



**NSE**

Nuclear Science & Engineering at MIT

science : systems : society

Politecnico di Milano - Friday, May 17, 2013

# Novel experimental and CFD analysis of two-phase flow in support of reactor safety



Massachusetts  
Institute of  
Technology

Emilio Baglietto

# CFD Modeling of Multiphase Flow

There is no generally applicable model, but models are driven by needs and limitations:

- **Flow characteristics**
  - ✓ Bubbly slug
  - ✓ Annular
  - ✓ Droplets
- **Process characteristics**
  - ✓ Separation
  - ✓ Boiling
  - ✓ Mixing
- **Parameter of interest**
  - ✓ Void Fraction
  - ✓ Wall temperatures

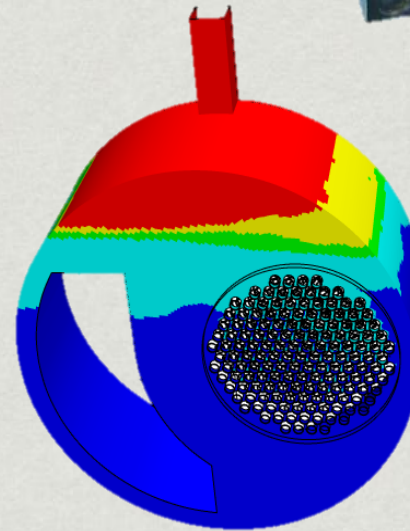


# An important distinction

- Computational fluid dynamics as a research tool for multi-phase flows.
- Computational fluid dynamics as a design tool for multi-phase flows



[www.nd.edu](http://www.nd.edu)



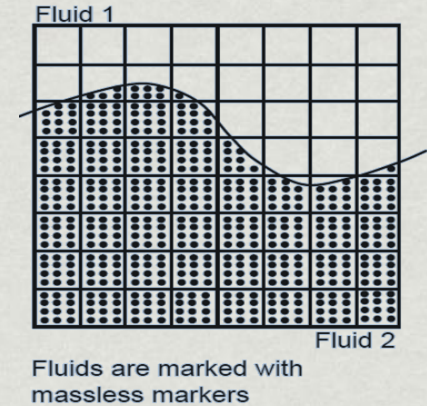
# MULTIPHASE CFD (M-CFD) METHODS

- **Lagrangian (Eulerian/Lagrangian)**
  - Track individual point particles.
  - Particles do not interact.
- **Discrete element method (DEM)**
  - Solve the trajectories of individual objects and their collisions, inside a continuous phase.
- **Homogeneous 2-P**
  - Dispersed phase in a continuous phase.
  - Solve one momentum equation for the mixture.
- **Eulerian Multiphase (Eulerian/Eulerian)**
  - Solve as many momentum equations as there are phases.
- **Interface Tracking/Capturing (ITM)**
  - Requires capturing the sharp interface, resolving the 2-P flow structures.



# Markers in Fluid Particle Method

- Marker and Cell (MAC) method - Harlow and Welch (1965).
- One of the earliest methods to resolve free surface problems.
- Based on Eulerian mesh of control volumes, massless markers are transported in a Lagrangian fashion to distinguish between fluids.



One of the most significant and commonly requested areas of real world simulation is fluid simulation.



*MAC Method used for 'X-Men: First Class'*

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Beyond the Fukushima nuclear power plant accident



# Front Tracking Method

- **Unverdi and Tryggvason (1992)** introduced the **Front Tracking Method**
- The Lagrangian interface is represented by a set of connected line segments, and is explicitly tracked and used to reconstruct a representation of the fluid property fields on an Eulerian mesh.
- Most successful method for DNS of bubbly flow



[www.nd.edu](http://www.nd.edu)

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# The “leap” for M-CFD:

## *“Safety analysis applications”*

### MESO-SCALE Representation of Multi-phase Flow

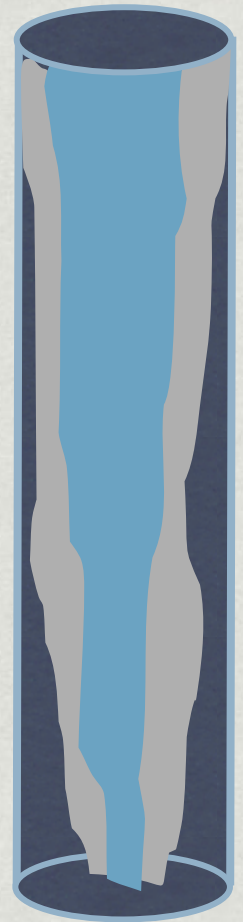
- While first principle representation of Multiphase Flow [quasi-DNS] is possible for specific limited simulations domains we must assemble a practical, robust, engineering approach to M-CFD.
- ***The challenge is to capture the dominant characteristics of the flow physics and to represent them with adequate and efficient models.***
- The framework is the two fluid model representation (aka EMP, 6-eq model... )

# MESO-SCALE “Interpenetrating continua”

- We consider the phases are mixed on length scales smaller than we wish to resolve and can be treated as continuous fluids.
- Both phases coexist everywhere, this concept is called “Interpenetrating continua”.
- Requires “Closure” to recover the information loss in the “Interpenetrating” assumption.



Instantaneous



Averaged



# Conservation of mass

- Conservation of mass for phase k is:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \sum_{j=1}^N (\dot{m}_{jk} - \dot{m}_{kj})$$

- $\alpha$ =volume fraction,  $\rho$ =density,  $\mathbf{u}$ =velocity,
  - $N$ =total number of phases,  $\dot{m}$ =mass transfer rate.
- Sum of volume fraction is unity,

$$\sum_k \alpha_k = 1$$

# Conservation of momentum

- Conservation of momentum for phase k is:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k u_k) + \nabla \cdot (\alpha_k \rho_k u_k u_k) \\ = -\alpha_k \nabla p + \alpha_k \rho_k g + \nabla \cdot \alpha_k (\tau_k + \tau_k^t) + M_k$$

- $p$  = pressure,
- $M$  = sum of interfacial forces (drag, turbulence drag, lift, virtual mass) and momentum transfer associated with mass transfer.

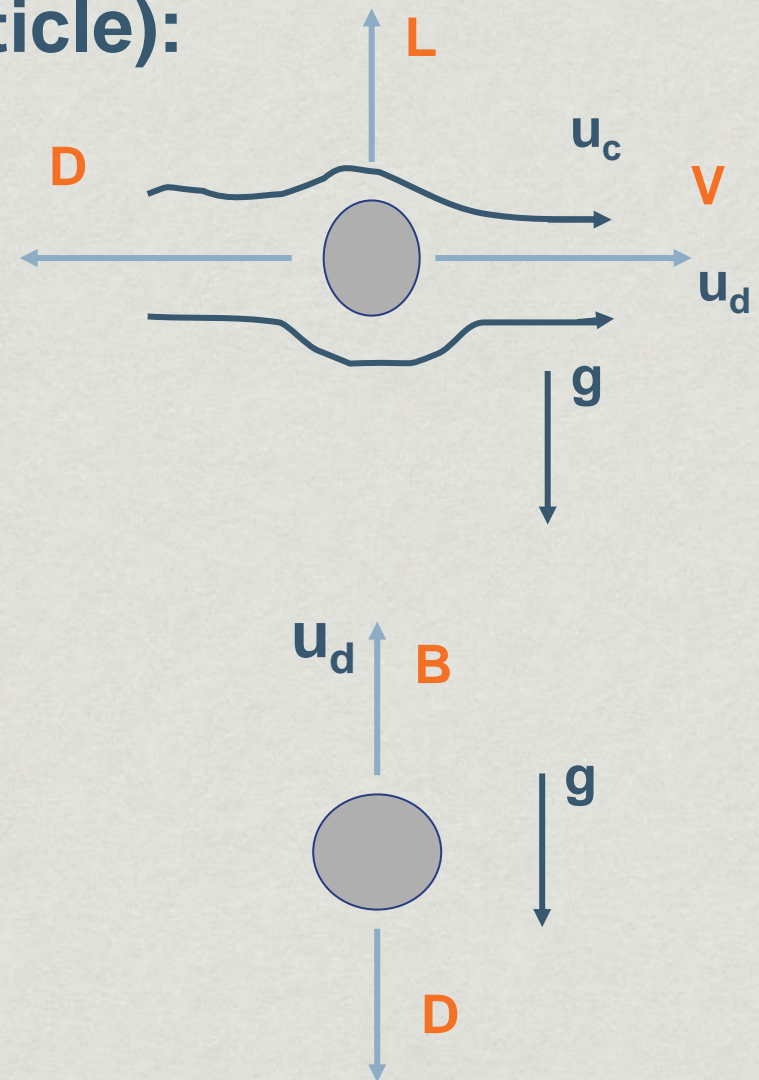
$$M = F_D + F_{TD} + F_L + F_{VM} + \sum_{j=1}^N (\dot{m}_{jk} u_j - \dot{m}_{kj} u_k)$$

$M$  = sum of interfacial forces (drag, turbulence drag, lift, virtual mass) and momentum transfer associated with mass transfer.



