Collecting and Characterizing Validation Data to Support Advanced Simulation of Nuclear Reactor Hydraulics

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Multi-Physics, Multi-Scale Problem

TH: Multiphase flow
Sub-cooled boiling

MP: Multi-Physics Interactions
FC: Fuels and cladding behavior

Micro-scale physics
Meso-scale
Macro-scale

RT-TH (strong)
TH-CC
FC-RT
RT-CC (strong)

Micro-scale physics
Meso-scale
Macro-scale

RT: Radiation transport
Core neutronics

CRUD formation

System-Level Code
(RETRAN, RELAPS, BOA)

10^4

T \sim \text{months}
L \sim 10 \text{m}

Sub-system-Level Code
\text{e.g., VIPRE for full core}

10^3

T \sim \text{hr}
L \sim \text{m}

"Snapshot" simulation with higher-resolution models

Component-Level Code
\text{e.g., Multiphase CFD for FA}

10^1

T \sim \text{mins}
L \sim \text{dm}

Control Volume-Level Code
"DNS", LES/ITM

10^1

T \sim \text{s}
L \sim \text{cm}

Microphysics (MP)
Mesoscale Code

10^1

T \sim \text{ms}
L \sim 10 \text{ \mu m}
Validation Hierarchy (Validation Pyramid) of Subcooled Boiling Flow Model
Bayesian Framework for Data Integration
Nuclear System Analysis – Subcooled Boiling Flow Example

- Underlying physics and models
  - Two-phase flow dynamics – drift-flux/two-fluid model
  - Subcooled boiling
    - Wall heat transfer – mixed forced convection and boiling heat transfers
    - Evaporation at wall – onset of nucleation, onset of significant void, nucleation density, bubble detachment radius and rate
  - Condensation in subcooled bulk fluid

- Data
  - Mostly at macro level, i.e., void fraction distribution, input/output pressure/temperature/flow rate
  - Mostly obtained at conditions (pressure, flow rate heat flux) much different from plant conditions
Sub-cooled Flow Boiling – Complex Modeling

Each circle is a model, which may comprises of one or more “daughter-layer” models (circles)
## Data Sources

### Low pressure

<table>
<thead>
<tr>
<th>Authors</th>
<th>Geometry (m) D or Dh</th>
<th>Pressure (kPa)</th>
<th>Heat flux (MW m(^{-2}))</th>
<th>Mass flux (kg m(^{-2}) s(^{-1}))</th>
<th>Measurement instrument</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferell (1964)(a)</td>
<td>Circular 0.0118</td>
<td>410</td>
<td>0.36</td>
<td>540–1060</td>
<td>–</td>
</tr>
<tr>
<td>Costa (1967)(a)</td>
<td>Rectangular 0.0038–0.0066</td>
<td>174–499</td>
<td>1.0–4.2</td>
<td>3000–7500</td>
<td>–</td>
</tr>
<tr>
<td>Staub (1968)(a)</td>
<td>Rectangular 0.01</td>
<td>500</td>
<td>0.6</td>
<td>1500–3000</td>
<td>–</td>
</tr>
<tr>
<td>Whittle and Forgan (1967)</td>
<td>Circular 0.065</td>
<td>1200</td>
<td>0.24</td>
<td>320–2000</td>
<td>–</td>
</tr>
<tr>
<td>Evangelisti and Lupoli (1969)</td>
<td>Circular 0.0064</td>
<td></td>
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<tr>
<td>Sekoguchi et al. (1974)</td>
<td>Circular 0.0136–0.0150</td>
<td>1000</td>
<td>0.5</td>
<td>1600–2800</td>
<td>–</td>
</tr>
<tr>
<td>Edelman and Elias (1981)</td>
<td>Circular 0.113</td>
<td>1000</td>
<td>1.0</td>
<td>2000–3000</td>
<td>–</td>
</tr>
<tr>
<td>McLeod (1986)</td>
<td>Annular 0.0089–0.0095</td>
<td>500</td>
<td>0.3</td>
<td>870–900</td>
<td>–</td>
</tr>
<tr>
<td>Rogers et al. (1987)</td>
<td>Annular 0.0089</td>
<td>500</td>
<td>0.3</td>
<td>870–900</td>
<td>–</td>
</tr>
<tr>
<td>Dougherty et al. (1990a, b)</td>
<td>Circular 0.0091–0.0094</td>
<td>500–1000</td>
<td>0.5–1.0</td>
<td>870–900</td>
<td>–</td>
</tr>
<tr>
<td>Bibeau and Salcudean (1994a, b)</td>
<td>Annular 0.0091</td>
<td></td>
<td></td>
<td></td>
<td>–</td>
</tr>
<tr>
<td>Zeitoun and Shoukri (1997)</td>
<td>Annular 0.0127</td>
<td>2000</td>
<td>0.25–0.30</td>
<td>500–700</td>
<td>–</td>
</tr>
<tr>
<td>Bartel et al. (1999)</td>
<td>Annular 0.0195</td>
<td>1000–2500</td>
<td>0.14</td>
<td>4400–8400</td>
<td>–</td>
</tr>
</tbody>
</table>

