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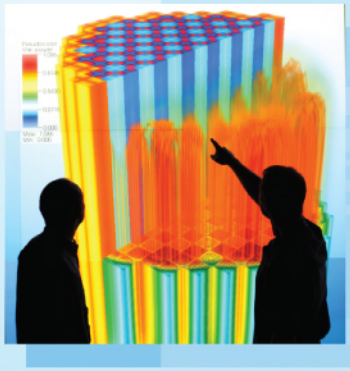

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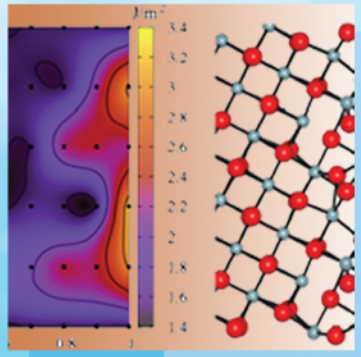

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Consortium for Advanced Simulation of LWRs

Validation Data Plan Implementation: Subcooled Flow Boiling Case Study

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Validation Data Plan Implementation: Subcooled Flow Boiling Case Study

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ABSTRACT

This report presents a step forward in the development and realization of a novel model-data integration approach that supports the validation and data assimilation framework currently being developed at the Consortium for Advanced Simulation of LWRs (CASL) to enable quantitative assessment of the CASL predictive capabilities [**1**]. The approach is designed and applied to the analysis of a subcooled boiling flow model which is an essential component in the CASL case study modeling of crud-induced power shift (CIPS) phenomenon. The validity of the boiling two-phase flow modeling depends not only on the robustness and accuracy of the numerical treatments (for discussion, see, e.g., [**2**]), but also on the correctness of the conservative laws-based models and various constitutive models or closure laws which are the simplified representations of micro-/meso-scale physics not resolved by the main conservation laws, i.e. vapor-liquid interactions, wall heat flux partitioning, bubble nucleation and detachment dynamics, etc. [**3**]. The closure laws are usually derived based on experimental data and can not be universally applied to all ranges of flow conditions.

Although measurement data have been used in the past for model calibration, a new trend has emerged which focuses on even more tightly integration of model and data in an effort to improve the predictive capability of modern complex multiphysics models. Data also needed for model validation and quantification of model prediction uncertainty. For complex hierarchical multiphysics systems, data availability, quality and uncertainty may vary widely depending on the scale, physics, and system level, which poses a significant challenge to model-data integration methods.

In this work a model calibration/validation approach based on Bayesian networks and Bayesian inference is proposed and developed which is used in the analysis of a subcooled boiling flow model. This approach is based on total data assimilation concept and allows the integration of different datasets obtained from different type of experiments and observations. Technical details about this Bayesian model-data integration approach as well as its capability and limitations in application to the considered subcooled boiling flow and the CASL case-study CIPS modeling are present and discussed. The proposed model-data integration approach is developed in conjunction with and support of the implementation of the CASL's VUQ-guided data collection, characterization and qualification concept [**1**].

This report is prepared for the Department of Energy's Consortium for Advanced Simulation of LWRs (CASL) program's VUQ Focus Area.

SUMMARY

In this CASL CIPS Validation Data Plan implementation case study, a model calibration/validation framework based on Bayesian inference for the analysis of a subcooled boiling flow model is outlined and analyzed. The framework based on the total data assimilation concept allows the calibration/validation of complex multiphysics models using heterogeneous data obtained from different types of experiments, i.e. SETs, METs, IETs and PMOs. Data quality defined by the relevancy, scalability and uncertainty are accounted for in the model analysis allowing the quantification of uncertainty in model predictions and parameter determination. Such a process of model-data integration could form a basis for advanced multiphysics model VUQ, data characterization and identification of the values of both available and missing data.

The couplings of multiple physics of different fidelity levels and based on both first-principle conservation laws or simplified empirical representations of physics are realized in this study using a Bayesian network which facilitates the propagation of uncertainty information between the coupled models. Bayesian inference conducted on such a network allows both the forward propagation of uncertainty in model form and parameters to model predictions and the backward propagation of data uncertainty to parameter estimates. Uncertainties of both parameter estimates and model form are therefore accounted for in the process.

A preliminary workflow has been established for the proposed model calibration/validation method which is “application-oriented” to the analysis of a subcooled boiling flow model. Currently, this test-case model comprises a drift-flux two-phase flow and other submodels representing wall convective heat transfer, wall evaporation, bulk flow condensation, etc. Except for the flow model which is conservation laws-based, the other models are semi-empirically derived which require parameter calibration. In this preliminary analysis, only data on axial distributions of void fraction and temperature have been used, but further extension of this calibration/validation framework will enable the use of the small-scale data on wall evaporation dynamics.

Based on the present study, the following conclusions and recommendations for the CASL validation data plan (VDP) can be made:

- CASL CIPS problem in particular and other nuclear power system and safety problems in general are characterized by presence of multiple scales and non-linear couplings of multiple parallel/nested physics which involve different modeling approaches based both on first-principle and empirical/semi-empirical derivations;

- Both high-fidelity spatio-temporal conservation-laws based and evidences-based local-interactions (characteristically, lower-fidelity) constitutive models are used in multiphysics system modeling. Such a mixture of models constitutes a major new complication in the validation and calibration tasks of advanced simulation capability;
- Conservation laws based models represented by PDEs are more credible and scale-independent which constrain the constitutive model calibration. However, the potential bias in selecting model forms could cause significant off-settings that render the model un-amenable for parameter calibration;
- Data of multiphysics 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;
- Data uncertainty must be accounted for and used in quantification of prediction uncertainty;
- A flexible model-data integration framework is needed which can
  - represent the complex hierarchy of coupled multiphysics models
  - account for model form inadequacy and biases
  - account for data relevance, scaling and uncertainty (represented by "weight" factor [**1**])
  - assimilate heterogeneous data available at different levels of model hierarchy
  - not be rendered unworkable when data are missing or not directly applicable for some constituent models
- Bayesian inference in combination with Bayesian influence networks is a promising approach to multiphysics model VUQ which satisfies the above requirements;
- Data homogenization, grading and characterization are required before the data can be used in the proposed "unified" VUQ framework;
- It is recommended that the present case study (subcooled flow boiling) be continued and extended in a close collaboration with THM, AMA, NE-KAMS team and the CDC initiative, with the objective to enable a VUQ-aided, data-cognizant development of advanced capability in Computational Multiphase Fluid Dynamics for CASL.

ACRONYMS

	Description
AMS	Advanced Modeling and Simulation
CASL	Consortium for Advanced Simulations of LWRs
CDC	CASL Validation Data Center
CFD	Computational Fluid Dynamics
CHF	Critical Heat Flux
CILC	Crud Induced Localized Corrosion
CIPS	Crud Induced Power Shift
CMFD	Computational Multi-phase Fluid Dynamics
CRUD	Chalk River Unidentified Deposit
DA	Data Assimilation
DNB	Departure from Nucleate Boiling
DNS	Direct Numerical Simulation
EMU	Experimental Measurement Uncertainty
FA	Focus Area (in CASL)
IET	Integral Effect Test
MCMC	Markov Chain Monte Carlo sampling
MET	Multiple Effect Test
ONB	Onset of Nucleate Boiling
OSV	Onset of Significant Void
PCD	Principal Component Decomposition
PDE	Partial Differential Equation
PMO	Plant Measurements and Observations
RPP	Reactor Prototypicality Parameter
SET	Separate Effect Test
SFB	Subcooled Flow Boiling
SNB	Subcooled Nucleate Boiling
THM	Thermal-Hydraulics Method (FA)
VDP	Validation Data Plan
V&V	Verification and Validation
VERA	Virtual Environment for Reactor Applications
VUQ	Validation & Uncertainty Quantification
UQ	Uncertainty Quantification

NOMENCLATURE

Latin letters

A	Area
c_p	Specific heat
D	Diameter
E	Total energy
f	Friction factor
g	Gravity
h	Enthalpy/Heat transfer coefficient
i	Internal energy
j	Volumetric flux
k	Heat conductivity
$\mathcal{L}$	Likelihood function
$\mathcal{N}$	Normal probabilistic distribution
p	Pressure/Probability
Pe	Peclet number
q,Q	Heat flux
t	Time
T	Temperature
u	Velocity
V_{gj}	Drift velocity

Greek letters

α	Volume fraction
Γ	Mass generation rate
η	Surface roughness
ρ	Density
σ	Surface tension
τ	Stress tensor

Superscripts

T	Turbulence/Transpose (of matrix)

Subscripts

f	fluid
FC	Forced Convection
I	Interface
fg	Transition from fluid to gas
g	vapor
m	mixture
NB	Nucleate Boiling
x	spatial direction x
w	wall

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1. INTRODUCTION

Advanced modeling and simulation of nuclear reactor systems increasingly involve high-fidelity/high-resolution multi-physics, multi-scale methods and tools. On one hand, it appears that the advent of these capabilities has surpassed the pace at which experiments could be designed, constructed, and performed to produce VUQ-grade data suitable for calibration and validation of advanced codes. On the other hand, extraordinary progress in experimentation and instrumentation allows visualization and characterization of various phenomena and processes at a level of resolution not imaginable decades ago. Most notably, experiments use different working fluids and are conducted under a broad range of test conditions which may or may not be similar to the plant conditions. For an engineering application and conditions of interest, different experiments (and their resulting datasets) are characterized by their individual relevance and applicability. Because a typical nuclear energy system is characteristically complex, involving multiple phenomena, some enveloping many others, measurement data are often heterogeneous, varying greatly from experiment to experiment. Correspondingly, each experiment may have unique values to calibration and validation of computer models and codes. The heterogeneity of data presents a challenge to the characterization of datasets and their assimilation for the purpose of integrated assessment of the predictive capability in question.

The crud-induced power shift (CIPS) and crud-induced localized corrosion (CILC) have been chosen by the DOE Consortium for Advanced Simulation of Light Water Reactor (CASL) to be challenge problems to assess the CASL predictive capabilities which are under continuing development [**1**]. These problems are caused by localized evaporation of coolant and deposition of corrosive boron and corrosion products on fuel rods leading to distorted axial and radial distributions of neutrons and power in a PWR reactor core. Such phenomena involve a range of different interacting physics and chemistries, such as thermal hydraulics of single/multi-phase flow, subcooled boiling, boron transport and deposition, corrosion product formation and convection, core neutronics, etc. In this context, the dynamics of subcooled boiling flows plays a prominent role and, by itself, is a multiphysics phenomenon involving two-phase fluid dynamics, heat transfer and phase changes (boiling and condensation) (*Figure 1.1*).

As a result of the study on "CIPS Validation Data Plan" [**1**], a comprehensive (application-oriented, VUQ-guided) strategy to validation data support for the CIPS challenge problem was formulated. The study also suggests that implementation of the proposed approach (namely, Bayesian data assimilation framework, aided by a validation data management system, or CASL Data Center) be started with a case study, which is complex enough

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to reflect all key aspects requiring consideration in a validation data plan (VDP), while simple enough to allow an integrated treatment, from data collection to model calibration. Based on a detailed review of CIPS-related data and models performed in Chapter 4 of [**1**], subcooled flow boiling was found to best meet these requirements and recommended for VDP case study[1]. Furthermore, reliable prediction of subcooled flow boiling is a much-needed capability for solving the CIPS challenge problem and is a focal point of development in CASL Thermal-Hydraulics Method (THM) area.

