Computational Approach to Multiscale Multiphysics Modeling of Nuclear Reactors

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Presentation Outline

- Background: *Modeling framework*
- Modeling and computational challenges in "DOE University Consortium" project
- Research challenges associated with new projects (DOE/NEUP, DOE/CASL)
- Conclusions

Modeling framework

- Multiscale
  - molecular/nano;
    - *radiation-induced molecular fuel structure evolution and damage*
    - *thin films*
    - *interfacial phenomena*
  - micro
    - *continuum fluid mechanics and heat transfer (DNS)*
  - macro
    - *reactor-scale fluid mechanics and heat transfer,*
    - *ensemble-averaged models of two-phase fluids*

Modeling framework (continued)

- Multiphysics:
  - solid mechanics (reactor fuel performance: microstructure, effect of fuel burnup on fuel/cladding interaction; fuel/core deformation and failure mechanisms)
  - single-phase fluid mechanics in complex geometries (turbulence, heat transfer)
  - two-phase flow and heat transfer (level of complexity orders of magnitude higher than in single-phase flow)

DOE University Consortium

Deployment of a Suite of High Performance Computational Tool for Multiscale Multiphysics Simulation of Generation-IV Reactors

Consortium Members

- Universities:

  - RPI, Columbia University, SUNY at Stony Brook

- National Laboratory:

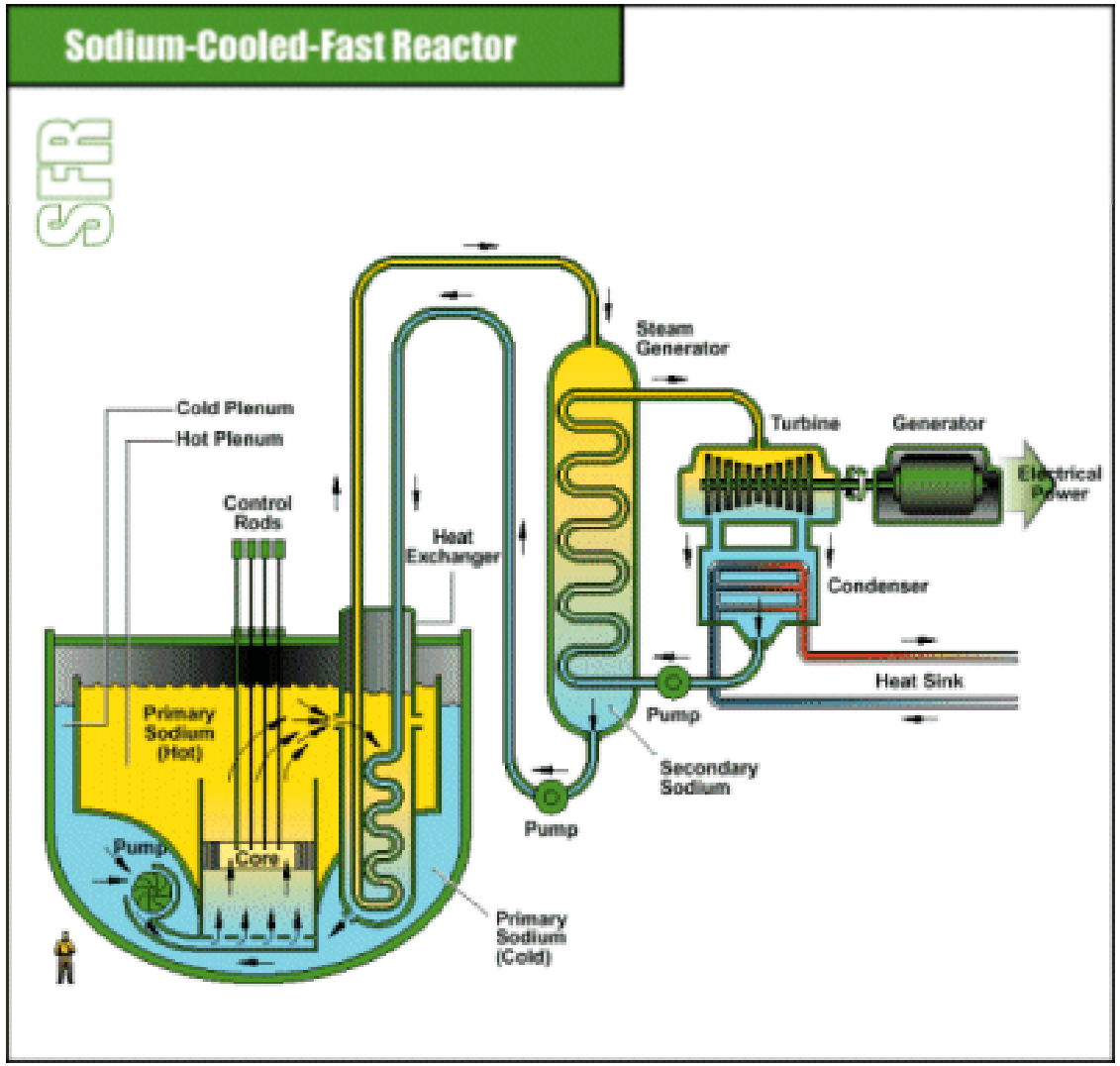
  - BNL

Consortium Team

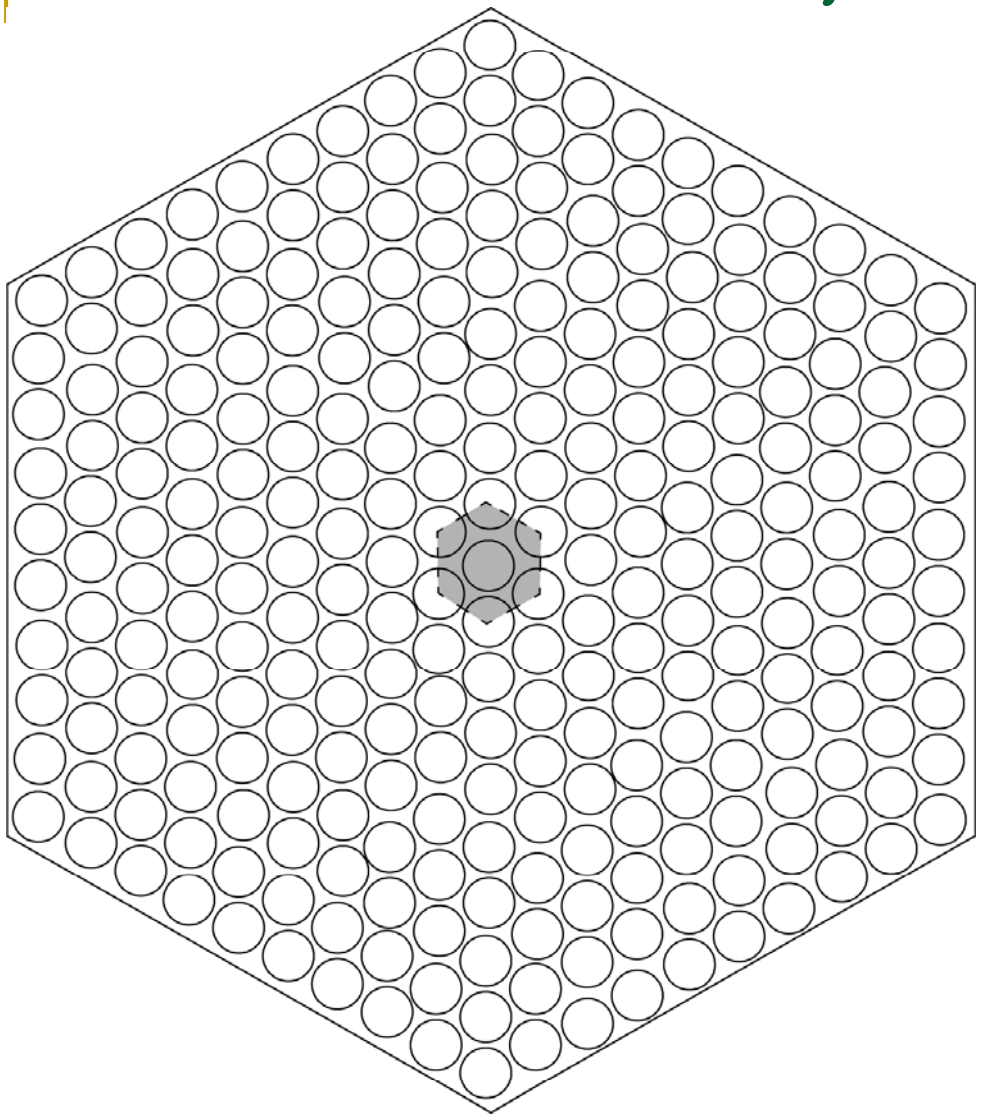
Project Objectives

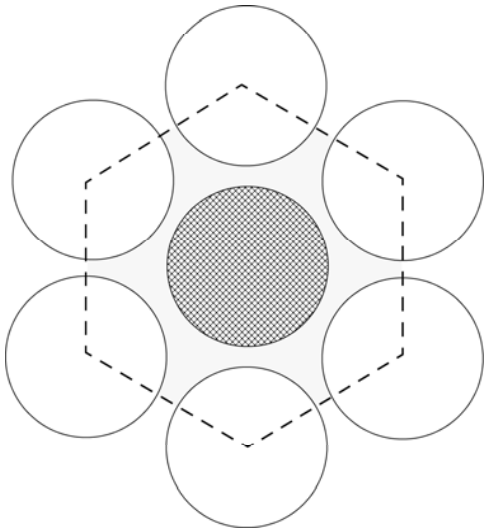
- *The overall objective is to develop a multiple computer code platform for advanced multiscale/multiphysics simulations of Generation IV reactors*
- *Apply proposed methodology to local channel blockage accident analysis for Sodium Fast Reactor (SFR)*

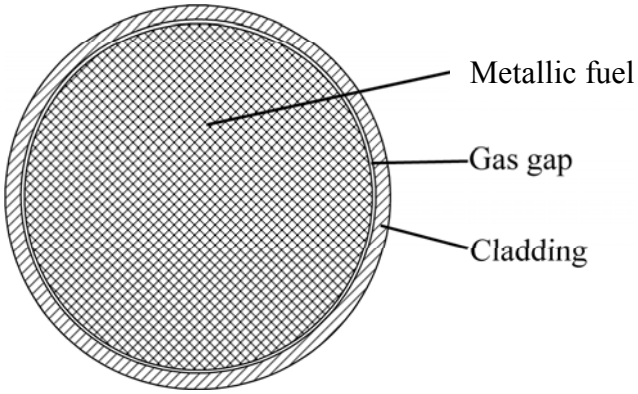
Sodium-Cooled Fast Reactor (SFR)



