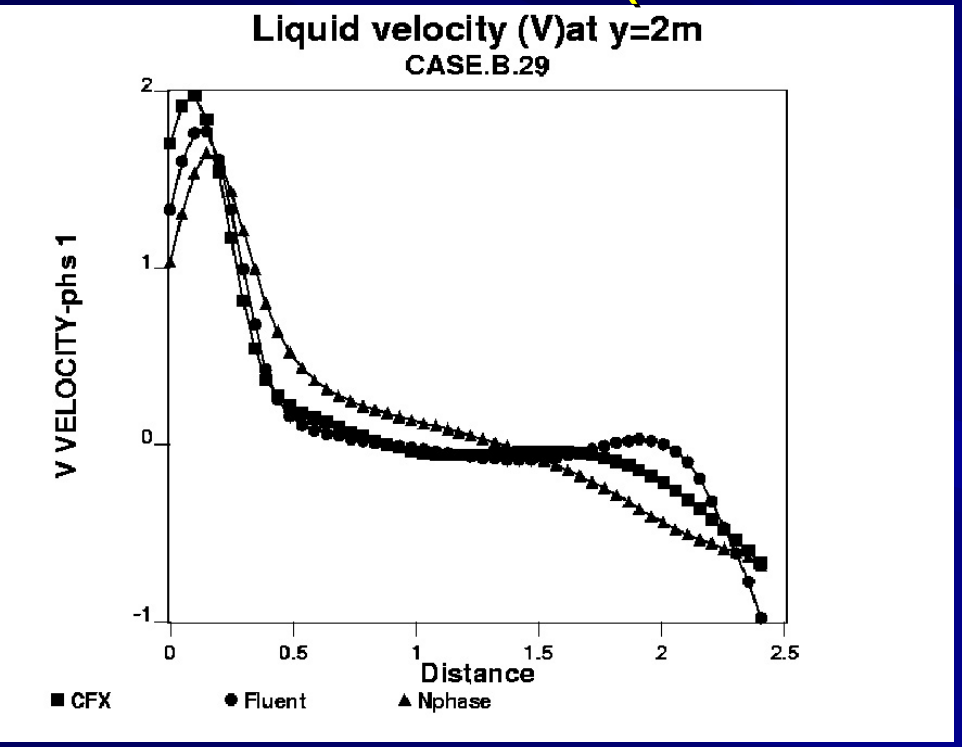


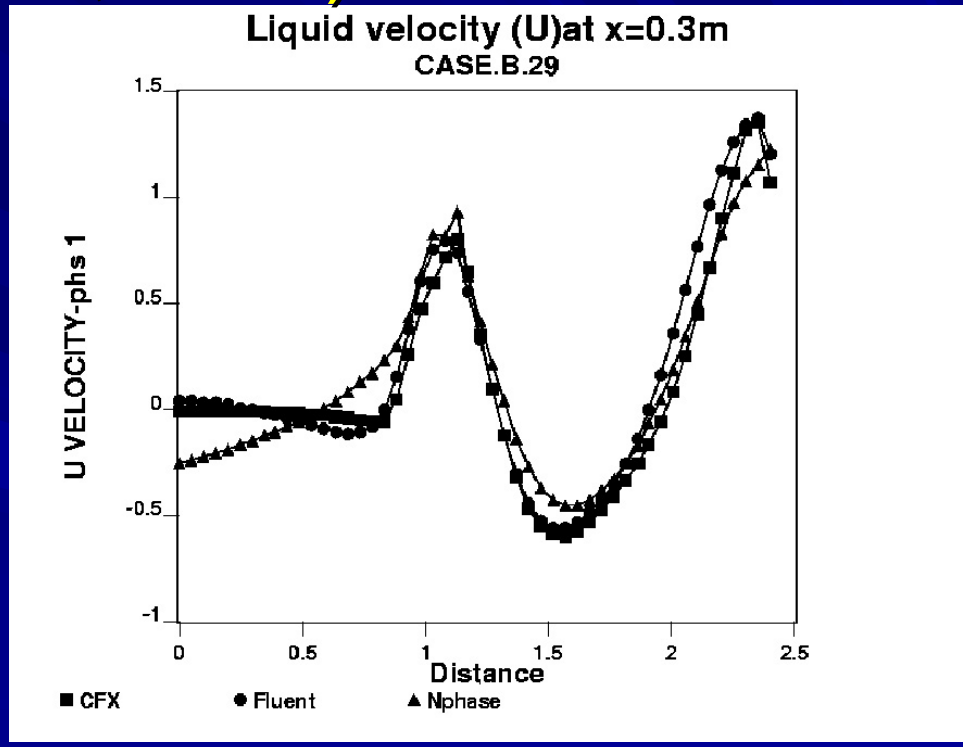
CFX



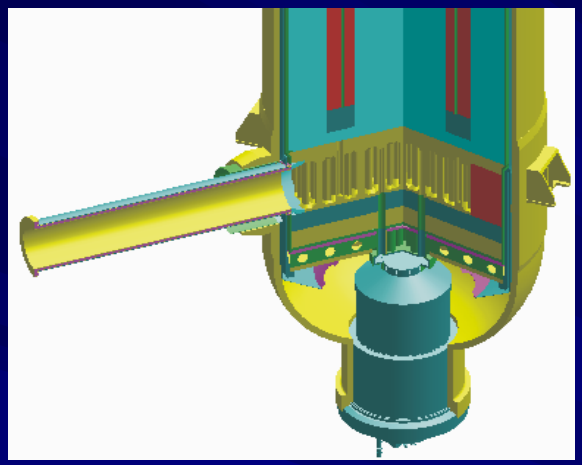
NPHASE

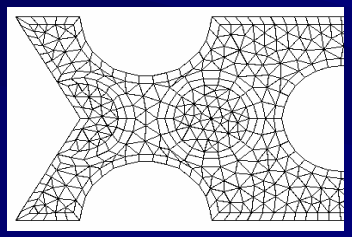
Planary Velocity Profiles in IRWST Calculated by CFX, Fluent and NPHASE for 