### High pressure

<table>
<thead>
<tr>
<th>Author</th>
<th>Geometry (m) D or Dh</th>
<th>Pressure (kPa)</th>
<th>Heat flux (MW m(^{-2}))</th>
<th>Mass flux (kg m(^{-2}) s(^{-1}))</th>
<th>Measurement instrument</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bartolemei and Chanturiya (1967)(a)</td>
<td>Circular 0.0154–0.0240</td>
<td>1500–4500</td>
<td>0.38–0.80</td>
<td>870–900</td>
<td>Gamma-ray</td>
</tr>
<tr>
<td>Bartolemei et al. (1982)</td>
<td>Circular 0.012</td>
<td>3000–14 800</td>
<td>0.34–2.20</td>
<td>440–2200</td>
<td>Gamma-ray</td>
</tr>
<tr>
<td>Christensen (1961)(a)</td>
<td>Rectangular 0.0178</td>
<td>2760–6890</td>
<td>0.21–0.50</td>
<td>640–850</td>
<td>–</td>
</tr>
<tr>
<td>Dix (1971)</td>
<td>Annular 0.00914</td>
<td>314–848</td>
<td>0.004–0.03</td>
<td>65–140</td>
<td>Hot-film anemometer, photography</td>
</tr>
<tr>
<td>Egen et al. (1957)(a)</td>
<td>Rectangular 0.00475</td>
<td>13 800</td>
<td>0.25–1.60</td>
<td>400–870</td>
<td>–</td>
</tr>
<tr>
<td>Griffith et al. (1958)</td>
<td>Rectangular 0.0127</td>
<td>8270–13 800</td>
<td>0.31–1.90</td>
<td>450–870</td>
<td>Photography</td>
</tr>
<tr>
<td>Labuntsov et al. (1984)</td>
<td>Circular 0.012</td>
<td>2000–7000</td>
<td>0.58–1.2</td>
<td>850–3000</td>
<td>Gamma-ray</td>
</tr>
<tr>
<td>Martin (1972)</td>
<td>Rectangular 0.0038–0.0053</td>
<td>7848</td>
<td>0.4–1.7</td>
<td>750–2200</td>
<td>X-ray</td>
</tr>
<tr>
<td>Rouhani (1965)(a)</td>
<td>Annular 0.013</td>
<td>980–5000</td>
<td>0.3–1.20</td>
<td>130–1200</td>
<td>–</td>
</tr>
<tr>
<td>Mauer (1960)</td>
<td>Rectangular 0.0041</td>
<td>8550–14 300</td>
<td>0.79–7.70</td>
<td>560–4800</td>
<td>Diff pressure, gamma-ray</td>
</tr>
<tr>
<td>Celata et al. (1997)</td>
<td>Circular 0.008</td>
<td>1000–2500</td>
<td>0–14</td>
<td>4400–8400</td>
<td>Differential pressure</td>
</tr>
<tr>
<td>St. Pierre and Bankoff (1967)</td>
<td>Rectangular 0.0178</td>
<td>1400–5500</td>
<td>0.072–0.29</td>
<td>670–880</td>
<td>Gamma-ray</td>
</tr>
</tbody>
</table>
Subcooled Boiling Flows – Data Sources