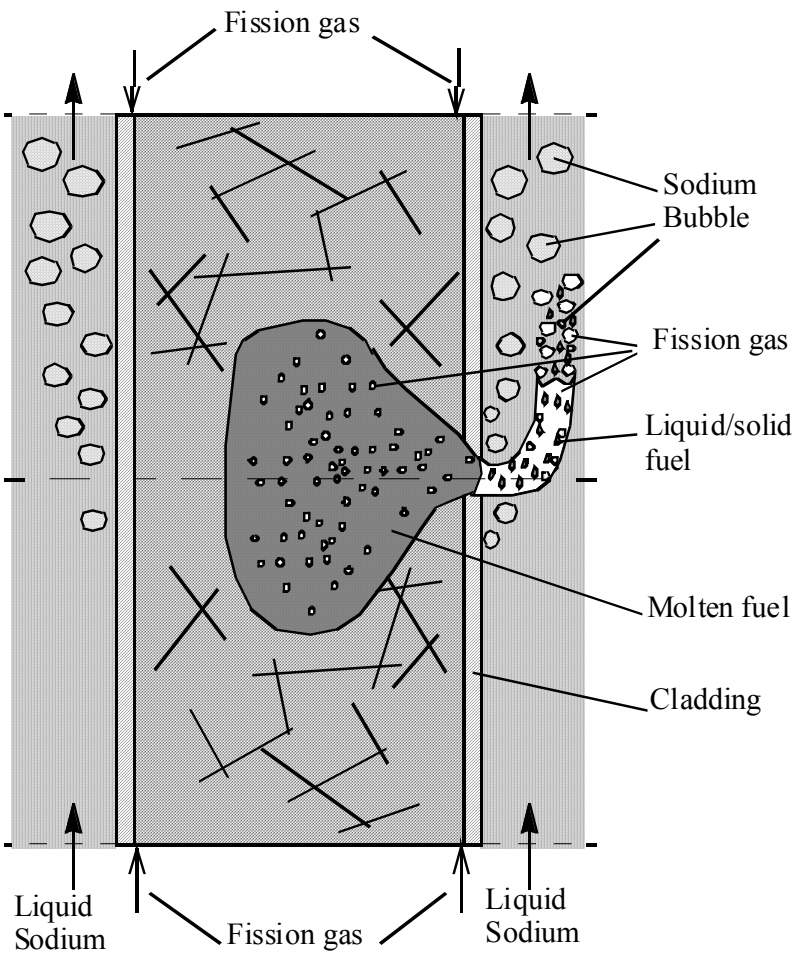
SFR Core Geometry

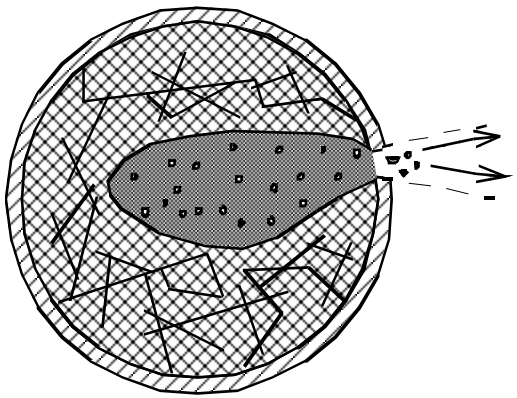






Schematic of fuel degradation and transport in SFR during fuel rod failure accidents

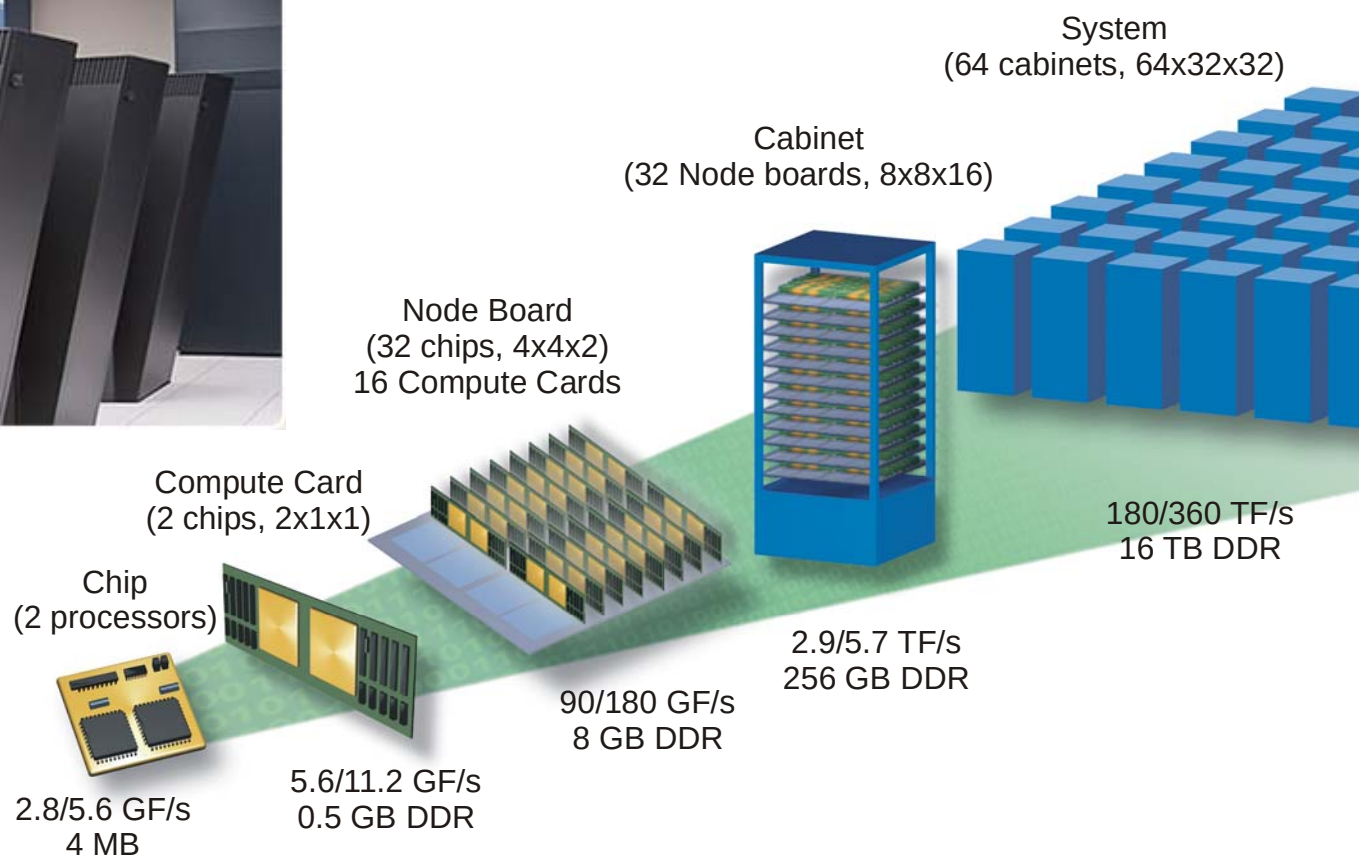




Tools and Approach

- Application of three existing computer codes
  - FronTier (SUNY-SB)
  - PHASTA (RPI)
  - NPHASE-CMFD (RPI)
- Development of advanced numerical modeling methods and their implementation in the computer codes used in the project (e.g.: coupling between NPHASE-CMFD and PETSc)
- Integration of individual models/computer codes
- Demonstration of capabilities of the new computer platform using IBM supercomputers

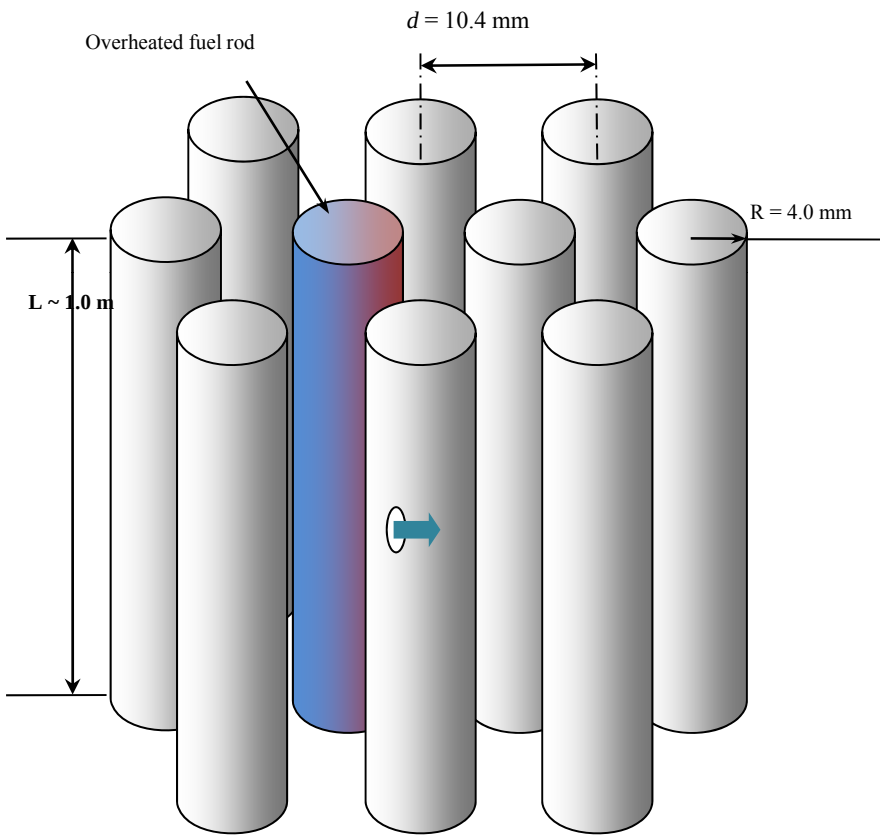
IBM Blue Gene Supercomputer



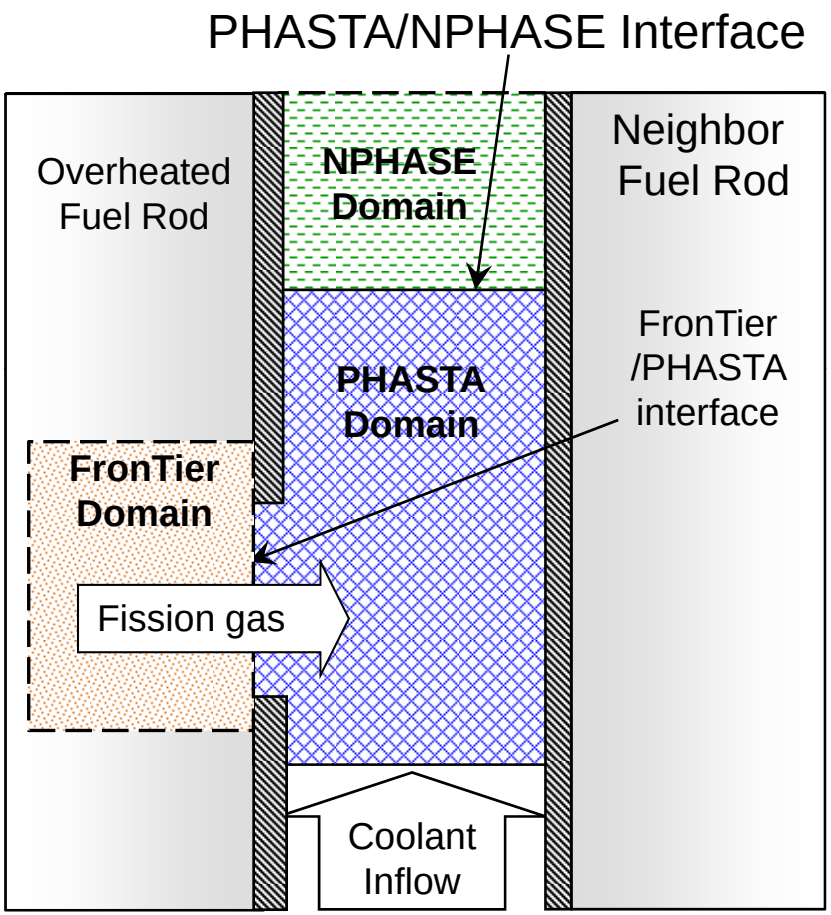
BNL: 18,432 nodes (36,864 processors) with 1GB/node 300TB of disk

RPI: 32,768 processors

Geometry and dimensions of a section of SFR fuel rod assembly with cladding failure location