40% Inlet Vapor Volumetric Fraction (Antal et al., 2001)

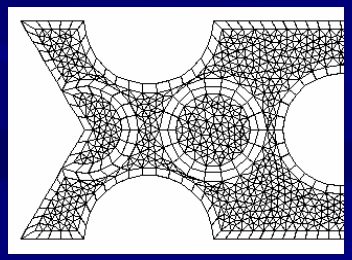


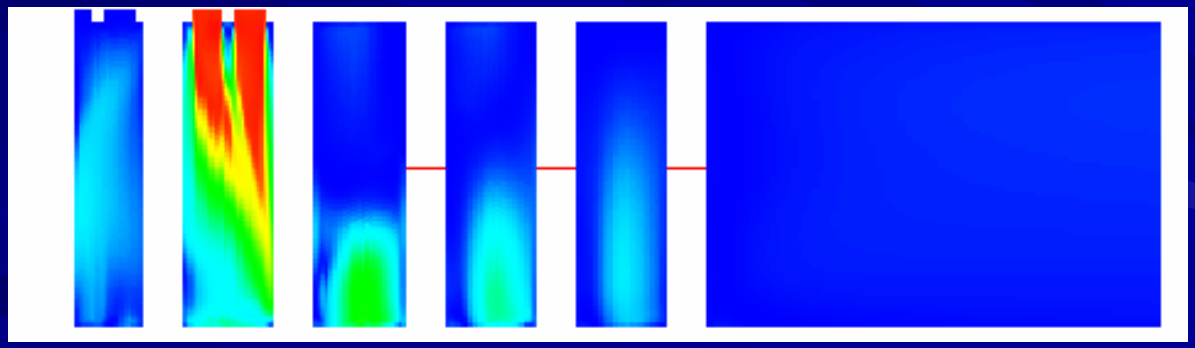


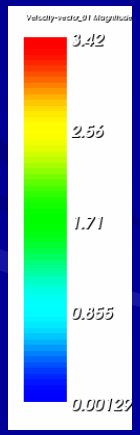
NPHASE Simulation of VHTR Outlet Plenum (Gallaway et al., 2007)