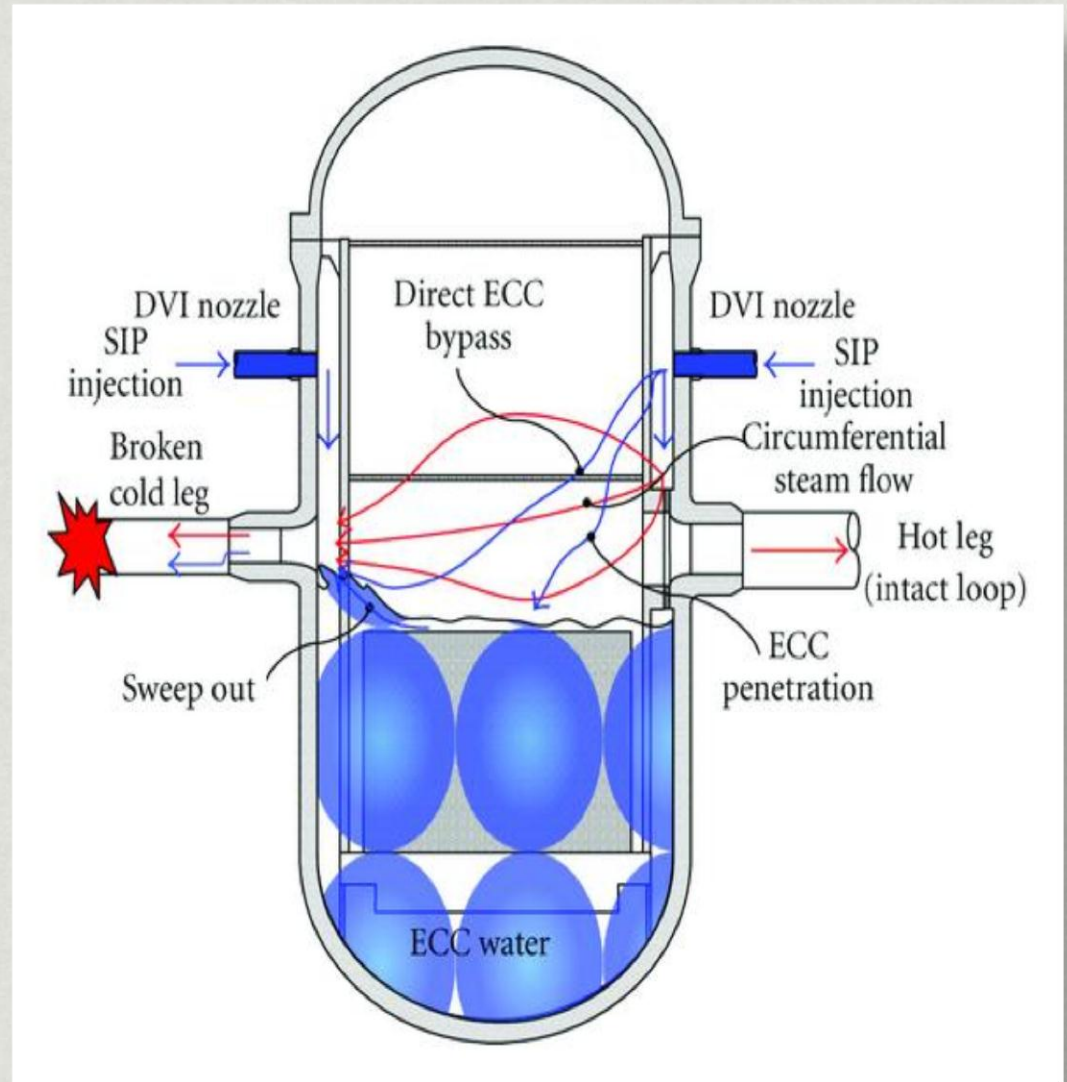
## ▪ Interfacial forces (on a particle):

- Buoyancy,  $B$ .
- Viscous Drag,  $D$ .
- Lateral Lift,  $L$ .
- Virtual mass,  $V$ .
- Basset force.
- Turbulence Dispersion.
- Wall Lubrication.
- ...



# Why do we need Multiphase-CFD ??

A schematic diagram of the direct ECC bypass.



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Beyond the Fukushima nuclear power plant accident





# CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub for Modeling & Simulation of Nuclear Reactors

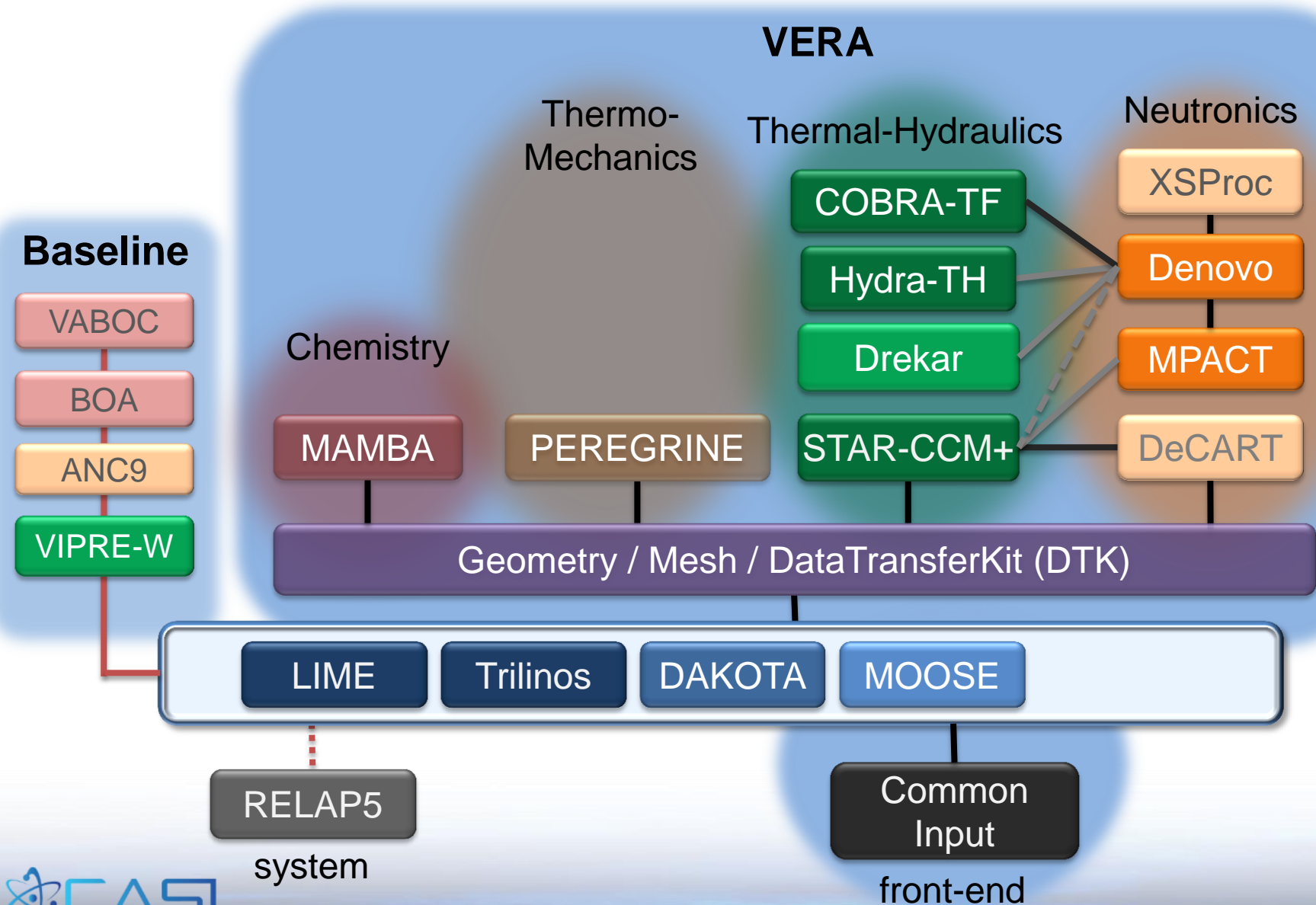


**Task 1:** Develop computer models that simulate nuclear power plant operations, forming a “virtual reactor” for the predictive simulation of light water reactors.

**Task 2:** Use computer models to reduce capital and operating costs per unit of energy, .....



# Virtual Environment for Reactor Applications







Prof. Emilio Baglietto



Lindsey Gilman  
(PhD student)

THM.CLS.P7.09 - 8/30/2013

Development of hardened CMFD boiling model. –  
Release and testing of new approach aiming at robust  
sensitivity to surface and flow parameters, with built-in  
extension to DNB.

## Boiling Model Development



Rosie Sugrue  
(graduate student)

THM.CLS.P7.10 - 8/30/2013  
Advanced M-CLs based on  
ITM/DNS and experiments

## Momentum Closures



Prof. Jacopo Buongiorno



Dr. Thomas McKrell  
(research scientist)



Bren Phillips  
(PhD student)

THM.CLS.P7.01 - 6/28/2013

Experimental database for  
subcooled flow boiling

## Dedicated Experimental Database



Dr. Gustavo Rabello  
(post-doc)



Alexandre Guion  
(graduate student)

THM.CLS.P6.01 - 3/29/2013

Dedicated model for microlayer heat transfer

THM.CLS.P7.03 - 9/30/2013

Challenge Simulations of Boiling Phenomena.  
Nucleation, growth and bubble departure.

## DNS/ITM Database

# Novel Mechanistic Flow Boiling Model

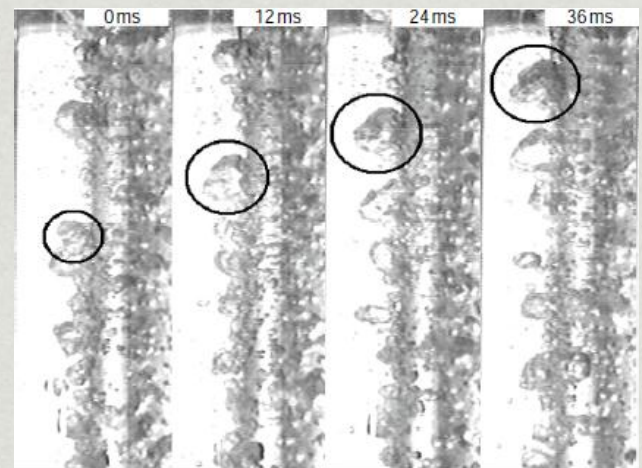
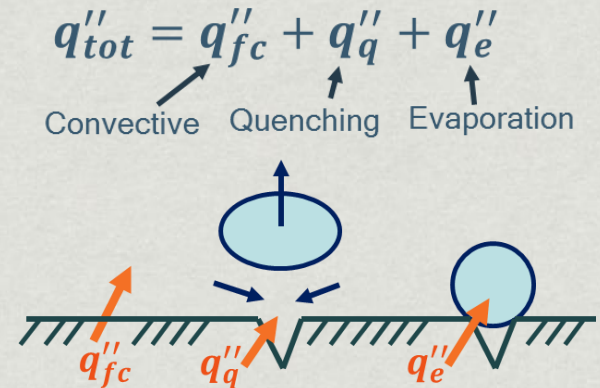
## Kurul and Podowski Partitioning