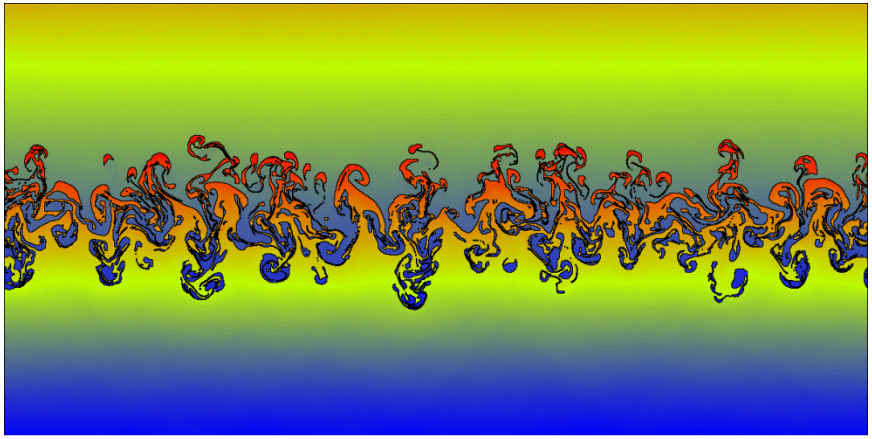


Computational domains overview (side view)

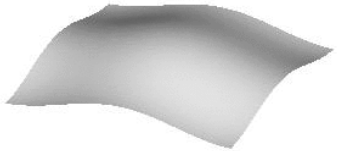


Software Overview

- FronTier
  - Parallel 3D multiphysics code based on front tracking
  - Explicit tracking of material interfaces
  - Compressible and incompressible fluid dynamics
  - MHD
  - Flow in porous media
  - Elasto-plastic deformations
  - Phase transition models



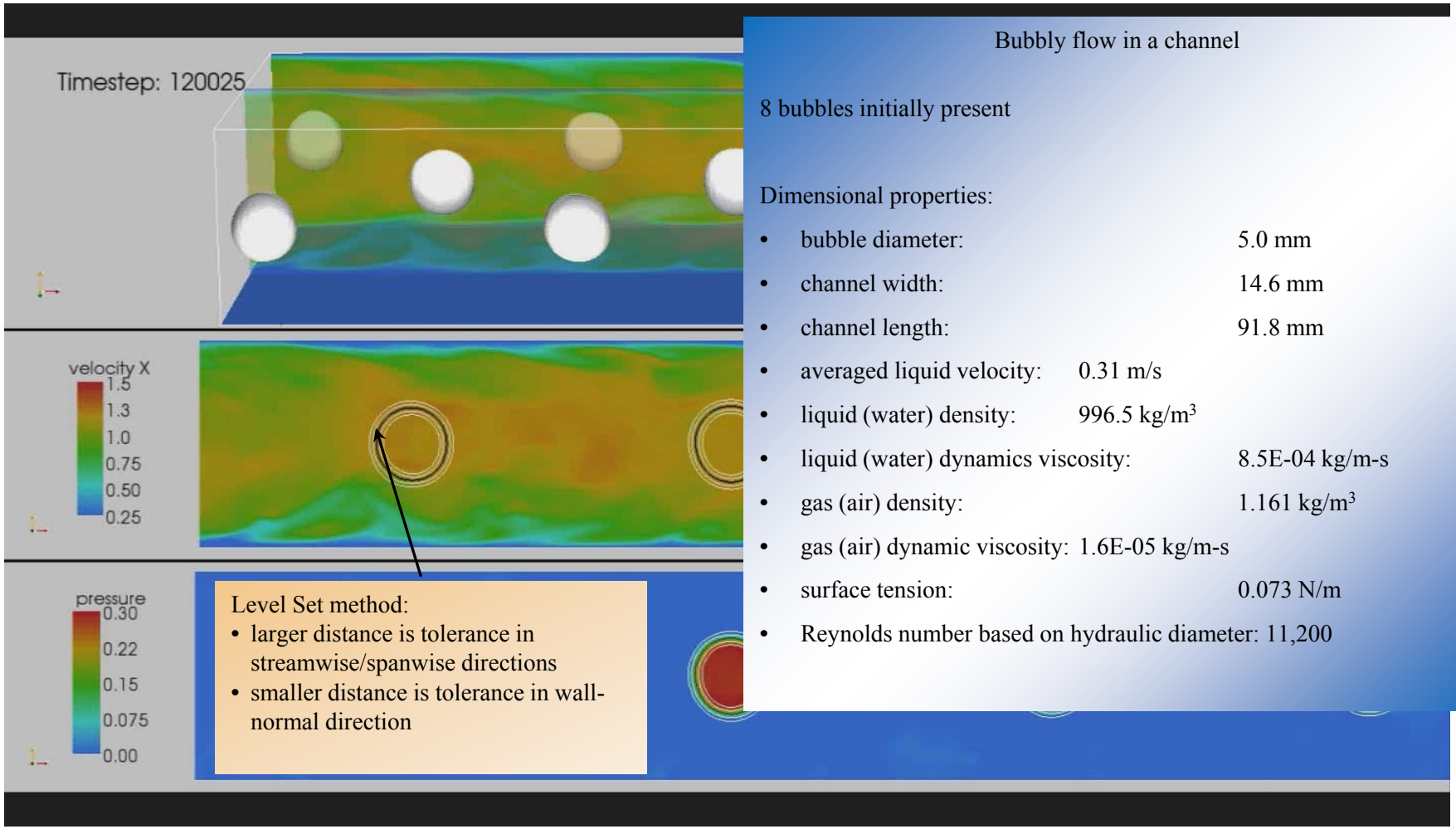
Turbulent fluid mixing



Software overview

- PHASTA
  - **P**arallel, **H**ierarchic, **A**daptive, **S**tabilized (finite element) **T**ransient **A**nalysis flow solver developed at RPI
  - Effective tool for bridging a broad range of length scales in turbulent flows: RANS, LES, detached eddy simulation (DES), DNS
  - Uses advanced anisotropic adaptive algorithms
  - Uses anisotropically adapted unstructured grids
  - Capable of simulating two phase flows with level set method
  - Highly scalable performance on massively parallel computers (e.g.,IBM Blue Gene)

PHASTA DNS simulation of bubbly flow



Level Set method:
- larger distance is tolerance in streamwise/spanwise directions
- smaller distance is tolerance in wall-normal direction

Bubbly flow in a channel

8 bubbles initially present

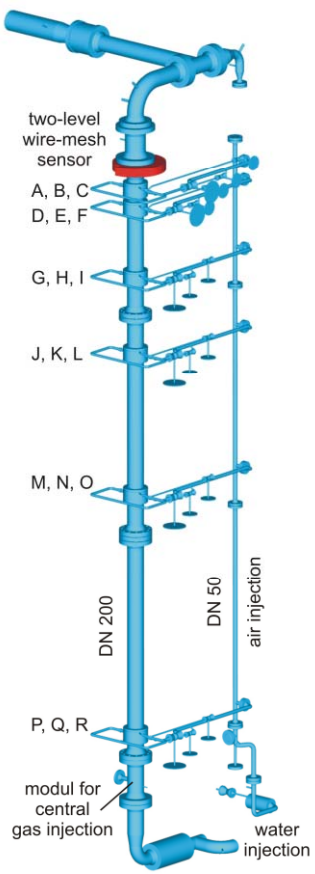
Dimensional properties:

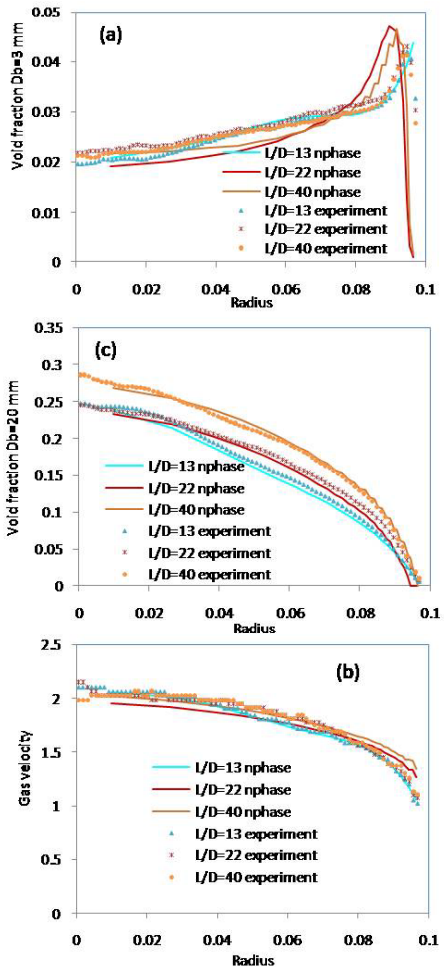
- bubble diameter: 5.0 mm
- channel width: 14.6 mm
- channel length: 91.8 mm
- averaged liquid velocity: 0.31 m/s
- liquid (water) density: 996.5 kg/m^3
- liquid (water) dynamics viscosity: 8.5E-04 kg/m-s
- gas (air) density: 1.161 kg/m^3
- gas (air) dynamic viscosity: 1.6E-05 kg/m-s
- surface tension: 0.073 N/m
- Reynolds number based on hydraulic diameter: 11,200

Software overview

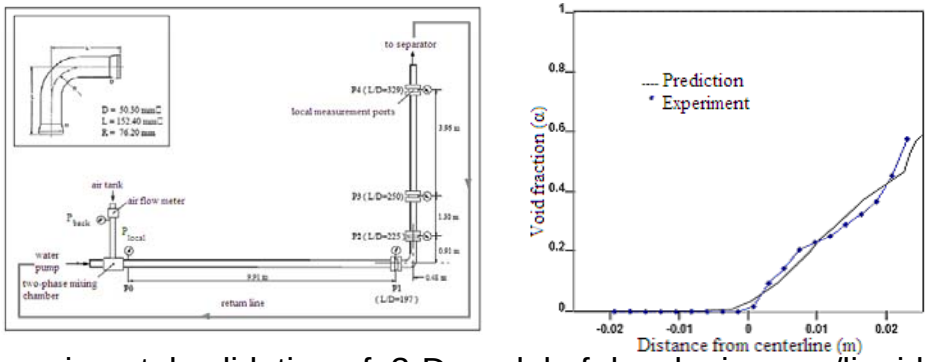
- NPHASE CMFD
  - Computational Multiphase Fluid Dynamics solver
  - Uses unstructured grids with arbitrary element types
  - Capable of modeling an arbitrary number of fields (fluid components and/or phases)
  - Has built-in mechanistic modeling, integrated with numerics
  - Characterized by improved robustness and numerical convergence
  - Can be used to model gas/liquid interfaces using Level-Set method
  - Uses state-of-the-art multiphase models which have been extensively validated

Examples of NPHASE-CMFD validation

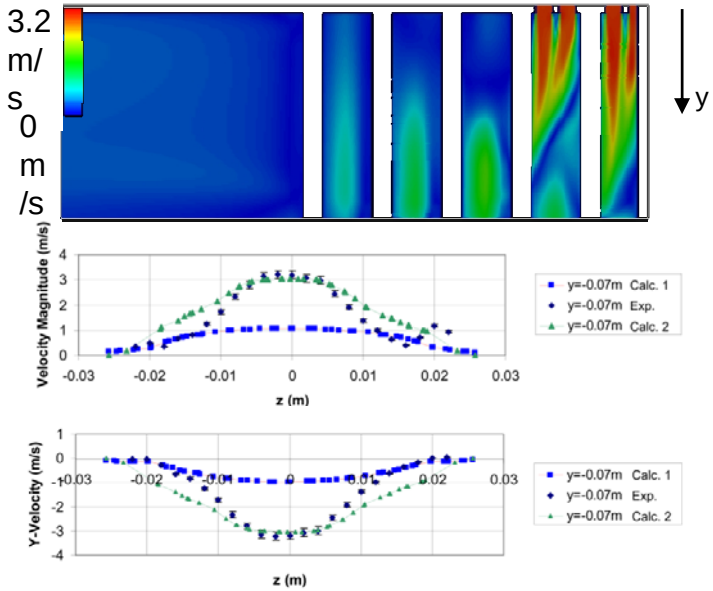




- Validation of 3-D model of developing gas/liquid flow against TOPFLOW experiments (Tselishcheva et al., 2010)



Experimental validation of 3-D model of developing gas/liquid flow in horizontal pipe with 90° elbow (Tselishcheva et al. 2010)