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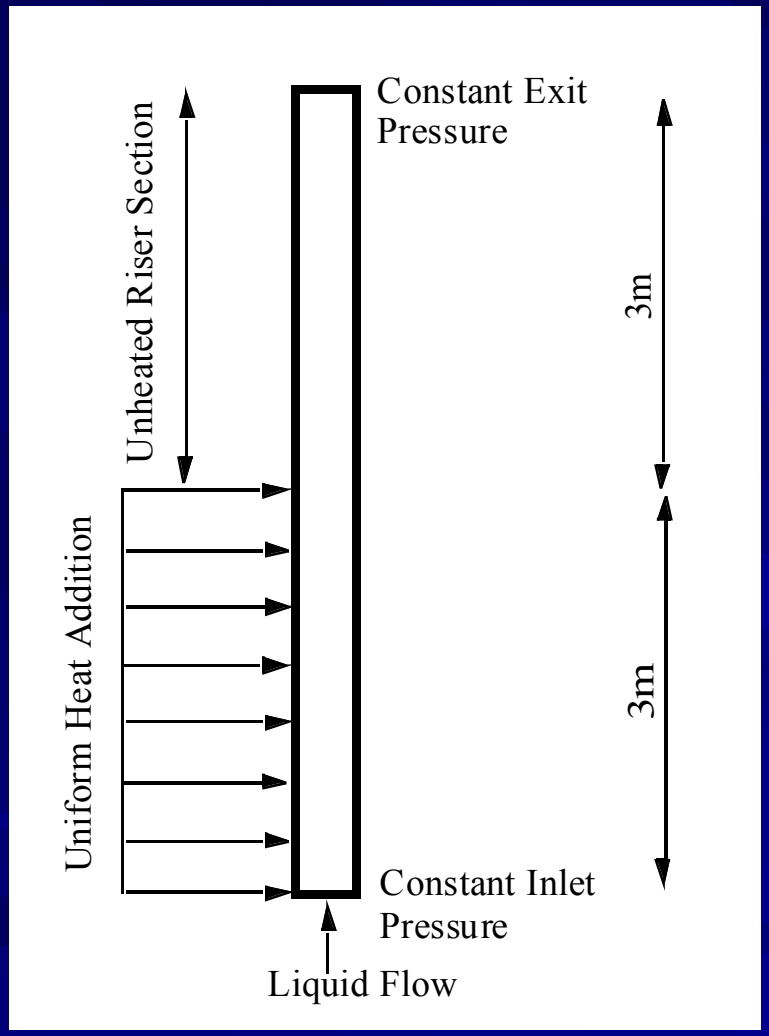
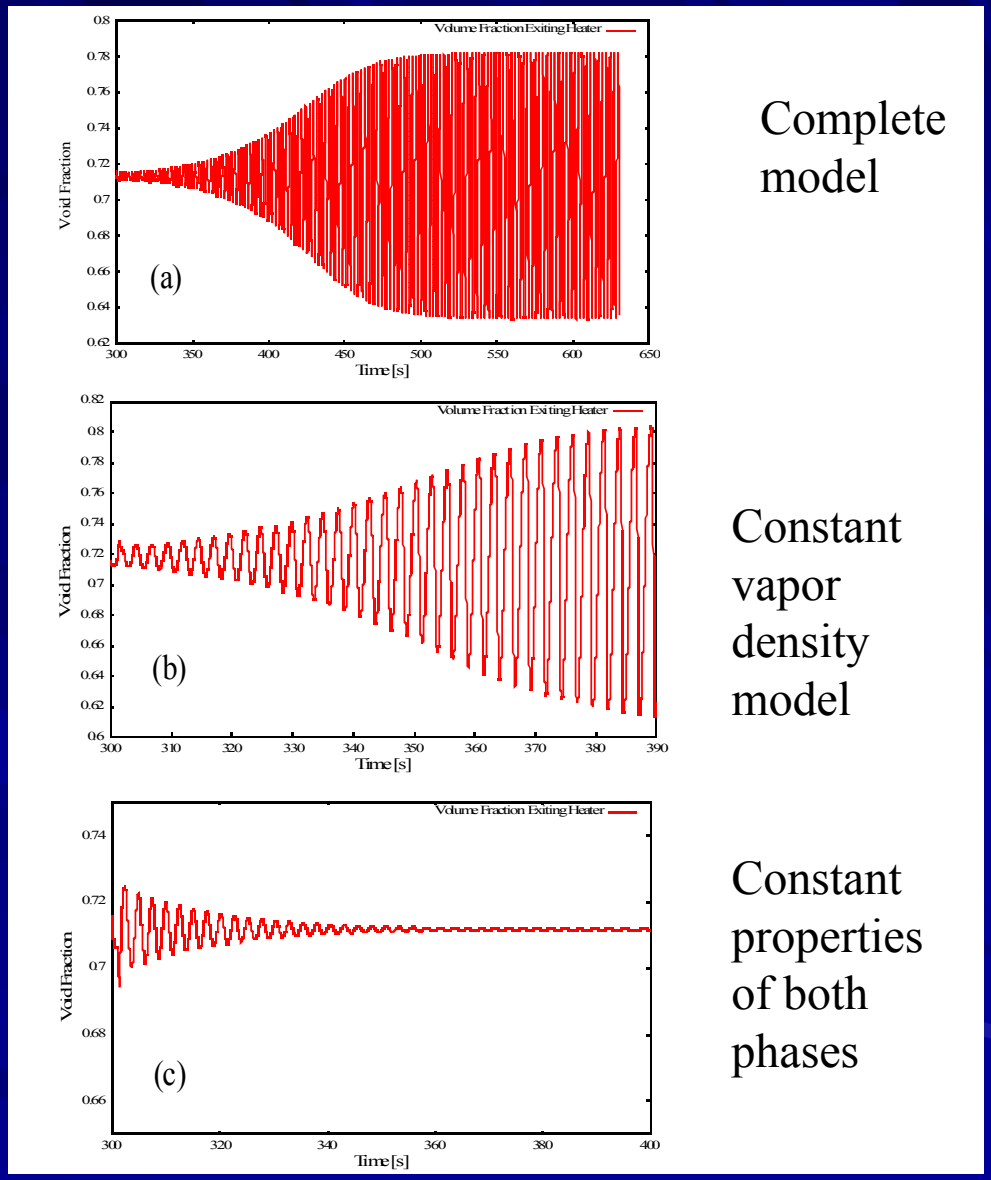
Transients and Instabilities