### Mechanistic approach

- *Flexible model*
- *Proven application record*
- *First deployment option for Hydra-TH*

So why a new model? (*hopefully start addressing Nam's fundamental question*)

- I will go through this “one piece at a time”, but first things first, the final target:
- *Increased synergy with experimental “micro” measurements*
- *Extended applicability (lower/ higher vapor generation)*
- *Include modeling toward limiting behavior (CHF)*



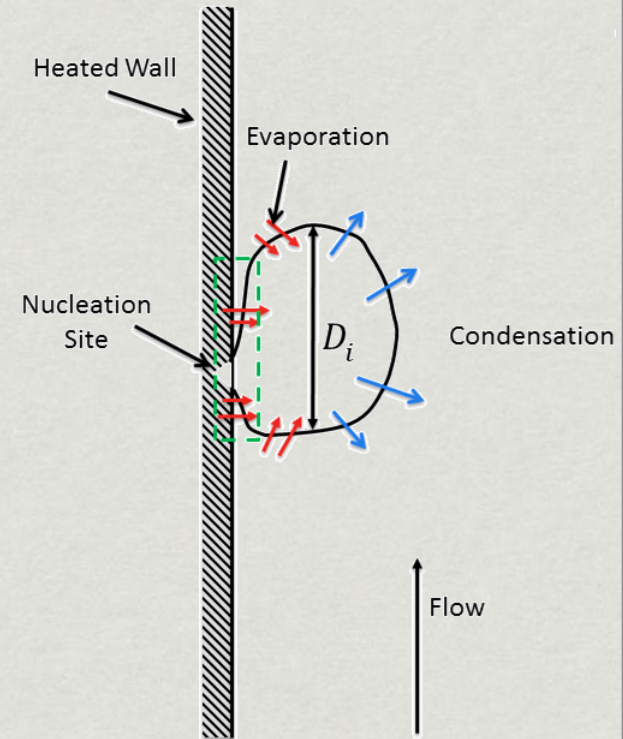


# Novel Mechanistic Flow Boiling Model (2)

## Key Components - 1

### Evaporative Heat Transfer $q''_e$

- Kurul-Podowski is “a posteriori” concept
- $D_d^3$  behavior
- e.g.  $\rightarrow q''_e = 0$  until OSV
- New model targets capturing the real evaporative  $q''_e$
- Builds in tracking of physical limits  $\rightarrow$
- Naturally extends to limit behavior without need for new empirical model



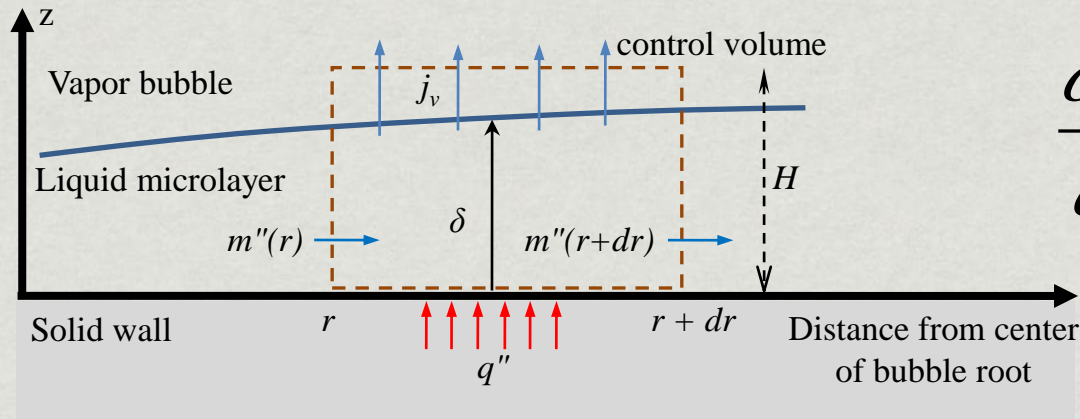
$$q''_e = \rho_v h_{fg} \frac{\pi}{6} D_d^3 N'' f \propto S_{\text{microlayer}}$$

Need to model the microlayer evaporation – *leverage ITM\_DNS*

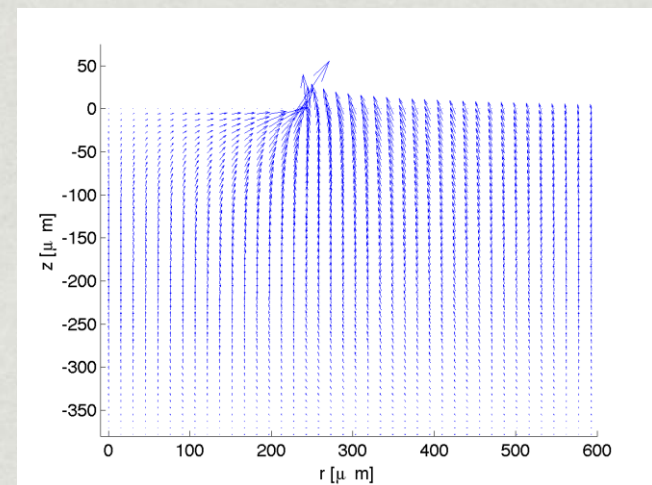
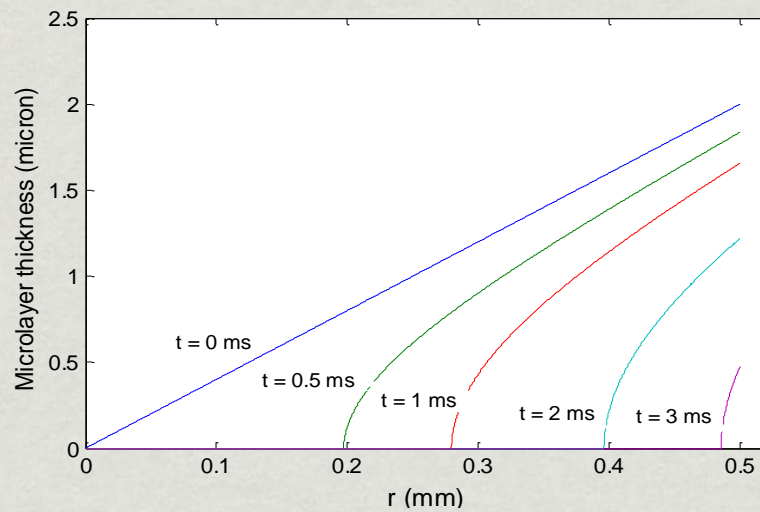
# Microlayer Model

Rosie Sugrue, Alex Guion,  
Gustavo Rabello

Axisymmetric, time-dependent model:



$$\frac{\partial \delta}{\partial t} = - \frac{k_l (T_w - T_{sat})}{\delta \rho_f h_{fg}}$$



Model predicts time evolution of microlayer shape + heat flux associated with microlayer evaporation

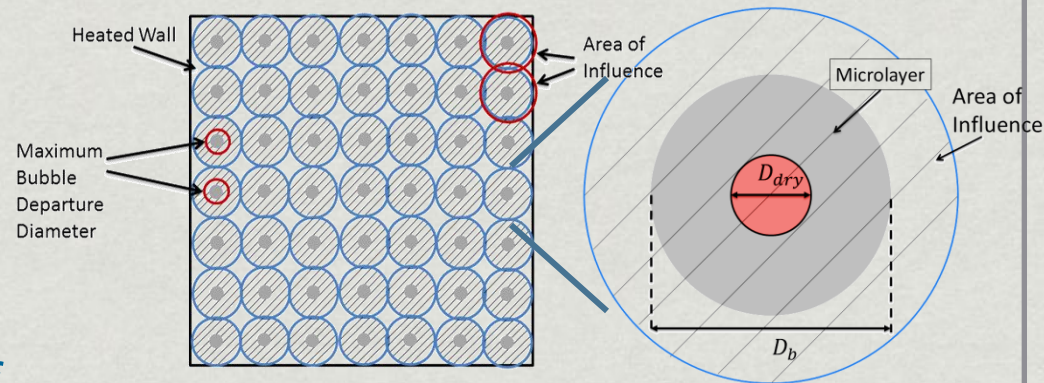


# Novel Mechanistic Flow Boiling Model (3)

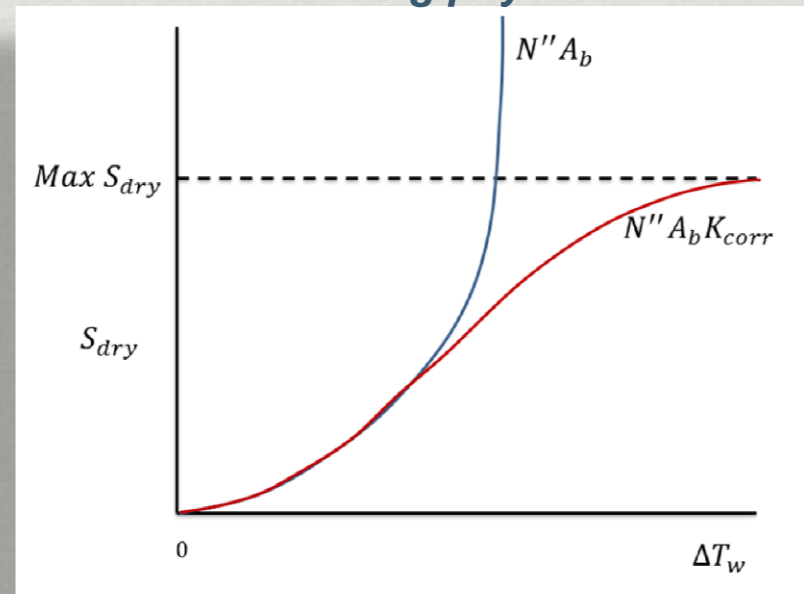
## Key Components - 2

### Effects of bubble crowding

- *Current models are strongly sensitive to active nucleation site density (require the use of experienced based limiters)*
- *Built in crowding effect eliminates need for limiters*
- *Prediction of dry surface can be directly verified against experimental measurements*
- *DNB can be expressed as the limit of this behavior*
- *Potentially local/scalable model for DNB*