Modeling of subcooled boiling flows in nuclear power systems is commonly based on the first-principle descriptions of mass, momentum and energy conservations and various empirical/semi-empirical constitutive correlations which describe the physics and interactions at the micro- and meso-scopic scales. As such, constitutive laws are also models which represent the real physics in a simplified manner. Given the incomplete understanding of micro-/meso-scale physics, the constitutive models are mostly stochastic with many uncertainties involved. The model of subcooled boiling flows therefore is a hierarchy of nested models of different reliabilities and the predictive capability of the model as a whole greatly depends on the reliability and accuracy of the constituent models. The constitutive laws – being crude representations of physics and in many cases derived from particular experimental datasets obtained for certain flow configurations and conditions – have lower reliability (compared to the first-principle conservation laws) and are the weakest links in such a hierarchy. Their presence in the model necessitates extensive model calibration and validation before it can be applied in analyses of realistic operational, transient and accident scenarios in (full-scale) nuclear power plants.

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[1] The case study's technical approach includes the following steps [1]:

i. Review modeling approaches, data bases and simulation capability for crud-related thermal-hydraulics and material-chemistry processes in subcooled flow boiling (SFB) at all relevant scales.
ii. Identify, assess and treat various sources of uncertainty in SFB experimental data related to their application in a PWR crud analysis.
iii. Evaluate sub-cooled flow boiling models and their hierarchical decomposition for modeling/ experimentation/ validation consistency.
iv. Design, initial implementation and application of a framework (including infrastructure) for SFB model calibration and validation.
v. Document the implementation of SFB thermal-hydraulics validation data plan, lessons learned, and recommendations for improvements.
vi. The work is to be performed in close collaboration with THM, MPO, and AMA experts, and with the CASL Data Center initiative.

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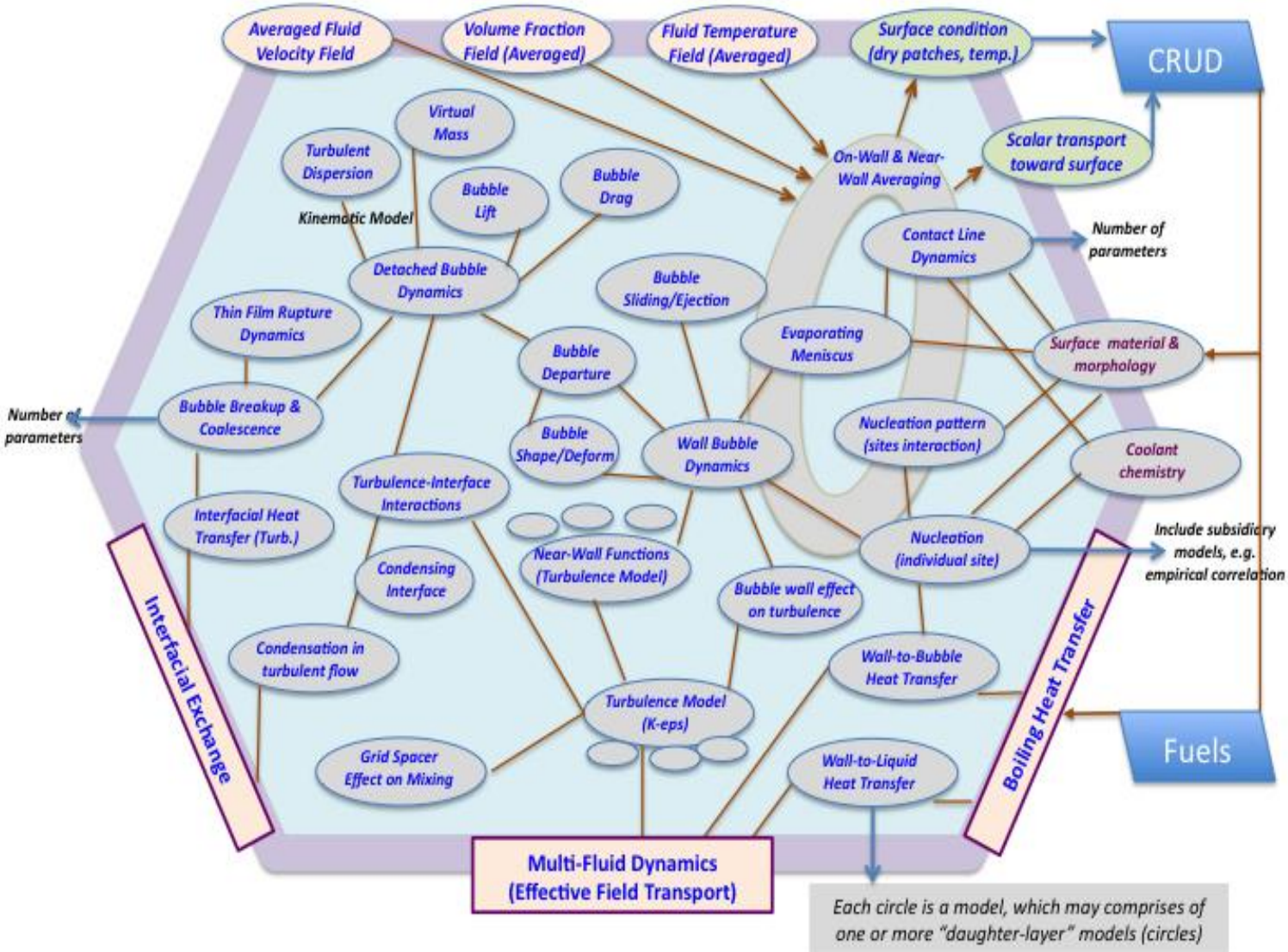

Figure 1.1. Complex interactions of multiple thermal-fluid phenomena at different scales involved in subcooled boiling flows, and their interactions with other physics (fuels/cladding/heat/neutronics; CRUD/corrosion/ system) that govern the CASL CIPS problem; see detail discussion in [**1**].

The phenomenology of subcooled boiling flows has been extensively investigated in the past decades. In parallel to numerical modeling, experiments have been conducted for boiling flows with different flow orientations (vertical and horizontal), conditions (low/high pressure, heat flux, flow rate, etc.) and geometric configurations (pipe, annular, duct, tube bundles). Data have been obtained at both system (integral) level, e.g. radial and axial distribution of temperature, void fraction, interfacial concentration, flow regime, etc., and smaller scales, e.g. bubble size, nucleation site density, bubble growth rate, bubble detachment frequency and diameter, etc. [**4**,**5**,**6**]. In

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the current practice of model calibration/validation, separate effect experimental data are used to derive and calibrate constitutive relationships (via data fitting), whereas integral level data are employed to validate the whole model (by direct comparison of simulation results and data). A physical model calibrated and validated in such ways are capable of providing reasonable predictions only for system configurations and conditions not too different from the configurations and conditions of the experiments which provide the calibration/validation data. Such a constraint significantly reduces the credibility and applicability of the model, especially when in extrapolative predictions.

The above-mentioned practice of computer model calibration and validation is cumbersome and may become intractable when applied to increasingly complex multiphysics system models and codes where no data may be available for calibration/validation of constitutive models of interacting or individual physics. Moreover, it can't take into consideration the effect of data unreliability/uncertainty and/or allows a full use of different types of measurement data in individual and overall model calibration.

Calibration based on data assimilation [**7**] and Bayesian inference [**8**] offers a better framework for complex model calibration and data integration. Such a framework allows to account for data uncertainty and, most importantly, to utilize the whole spectrum of available data in the calibration process. Moreover, the framework offers a mechanism for data grading and characterization, i.e. assessing the values of available and "missing" data of different types in overall model improvement. Until now, there are few reported applications of Bayesian inference in analysis of complex multiphysics models [**9**].

The goal of this study is to develop a more concrete solution for the project implementation strategy shown in *Figure 1.2* where integration of models and data plays a central role. In this study, the multiphysics model of subcooled boiling flows is the application to be considered.

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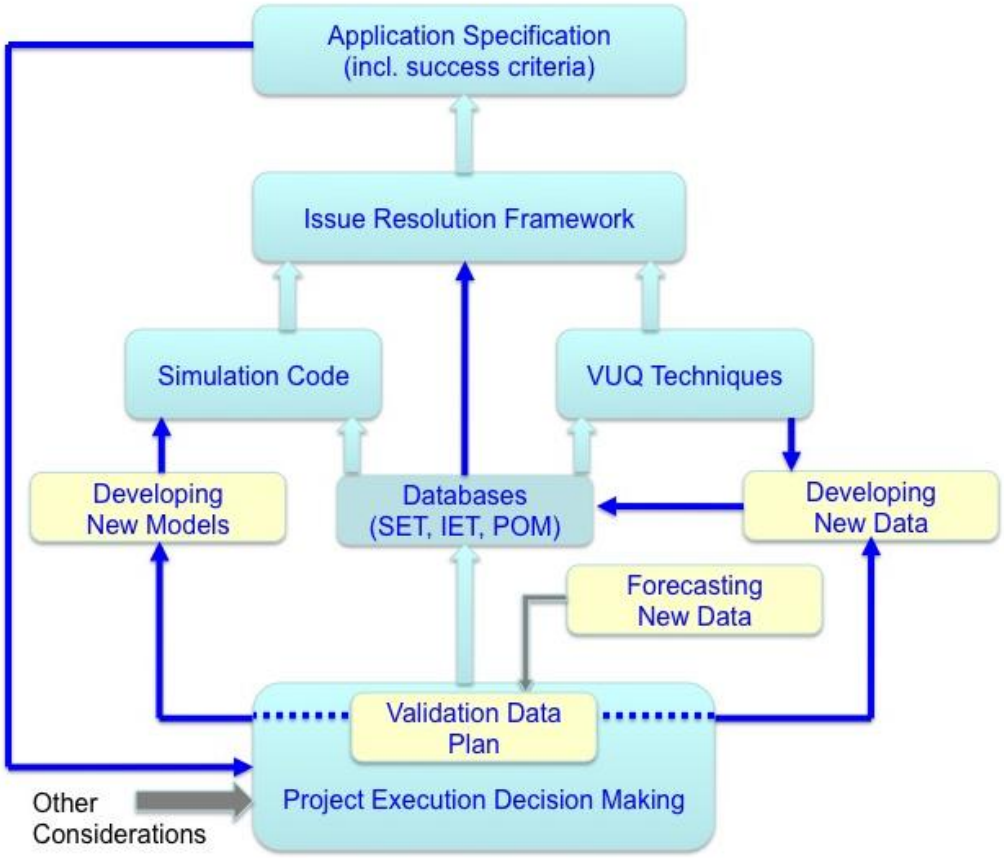

Figure 1.2. The project implementation chart for a specified application (challenge problem) [**1**]. *The key distinction between engineering solution-oriented model calibration/validation effort and predictive capability-oriented (such as a general purpose CFD or CSM code) V&V effort is the latter has a convergence point to compare with (a scientifically accepted truth, e.g. Navier-Stokes equations DNS), while the former is an open-ended enterprise, judged by experts' confidence (in issue being resolved) and ultimately by engineering practice.*

The present development aims to bring together the knowledge of the capability of the modern data-model fusion techniques, the phenomenology of subcooled boiling flows, the relevant experimental studies/data and the current modeling practices applicable to such a multiphysics problem. Extension of this example study to the CASL CIPS challenge problem is discussed.

2. SUBCOOLED BOILING FLOW MODELING AND EXPERIMENTAL STUDIES

Subcooled boiling flows involve a number of interacting physics (*Figure 2.1.*) which usually require different approaches to modeling. Whereas the heat-mass transfers by flows can be represented using mathematically rigorous ensemble-averaged conservation laws-based models, a range of smaller (micro-/meso-) scale physics, e.g. vapor-fluid and near-wall thermal hydrodynamic interactions, are described by empirical/semi-empirical constitutive models which are normally derived from specific datasets and for certain ranges of conditions (flow configuration, pressure, temperature, wall heat flux, etc.).The conservation laws-based models are more credible and universal than the constitutive models, but they are also responsible for model form inadequacy/biases which may lead to consistently inaccurate predictions. The constitutive models being derived from experimental data obtained under certain conditions have a scaling problem and their tuning parameters are required to be calibrated when the models are applied to different problems with different conditions.