Density-Wave Oscillations in Core-Riser of BWR

(Antal & Podowski, 2003)





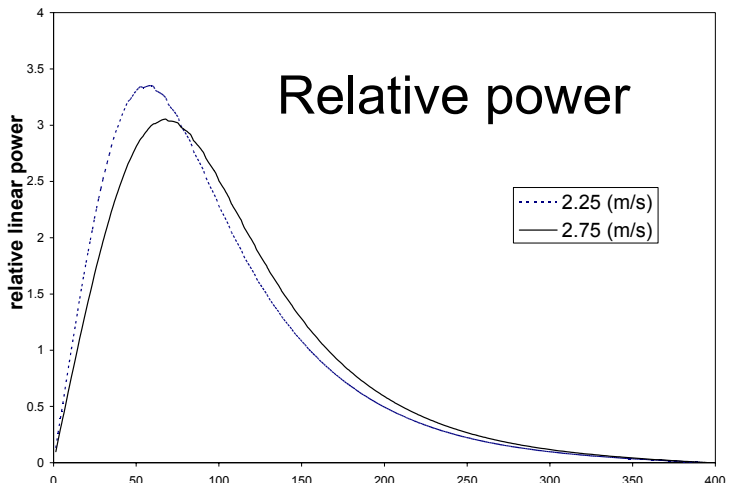
Complete model

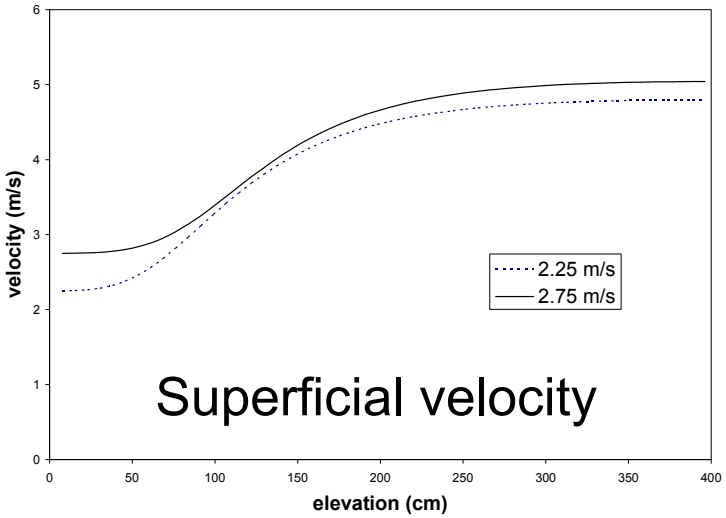
Constant vapor density model

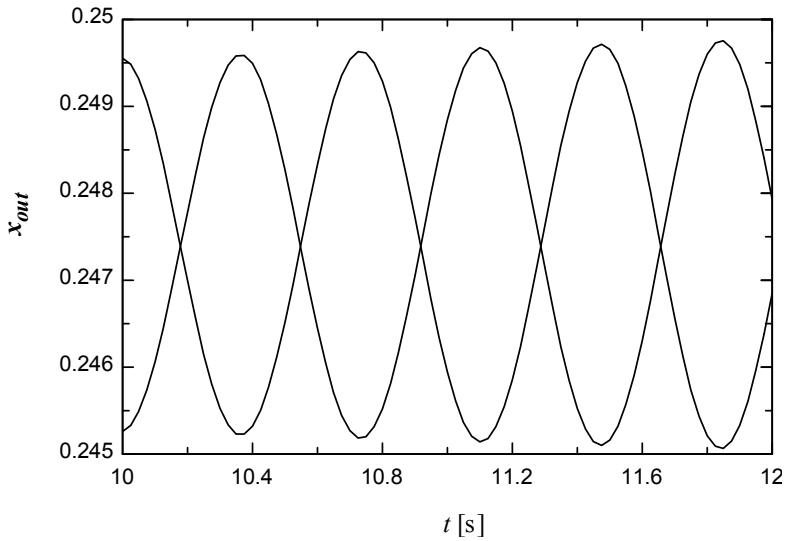
Constant properties of both phases

Coupled Thermal-Hydraulics/Neutronics Model

(Podowski & Aniel-Buchheit, 2006)







Stable limit-cycle oscillations in two-zone/two-parallel-channel point kinetics core model

Summary

- Selected multiphase flow modeling and computational issues have been discussed
- Details can be found in published papers
- Most-recent results have been submitted for publication (journals and/or 2007 conferences)

Recent Publications

- "On the Modeling of Dispersed Particulate Flows using a Multifield Model", P. Tiwari, S.P. Antal and M.Z. Podowski, *Computational Solids and Fluids Mechanics*, Elsevier (2003)
- "Multifield Computational Fluid Dynamics Model of Particulate Flow in Curved Circular Tubes" P. Tiwari, S.P. Antal, G. Belfort, A. Burgoyne and M.Z. Podowski, *Theoretical and Computational Fluid Dynamics* (2004)
- "The Modeling of Thin Liquid Films along Inclined Surfaces", M.Z. Podowski and A. Kumbaro, *Journal of Fluids Engineering* (2004)
- "Theoretical Model of Contact Angle and Shape of Droplets on Solid Substrates", S. Vafaei and M.Z. Podowski, *Nuclear Engineering and Design* (2005)

Recent Publications (*continued*)

- "Understanding Multiphase Flow and Heat Transfer: Perception, Reality, Future Needs", M.Z. Podowski, *Archives of Thermodynamics* (2005)