- *Allows tracking physical limits*

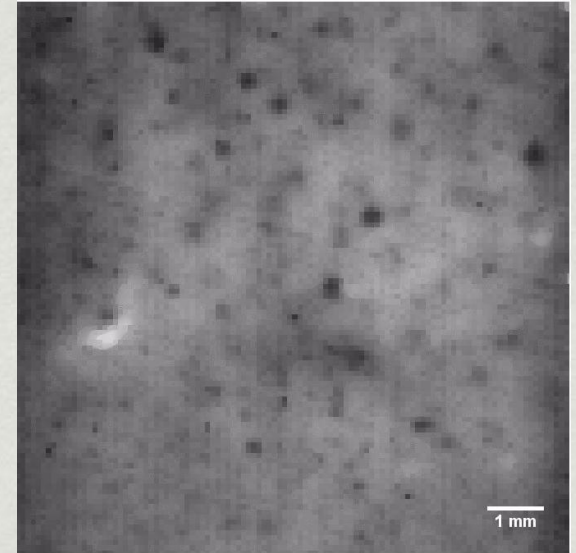


# Nucleation Site Density

*(hope to leverage as validation rather than calibration)*

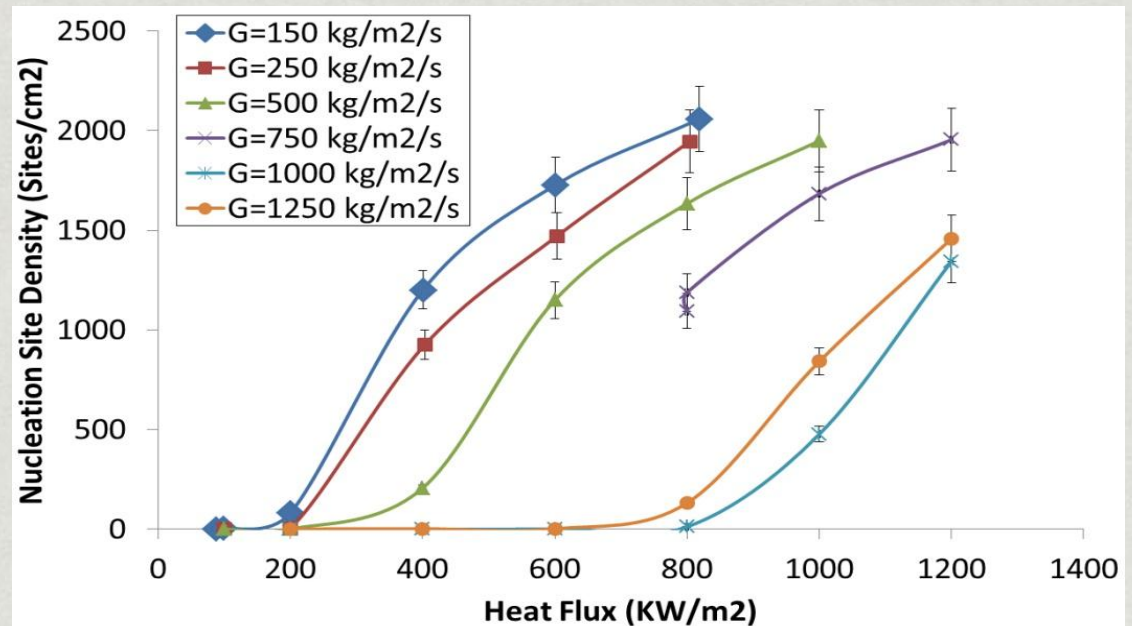
Bren Phillips, Rosie Sugrue,  
Tom McKrell

- Automated routine for counting nucleation sites from IR data
- Verified with manual counting
- Currently investigating statistical correction for measurement resolution



Data follow  
expected trends  
with heat and  
mass flux

Note plateauing  
at high heat flux



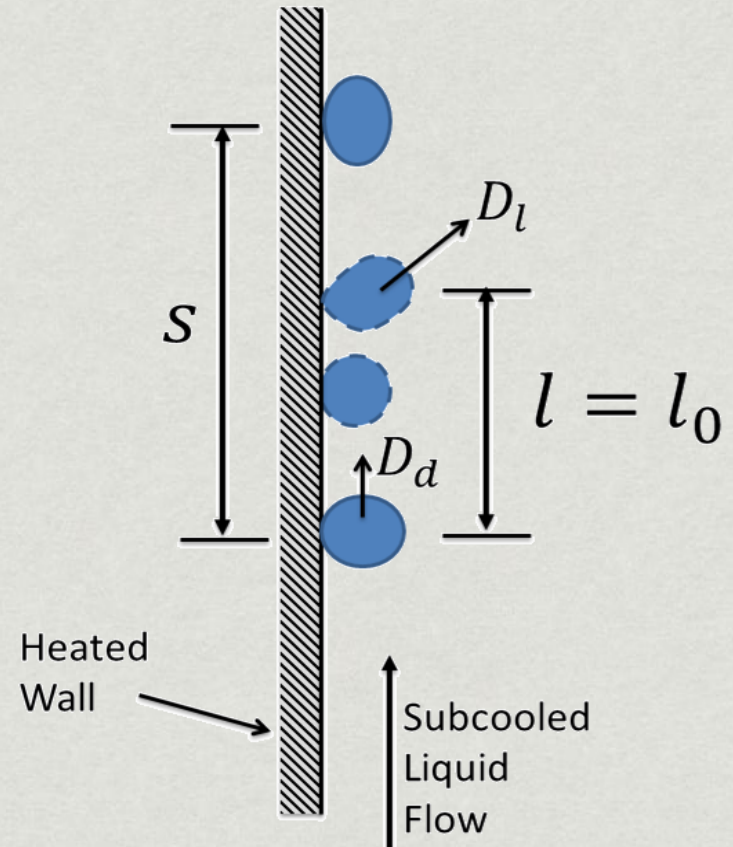


# Novel Mechanistic Flow Boiling Model (4)

## Key Components - 3

### Bubble departure and sliding - I

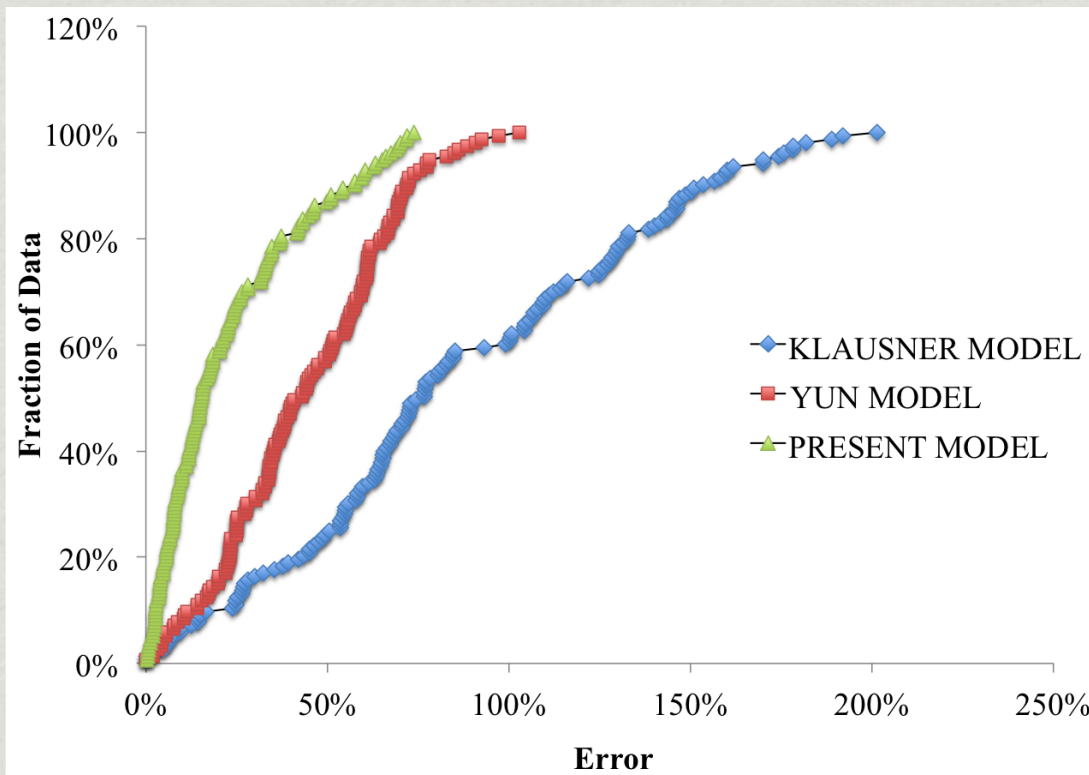
- *Leverage improved mechanistic force balance model a la Klausner:*
  - ✓ Sugrue, Buongiorno 2013
- *MIT implementation shared among CASL partners (external C routine)*
- *Optimal estimation of departure diameter ( $D_d$ )*
- *Allows quantifying lift off diameter ( $D_l$ )*
- *Includes wall inclination effects*



