Subgrid Scale Modeling and the art of CFD

Emilio Baglietto, NSE
Multiphase-CFD: a full-scope redesign

Challenges:
- Complex physical phenomenon
  - Complex interfaces
  - Multiple flow regimes
- Undeveloped physical laws & mathematical treatment of two phase phenomena
  - Lack consistent experimental validation
- Complex interaction of numerics and closure forces
  - Unstable solutions, oscillatory behavior, etc.

Approach:
- Wall Boiling
  - Novel Physical Representation
- Extension to CHF
- Multiple flow regimes
- Hydrodynamic Closures
  - Account for vapor morphology
  - Account for group behavior
  - Implement physical under-relaxation
- 2-Phase wall Functions
  - Extend to include unresolved lubrication effect
- Multiphase turbulence
  - Leverage recent ITM/DNS and experimental data
GEN-II Heat Partitioning: Improved Physical Understanding

**Key challenges/approach:**
Tremendously complex surface interactions, cannot be resolved by first principle:

- Selection of local characteristic in the CFD solution to drive the SGS Model representation
- Fully Mechanistic representation to extend generality and allow leveraging experimental microscale measurements
- Tracking of subgrid surface characteristics to:
  - Include influence of surface evolution (oxidation, crud, etc.)
  - Extension to CHF description as surface hydrodynamic phenomenon

- Mechanistic model proposed by Judd and Hwang (1976)
- Adapted by Kurul and Podowski (1990) for wall heat flux partitioning during pool nucleate boiling.
- While limited it is de-facto the only model in M-CFD.
- Erroneous representation of physical boiling.

\[ q''_{tot} = q''_{fc} + q''_q + q''_e \]

Convective Quenching Evaporation

\[ q''_{fc} \quad q''_q \quad q''_e \]
GEN-II Heat Partitioning: Quick Overview

1. Mechanistic Representation of Bubble Lift off and Departure Diameters

2. Accurate evaluation of evaporation heat flux by modeling effective microlayer

3. Account for sliding bubble effect on heat transfer and nucleation sites

4. Account surface quenching after bubble departure

5. Account for bubble interaction on surface

Emilio Baglietto - NSE Nuclear Science & Engineering at MIT
GEN-II Heat Partitioning: assessment

- Validation performed against MIT boiling curves
- Allows validating separate model components
- Calibration-free – demonstrated generality deriving from improved physical representation

Pressure = 1.0 bar and 10°C Subcooling

- Evaporation term is not dominant contribution
- Effect of bubble sliding dominates Flow Boiling Heat Transfer (previously postulated by Basu)
- The new model demonstrates improved predictions at all conditions
- Enhanced robustness at higher heat fluxes
EXTENSION TO DNB

Etienne Demarly
Extension to DNB

Dr. Yadigarouglu’s recent statement (IJMF, 2014): “After over 60 or 70 years of efforts by many researchers [..], the CHF problem has not found yet a definitive general solution and it may never find one”.

* Look-Up Table:

8 correction coefficients needed for reactor predictions!

**BUT:** I have an advantage, I need to predict conditions that have high probability of CHF, I don’t need to predict the perfect Local CHF

- I do not need to “depend” on a CHF model, I can implement a CHF mechanism
- I can afford to be off in the model, but my energy balance will make it so that one of the mechanisms to identify CHF conditions will kick in
A simple but powerful mechanism

- Bubbles merge on heater surface prior to departure
  - Indicates size of dry surface patches

\[ N_{b}'' = f t g N'' \]
\[ P = 1 - e^{-N_{b}'' \pi D_{d}^2} \]

I can track the wet and dry surface in a “cell”
- This allows me to split the heat transfer into 2 components where

\[ q''_{tot} = A_{dry} q''_{vapor\_film} + (1 - A_{dry})q''_{Nucleate} \]

.. as the heat flux increases, heat removed by the wetted area can’t keep up, leading to larger coalescence between bubbles, and further decreases in wetted area, resulting in surface dryout.
A simple but powerful mechanism ...

- Some evidences that, at least for pool boiling, the simple mechanism seems reasonable*

- Supporting assumption that CHF is largely governed by the micro-hydrodynamics of the thin liquid film on heating surface. [Scale Separation, Theofanous (2002) and Dinh (2007)]


- We can extend to include the treatment of introducing a representation of the contact line speed, based both on the surface characteristics and the near wall velocity distribution...

- But I have not yet been convinced that this is necessary.
DNB Models / Validation

Jin Yan - ISACC-2013, Xian, China
HYDRODYNAMIC CLOSURES FOR PWR +

Rosie Sugrue
(Ben Magolan)
(Nazar Lubchenko)
Quickly ... hardened hydrodynamic closures

- 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

Each region adopts specific Lift and Drag Formulations (continuous)
Interfacial Forces in Momentum Conservation

Buoyancy, B
Viscous Drag, D
Lateral Lift, L
Virtual Mass, VM

Basset Force
Turbulence Dispersion, TD
Wall Lubrication, WL

\[ M = F_B + F_D + F_{TD} + F_L + F_{VM} + F_{WL} + \sum_{j=1}^{N} (\hat{m}_{jk} u_j \hat{m}_{kj} u_k) \]
Drag Test Case: Results

Bubble Velocity [m/s] vs. Bubble Diameter [mm]

- Constant
- Schiller-Naumann
- Bozzano-Dente
- Tomiyama (cont.)
- Tomiyama (clean)
Complexity: Lift Coefficient

Thought this would be easy...