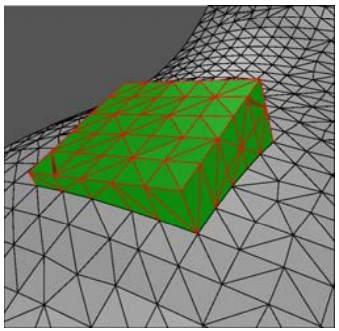
Experimental validation of 3-D model of single-phase flow distribution in scaled lower plenum of VHTR (Gallaway et al,. (2007)

Examples of solved computational issues

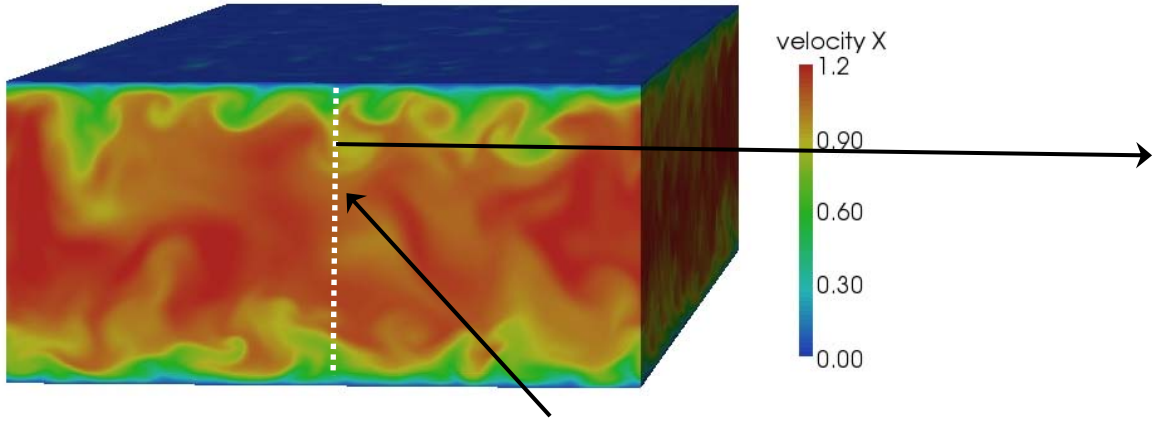
- Cladding failure model
- DNS data averaging
- DNS simulation of gas jet injection
- RANS simulation of gas/liquid metal flow

Development of mesoscale solid failure models for FronTier

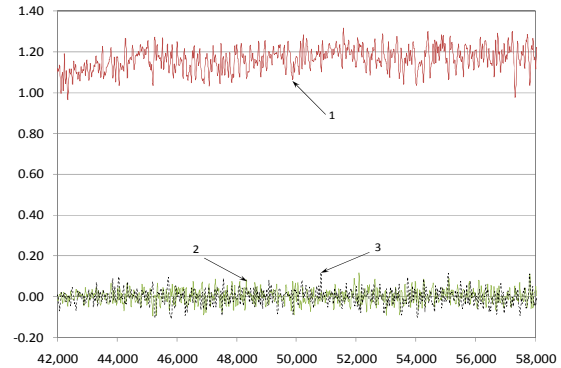
- *Finite element meshes conforming to interfaces of solid structures*
- *The medium is represented by a network of nodes connected by bonds satisfying some stress - strain relation*
- *Bonds are present with the probability p. The probability of initial defect is p-1*
- *The process consists of the energy minimization and sequential breaking of bonds which exceed the critical stress threshold*



Single-phase channel flow: Steady-state DNS data averaging



Set of virtual probes which collect fluctuating velocity at various wall distances



Velocity evolution, $u_i(\underline{t})$, is recorded for each probe

Post-processing code computes:

- Mean velocity

$$U_i = \frac{1}{N}\sum_{j=1}^{N} u_i(t_j)$$

- Turbulent dissipation rate

$$\varepsilon = \nu \frac{1}{N}\sum_{j=1}^{N}\sum_{i=1}^{3}\sum_{k=1}^{3}\frac{\partial u_i'(t_j)}{\partial x_k}$$

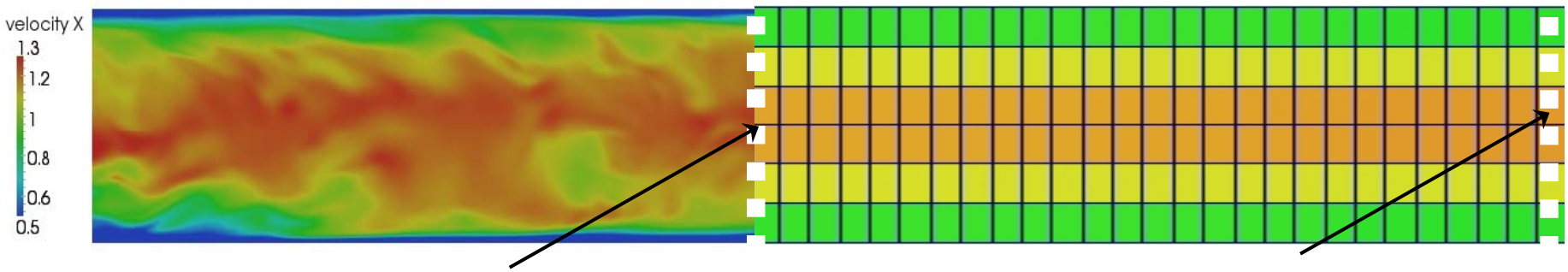
- Turbulent kinetic energy

$$k = \frac{1}{N}\sum_{j=1}^{N}\sum_{i=1}^{3}\left(u_i'(t_j)\right)^2, \quad u_i'(t_j) = u_i(t_j) - U_i$$