# Bubble Departure Diameter Model

Bren Phillips, Rosie Sugrue, Tom McKrell

**Prediction statistics for present model are much better than Klausner's original model and Yun's modified model**



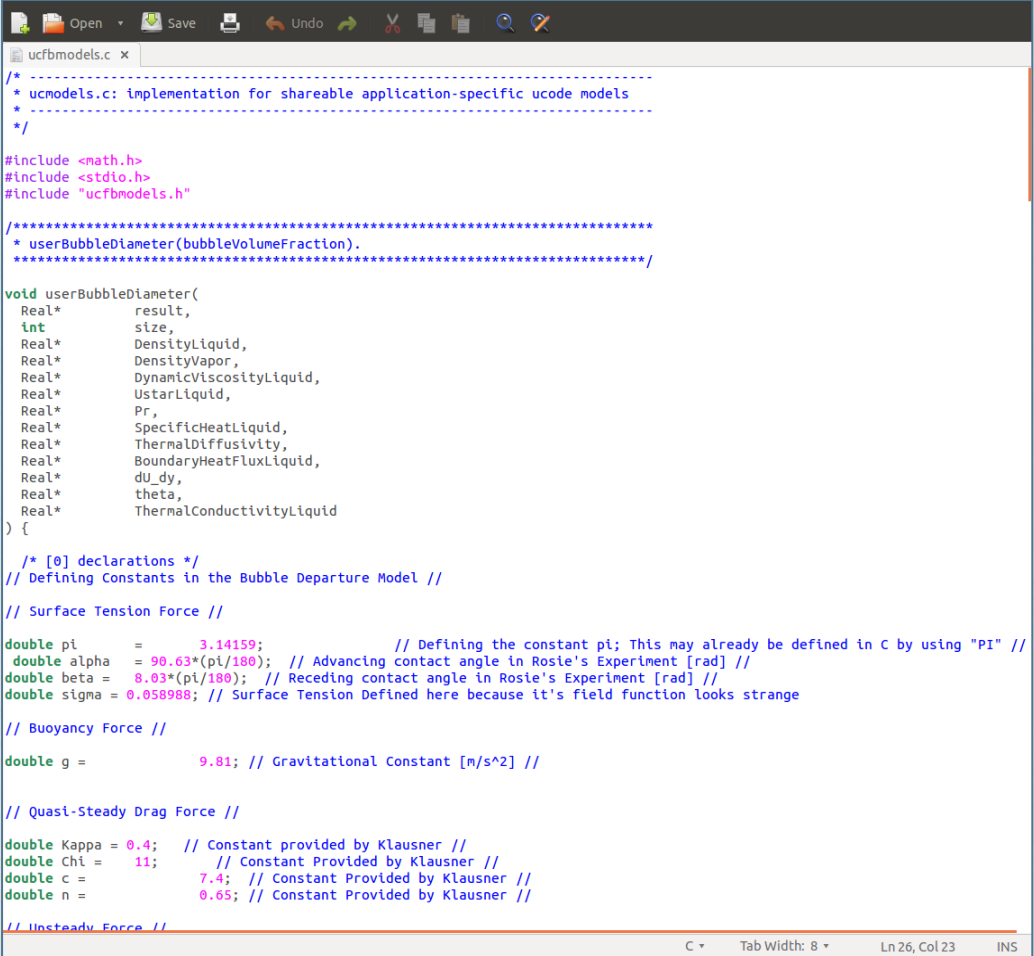
Aggregate Errors<sup>1</sup>:  
Klausner Model: 85.5% ( $\sigma=49.7\%$ )  
Yun Model: 43.9% ( $\sigma=23.1\%$ )  
**Present Model: 22.4% ( $\sigma=19.9\%$ )**

<sup>1</sup>Errors across experimental databases of Klausner et al., Sugrue et al., Zeng et al., Prodanovic et al., and Situ et al.



# A CFD Implementation

- Improved Mechanistic Departure Model fundamental component for all partitioning models.
- First Implementation an testing priority.
- Currently being tested
- Subroutine written in C
- Linked to STAR-CCM+ by building a user code library
- Employs multiple field functions available in STAR-CCM+, but fully commented for quick adaptability



```
ucfbmodels.c x
/*
 * ucbmodels.c: implementation for shareable application-specific ucode models
 */

#include <math.h>
#include <stdio.h>
#include "ucfbmodels.h"

/*****
 * userBubbleDiameter(bubbleVolumeFraction).
 *****/

void userBubbleDiameter(
    Real*    result,
    int      size,
    Real*    DensityLiquid,
    Real*    DensityVapor,
    Real*    DynamicViscosityLiquid,
    Real*    UstarLiquid,
    Real*    Pr,
    Real*    SpecificHeatLiquid,
    Real*    ThermalDiffusivity,
    Real*    BoundaryHeatFluxLiquid,
    Real*    du_dy,
    Real*    theta,
    Real*    ThermalConductivityLiquid
) {
    /* [0] declarations */
    // Defining Constants in the Bubble Departure Model //

    // Surface Tension Force //

    double pi      = 3.14159; // Defining the constant pi; This may already be defined in c by using "PI" //
    double alpha   = 90.63*(pi/180); // Advancing contact angle in Rosle's Experiment [rad] //
    double beta    = 8.03*(pi/180); // Receding contact angle in Rosle's Experiment [rad] //
    double sigma   = 0.058988; // Surface Tension Defined here because it's field function looks strange

    // Buoyancy Force //

    double g = 9.81; // Gravitational Constant [m/s^2] //

    // Quasi-Steady Drag Force //

    double Kappa = 0.4; // Constant provided by Klausner //
    double Chi = 11; // Constant Provided by Klausner //
    double c = 7.4; // Constant Provided by Klausner //
    double n = 0.65; // Constant Provided by Klausner //

    // Unsteady Force //
```

# Novel Mechanistic Flow Boiling Model (5)

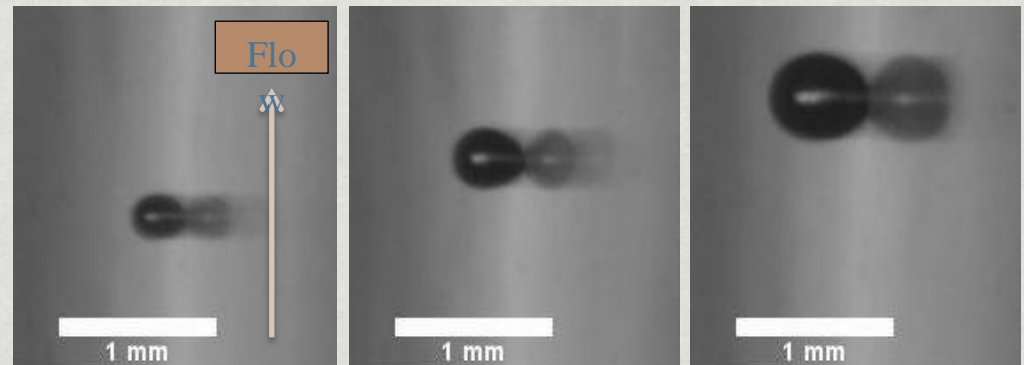
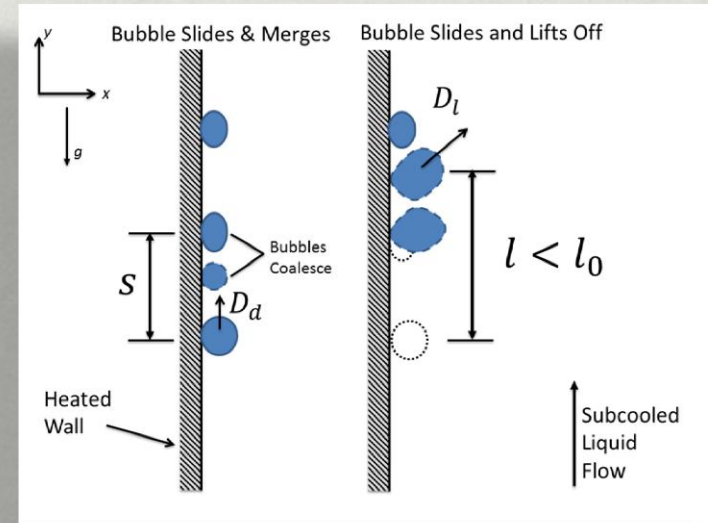
## Key Components - 3

### Bubble departure and sliding (and coalescence)

*Not included in K-P model*

#### Transient conduction: $q''_{tc}$

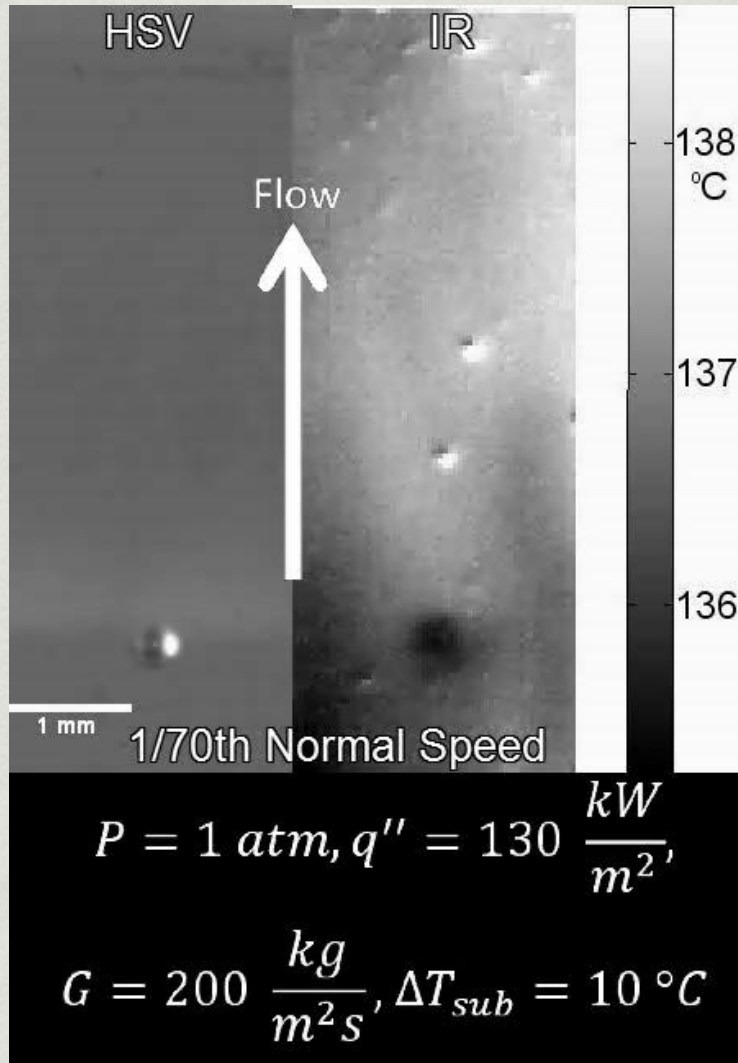
- *Active in areas swept by bubbles.*
- *Conduction through thin liquid film (experiment to confirm area of influence)*
- *“Local cooling roughly independent of mass flux”*
- *Mass flux enters in the “average area swept by bubbles”*
- *Captured using enhancement factor dependent on number of bubbles and time over which the transient conduction mode occurs.*