- **Data heterogeneity**: (i) measurement data available at the “system” level – left-most panel – and also at the “sub-model” level – nucleation site density, bubble detachment rate/radius, etc. Missing data at some levels; (ii) differences in data scalability, relevancy and uncertainty.
Subcooled Boiling Model Hierarchy

Flow regime

Vapor distribution

Pressure distribution

Flow velocity distribution

Flow temperature distribution

Wall temperature

Reynolds stress distribution

Fluid/vapor properties

Initial/boundary conditions

Vapor/Liquid mass conservation

Momentum conservation

Energy conservation

Turbulence

Bulk flow condensation rate

Wall evaporation rate

Wall convective heat flux

Wall conductive heat transfer

Wall turbulence

Nucleation site density

Bubble growth rate

Bubble detachment rate

Bubble detachment radius

Near-wall convective heat transfer

Near-wall turbulence

Wall material properties

Wall roughness

Wall heat flux

Inputs and parameters

Observable responses

Conservation laws-based models

Unobservable responses

Constitutive models
Representation of Multi-physics/Multi-level Subcooled Boiling Flow Model

- Hierarchical regression
- Bayesian influence networks - relationships represented by directed acyclic graphs (DAGs)
- Bayesian Structural Equation Modeling (BSEM) – permits hierarchical/non-hierarchical, recursive/non-recursive structural equations
Subcooled Boiling Flows – Data Heterogeneity

- Data Identification
- Data Collection
- Data Review

• Data Characterization
• Data Assimilation
Flow of information in traditional approach to calibration of multi-physics models

“Total data model integration” approach

Modeling of Multi-Scale & Multi-Physics Subcooled Boiling Flows – Calibration/Validation

Calibration

Model 1

SET Data 1

Model 2

SET Data 2

Model ..

SET Data ..

Whole model

IET Data

Validation

Predictions

Predictions

Conservation Law Models

Constitutive Models

SET Data

IET Data

Uncertainty

Uncertainty

Uncertainty

Uncertainty
The Total Data-Model Integration Approach for Model Calibration, Validation and Uncertainty Quantification

- Technical implementation of the proposed “total model-data integration” approach is difficult as it requires a combining of multiple heterogeneous data streams and dealing with multidimensional, multivariate model inputs/outputs.
- A preliminary realization of the approach was delineated in this presentation and employs a range of statistical modeling methods and techniques:
  - Surrogate model construction using a process convolution technique based Principal Component Analysis (PCA) and Gaussian processes (GPs), and Bayesian calibration using Markov Chain Monte Carlo (MCMC) sampling.
- Extension of this approach is envisioned to allow the use of 2D/3D data and data of other scale levels (from SETs) in calibration, validation, and uncertainty quantification of models of higher dimensionality. While proposed and developed for the subcooled flow boiling case study, this approach is intended to be applicable without much modification in the development of any multi-physics models and software.
- The proposed calibration, validation, and uncertainty quantification approach, while offering some flexibility in data usage (i.e., allowing the use of data of different origins, types, quality, etc.), does impose requirements on data collection, validation and characterization.
Strategy for Quantification of Data Needs, Data Collection, Validation, and Characterization

- With the total data-model integration approach for model calibration, validation and uncertainty quantification as proposed, data are desirable to be accompanied with:
  - Information about measurement error estimate and data acquisition/derivation methods – to quantify uncertainty;
  - Information needed for “application-oriented” data valuation – to determine relevancy and scalability.