Non-spherical Bubbles:
Consider the influence of bubble shape; can use Eotvos and Morton numbers

Reality:
Drag: easy
Lift: NOT easy
Understanding Lift: What’s Important

1. Coefficient Sign: *why it changes & when*
   - Understand bubble deformation
   - Still an open issue: how to represent lift for a group of bubbles – only depends on sign?

*Courtesy of G. Tryggvason*
Understanding Lift: What’s Important

2. Coefficient “Magnitude”
   - Work needs to be done!
   - Starting point: Tomiyama lift coefficient for deformed bubbles

![Chart showing lift coefficient vs. maximum bubble diameter](chart.png)

- Tomiyama Lift Coefficient
- PHASTA Values
- Tomiyama et al. (2002) Prediction

**Courtesy of I. Bolotnov**

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Future work: validation and testing

- Validation of separate effects
- Evaluate Robustness of Closures
- Evaluate computational cost of GEN-I vs. GEN-II

TAMU Freon Data

- Shadowgraphy experimental images - Carlos Estrada Texas A&M

Synthetic CRUD Boiling Curves

- Carolyn Coyle, Jacopo Buongiorno, Thomas McKrell
CLOSURES FOR BWR FUEL ASSEMBLIES

Giulia Agostinelli
# Baseline Boiling Models

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![2D topology specification](image)

- **Mist**
- **Sharp interface**
- **Bubble**

Emilio Baglietto - NSE Nuclear Science & Engineering at MIT
BFBT benchmark case

Experiment 4101-61

MESH

BCs

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Preliminary Results

Pixel void fraction

Sub-channel void fraction

Void Fraction Error (Predicted - Measured)

E[\%] = \alpha_{predicted} - \alpha_{measured}

experiment

CFD – Argonne Model

Sub-channel location

Emilio Baglietto - NSE Nuclear Science & Engineering at MIT
SINGLE AND MULTIPHASE TURBULENCE

Ben Magolan
Fuel Applications 1: Press. Drops
Extensive validation/application

- A 10 year experience
- Validated on large range of PWR/BWR design

- System and BOP
  ✓ Transient Mixing
  ✓ Hot Leg Streaming
  ✓ Thermal Striping
  ✓ SG performance
  ✓ Cooling Towers Interference

- Fuel Cycle and Beyond Design Basis Applications
  ✓ Spent fuel transportation and Storage

K. Ikeda et al. “Study Of Spacer Grid Span Pressure Loss Under High Reynolds Number Flow Condition” - Proceedings of ICONE17

Fuel Applications 1: Press. Drops

![Graph showing pressure drop vs. Reynolds number]

- **Strong Influence of Anisotropic Turbulence**
- **Necessary to Adopt an Accurate Anisotropic Turbulence Model** – current optimal solution is NLEVM

Fuel Applications 1: Press. Drops
Application of ASME V&V20 to Predict Uncertainties in CFD Calc.

• First-of-kind calculation of uncertainties related to a CFD calculation for nuclear fuel application in the open literature with the ASME V&V20 method

• CFD modeling to predict pressure losses in rod bundle is optimal
  • $E < U_{val}$: $E$ is lower than the upper limit of the possible error due to the CFD modeling assumptions and approximations
  • Modeling error within the "noise level" imposed by the numerical, input, and experimental uncertainties
  • Improving the CFD modeling is not possible without an improvement on the numerical, geometric and experimental errors

Fuel Applications 2: Accuracy
Importance of mesh quality and turbulence modeling

- Grid quality and consistency is “essential” for robust application [experience!, no tests!!]
- Industry Closure approach based on physical representation [Baglietto et al. 2006-2013]
- Demonstrates improved prediction at all locations, including Turbulence Levels

**Physically Based Closure Coefficient**

\[
\mu = \frac{\nu}{\frac{1}{3} \rho (\nabla u) \cdot (\nabla u)}
\]

Anisotropy

\[
\frac{\nu}{\frac{1}{3} \rho (\nabla u) \cdot (\nabla u)}
\]

Curvature Rotation

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EPRI Industrial Benchmark confirms 2006-NLEVM state-of-the-art modeling

RMS errors of the axial fluctuation velocities.
Anisotropic k-e models in Hydra-TH

Restructuring permits addition of multiple variants of the k-\(\varepsilon\) model
- Standard model
- RNG model
- Non-linear model (anisotropic viscosity model)
  - Captures secondary rotational flows damped by other k-\(\varepsilon\) models
CFD4NRS-6
hosted by
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science : systems : society

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Photo by John Stempien