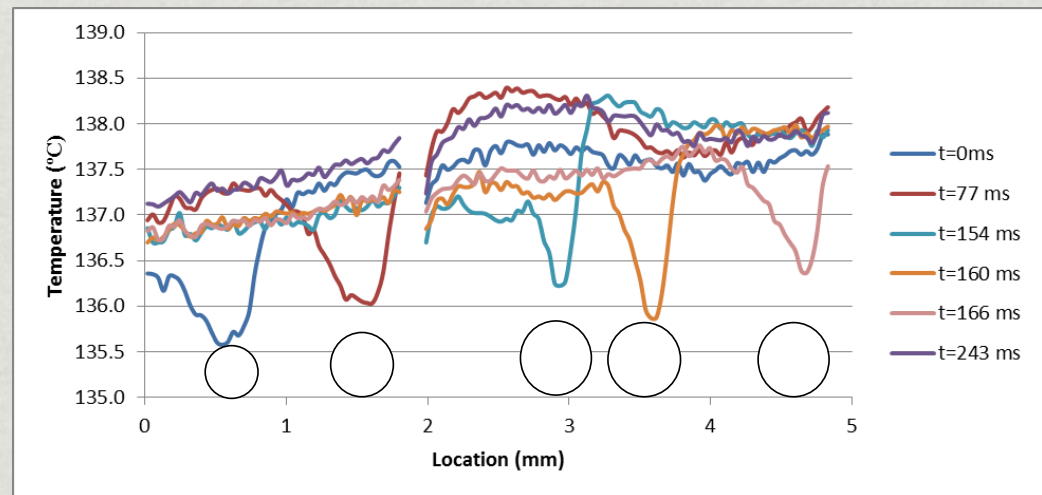


# Sliding Bubbles in Subcooled Flow Boiling

Bren Phillips, Rosie Sugrue, Tom McKrell



Synched IR and HSV  
allow measurement of  
sliding bubble velocity  
and local cooling



# Novel Mechanistic Flow Boiling Model (6)

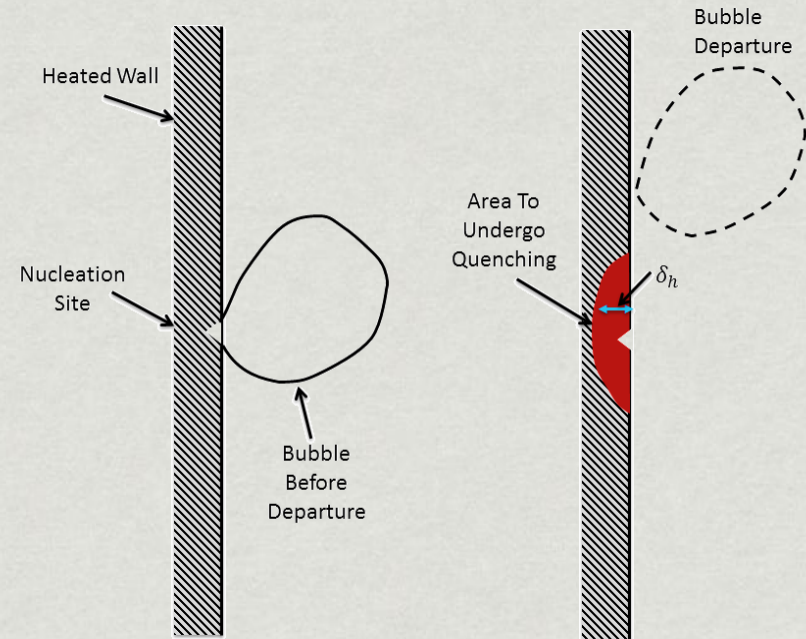
## Key Components - 4

### Quenching of “walls”

- *Currently related to fluid properties (can be combined into evaporative)*

### Influence of heater material

- *Semi-analytical representation of the influence area of the bubble on the heater back to the wall superheat and temperature distribution prior to bubble departure*
- *Unclear relevance, but minor implementation cost*



$$q''_q = \rho_h c_{p,h} (T_a - T_w) \delta_h$$



# Novel Mechanistic Flow Boiling Model (7)

## Key Components – 5

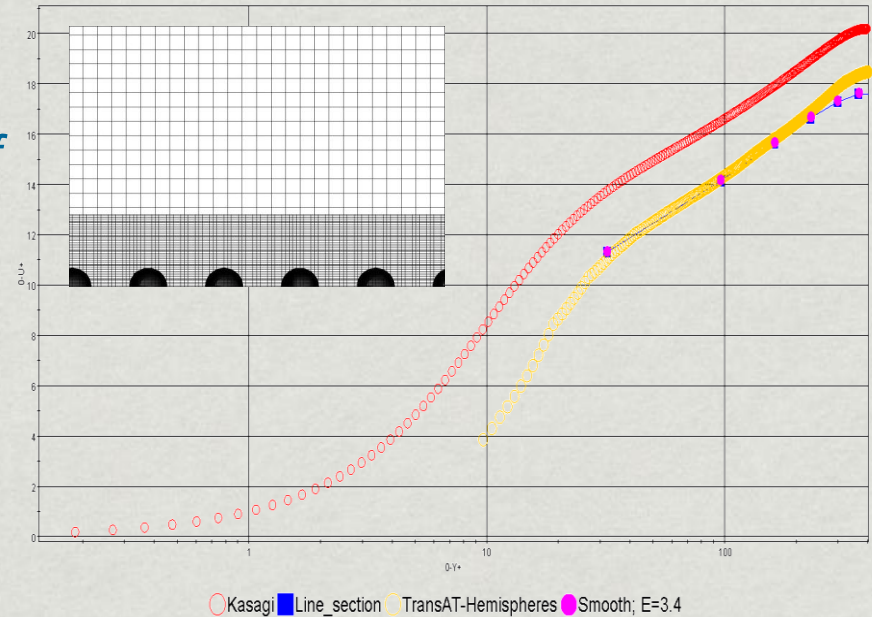
### Law of the “boiling” wall

- *Forced convection should be modified to account for presence of bubble (growing, sliding, departing)*
- *Common component to all CASL models*

### Generalized correction

- *Implement a “bubble aware” set of wall functions, for  $V$ ,  $T$ ,  $K$*
- *Start from DNS results from ITM-1*
- *Final corrections will require:*
  - ✓ MIT and TAMU experiments
  - ✓ ND and NCSU ITM/DNS

Demonstration of Wall Function correction DNS/LES data for hemispherical obstacles (ITM-1 results)



# Targeting generality

(simplified version.. more to come)

- *Microlayer Evaporation* → *DNS Simulations*
- *Active Nucleation Site Density* → *Experimental Meas.*
- *Departure diameter ( $D_d$ )* → *Sugrue et al*
- *Departure frequency* → *Consistent with Sugrue et al.*
- *Sliding (and coalesc.) Bubbles* → *Dedicated measurements*
- *Quenching* → *???*



## Subcooled Boiling Curves



# Subcooled Boiling Curves and Heat Transfer Coefficient

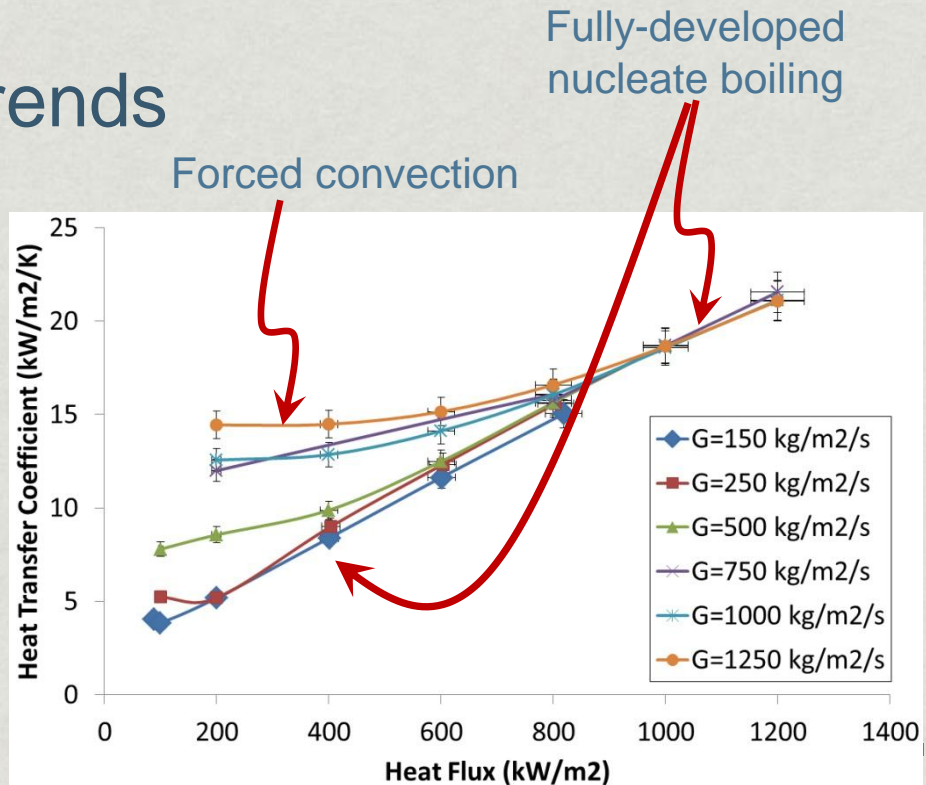
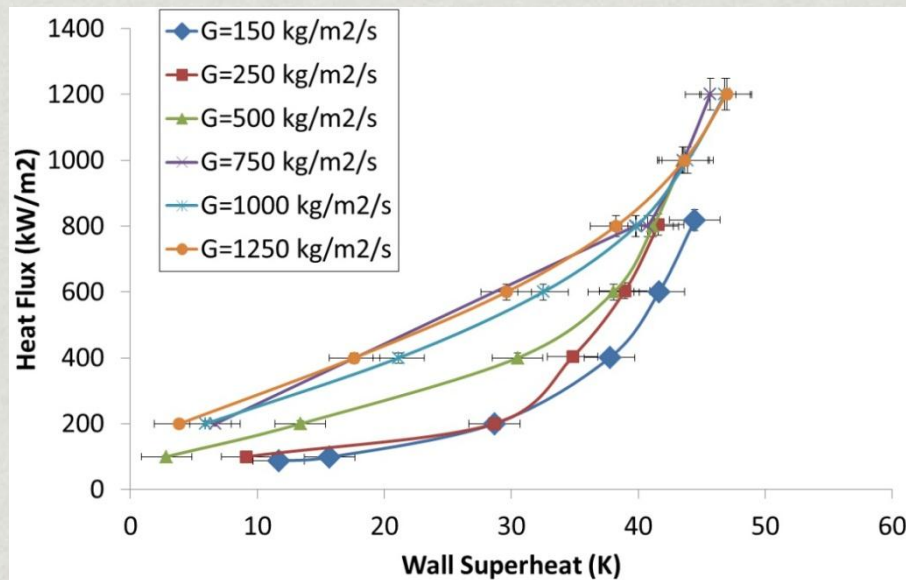
Bren Phillips, Rosie Sugrue, Tom McKrell