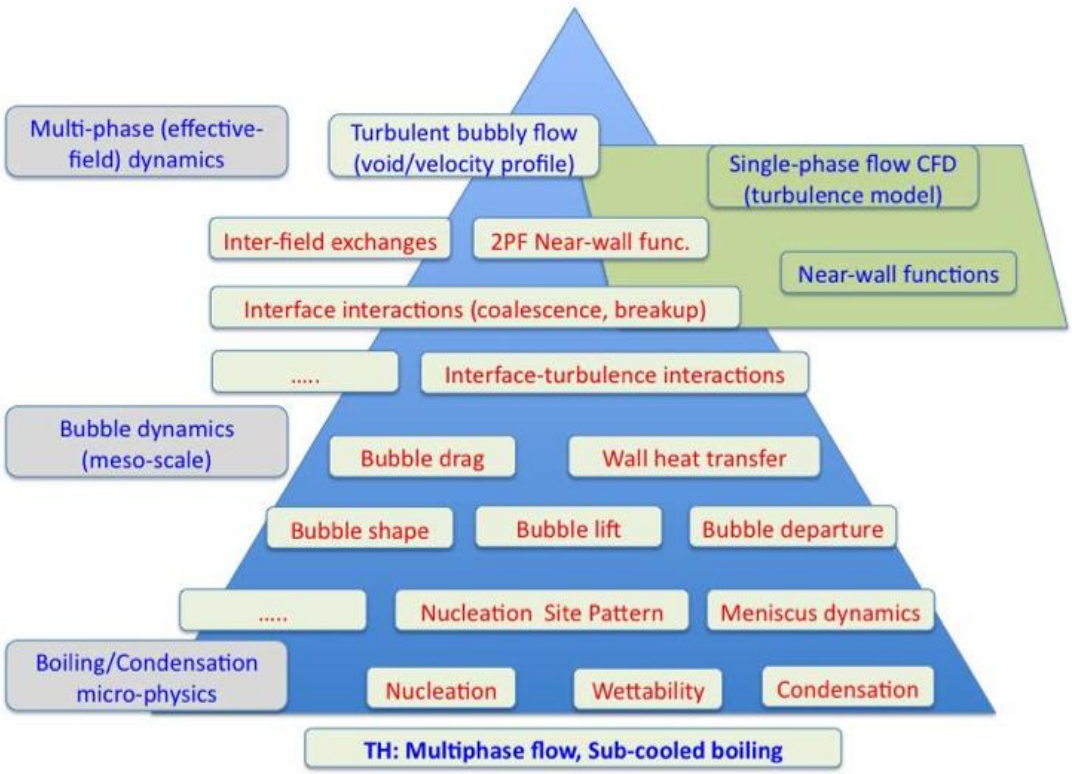

Figure 2.1. The pyramid of the subcooled boiling flow phenomenology [**1**].

2.1. Modeling approach

The most significant characteristic of, and critical requirement for, an advanced model for subcooled flow boiling subject to model calibration and validation is the use of PDE-based conservation laws (spatio-temporal balance equations) and constitutive relations (local non-equilibrium interactions). This can be achieved in a one-dimensional two-phase flow model known as drift-flux. The model provides a flexible physics-based mathematical framework for describing both thermal and mechanical non-equilibrium, and mass transfer between fields (fluids).

Ultimately, a computational multi-phase fluid dynamics (CMFD) may be used for the CIPS challenge problem. In fact, such a model and associated simulation capability are being developed in the CASL THM Focus Area's flagship product Hydra-TH code. The choice of modeling approach in the case study is, therefore, made with an eye on potential extension of the effort to Hydra-TH effort (as detailed in section 3.4 below). More importantly, the model choice is made such that it captures potential features in the CMFD, while amenable to an immediate implementation (without having to wait till Hydra-TH mature).

Conservation laws-based drift-flux two-phase flow model

The simplified one-dimensional (1D) drift-flux model is used in the present case study for simulation of heat-mass transports by subcooled boiling flows. This model can be derived from the two-fluid 6-equation model with the relative velocity between phases defined analytically. As a result, the total number of equations reduces by one and the resulted equation system allegedly becomes more well-posed and easier to be solved.

As noted in [**3**], the drift-flux model is acceptable when the dynamics of two phases are closely coupled. In many engineering systems, the large dimensionality of the systems may allow sufficient interaction times and, consequently, the two-phase flow phenomenon can be appropriately described by a drift-flux model. However, its application to the problems involving high-speed wave propagations, choking phenomena and high-frequency instabilities may be questionable [**3**].

Mixture mass conservation equation:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial}{\partial x}\ \rho_m u_m = 0$$

Fluid mass conservation equation:

$$\frac{\partial \alpha_f \rho_f}{\partial t} + \frac{\partial}{\partial x}\ \alpha_f \rho_f u_f = \Gamma_f$$

Mixture momentum equation:

$$\frac{\partial \rho_m u_m}{\partial t} + \frac{\partial}{\partial x}\left(\rho_m u_m^2\right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\tau_{xx,m} + \tau_{xx,m}^{\mathrm{T}}\right) - \rho_m g_x - \frac{f_m}{2D}\rho_m u_m \left|u_m\right| - \frac{\partial}{\partial x}\left[\frac{\alpha_g \rho_g \rho_f}{\alpha_f \rho_m} V_{gj}^2\right]$$

Fluid energy equation:

$$\frac{\partial \alpha_f E_f}{\partial t} + \frac{\partial}{\partial x}\left[\alpha_f u_f \left(E_f + p - \tau_{xx,f}\right)\right] = \frac{\partial}{\partial x}\left[\alpha_f \left(q_f + q_f^{\mathrm{T}}\right)\right] + \alpha_f \rho_f g_x u_f + Q_{w,f} + Q_{fI}$$

Relations between mixture and phase properties are defined as:

$$\alpha_g + \alpha_f = 1,$$

$$\rho_m = \alpha_g \rho_g + \alpha_f \rho_f ,$$

$$\rho_m u_m = \alpha_g \rho_g u_g + \alpha_f \rho_f u_f ,$$

$$\rho_m i_m = \alpha_g \rho_g i_g + \alpha_f \rho_f i_f .$$

The drift velocity of the gas phase is defined as:

$$V_{gj} = u_g - j = u_g - (\alpha_g u_g + \alpha_f u_f),$$

where j is the volumetric flux given by

$$j = \alpha_g u_g + \alpha_f u_f ,$$

and the relationships between the phase and drift velocities are defined as follows:

$$u_g = u_m + \frac{\rho_f}{\rho_m} V_{gj},$$

$$u_f = u_m - \frac{\alpha_g}{\alpha_f}\frac{\rho_g}{\rho_m} V_{gj}.$$

Constitutive models and scaling issue

Many complex physics of sub-cooled boiling flow thermal hydraulics (see §4.1.2 in [**1**]) at the micro-/meso-scopic scales are parameterized and described with use of simplified empirical/semi-empirical constitutive models. A list of the major constitutive models used in the present subcooled boiling flow model is given in the following table:

Model description	Reference	Comments
Drift velocity	[**10**]	Flow regime dependent
Mixture-wall friction factor	[**10**]	Flow regime dependent
Wall boiling – heat flux partitioning	[**11**] [**12**]	
Wall boiling - nucleation density	[**6**] [**13**] [**14**]	Nucleation boiling mode
Wall boiling - bubble detachment frequency	[**6**] [**15**]	Nucleation boiling mode
Wall boiling- bubble detachment size	[**6**] [**16**]	Nucleation boiling mode
Bulk flow condensation	[**6**] [**17**] [**18**]	
Flow regime transition model	[**3**] [**6**]	

The flow transition model is based on empirically derived flow regime maps which correlate the factors such as the local void fraction or quality, flow direction (upward, downward, horizontal), heat flux, temperature, etc. in determination of the local configuration of vapor and liquid [**6**]. Since many other constitutive models are flow regime-dependent (see above table), invalidity/uncertainty in determination of local flow regime contributes greatly to the incorrectness and uncertainty of overall model predictions.

Instead of defining wall evaporation in terms of meso-scale models describing, e.g., nucleation site density, bubble detachment frequency and radius [**16**,**13**,**15**], wall evaporation can also be calculated direction from the model of wall energy split, i.e. portions of heat flux going to fluid heating and to fluid evaporation [**12**].

It is constructive to note that most boiling closure laws described above have been empirically or semi-empirically derived using experimental data obtained at the laboratorial conditions which are far different from the LWR plant conditions (i.e. low pressure, low heat flux, simple flow geometry, etc.). In many experiments, working fluids have been refrigerants [**19**] which have thermodynamic properties much different from water. Consequently, the scaling issue may arise which necessitates the examination and quantification

of uncertainty related to the use of closure models derived/calibrated based on those experimental data.

The above scaling issue can be implicated from the dependencies of relevant physics on factors such as pressure, temperature, heat flux, etc. For instance, increase of pressure will change the thermodynamic properties of fluid and vapor, i.e. reduce the vapor-fluid density ratio, elevate boiling temperature, etc., and leads to the alterations of wall boiling and flow heat transfer factors as follows:

Wall boiling:

- Decrease of nucleation site density [**14**];
- Decrease of bubble growth rate [**20**,**21**];
- Decrease of bubble detachment frequency and diameter [**21**,**22**];
- Change of CHF threshold [**23**];

Heat transfer by flows:

- Smaller relative vapor-fluid density which reduces buoyancy force and relative velocity between phases (drift velocity);
- Smaller bubble size which reduces the bubble Reynolds number and increases the drag force;
- Stronger effect of bubble condensation in bulk flow;
- Change of forced convection heat transfer.

In overall, pressure increase leads to increase in the boiling heat transfer coefficient (*Figure 2.2*) and change of the CHF threshold (*Figure 2.3*).

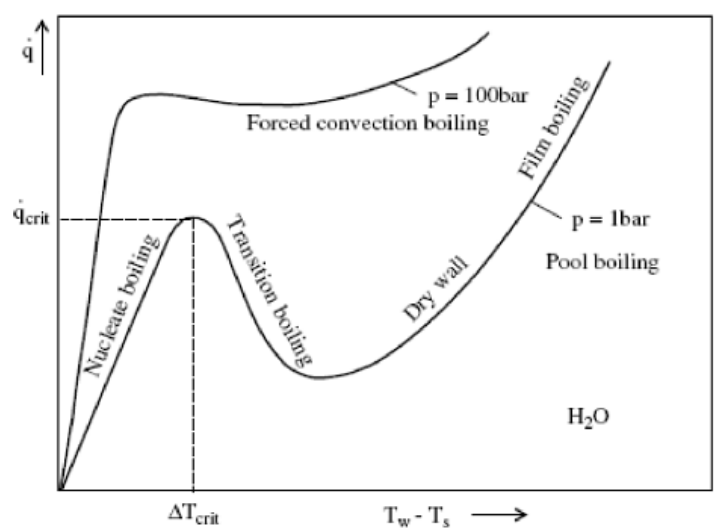

Figure 2.2.Change of boiling curve with pressure [**24**].