Single-phase channel flow: Link with high-Re k-ε model case

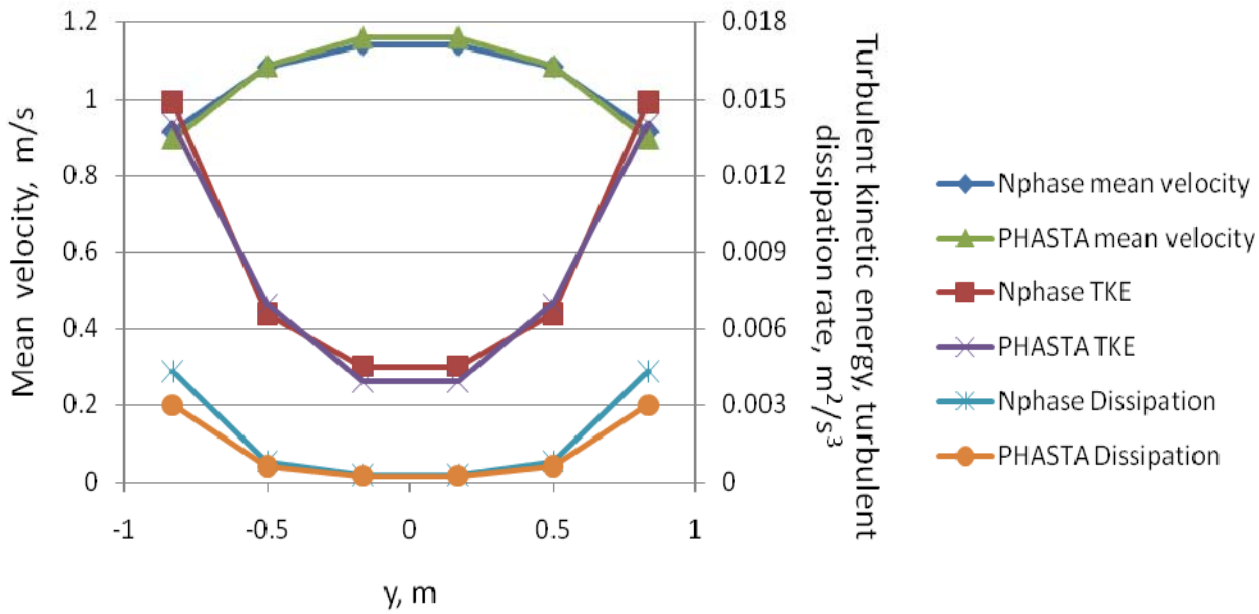
Channel flow DNS at Re_{hd} = 11,200

High-Re k-ε model: Re_{hd} = 11,200



PHASTA-DNS probe points

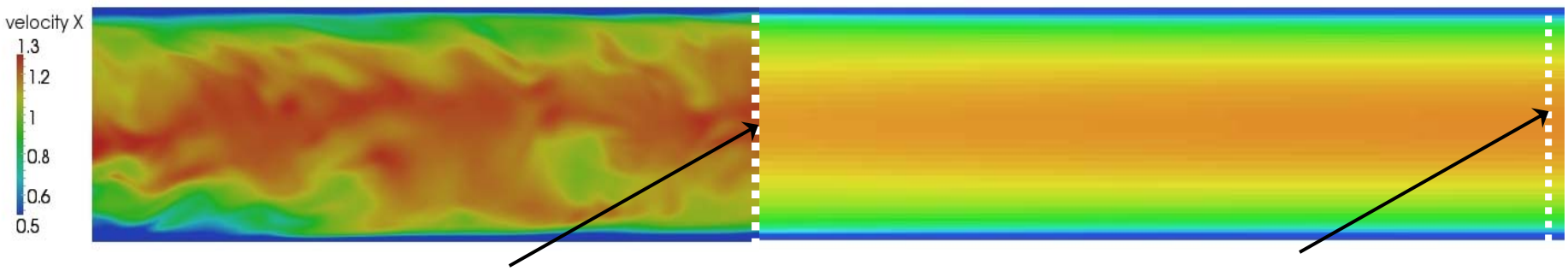
NPHASE outflow result



Single-phase channel flow: Link with low-Re k-ε model case

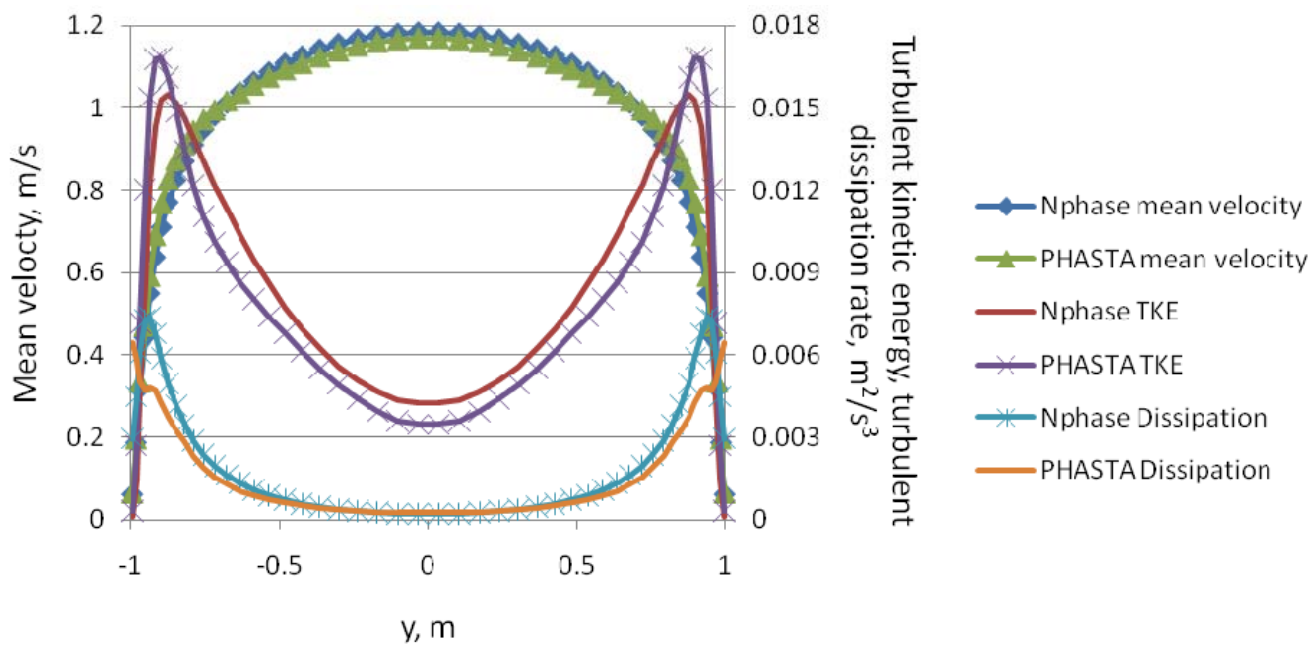
Channel flow DNS at Re_{hd} = 11,200

Low-Re k-ε model: Re_{hd} = 11,200



PHASTA-DNS probe points

NPHASE outflow result



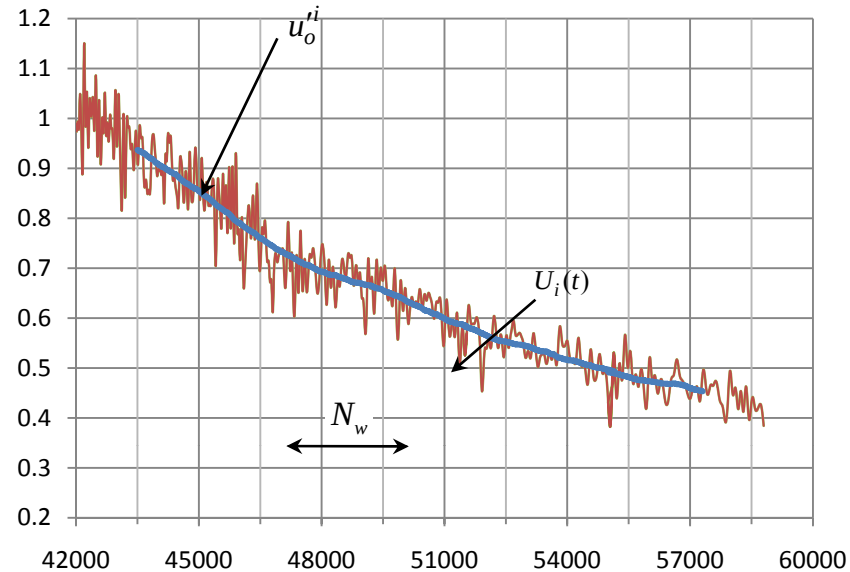
DNS data averaging in transient flows

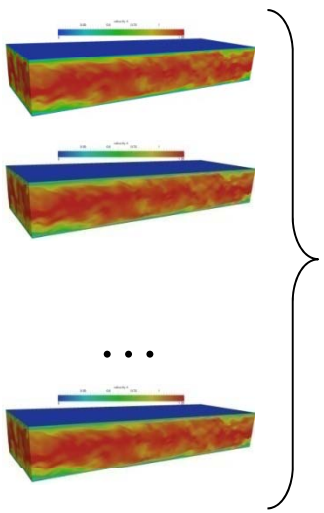
Time-window averaging is not appropriate solution in case of rapid transient flows.

Although mean velocity computation does not require significant statistics, second-order quantities, such as turbulent kinetic energy and turbulent dissipation rate does.

In order to compensate the restriction on the averaging window length we can employ ensemble averaging combined with small window-averaging.

Different runs are performed with slightly different initial conditions in order to develop a random fluctuating velocity field for each case to be cross averaged.





N_e runs are cross averaged

$$U_i(t) = \frac{1}{N_e}\sum_{o=1}^{N_e}\left(\frac{1}{N_w}\sum_{j=1}^{N_w} u_o^i\left(t+t_j\right)\right)$$

$$k(t) = \frac{1}{N_e}\sum_{o=1}^{N_e}\left(\frac{1}{N_w}\sum_{j=1}^{N_w}\sum_{i=1}^{3}\tfrac{1}{2}\left(u_o'^i(t+t_j)\right)^2\right),$$

$$u_o'^i(t+t_j) = u_o^i(t+t_j) - U_i(t)$$

$$\varepsilon(t) = \nu\frac{1}{N_e}\sum_{o=1}^{N_e}\left(\frac{1}{N_w}\sum_{j=1}^{N_w}\sum_{i=1}^{3}\sum_{k=1}^{3}\frac{\partial u_o'^i(t+t_j)}{\partial x_k}\right)$$

where:
N_e is the number of ensemble members,
N_w is the number of velocity samples in each window,
t is the current time,
$t_j = \left(j - N_w/2\right)\Delta t$ is the local window time,
Δt is the time step.

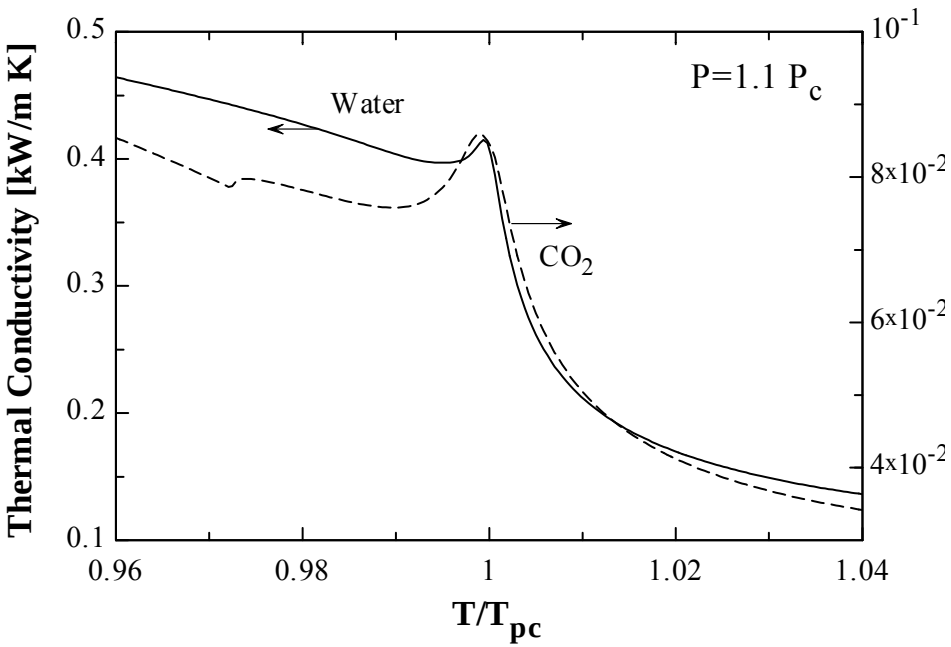
Coming Research Challenges

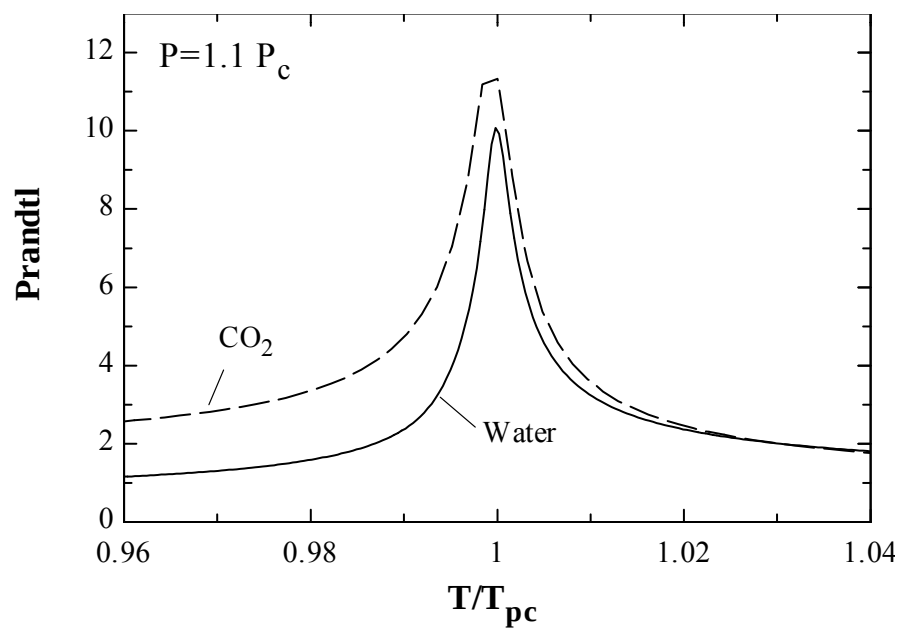
- DOE Nuclear Energy University Programs (NEUP): ***Development and Validation of Multidimensional Models of Supercritical CO_2 Energy Conversion Systems for Nuclear Power Reactors***

- DOE Energy Innovation Hub ***Consortium for Advanced Simulation of Light Water Reactors (CASL)***

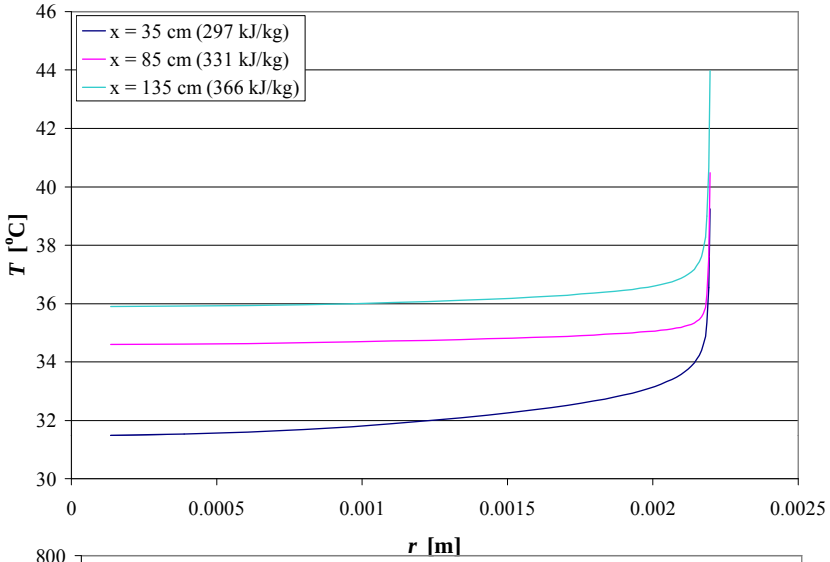
DOE/NEUP

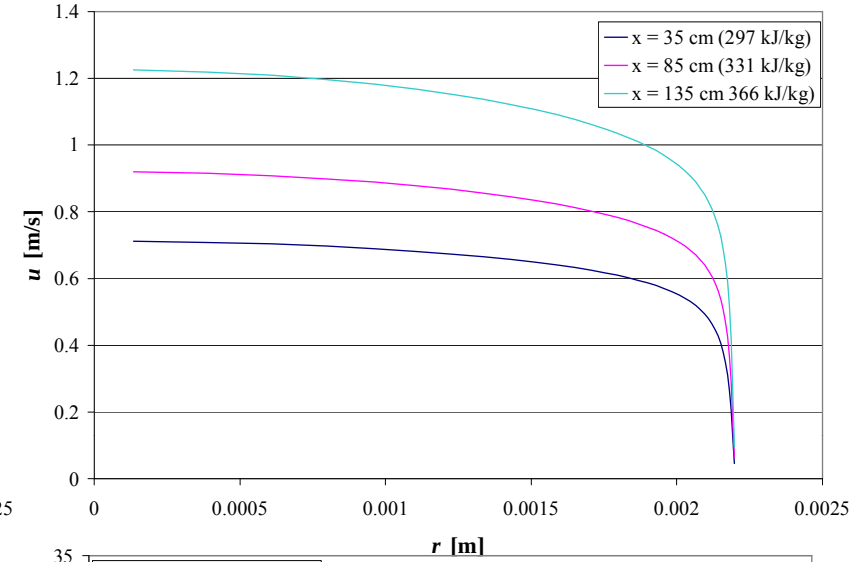
Development and Validation of Multidimensional Models of Supercritical CO_2 Energy Conversion Systems for Nuclear Power Reactors