- Quantification of data value/quality can be based on the following criteria:
  - Relevancy
  - Scalability
  - Uncertainty

- Data classification and characterization can be based on factors, such as:
  - Scope of involved physics and strength of their couplings – turbulence, boiling, heat transfer mode, convection mode, etc.; single physics (SETs) or multi-physics (IETs);
  - Temporal/spatial dimensionality and resolution of data;
  - Relevancy (in physics involvement sense) to an application or a scenario of interest – SFB, LOCA, Feed-and-Bleed, etc.;
  - Data quality – measurement method, error/uncertainty assessment;
  - Scalability – size, geometry, material properties, pressure, temperature, flow rate, etc.
### Example of Quantification of Data Needs, Data Classification and Characterization to Support SFB model Validation and Calibration

<table>
<thead>
<tr>
<th>Physics</th>
<th>Exp. data acquisition method</th>
<th>Data availability</th>
<th>Exp.</th>
<th>DNS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two-phase fluid dynamics</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Turbulence</td>
<td>Direct</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>(Dispersed) phase transport</td>
<td>Direct</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Wall friction</td>
<td>Indirect</td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Two-phase flow instability</td>
<td>Direct</td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mechanical interactions between phases</td>
<td>Indirect</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Interfacial tension force - bubble breakup &amp; coalescence</td>
<td>Direct</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Two-phase heat-mass transfer</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Convective heat transfer</td>
<td>Indirect</td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wall heat flux partitioning</td>
<td>Indirect</td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wall evaporation</td>
<td>ONB, OSV</td>
<td>Direct</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Nucleation</td>
<td></td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bubble growth dynamics</td>
<td></td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Bubble detachment</td>
<td></td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Boiling crisis (CHF)</td>
<td>Indirect</td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal interactions between phases</td>
<td>Indirect</td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vapor condensation in bulk flow</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Notes:

ONB – Onset of Nucleate Boiling  
OSV – Onset of Significant Void  
CHF – Critical Heat Flux

Indirect – indirect determination  
Direct – direct measurement or observation
Implication to the CASL Validation and Data Plan Strategy

• A first step forward to implement the CASL “application-oriented, total data assimilation” strategy for multi-physics model calibration and validation

• The proposed Bayesian model calibration and data assimilation framework is intended to realize several goals stated in the CASL validation data plan, in particular,
  – “consistent integrated treatment of uncertainty across physics and scales”;
  – “Data Realism” concept, i.e., maximal usage of data of different origins, types, scales and qualities;
  – (continuing) incremental update of models with more data becoming available.

• The framework helps to establish the requirements and templates for data in support of the realization of the “VUQ-guided data collection, characterization & qualification”:
  – Model of data inaccuracy/uncertainty should be provided together with data, i.e., distributions instead of ± error range;
  – Conversion/homogenization of data to the formats acceptable to VUQ;
  – Reconciliation of conflicting/contradicting data;
  – Data validation/grading/comparison to provide the “weight” factor of a dataset (to be used in VUQ).
CASL Data Center (CDC)

- The CDC functions include
  1. Validation data inventory and warehouse;
  2. VUQ-guided data qualification, and
  3. Data processing for interface with users’ data operation, with CASL codes and with VUQ workflow, including data assimilation.
Summary

• “Calibration in the narrow sense may corrupt a model by ignoring information” → a need for “calibration in the broad sense of combining all relevant information about the parameters” (Jansen & Hagenaars) (including physically meaningful interpretation of the parameters)

• Validation/calibration of complex multi-physics models using heterogeneous data require a hierarchical representation of interdependency between multiple submodels and parameters.

• Modern nuclear multi-scale multi-physics models are based both on
  – more reliable and scalable conservation laws represented by PDEs
  – less reliable/universal constitutive (closure) laws having a number of tuning parameters

Both inadequacy of the model form represented by PDEs and uncertainty of model parameters are needed to be assessed in the VUQ process. Closure model parameter calibration needs to be somehow “constrained” by the validity/bias of the conservation laws-based models.

• Data of multi-physics systems are heterogeneous, multivariate, multidimensional and data availability varies greatly depending on scales and physics.

• A total data assimilation approach to VUQ is needed to take the advantage of all available data regardless of their origin, uncertainty and characteristics.

• “Total data-model integration” can be realized with use of model analysis approaches based on Bayesian inference.