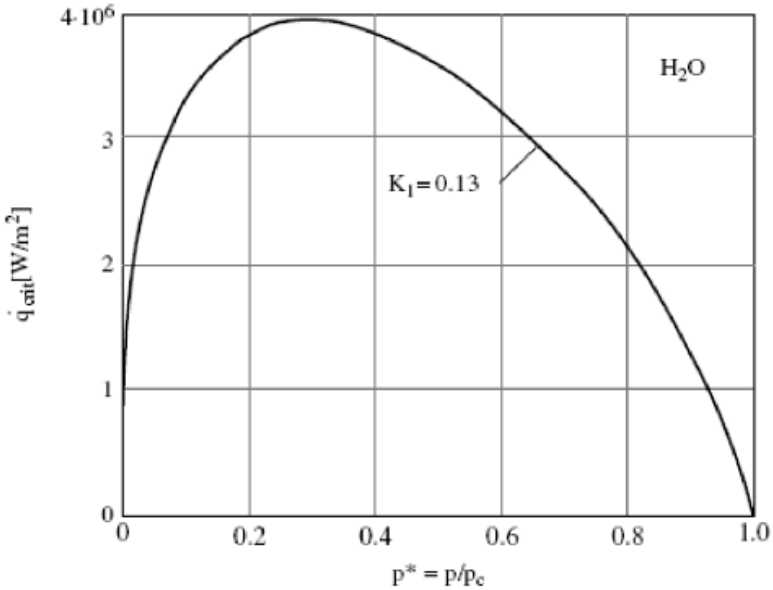

Figure 2.3. Variation of CHF with pressure in pool boiling [**24**].

2.2. Experimental studies and data

For the considered subcooled boiling flows which involve a range of physics occurring at different scales (*Figure 2.1*), experimental studies can be classified into Separate-Effect Tests (SETs), Multiple-Effect Tests (METs) and Integral-Effect Tests (IETs). IETs have been conducted to obtain data at the large-scale level regarding, for instance, void fraction/temperature/velocity distributions, pressure drop and inlet/outlet flow rate, etc. [**25**]. With the advance of modern experimental methods, measurements of small-scale phenomena such as bubble growth/departure dynamics, wall nucleation, and bubble-flow interactions become feasible which provide data to *derive* the closure laws used in boiling flow modeling (see reviews in [**1**] and [**26**]). Those METs/SETs/small-scale IETs however have been conducted mainly under laboratorial conditions which are far from the realistic plant conditions (i.e. low pressure, low and uniform wall heat flux, simple flow geometry, etc.). Consequently, the scaling issue may arise for the computer models which employ the closure laws derived from those experimental data.

The practice of using SET data for derivation/validation of closure models and IET data for validation of overall models fits into the so-called "traditional" concept of calibration/validation of multiphysics models (illustrated in *Figure 2.5*).

In the so-called "total data assimilation" approach proposed in [**1**], the whole spectrum of available data provided by IETs, METs, SETs, etc., is going to be used in the calibration/validation process and, in particular, includes data (see *Figure 2.4*):

From IET measurements:

- Void temporal and spatial (axial and radial) distributions [**25**]
- (Axial) interfacial area distribution [**27**,**28**]

From SET measurements: (mostly under atmospheric pressure) [**16**,**13**,**15**]

- nucleation site density;
- bubble growth rate;
- bubble detachment frequency and diameter;
- bubble Sauter diameter.

Those data are highly heterogeneous, being very different in their origin, dimensionality, uncertainty, reliability, scalability, etc., which poses a significant challenge to the data assimilation/integration method. Specifically, IET data on subcooled boiling flows are often multi-dimensional (e.g. 1D/2D void fraction/temperature distributions) and featuring the time variations of flow characteristics. The model calibration method therefore should be able to handle such dynamic and multi-dimensional data.

In addition to the "true" experimental measurements described above, Direct Numerical Simulation (DNS) models, which rely mostly on first-principle physical laws and inherently possess high predictive capability, can also be used to generate data needed in the calibration and validation of less accurate models. The DNS study presented in [**16**], for instance, provides valuable information about of bubble dynamics which can be used in calibration/validation of the subcooled boiling flow model proposed in this work. DNSs however are very computationally intensive/expensive. Moreover, like all other modeling, DNSs may incur significant uncertainty in their predictions due to inadequate/biased model form.

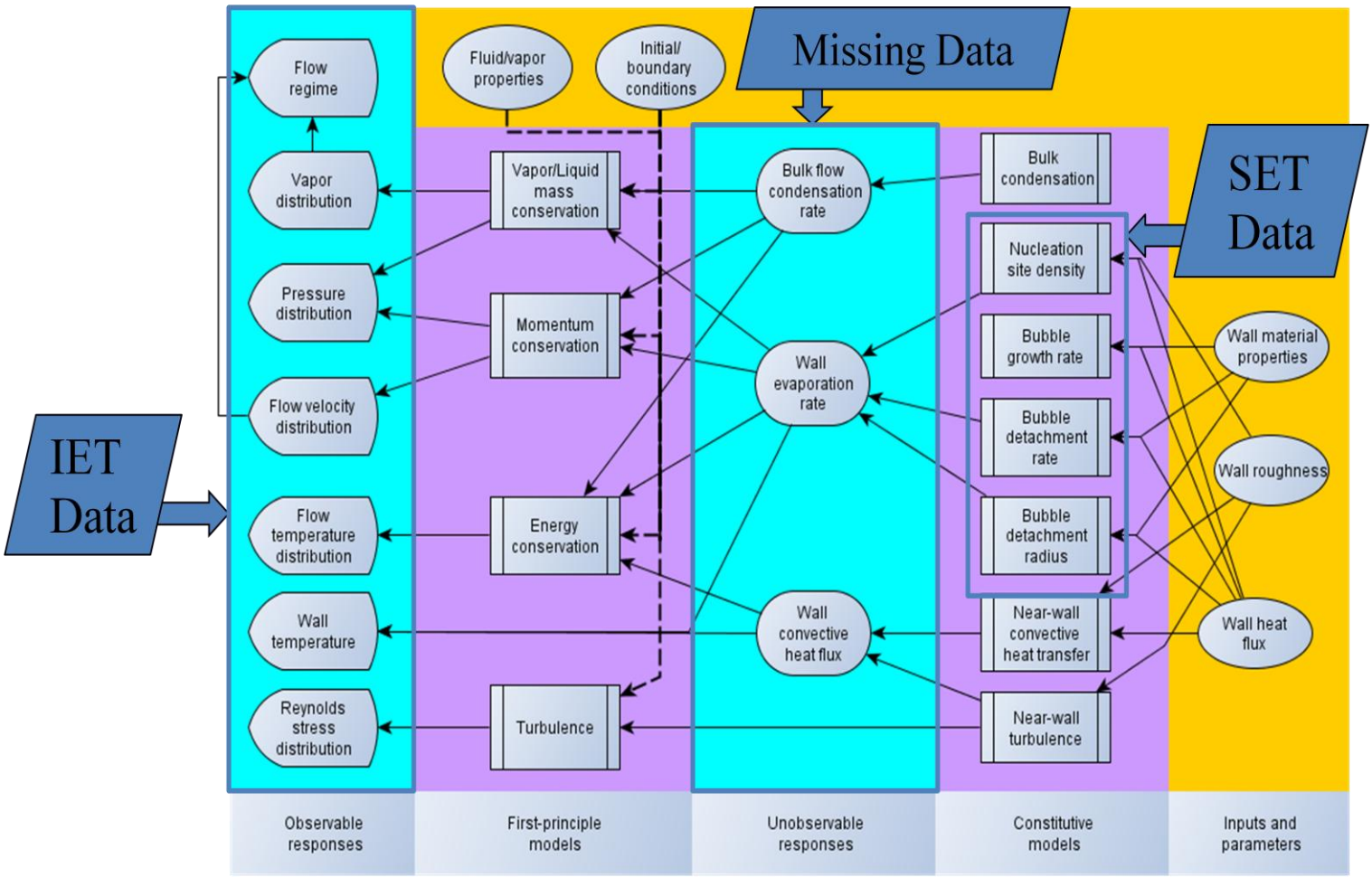

Figure 2.4.Interrelationship of conservation-laws based and constitutive models and data available for calibration/validation of the proposed subcooled boiling flow model.

A strategy to deal with data heterogeneity involves data validation and data homogenization. As described in [**29**], data validation may include:

- Faulty data detection: identifies doubtful or missing data;
- Data correction: modifies doubtful data or estimates missing data – interpolation, data smoothing, data mining, data reconciliation, etc.;
- Data quality quantification: UQ, scalability assessment, etc.

Data homogenization is required to remove the factors which cause data variations/biases which are not related to the physics of the subcooled boiling phenomenon. These factors include, for instance, instrumental inaccuracies, variations in data acquisition and processing methods/procedures, changes in experimental settings and conditions, etc. If DNS is used for data generation, grid resolution/dependency would be the factor which needs to be addressed.

More detailed discussion about data strategy needed to realize the total data assimilation concept can be found in [**1**].

Notably, data depending on their relevance, scalability and uncertainty can be graded as outlined in [**1**]. A Reactor Prototypicality Parameter (RPP) and an Experimental Measurement Uncertainty (EMU) have been introduced (see [**1**]) which can be used as a means to "harmonize (influence of) different experiments, different types and quality of evidence" [**1**].

A weight factor can be then determined on the basis of RPP and EMU and used in the Bayesian model analysis as discussed below. Given the objective of the capability for SFB simulation being prediction of CIPS phenomena in a PWR, system pressure itself p (in dimensionless form of $[p / p_{cr}]$ where p_{cr} is the coolant (water) critical pressure, can be considered as the scaling parameter. This choice reflects a vast knowledge base on the effect of system pressure on two-phase flow phenomena. The effect can be traced to pressure dependence of coolant's thermo-physical and thermodynamic properties, most notably liquid and vapor density, and their density ratio.

The table below (from [**1**]) lists references of relevant experiments on mesoscale mechanisms involved in SFB. It was noted [**1**] that – with one exception, the available experiments were poorly scalable to PWR-CIPS conditions, as characterized by their low scaling grade (see [**1**], Table 3.1 for definition of scaling grades). The tests conducted also had limited diagnostics, without resolving near-wall structures and detail dynamics.

Authors (year)	Phenomena investigated	Scaling
Bertel et al (2001)	Interfacial area in SFB	1 (1 atm)
Garnier et al (2001)	Local measurements	1 (R12)
Kang et al (2002)	Vapor phase measurements SFB	1 (R113)
Warrier et al (2002)	Interfacial heat transfer	1 (low P)
Roy et al (1992, 1997)	Turbulence, void fraction	1 (R133)
Chen et al (2003)	Bubble coalescence	1 (1 atm)
Yeoh et al (2004)	Bubble departure, bubbly flow	1 (1-2 atm)

Okawa et al (2005a,b)	Bubble slide	1 (1 atm)
Mauruset al (2006)	Bubble; boundary layer	1 (horiz.)
Bang et al (2004)	Visual bubble	1 (R134a)
Situ et al (2004a,b)	Bubble dynamics	1 (1 atm)
Unal (1976)	Bubble growth	3 (full P)
Chang et al (2002)	Wall bubble	1 (R134a)
Basu et al (2005)	Wall heat partitioning in SFB	1 (low P)
Basu et al (2002)	Boiling onset, nucleation site density	1 (low P)
Hibiki& Ishii (2003)	Nucleation site	1 (1 am)
Theofanous et al (2001)	Nucleation on different surfaces	1 (1 atm, PB)
Dinh et al (2004)	Nucleation	1 (1 atm, PB)

* PB – pool boiling

More review on the diversity of experimental data relevant to subcooled boiling flows is provided in Appendix C.

2.3. Traditional model calibration and validation

As mentioned earlier, traditional approach of data-model integration involves calibrations of constitutive sub-models using SET data and whole model validation using IET data (see *Figure 2.5*). The shortcomings of such an approach include, but not limited to:

- Not accounting for data uncertainty;
- Inability to quantify prediction uncertainty;
- Ambiguity in determination of the reasons of "wrong" model predictions;
- Difficulty in using IET data for submodel calibration/validation;
- Not allowing incremental model update based on newly available data.