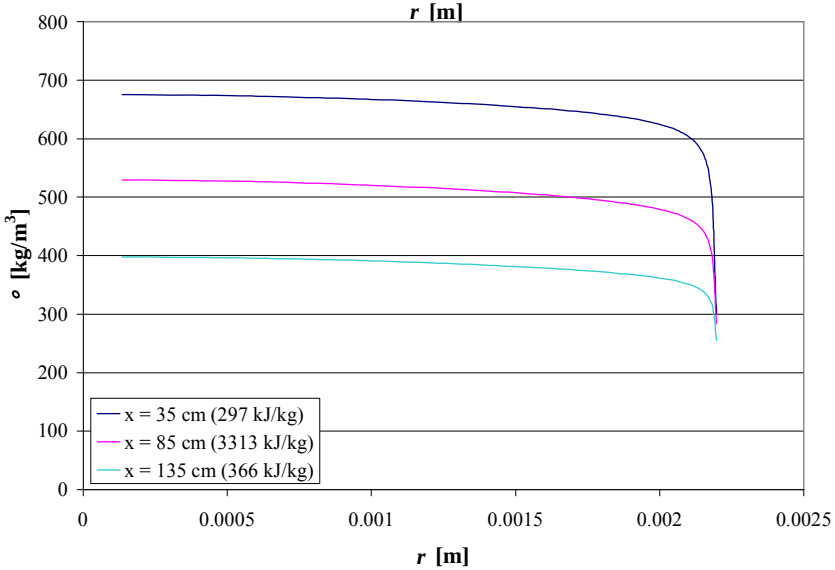


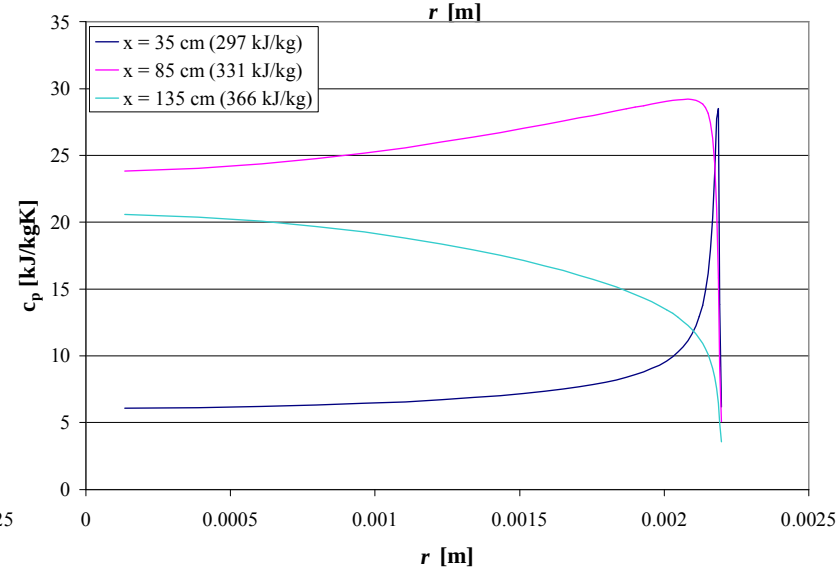


Radial Distributions of SCO_2 Properties using LRe k-ε Model

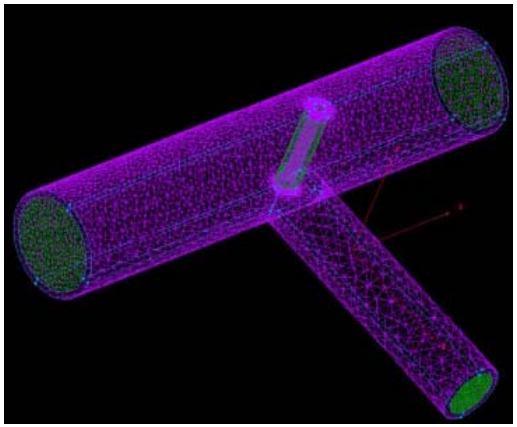


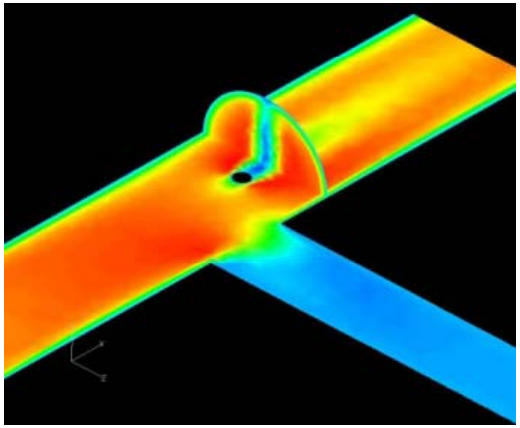




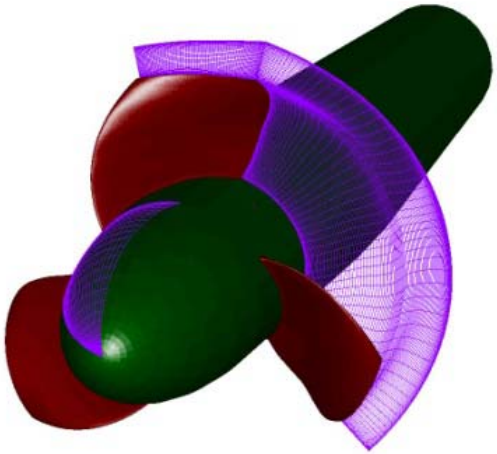


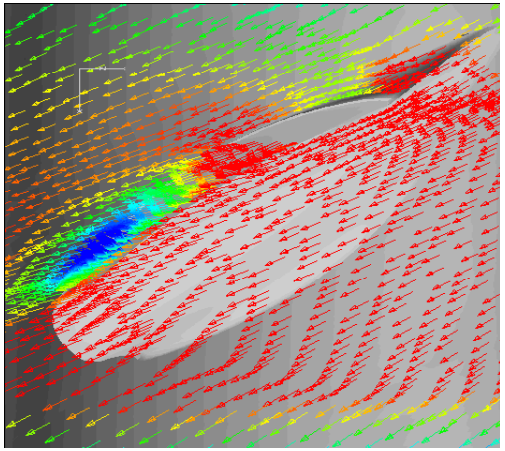
Modeling Challenges: Flow of Variable-Property SCO_2 in Complex Geometry Systems





Flow junctions and dividers





Rotating machinery

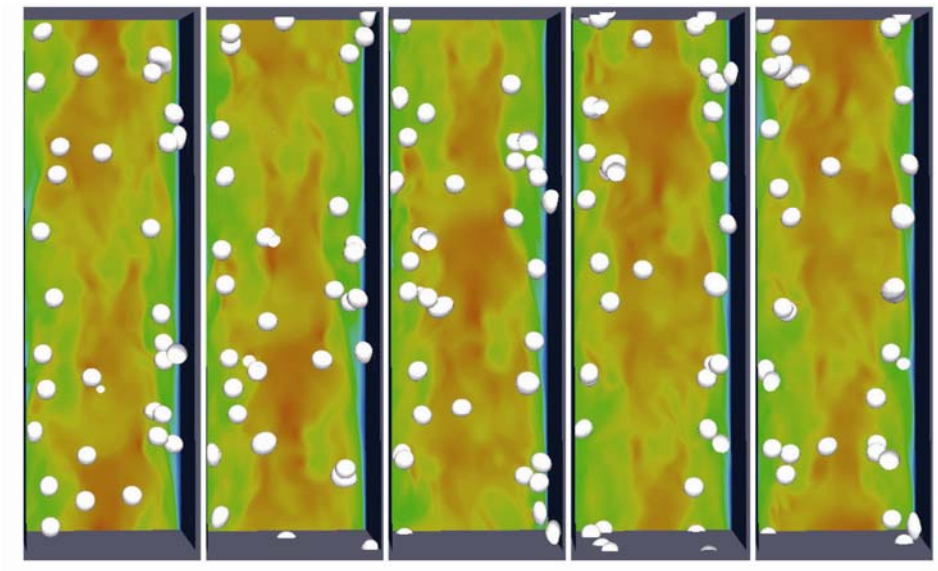
DOE Energy Innovation Hub

Consortium for Advanced Simulation of Light Water Reactors (CASL)

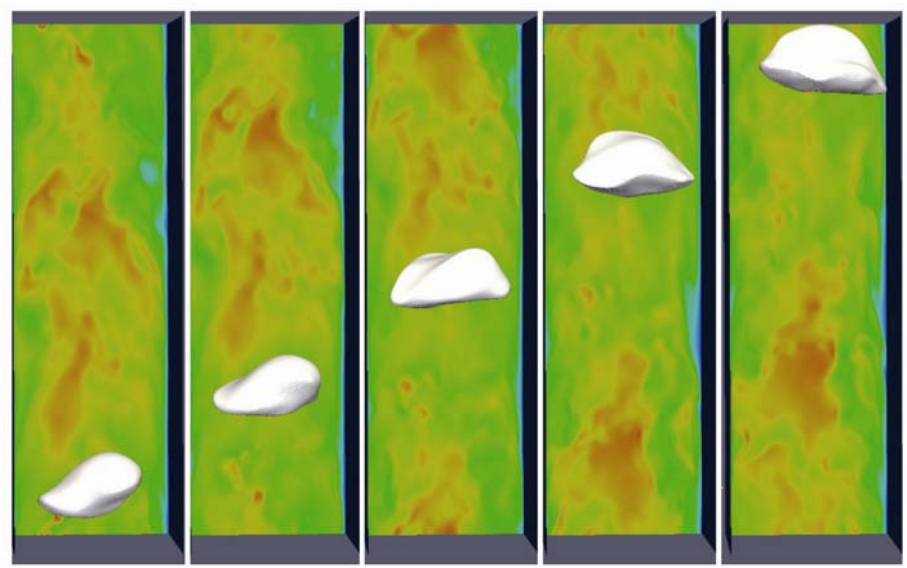
Key fluid mechanics and heat transfer issues:

- *Turbulence in complex geometries and in two-phase flows*
- *Subcooled (thermal non-equilibrium) boiling*
- *Boiling Crisis (Critical Heat Flux – CHF)*

Snapshots of DNS simulations of turbulent bubbly flows (Bolotnov et al., 2010)