- "Three-Dimensional Fluid Mechanics of Particulate Two-Phase Flows in U-bend and Helical Conduits", P. Tiwari, S.P. Antal and M.Z. Podowski, *Physics of Fluids* (2006)
- "On the Modeling of Bubble Evolution and Transport using Coupled Level-Set/CFD Method", B.W. Wierzbicki, S,P. Antal and M.Z. Podowski, Proc NURETH-11 (2005), also: *Nuclear Technology* (2006, in print)
- "Multidimensional Modeling of Developing Two-Phase Flows in a Large Adiabatic Riser Channel", S. P. Antal, M.Z. Podowski, R.T. Lahey, D. Barber and C. Delfino, Proc NURETH-11 (2005)
- "Development of Mechanistic Modeling Capabilities for Generation-IV Supercritical Water-Cooled Reactor", M.Z. Podowski, S.P. Antal and H. Anglart, Proc. ICAPP (2006)

Recent Publications (*continued*)

- "Multidimensional Model of Fluid Flow and Heat Transfer in Generation-IV Supercritical Water Reactors", T. Gallaway, S.P. Antal and M.Z. Podowski, Proc. ICONE-14 (2006). Also: *Nuclear Engineering and Design* (in print)
- "On The Modeling of Local Neutronically-Coupled Flow-Induced Oscillations in Advanced Boiling Water Reactors", S. Aniel-Buchheit and M.Z. Podowski, Proc. ICONE-14 (2006)
- The Effect of Bubble/Bubble Interactions on Local Void Distribution in Two-Phase Flows", A. Kumbaro and M.Z. Podowski, Proc. 13th IHTC (2006)
- "On the Consistency of Multifield Formulation for Modeling Two-Phase Flow and Heat Transfer", M.Z. Podowski, Proc. 13th IHTC (2006)