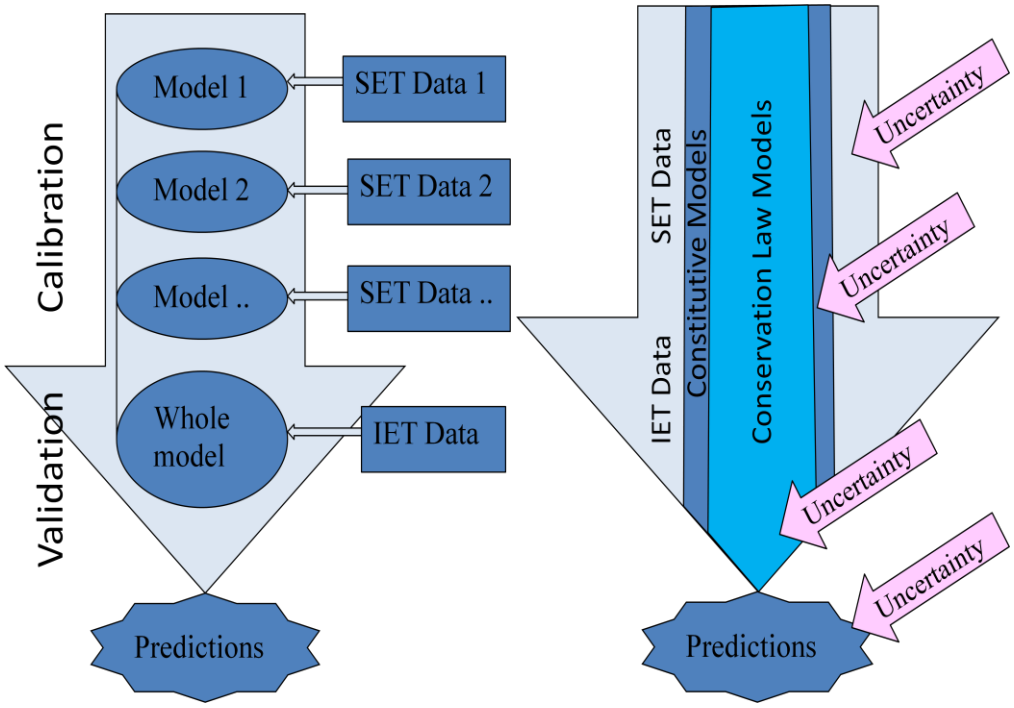

Figure 2.5. "Traditional" approach to multiphysics model calibration & validation (left) versus "total data assimilation" approach (right).

The so-called "naïve" validation approach has been employed until now where the validity of a computer model is judged based on the comparability of model predictions and experimental data (see example in*Figure 2.6*). However, values of such ad-hoc validations are hard to be quantified and successful validations do not necessarily warrant equally successful application of the model to real plant simulations.

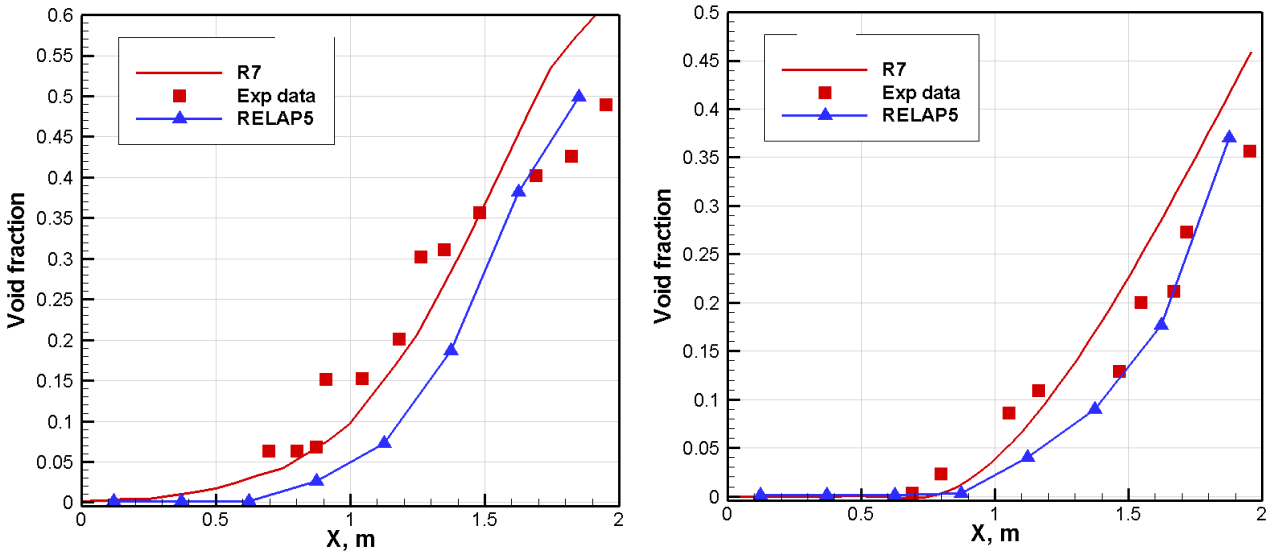

Figure 2.6. "Traditional" validation of the subcooled boiling flow model proposed in this study (Red line – this model's predictions; Experimental data from [**25**]*; RELAP5 predictions from* [**30**] *– Conditions: flow rate – 890 kg/s; heat flux – 790 kW/m^2; pipe diameter – 24 mm; subcooling – 49.2^{o}C (left) and 52.4^{o}C (right); pressure– 1.5 MPa (left) and 4.5 MPa (right)).*

Validation of the RELAP5/MOD3.2 subcooled boiling model was based mainly on high pressure data [**31**]. Modification of that model was suggested [**32**,**33**] and MOD3.3 had improved capability in predicting low-pressure cases and handling non-uniform heat flux profiles.

In [**34**], RELAP5 and COBRA-EN were shown to be able to provide relatively good predictions of void fraction axial distribution for pressure down to 1.5 MPa. Significant discrepancy between model predictions of wall temperature and experimental data was however observed even at the relatively high pressure of 4.5 MPa.

TRACE was found to over-predict evaporation in the OECD/NRC PSBT Benchmark simulations.

3. BAYESIAN FRAMEWORK FOR CALIBRATION AND VALIDATION OF SUBCOOLED BOILING FLOW MODELS

As can be seen from the model hierarchy shown in *Figure 2.1*, the subcooled boiling flow model is based on both conservation laws-based models and empirical/semi-empirical closure models. The validity of the model as a whole is therefore constrained by the validities of both the conservation laws and the closure laws models. With the conservation laws represented by a system of partial differential equations (PDEs), model calibration can be thought of as a PDE-constrained optimization process with the PDEs determining the "shape" of the response surface, whereas calibration helping to "move" that surface closer to the data.

The conservation laws-based models are relatively more credible and universal than the constitutive (closure) models and their validity can be scrutinized in a model comparison test. On the other hands, closure models normally have many parameters which require calibration. Compared to single-physics model calibration, the calibration of multiphysics models is more challenging because it may involve finding the optimized *correlations* or *dependencies* of model parameters (e.g. pressure/temperature-dependent nucleation site density) or *spatial distributions* of them (e.g. spatially varying thermal conductivity) rather than their single values [**35**].

For the subcooled boiling flow model described above, the calibration process entails both the assessment of the model form inadequacy/bias and the optimization of the constitutive model parameters. The optimization or calibration of the constitutive model parameters is constrained by the validity/adequacy of the conservation laws-based models, i.e. (i) if the conservation laws-based model is heavily inadequate, parameter calibration may become impossible, and (ii) valid and robust conservation laws-based models limit the impact of uncertainty/errors/ biases of poorly calibrated model parameters.

The involvement of multiple parallel (turbulence, flow dynamics) and nested (flow dynamics, wall evaporation) models in subcooled boiling flow simulations poses significant challenge to the VUQ framework. Without considering the complex structure of multiple coupled models, the full model of subcooled boiling flows can be thought of as a black box with multiple inputs and outputs and the calibration process is carried out using data at the system level, i.e. axial distributions of vapor fraction, fluid temperature, etc. Such an approach however would not allow to use data obtained at other scales, such as measurements of nucleation site density, bubble detachment

radius/frequency, etc. in the calibration process. Moreover, the issue of non-identifiability may also arise.

As illustrated in *Figure 2.5*, a traditional "hierarchical" calibration of multiphysics model may also applied to our problem, which consists of two steps [**36**]: (i) parameters of the sub-models are first calibrated independently from each other and then (ii) other parameters common for the whole model are subsequently calibrated. Such a calibration approach is only feasible if measurement data are available at every sub-/full-model levels. When data are less abundant and missing at some levels, the "top-down" calibration approach described in [**36**] is more appropriate, which is similar to the simple single-model calibration delineated previously.

The model calibration approach proposed in this work is based on the expression of inter-dependencies between the involved models, parameters and inputs using Bayesian influence networks as shown in *Figure 2.7* and *Figure 2.8.*It is noteworthy that Bayesian networks are directed and acyclic graphs (DAGs) and, consequently, two-way couplings between the nodes can't be described.

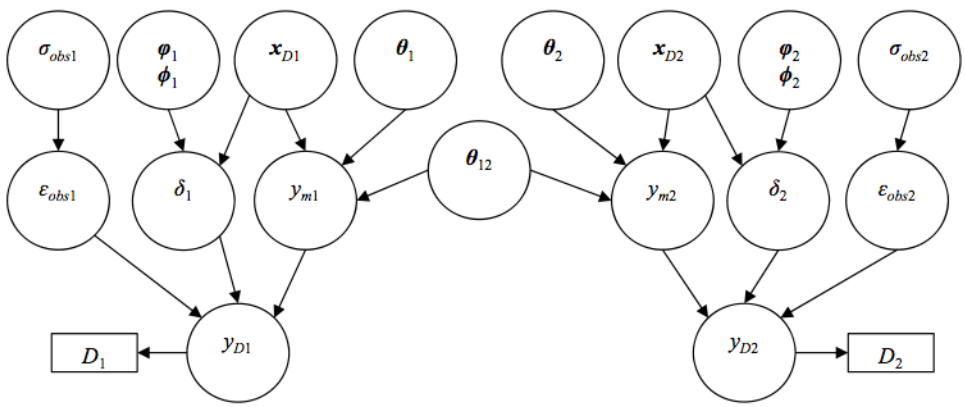

Figure 2.7. Example of a Bayesian influence network representing the relationships between two parallel physics sharing a common model parameter [**9**].