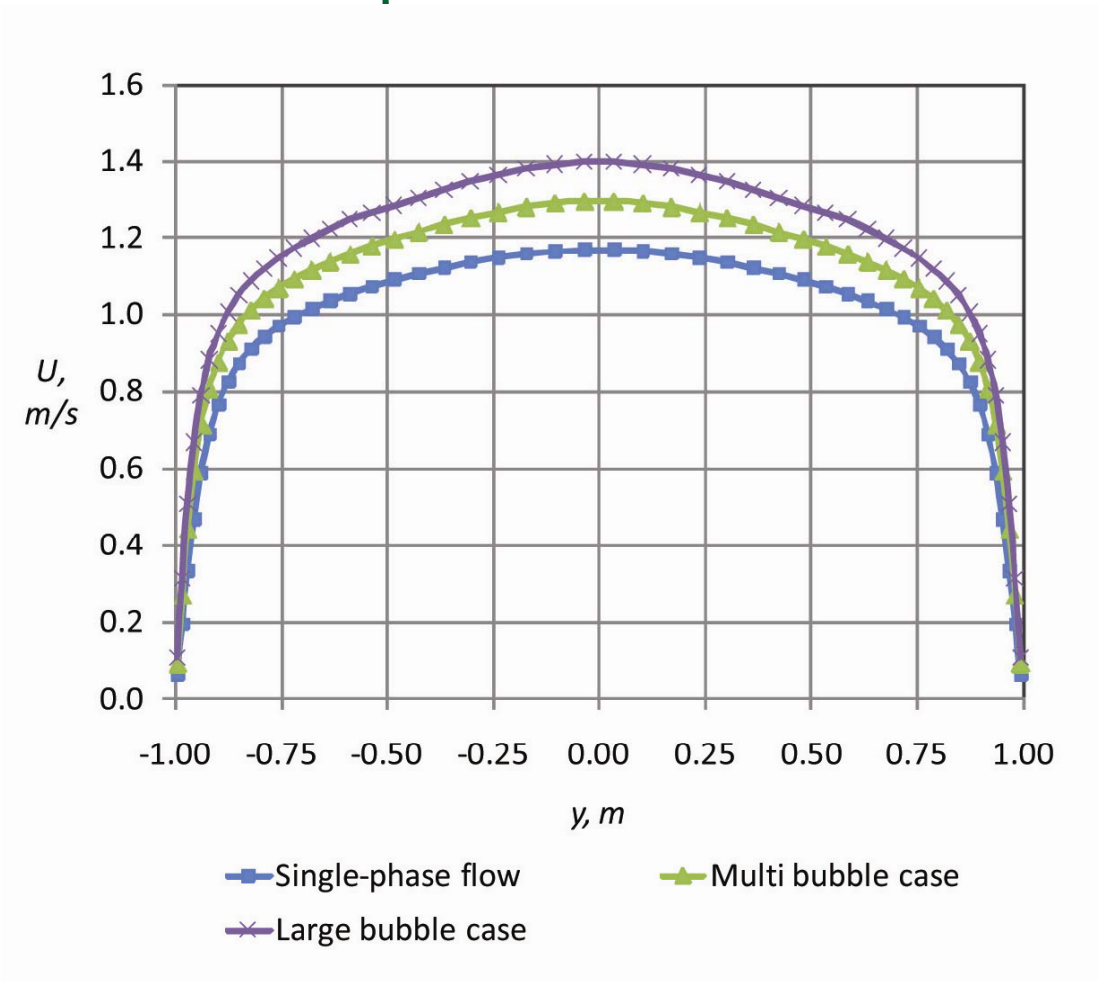


Small bubbles

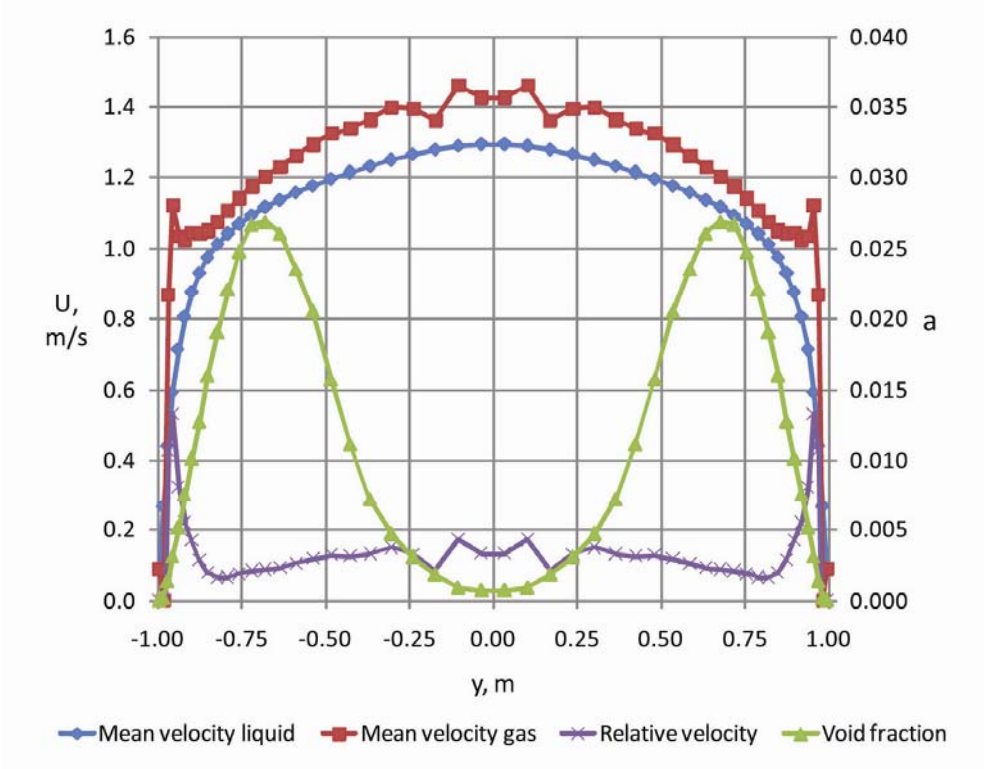


Large bubble

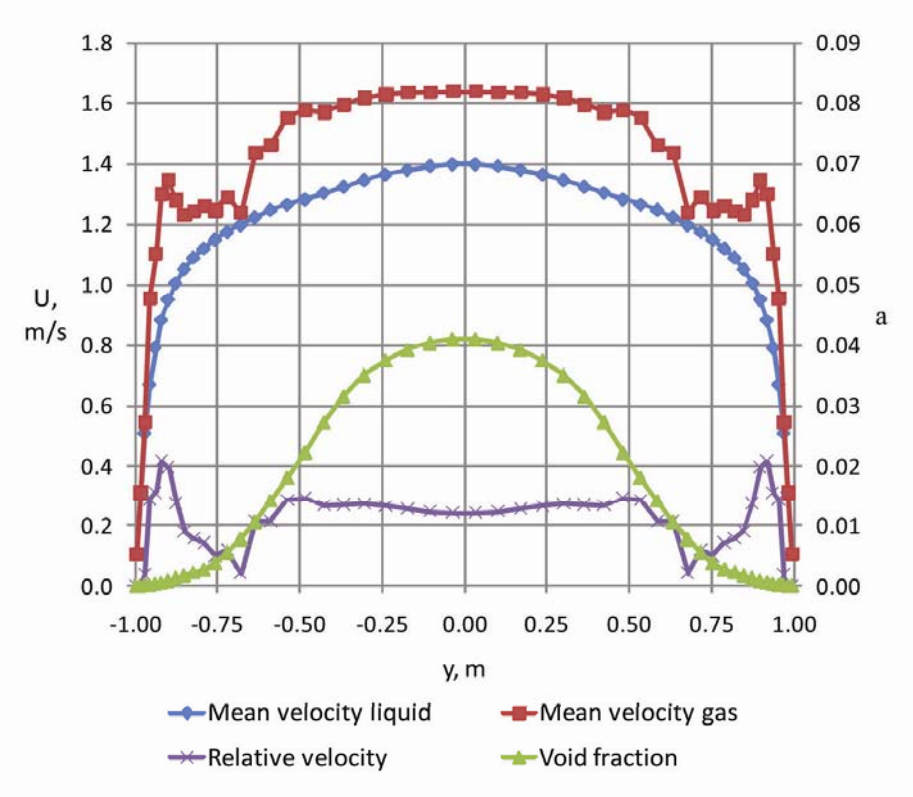
Axial liquid velocity for single-phase and two-phase flows