First data collected at:

- $q'' = 0\text{--}1300 \text{ kW/m}^2$
- $\Delta T_{\text{sub}} = 10^\circ\text{C}$

- $G = 150\text{--}1250 \text{ kg/m}^2\text{s}$
- $P = 0.101 \text{ MPa}$

Data follow all expected trends



# Subcooled Boiling Curves and Heat Transfer Coefficient

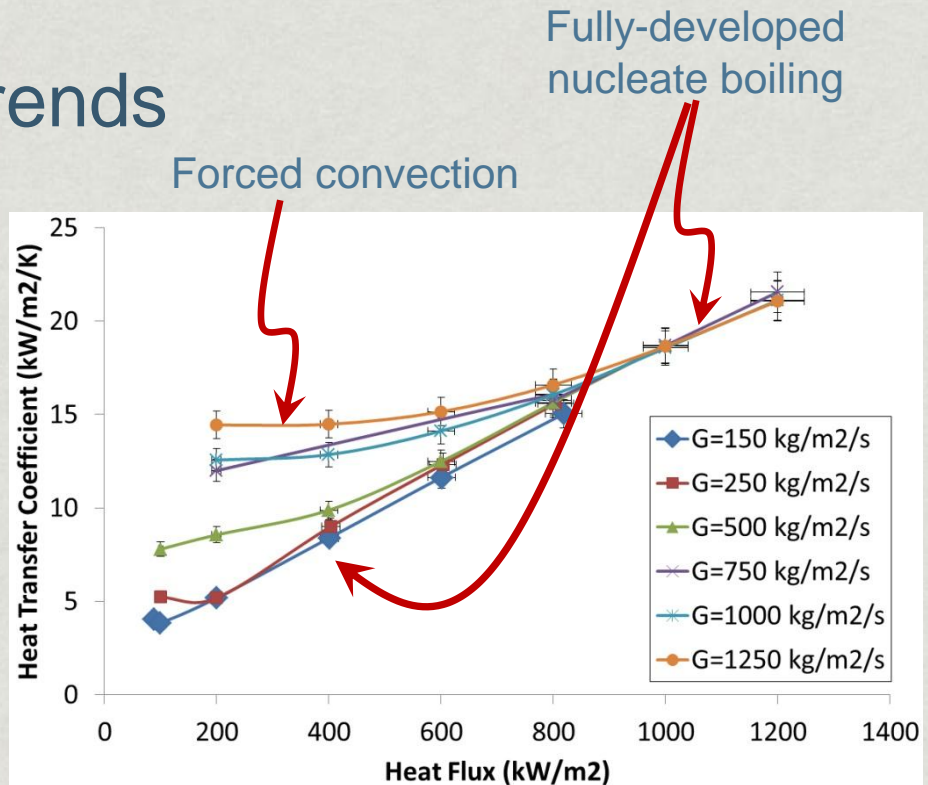
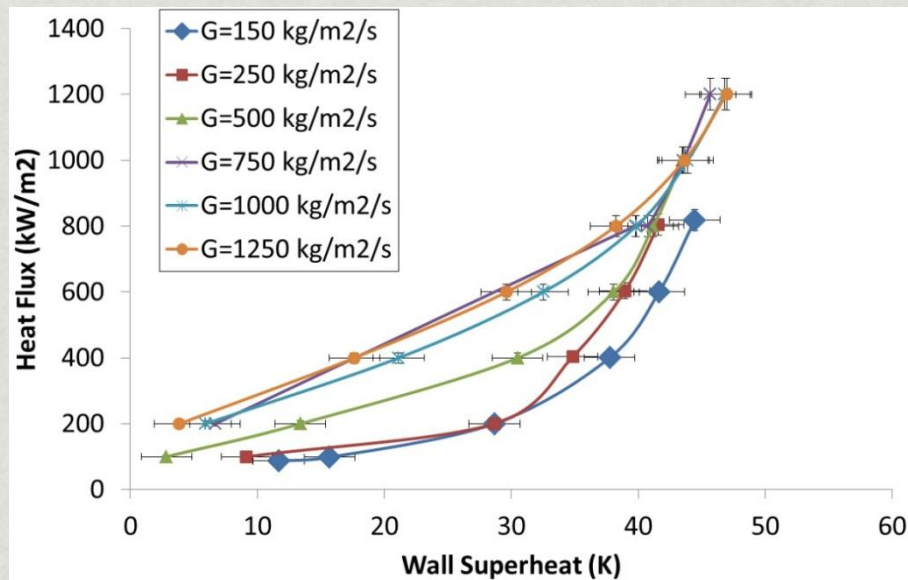
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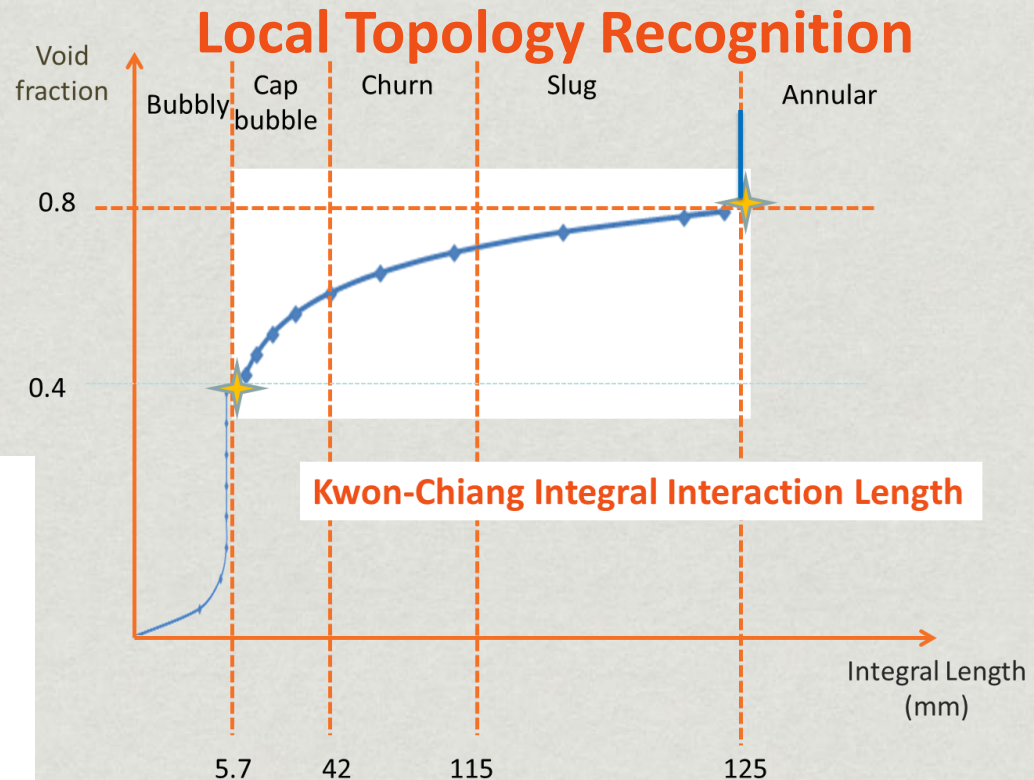
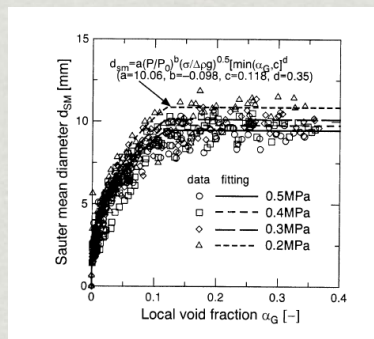
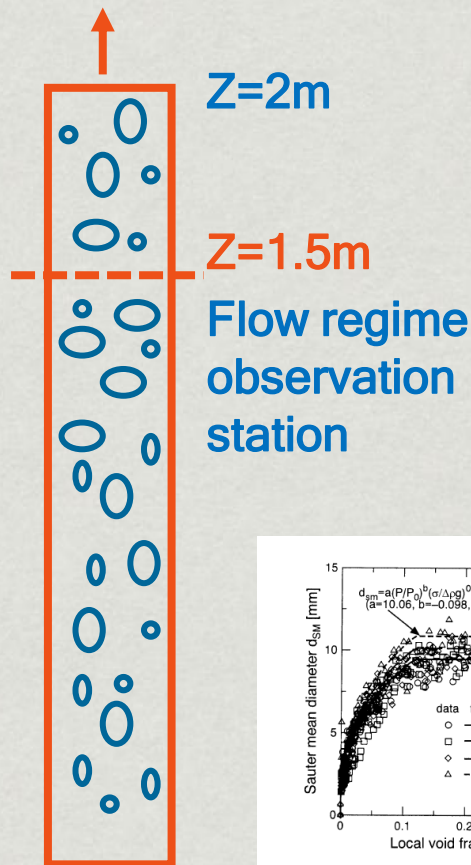