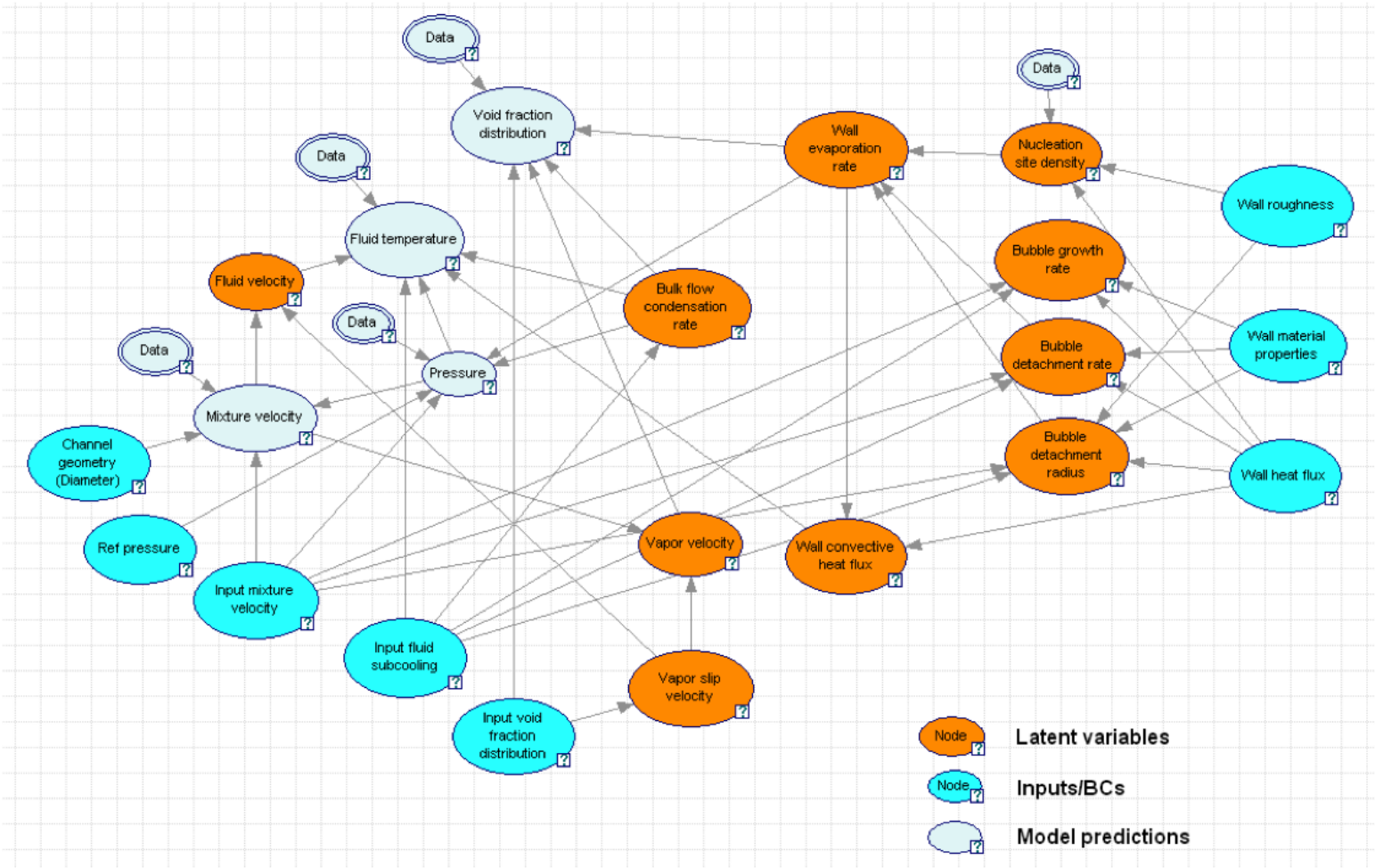

Figure 2.8. A simplified Bayesian network representing the nested physics of subcooled boiling flows. The Bayesian networks only link inputs and model parameters to the responses and the models are therefore hidden.

Bayesian inference is best equipped to incorporate/assimilate heterogeneous data with models for model and prediction improvement, since it can:

- account for uncertainty in observed data or take into consideration the "weight" or "values" of data given their uncertainty;
- quantify prediction uncertainty;
- exploit the results of past validations/calibrations (in construction of more informative priors for analysis), i.e. sequential model updating;
- handle "missing" data and allow the validation of unobserved quantity predictions;
- handle multiple (multiphysics) coupled models using Bayesian influence networks.

3.1. Overview of Bayesian data assimilation and model calibration

Bayesian calibration is based on the Bayes theorem, which computes a posterior probabilistic distribution of unknowns $\boldsymbol{\theta}$ (i.e. model parameters in our model calibration) from observed data $\boldsymbol{D}$ as follows:

$$p(\boldsymbol{\theta}|\boldsymbol{D}) \propto \mathcal{L}(\boldsymbol{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

where $p(\boldsymbol{\theta})$ is a prior probabilistic distribution of $\boldsymbol{\theta}$ and $\mathcal{L}(\boldsymbol{D}|\boldsymbol{\theta})$ is the "likelihood" of observations $\boldsymbol{D}$ given specific values of $\boldsymbol{\theta}$.

In Bayesian model calibration, the relationship between observed data and model predictions $\boldsymbol{M}$ can be expressed as [**8**,**37**]

$$\boldsymbol{D} = \boldsymbol{M}(\boldsymbol{x}, \boldsymbol{\theta}) + \delta(\boldsymbol{x}) + \epsilon$$

with $\delta(\boldsymbol{\theta})$ being a model inadequacy/bias function, ϵ indicating the observation error/uncertainty and $\boldsymbol{x}$ denoting the vector of known variable inputs.

Both δ and ϵ can be assumed to be normally distributed with ϵ having a zero mean, i.e. $\delta(\boldsymbol{x}) \sim \mathcal{N}[m_\delta(\boldsymbol{x}), c_\delta(\boldsymbol{x}, \boldsymbol{x}')]$ and $\epsilon \sim \mathcal{N}[0, c_\epsilon(\boldsymbol{x}, \boldsymbol{x}')]$ with m and c being the mean and covariance functions, respectively. A common choice for covariance function has the squared exponential form as follows:

$$c(\boldsymbol{x}, \boldsymbol{x}') = \sigma^2 \exp\left[-\sum_{i=1}^{k} \omega_i (\boldsymbol{x} - \boldsymbol{x}')^2\right].$$

where k is the dimension of $\boldsymbol{x}$ and $\boldsymbol{x}'$, σ is the variance and ω is the roughness parameter.

Given the above assumptions about the distributions of data, observation error, and model inadequacy, the 'likelihood' function is also a normal probability density function defined as

$$\mathcal{L}(\boldsymbol{D}|\boldsymbol{\theta}) \propto \exp\left[-\frac{1}{2}(\boldsymbol{D} - \boldsymbol{M})^T \boldsymbol{V}^{-1} (\boldsymbol{D} - \boldsymbol{M})\right]$$

with $\boldsymbol{V}$ being a matrix which combines the variance and covariance matrices of $\boldsymbol{D}$, $\boldsymbol{M}$, δ and ϵ [**8**].

Calculation of the likelihood function involves forward model simulations to determine $\boldsymbol{M}$ given specific inputs $\boldsymbol{x}$ and $\boldsymbol{\theta}$. When the likelihood function is intractable, approximate Bayesian calibration [**38**] and/or likelihood-free MCMC [**39**] can be applied.

As can be seen in its formulation, the likelihood function is where comparison of model predictions and data occurs and, when there are multiple observed data, a joint likelihood function can be derived which is simply a multiplication of the individual likelihood functions, i.e.

$$\mathcal{L}(\boldsymbol{D}|\boldsymbol{\theta}) = \prod_{i=1}^{n} \mathcal{L}_i(\boldsymbol{D}_i|\boldsymbol{\theta}_i),$$

where $\boldsymbol{D}_i$ and $\boldsymbol{\theta}_i$ being the subsets of the full data space $\boldsymbol{D}$ and parameter space $\boldsymbol{\theta}$, respectively.

In the model calibration that involves *maximum likelihood estimation*, the natural logarithm of the likelihood function is normally used, which is expressed as the sum of individual log-likelihoods:

$$\ln[\mathcal{L}(\boldsymbol{D}|\boldsymbol{\theta})] = \sum_{i=1}^{n} \ln[\mathcal{L}_i(\boldsymbol{D}_i|\boldsymbol{\theta}_i)].$$

As suggested in [**40**], the weighting factor ω_i of dataset $\boldsymbol{D}_i$ calculated based on the relevancy, scalability and uncertainty criteria (see §2.2) can be used to express the *variance* of $\boldsymbol{D}_i$ in terms of a *common variance* determined for all datasets.

When data and models have hierarchical structures, e.g. both IET and SET data are available as shown in *Figure 2.4*, the calibration process becomes more complicated. For the two-level model hierarchy shown in *Figure 3.1* the relationships between responses and parameters are expressed as:

$$\boldsymbol{f} = \boldsymbol{M}(\boldsymbol{g}) + \epsilon$$

$$\boldsymbol{h} = \boldsymbol{N}(\boldsymbol{f}) + \zeta$$

where $\boldsymbol{M}$ and $\boldsymbol{N}$ are the predictions/responses provided by bubble dynamic and two-phase flow models, respectively, $\boldsymbol{f}$ and $\boldsymbol{h}$ are data with measurement errors ϵ and ζ, respectively. The model biases are ignored for simplification.

The likelihood functions are then given by

$$\mathcal{L}(\boldsymbol{h}|\boldsymbol{f},\boldsymbol{g}) \propto \exp\left[-\frac{1}{2}(\boldsymbol{h}-\boldsymbol{N})^T\boldsymbol{P}^{-1}(\boldsymbol{h}-\boldsymbol{N})\right]$$

$$\mathcal{L}(\boldsymbol{f}|\boldsymbol{g}) \propto \exp\left[-\frac{1}{2}(\boldsymbol{f}-\boldsymbol{M})^T\boldsymbol{Q}^{-1}(\boldsymbol{f}-\boldsymbol{M})\right]$$

with $\boldsymbol{P}$ and $\boldsymbol{Q}$ denoting the variance/covariance matrices.

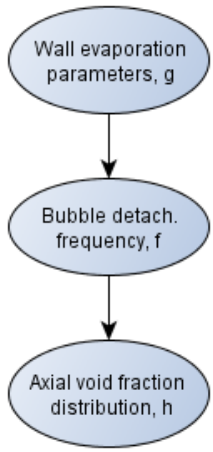

Figure 3.1. Example of two-level model hierarchy.

The posterior distribution of parameters $\boldsymbol{g}$ is then determined from

$$p(\boldsymbol{g}, \boldsymbol{f}|\boldsymbol{h}) \propto \mathcal{L}(\boldsymbol{h}|\boldsymbol{f}, \boldsymbol{g})\mathcal{L}(\boldsymbol{f}|\boldsymbol{g})p(\boldsymbol{g}).$$

Problems related to the application of Bayesian model calibration include [**41**]:

- When model bias is large, calibration may be impossible, as it is impossible to pinpoint what is the reason of discrepancy between model predictions and data – model bias or wrongly specified model parameters;
- Non-identifiability problem for models with multiple calibrating parameters may arise when a similar response can be caused by variations of different parameters. For multi-physics modeling, there is also a danger of calibration of "wrong" models or parameters, e.g. calibrating "wrong" friction model due to incorrect flow regime defined. This issue however can be alleviated when multiple responses are used in the calibration process [**42**]. Better prior information about parameters and/or model discrepancy may also help;
- If computer model is computationally expensive, calculation of likelihood function may become too costly. In this case, faster approximate or surrogate model may need to be constructed to replace the real physics-based model. Gaussian process (GP), polynomial chaos expansion (PC), support vector machine (SVM), Bayesian/artificial neural network [**43**] and Multiple Adaptive Regression Spline (MARS) [**44**] are common techniques used for surrogate model construction;
- Difficulty may also arise on how to assign priors when little or no information about them are available. The principle of maximum entropy may be applied in this case to determine the probabilistic distributions of priors.

Bayesian calibration using the Gaussian processes to approximate $\boldsymbol{M}$ and δ can use the method of maximum likelihood estimation (MLE) to directly calculate parameters. In this case, the estimated parameters do not have probabilistic distributions and their values are assumed to be unchanged during the rest of the Bayesian analysis.

The output of the subcooled boiling two-phase flow model and the data available for model validation are commonly multivariate and multidimensional (varying in time and space) which considerably complicates the application of Gaussian process for model approximation (due to enormous number of training points and big size of the covariance matrix) and the model calibration as a whole. Remedies to this situation can be:

- Dimensionality reduction via principal component analysis (PCT) [**45**,**46**,**47**] or QPIRT [**48**]
- Use of "Greedy algorithm" [**49**] – selectively choosing of candidate training points or training point selection with optimization
- Use of multiple independent Gaussian process surrogates for different subsets of data (different spatial location or time).