Mean flow parameters for gas/liquid two-phase flows

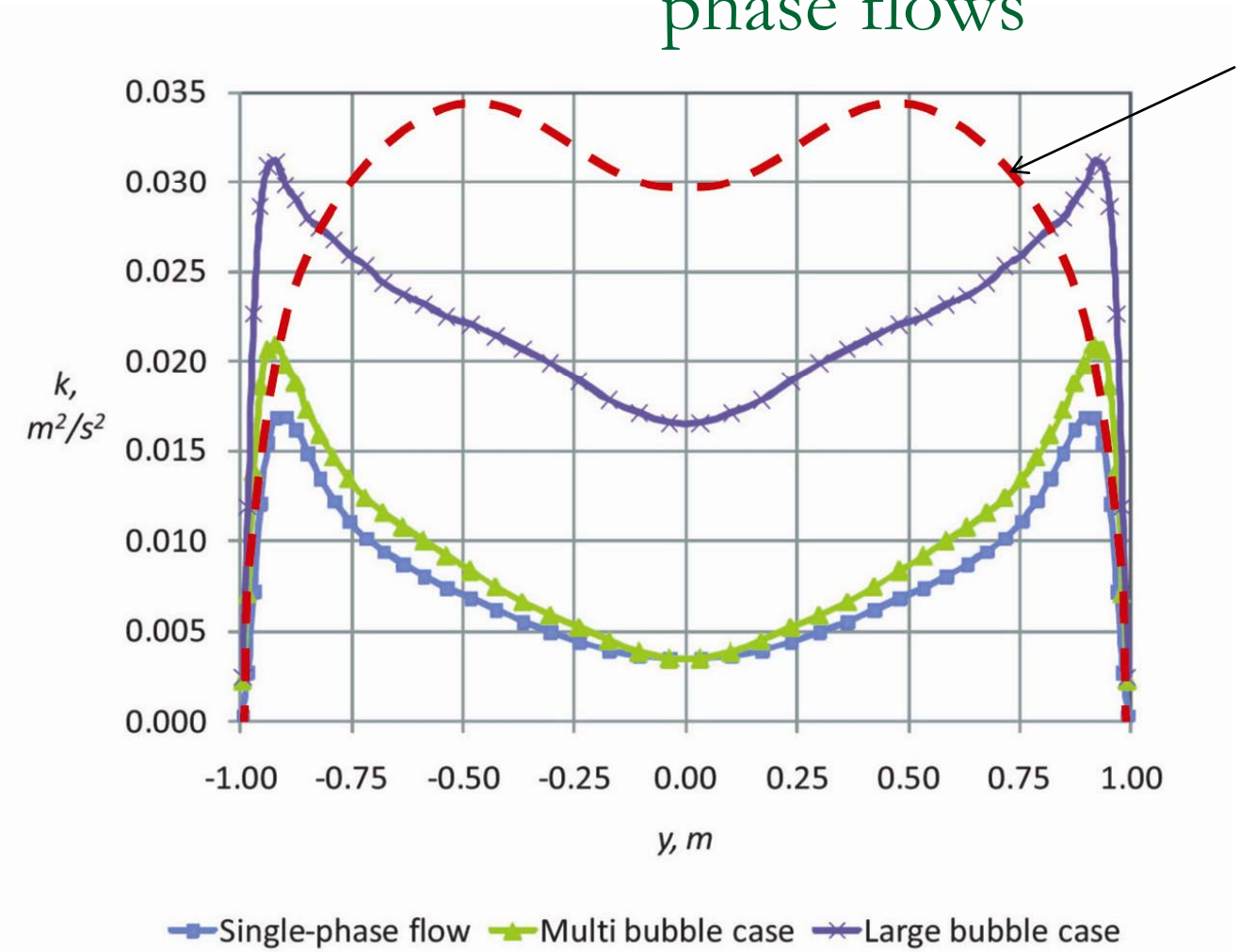


Small bubbles



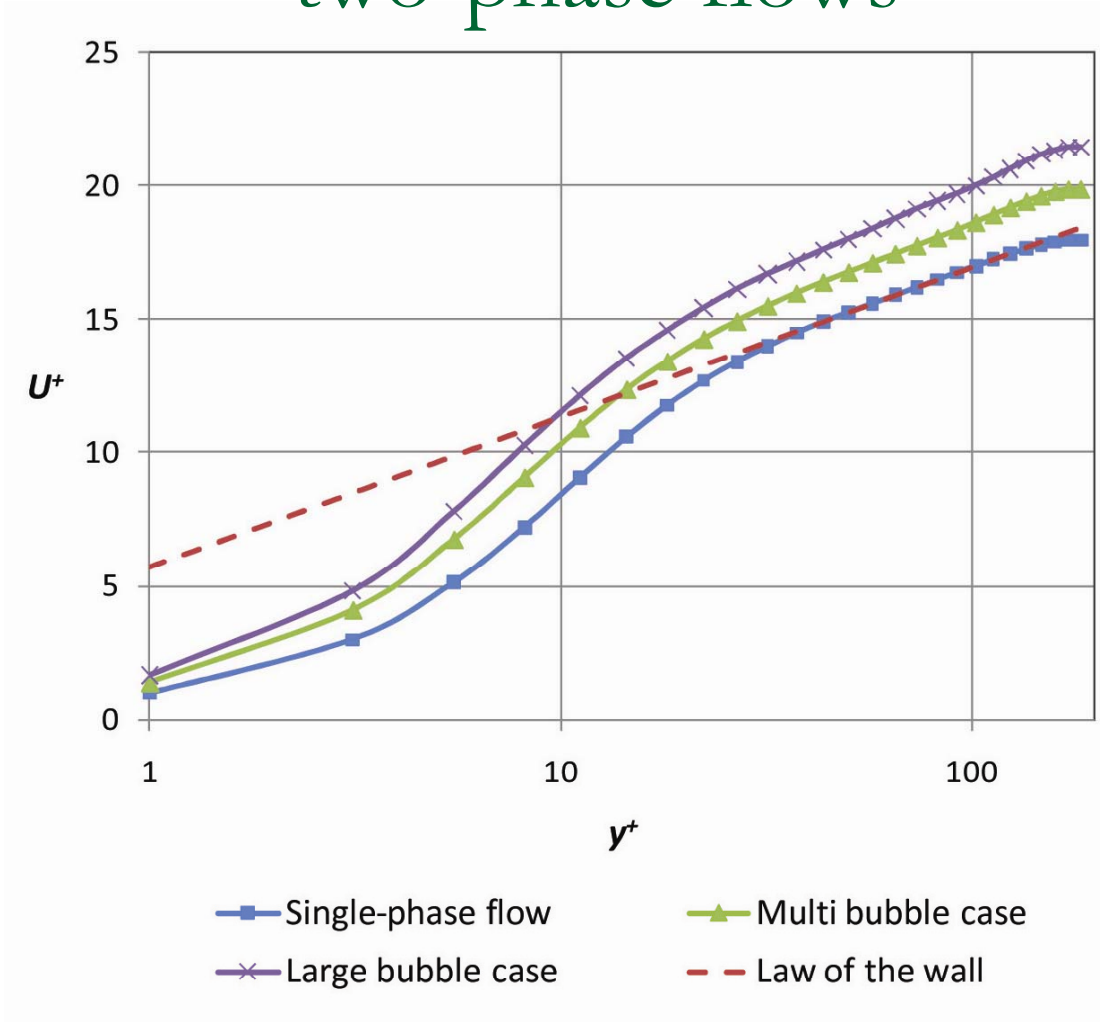
Large bubble

Turbulent kinetic energy for single-phase and two-phase flows



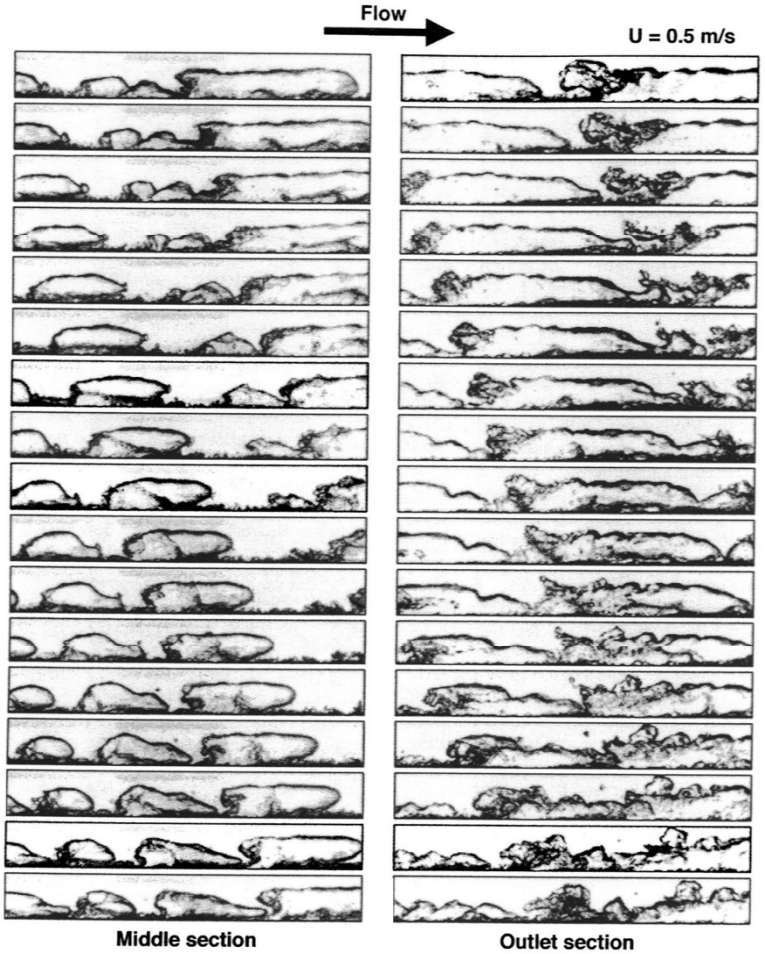
Typical result for large bubbles obtained using RANS single-phase *k*-ε model

Shear stress distribution for single-phase and two-phase flows

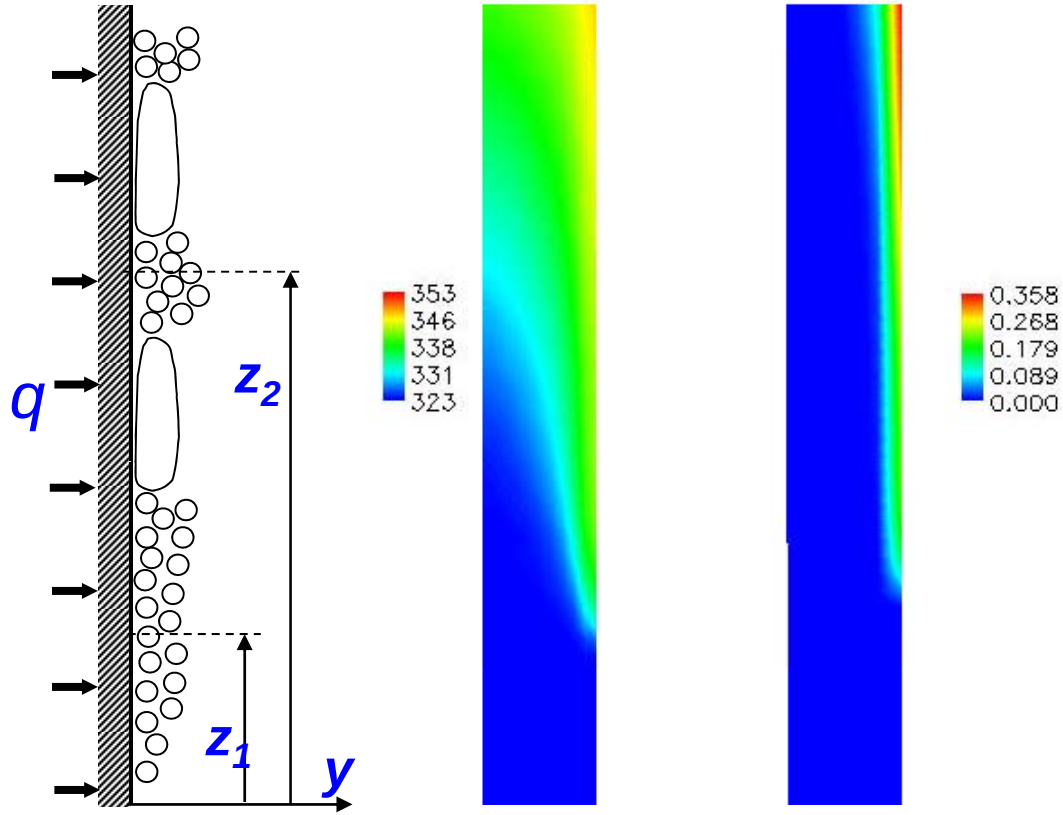


CHF in Subcooled Boiling

(Podowski & Antal, 2002)

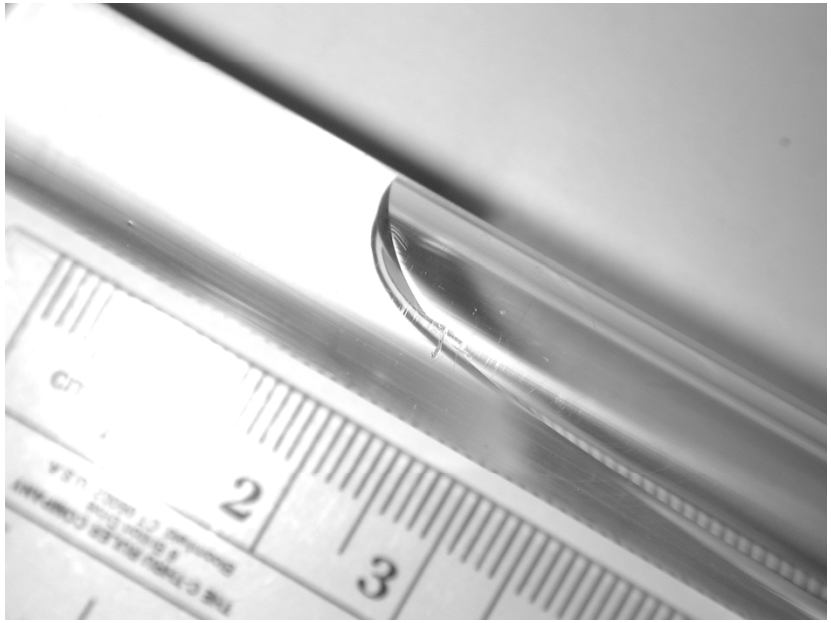


Flow visualization
(Moudawar et al., 2002)

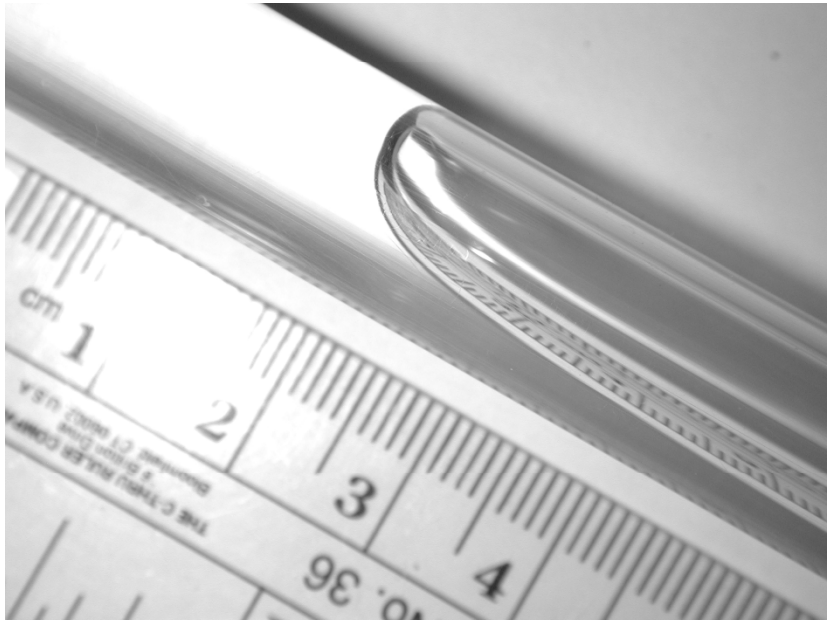


Mass Flux [kg/m^{2}s]	Liquid Subcooling [K]	Predicted CHF [kW]	Measured CHF [kW]	Error [%]
512	30	241	241	2
512	20	172	211	**16**
1236	30	305	332	8

Shape of air bubble in double-distilled water flowing along inclined polycarbonate tube



(a) Before runs with Alumina nanofluid ('**dewetted**' tube surface)



(b) After few runs with Alumina nanofluid ('**wetted**' tube surface)