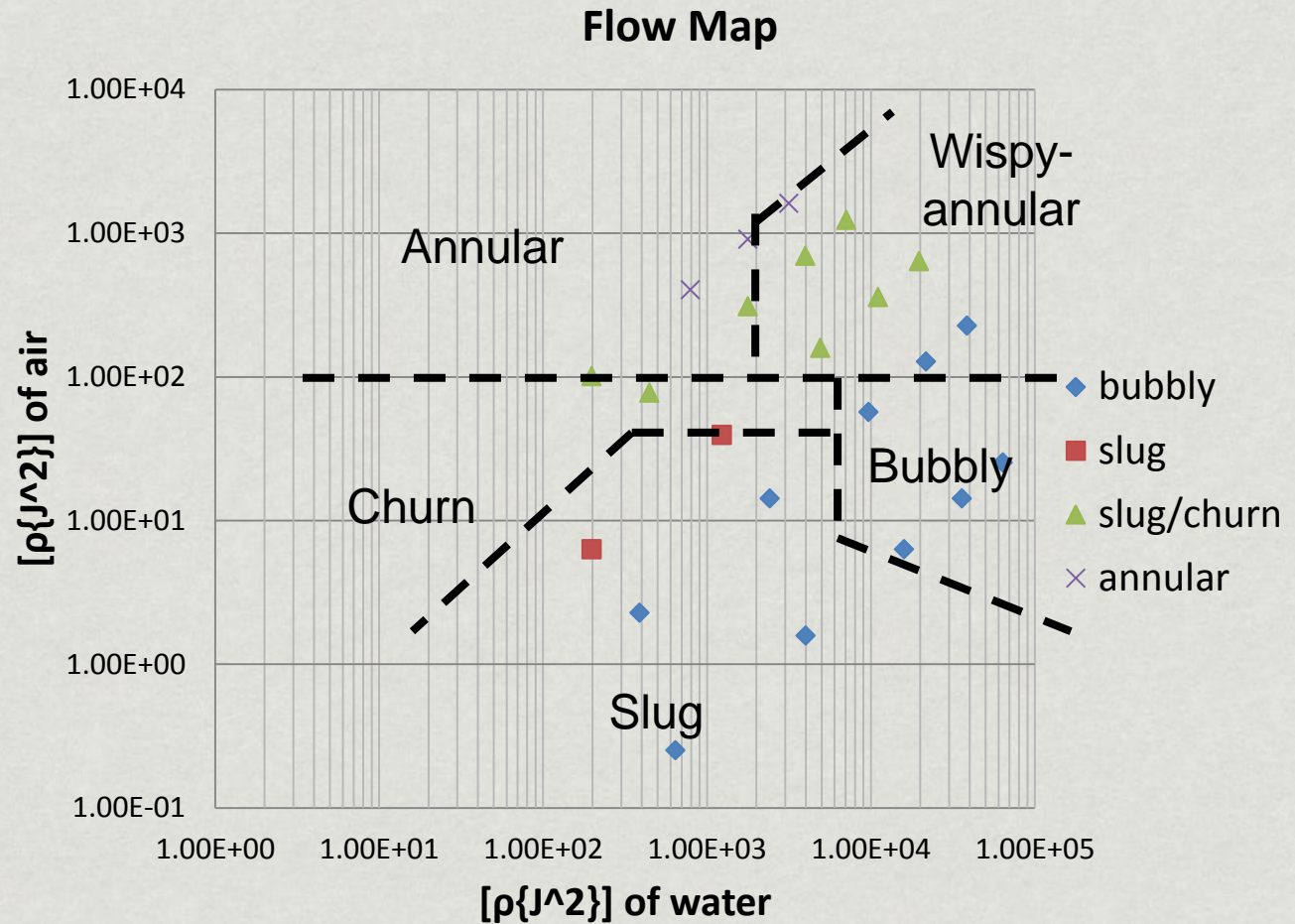
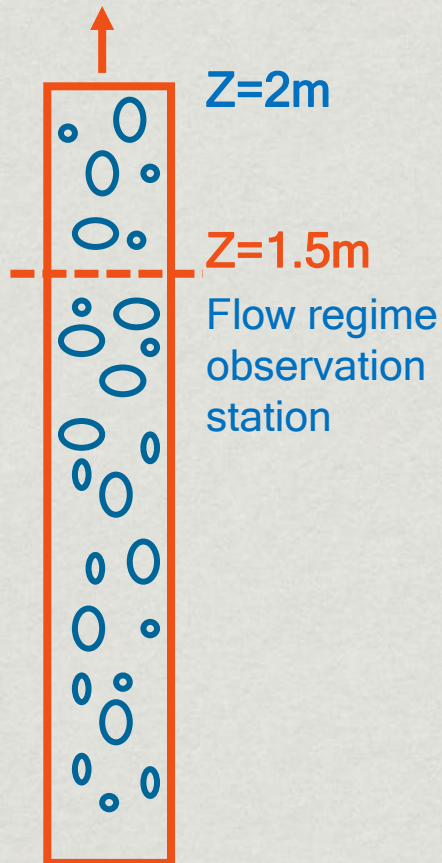
# Quickly ... on momentum closure

- We need a robust closure formulation for extended application
- *Robust* requires realistic physics, don't always blame the code
- The general approach requires a physical under-relaxation (which is simply physics) a homework example:

Each region adopts specific Lift and Drag Formulations (continuous)



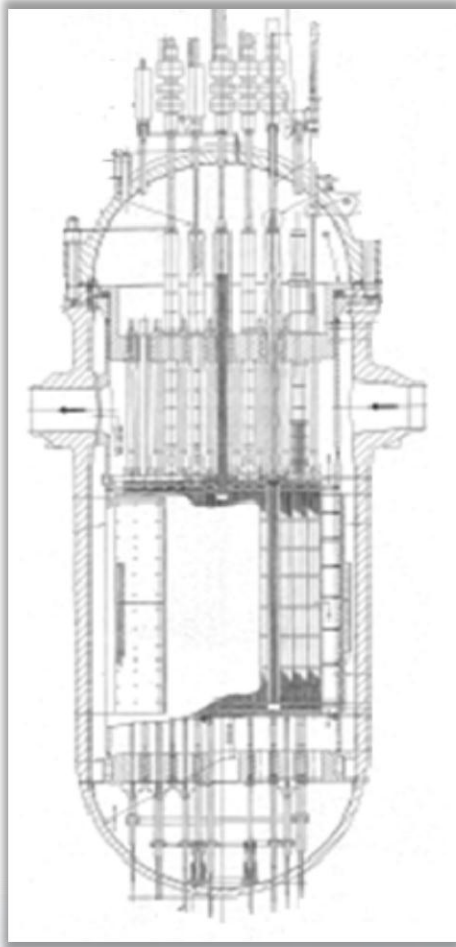
# Why physics based ??



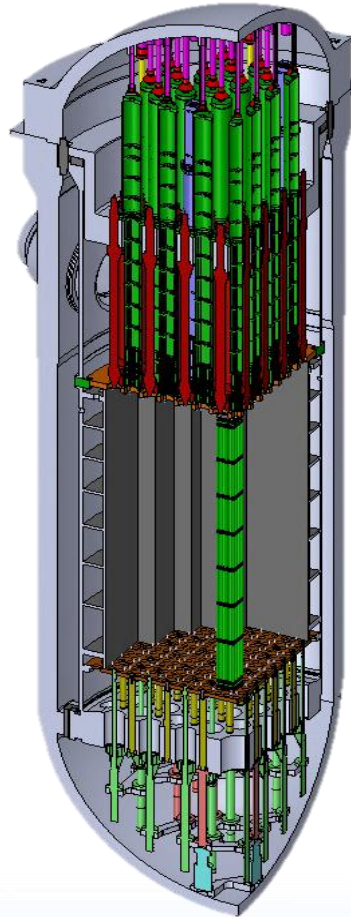


# 4-Loop Westinghouse PWR Multi-Physics Model Development

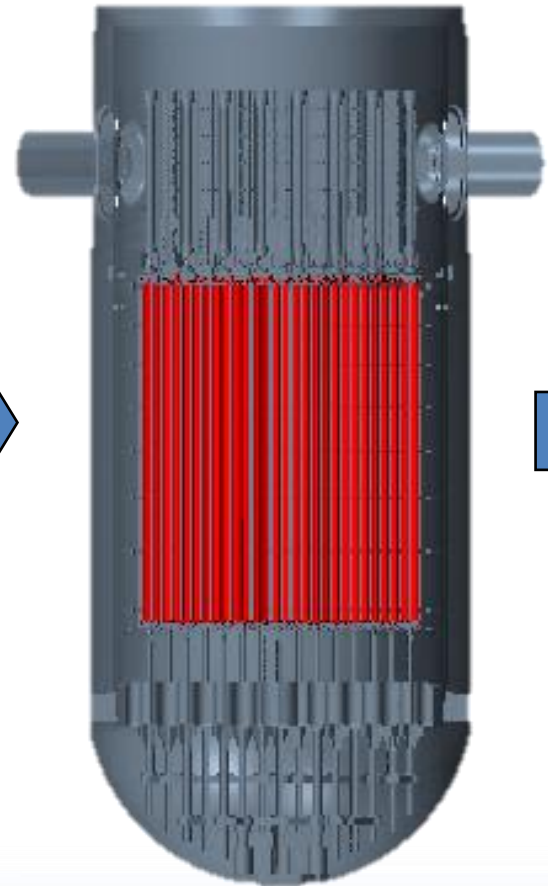
- RPV ID 173", 193/4 Fuel Assemblies, 13,944 fuel rods (fuel pellets, helium gap), 434 spacers, 148,224 mixing vanes; **1.2 billion cells**



Drawings



CAD Model



CFD Model



# 4-Loop Westinghouse PWR Multi-Physics Model Development

- RPV ID 173", 193/4 Fuel Assemblies, 13,944 fuel rods (fuel pellets, helium gap), 434 spacers, 148,224 mixing vanes; **1.2 billion cells**