Sampling of posterior distributions and integration of high-dimensional functions involved in the Bayesian model calibration are very computationally expensive. In such cases, an efficient statistical tool such as the Markov Chain Monte Carlo (MCMC) method [**50**] is needed. Different implementations of the MCMC algorithm can be found in many Bayesian/statistical software packages as shown in the next section.

3.2. Review of the Bayesian data-assimilation and model analysis software packages

An overview of select software packages available for Bayesian model analysis is given in the following table [**51**].

Software	Data Analysis	Bayesian Data Analysis	Space-Filling DOE	Model Emulation*	Variance-Based Sensitivity Analysis	Bayesian Model Calibration via Kennedy & O'Hagan Methods		Optimization	Uncertainty Analysis
						Single Response	Multiple Responses		
GEMSA			X	X	X				X
GEMCAL						X			
GPMSA			X	X	X	X	X		
DAKOTA			X	X	X			X	X
Isight			X					X	X
Matlab (Optimization Toolbox)								X	
Matlab (Statistics Toolbox)	X		X						X
R (BACCO Package)				X	X	X			
R (Base Package)	X							X	X
R (gptk Package)				X					
R (lhs, DiceDesign, DiceKriging Packages)			X						
R (mlegp Package)				X	X				
R (tgp Package)				X	X				
R (Sensitivity Package)					X				
R (LearnBayes package)		X							
WinBUGS		X							
JMP	X		X	X	X				X
SAS	X	X						X	X
Minitab	X								
SimLab (Matlab/R)					X				X
NESSUS/CENTAUR	X	X	X	X	X			X	X

Classification of the relevant software packages based on their application purpose is as follows:

- General Bayesian inference: OpenBUGS, R/BRUGS, R/jags
- Uncertainty quantification: DAKOTA, GEMSA, R/BACCO, PSUADE
- Gaussian regression: GPML, R/gausspr, Multi GP, GEMSA, GPMSA, DAKOTA
- Sensitivity analysis: GPMSA, DAKOTA, R/BACCO, SamIam
- Bayesian model calibration: GPMSA, (DAKOTA+GPMSA), R/BACCO, PSUADE, GEMCAL, BAT
- Bayesian networks:SamIam, GeNIe, Netica, Analytica, HuginLite
- MCMC: R/mcmc, R/MCMCHybrid, OpenBUGS, R/BRUGS, etc.

- Structural Equation Modeling (SEM): R/OpenMx, SmartPLS, R/sem, SMILE/GeNIe
- Data assimilation: OpenDA

Preliminary testing of the packages highlighted in red has been conducted and, as a result, the Matlab-library GPMSA (and the currently under-development joint DAKOTA/GPMSA package) and C++-library BAT are recommended for the simplified calibration of the proposed subcooled boiling flow model (see more details in the following section §3.3).The more advanced model calibration involving an integration of multi-level data and a coupling of Bayesian network representations of multiphysics models and Bayesian model analysis methods would require an extension of one of the Bayesian network software packages described above, e.g. GeNIe, or a development of a new software tool based on the above open-source libraries/software.

3.3. Total data assimilation in application to the subcooled boiling flow problem

The model-data integration strategy delineated above is currently being implemented and applied to the analysis of the case-study subcooled boiling flow model. The current implementation is based on the simplified models of wall evaporation and bulk flow condensation as described in the Appendices. An interface between DAKOTA [**52**] and this subcooled boiling flow mode has been developed and some DAKOTA runs were conducted to study the parameter sensitivity. The results shown in *Figures 3.2* indicate relatively high sensitivity of the void fraction prediction to the change of the bulk condensation parameter. The variation of the boiling heat transfer parameter however has a relatively smaller effect on the axial void fraction prediction shown in *Figures 3.3*.

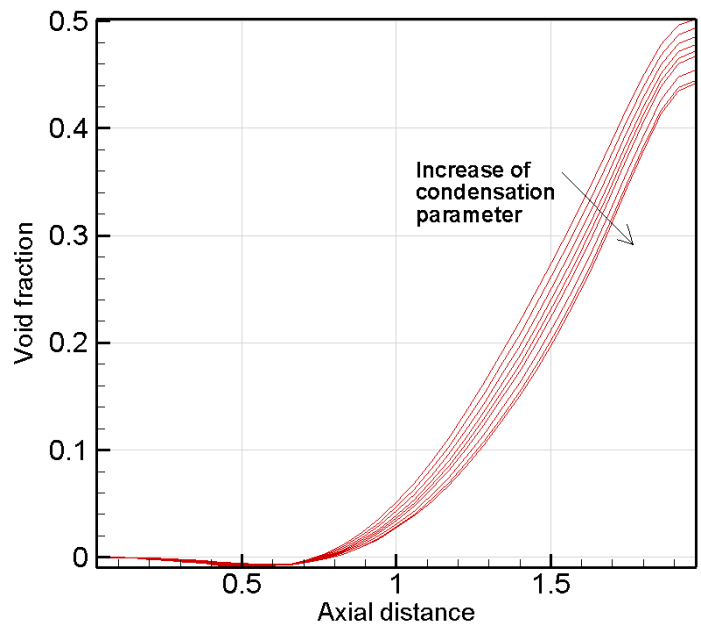

Figure 3.2. Effect of the variation of the bulk condensation parameter C_{cond} in the range (0.08-0.24)(standard value is 0.16).

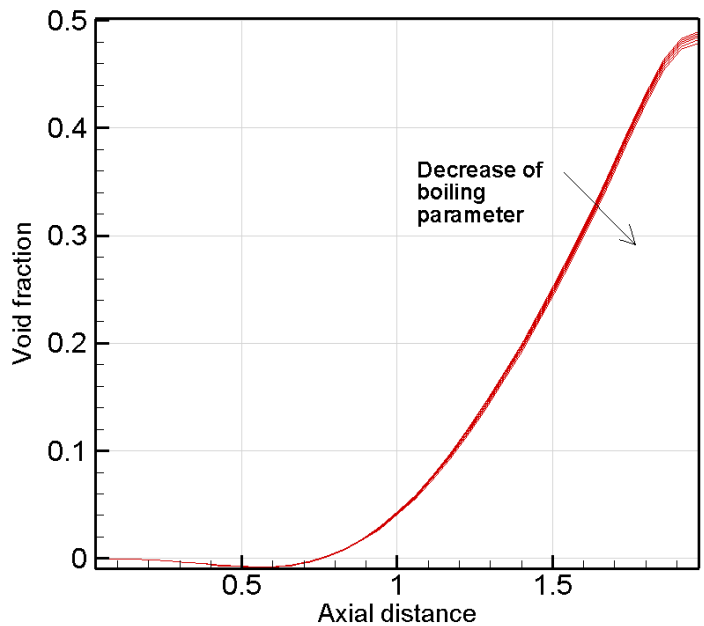

Figure 3.3. Effect of the variation of the boiling heat transfer parameter $h_{NB,0}$ in the range (4600-6600)(standard value is 5600 W/(m^2 K)).

For standard (non-Bayesian) model calibration, the non-linear least squares capabilities of DAKOTA can be employed.

The computational results generated in the DAKOTA parameter study are used to construct a Gaussian process (GP) emulator of the subcooled boiling flow model following the approach proposed by Higdon et al. [**45**,**47**].

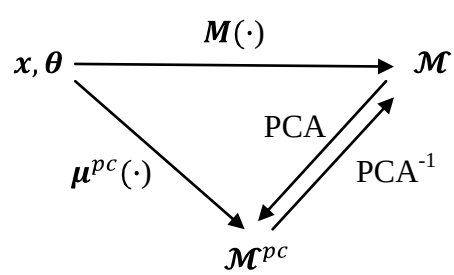

Figure 3.4. Application of principal component analysis (PCA) in GP emulator construction [**47**].

Given the high dimensionality of the outputs, the principal component analysis (PCA) technique [**53**] is used here for dimensionality reduction. As shown in *Figure 3.4*, an alternative path to model predictions is constructed using a GP-based emulator $\boldsymbol{\mu}^{pc}$ and a PCA mapping, thus avoiding costly $\boldsymbol{M}(\cdot)$ simulations.

The matrix of 25 (or 5×5, 5 per parameter) one-dimensional void-fraction distributions obtained in the parameter study described above is used in the principal component analysis (each row of this matrix contains the results of one simulation). The matrix is first standardized, so that the mean of each column is

zero and the variance of each column is one. The singular value decomposition (SVD) is then applied to the standardized simulation result matrix $\mathcal{M}'$(of 25×35 dimension) as follows:

$$\mathcal{M}' = \boldsymbol{U}\,\Sigma\,\boldsymbol{V}^*$$

where $\boldsymbol{U}$ is a 25×25 unitary matrix containing the left singular vectors, $\boldsymbol{V}$ ($\boldsymbol{V}^*$ - the complex conjugate transpose of $\boldsymbol{V}$) is a 35×35 unitary matrix containing the right singular vectors, and Σ is a 25×35 rectangular diagonal matrix with non-negative real principal values (or eigenvalues) on the diagonal.

The eigenvalues on the matrix Σ diagonal indicate that up to 99.2% of variance can be "explained" or represented by the first two principal components. Consequently, the principal subspace $\mathcal{M}^{pc}$ is constructed on the basis of two orthogonal vectors given by the first two columns of $\boldsymbol{V}$ [**47**] as follows

$$\mathcal{M}^{pc} = \mathcal{M}'\,\boldsymbol{V_1}$$

where $\boldsymbol{V_1}$ is the mapping matrix formed from the first two column of $\boldsymbol{V}$.

Following [**47**], the PC emulator μ^{pc} is constructed, which, in this case, comprises two independent Gaussian processes – one for each dimension of the principal subspace (i.e. $\mu^{pc} = (\mu_1^{pc}, \mu_2^{pc})$).

For Bayesian model calibration, either BAT – Bayesian Analysis Toolkit [**54**] – or GPMSA [**45**] software package can be used. The Bayesian calibration of the subcooled boiling flow model will primarily be based on the steady-state axial void fraction distribution data reported in [**25**] with information about measurement errors artificially introduced. To overcome the non-identifiability issue, other data such as fluid temperature axial distribution, mixture axial velocity or void fraction radial distribution may also be used in the so-called "multiple response" model calibration [**42**]. It is noted that, in the preliminary case study, model bias is not accounted for and calibration in such a way does not allow the use of data obtained at other (smaller-scale) levels.

The above whole (single)-model Bayesian calibration is then extended to include model bias which, as in a normal practice, is modeled using a Gaussian process.

More advanced implementation of the proposed data integration strategy in the future will rely on a Bayesian influence network to represent the connections between detailed models of wall evaporation (based on the constitutive models describing, for instance, nucleation site density, bubble growth/detachment dynamics, etc.) and related parameters (*Figure 2.8*). As shown in [**9**], even calibration of two single-level models joint by a simple Bayesian network entails complex information exchange on the network and, depending on the direction of the information flow, different calibration strategies can be adopted. A strategy for dimensionality reduction must and will also be developed to reduce the computational cost.

3.4. Implications to the CASL validation strategy and data plan

This work presents a first step forward to implement the CASL "application-oriented total data assimilation" strategy for multiphysics model calibration and validation which was established in [**1**]. The Bayesian model calibration and data assimilation framework proposed in this work has the potentials to:

a. study the propagation of uncertainty information on the networks of coupled multiple physical models based on both conservation laws and simplified empirical/semi-empirical representations of physics;
b. integrate data of different origins, types, scales and qualities in the process of model optimization and validation;
c. permit sequential model calibration/validation, i.e. incremental model improvement.

The goal of "consistent integrated treatment of uncertainty across physics and scales" stated in the CASL CIPS validation data plan [**1**] can be achieved with (a) which is based on the use of Bayesian influence networks to facilitate the exchange of uncertainty information between the physical models.

Capability (b) enables the realization of the "Data Realism" concept [**1**] which is a cornerstone feature of the CASL CIPS validation data plan. Recognizing the heterogeneity nature of available validation data as well as the scarcity/missing of data for certain scales and physics, the "Data Realism" concept calls for a flexible model calibration/validation approach which would maximize the use of past, current and future data of different origins, types, qualities, scales, and have the capability to deal with data shortage/missing.

As stated in [**1**], given the never-perfect states (availability, quality, etc.) of data and codes, model calibration/validation should be considered as a continuing process which assimilates newly available data to incrementally update model/code and reduce uncertainty both in model form and parameters. The capability described in (c) therefore permits this strategy to be employed.

The proposed model calibration/validation framework with its capability in assimilation of data uncertainty and "weights/grades" in model analysis would be able to support the "VUQ-guided data collection, characterization & qualification" process and the establishment of the CASL Data Center (CDC) delineated in [**1**]. Moreover, data characterization based on the principal component analysis (PCA) should be conducted in conjunction with the model emulator construction as described in §3.3.

As a next step, it is recommended to direct the present VUQ/VDP effort to support the development and assessment of CMFD capability Hydra-TH code being planned in the CASL THM Focus Area. Notably, the multi-phase flow capability in Hydra-TH code is being designed with subcooled flow boiling in mind, to support the CIPS challenge problem. Boiling surface area (in subcooled flow boiling regime) is found to be a leading uncertainty for crud prediction (along with the primary reactor system's crud source, and crud deposition/growth rate) identified by a DAKOTA-aided sensitivity/uncertainty analysis performed for the suite of CIPS baseline codes (ANC/VIPRE/BOA). It is expected that the finding remains applicable to the advanced capability under development (DeNOVO/Hydra-TH/MAMBA). In fact, the development of Hydra-TH capability stems from a premise that high-fidelity CMFD capability is foundational to reducing uncertainty in predicting the SFB boiling area.

On one hand, this (uncertainty reduction) goal is a challenge, given all we know about (lack of) supporting data and resulting model uncertainty (see also discussion of "CIPS predictability" in section 4.2.1 in [**1**]).Furthermore, an effective implementation of VDP approach requires database infrastructure such as outlined in CASL Data Center (CDC) section in [**1**]. It is expected that in FY 2013, the CDC functions in Validation Data Management System (VDMS) will largely rely on database capability provided by the NE-KAMS platform, which in itself is subject to programmatic uncertainty.

On the other hand, the circumstance presents a unique opportunity to apply VUQ methodology to support the development of a new CMFD capability. The most pronounced impact to be expected in this approach is to minimize, and hopefully avoid, late surprises in finding out about lack of supporting (relevant, scalable, VUQ-grade) data, data-model inconsistencies, and/or data-software incompatibilities for effective VUQ operations (e.g., total data assimilation, dealing with non-traditional data types, such as multi-dimensional and multi-scale data). As a result, the developed capability would become cumbersome or even not be amenable to necessary calibration, validation and application under system conditions of interest. Another important benefit of the proposed VUQ-aided data-cognizant development of CMFD capability is that first-hand insights and lessons learned from the THM-VUQ collaboration can help guide the development of NE-KAMS VDMS in a way that is both beneficial for meeting NE-KAMS objectives and CASL needs.

As an extension from 1-D formulation evaluated in the present study into 3-D formulation of CMFD, a next step can be made to focus on assessing components of SFB models and their integration in the CMFD formulation, including the following steps:

1. Extend the initial review of modeling approaches, data bases and simulation capability for subcooled flow boiling (SFB) (for 1-D,

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drift-flux model) into that of CMFD SFB (two-fluid three-dimensional formulation).

2. Assess relevance, scalability and uncertainty, and provide VUQ grading, for SFB experimental data related to their application in a PWR operating condition, in CMFD formulation.

3. Assess architecture, functions and software platform of NE-KAMS VDMS and CDC for their compatibility and usability with CMFD SFB databases.

4. Provide a summary on data collection, characterization, and integration of validation data, and their adequacy, for support of CMFD capability for SFB regime in PWR CIPS-related analysis.

5. Evaluate consistency of constitutive models (closures) selected for CMFD sub-cooled flow boiling models and supporting databases.

6. Design, initial implementation and application of a framework for calibration and validation of SFB closure models in CMFD.

7. Continue close collaboration and interactions with THM and AMA experts, the NE-KAMS team and the CASL Data Center initiative.

8. Document outcomes, lessons learned, and recommendations for improvement in the task of VUQ support for CMFD development in the form of a PoR-7 milestone report (tentative title: "VUQ-aided data-cognizant development and assessment of constitutive models for CMFD in PWR CIPS-related subcooled flow boiling").

4. CONCLUSIONS AND RECOMMENDATIONS

In this CASL CIPS Validation Data Plan implementation case study, a model calibration/validation framework based on Bayesian inference for the analysis of a subcooled boiling flow model is outlined and analyzed. The framework based on the total data assimilation concept allows the calibration/validation of complex multiphysics models using heterogeneous data obtained from different types of experiments, i.e. SETs, METs, IETs and PMOs. Data quality defined by the relevancy, scalability and uncertainty are accounted for in the model analysis allowing the quantification of uncertainty in model predictions and parameter determination. Such a process of model-data integration could form a basis for advanced multiphysics model VUQ, data characterization and identification of the values of both available and missing data.

The couplings of multiple physics of different fidelity levels and based on both first-principle conservation laws or simplified empirical representations of physics are realized in this study using a Bayesian network which facilitates the propagation of uncertainty information between the coupled models. Bayesian inference conducted on such a network allows both the forward propagation of uncertainty in model form and parameters to model predictions and the backward propagation of data uncertainty to parameter estimates. Uncertainties of both parameter estimates and model form are therefore accounted for in the process.

A preliminary workflow has been established for the proposed model calibration/validation method which is “application-oriented” to the analysis of a subcooled boiling flow model. Currently, this test-case model comprises a drift-flux two-phase flow and other submodels representing wall convective heat transfer, wall evaporation, bulk flow condensation, etc. Except for the flow model which is conservation laws-based, the other models are semi-empirically derived which require parameter calibration. In this preliminary analysis, only data on axial distributions of void fraction and temperature have been used, but further extension of this calibration/validation framework will enable the use of the small-scale data on wall evaporation dynamics.

Based on the present study, the following conclusions and recommendations for the CASL validation data plan (VDP) can be made:

- CASL CIPS problem in particular and other nuclear power system and safety problems in general are characterized by presence of multiple scales and non-linear couplings of multiple parallel/nested physics which involve different modeling approaches based both on first-principle and empirical/semi-empirical derivations;
- Both high-fidelity spatio-temporal conservation-laws based and evidences-based local-interactions (characteristically, lower-fidelity) constitutive models are used in multiphysics system modeling. Such a

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mixture of models constitutes a major new complication in the validation and calibration tasks of advanced simulation capability;

- Conservation laws based models represented by PDEs are more credible and scale-independent which constrain the constitutive model calibration. However, the potential bias in selecting model forms could cause significant off-settings that render the model un-amenable for parameter calibration;
- Data of multiphysics 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;
- Data uncertainty must be accounted for and used in quantification of prediction uncertainty;
- A flexible model-data integration framework is needed which can
  - represent the complex hierarchy of coupled multiphysics models
  - account for model form inadequacy and biases
  - account for data relevance, scaling and uncertainty (represented by "weight" factor [**1**])
  - assimilate heterogeneous data available at different levels of model hierarchy
  - not be rendered unworkable when data are missing or not directly applicable for some constituent models
- Bayesian inference in combination with Bayesian influence networks is a promising approach to multiphysics model VUQ which satisfies the above requirements;
- Data homogenization, grading and characterization are required before the data can be used in the proposed "unified" VUQ framework;
- It is recommended that the present case study (subcooled flow boiling) be continued and extended in a close collaboration with THM, AMA, NE-KAMS team and the CDC initiative, with the objective to enable a VUQ-aided, data-cognizant development of advanced capability in Computational Multiphase Fluid Dynamics for CASL.

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Appendix A

Subcooled boiling model

Under the sub-cooled boiling condition, evaporation starts on the heating wall long before the average fluid temperature reaches the boiling temperature. The onset of nucleate boiling (ONB) is defined as the wall superheat at that point bubble nucleation starts. From this point to the point of onset of significant void (OSV), partial boiling occurs and both bubble nucleation and condensation happen due to the thermodynamic non-equilibrium between vapor and subcooled liquid.

The ONB is dependent on many factors including wall heat flux and material as well flow conditions (flow rate and subcool). According to Basu et al. [**13**], the wall superheat at the ONB is empirically defined as:

$$\Delta T_{ONB} = (T_w - T_{sat})_{ONB} = \frac{\sqrt{2}}{G(\phi)}\left(\frac{\sigma T_{sat} q_{w,ONB}}{\rho_g k_f h_{fg}}\right)^{1/2}$$

with factor $G(\phi)$ being a function of the wetting contact angle ϕ

$$G(\phi) = 1 - \exp[-\phi^3 - 0.5\phi].$$

With the wall heat flux at the ONB $q_{w,ONB}$ defined by

$$q_{w,ONB} = h_{FC}(\Delta T_{ONB} + \Delta T_{f,sub}) \ ,$$

where h_{FC} is the forced convection heat transfer coefficient and $\Delta T_{f,sub} = T_{sat} - T_f$, the wall heat flux is expressed as follows

$$q_{w,ONB} = \frac{h_{FC}}{4}\left(\sqrt{\Delta T_{ONB,sat}} + \sqrt{\Delta T_{ONB,sat} + 4\Delta T_{f,sub}}\right)^2$$

where

$$\Delta T_{ONB,sat} = \frac{2h_{FC}}{G^2(\phi)}\frac{\sigma T_{sat}}{\rho_g k_f h_{fg}}.$$

Superposition of the wall forced convection heat flux $q_{w,FC}$ and boiling heat flux $q_{w,NB}$ is given by

$$(q_w)^3 = \left(q_{w,FC}\right)^3 - \left(q_{w,NB} - q_{w,NB}\left(T_{w,ONB}\right)\right)^3$$

In this work, the formulation of boiling heat flux proposed for water by Gorenflo [**6**] is used which is expressed as

$$q_{w,NB}(T_w) = h_{NB}(T_w - T_{sat})$$

with

$$h_{NB} = h_{NB,0} F_{PR}\left(\frac{q_w}{q_0}\right)^n \left(\frac{\eta_w}{\eta_0}\right)^{0.133}$$

$$F_{PR} = 1.73\, P_r^{0.27} + \left(6.1 + \frac{0.68}{1 - P_r}\right) P_r^2$$

$$n = 0.9 - 0.3\, P_r^{0.15}$$

and $h_{NB,0}$ = 5600 W/(m^2 K), q_0= 20000 W/m^2, η_0= 0.4 μm, P_r=p/p_{cr} , p_{cr} = 220.6 bar.

The rate of wall evaporation is then defined by the following correlation

$$\Gamma_{\text{evap}} = f_{sub} \frac{(q_w - q_{w,FC}) A_w}{h_{g,sat} - h_f}.$$

Due to fluid subcooling, wall evaporation is suppressed which is represented by a suppression factor f_{sub} defined by

$$f_{sub} = \max\left[\frac{(h_f - h_{fd})}{(h_{f,sat} - h_{fd})}, 0\right]$$

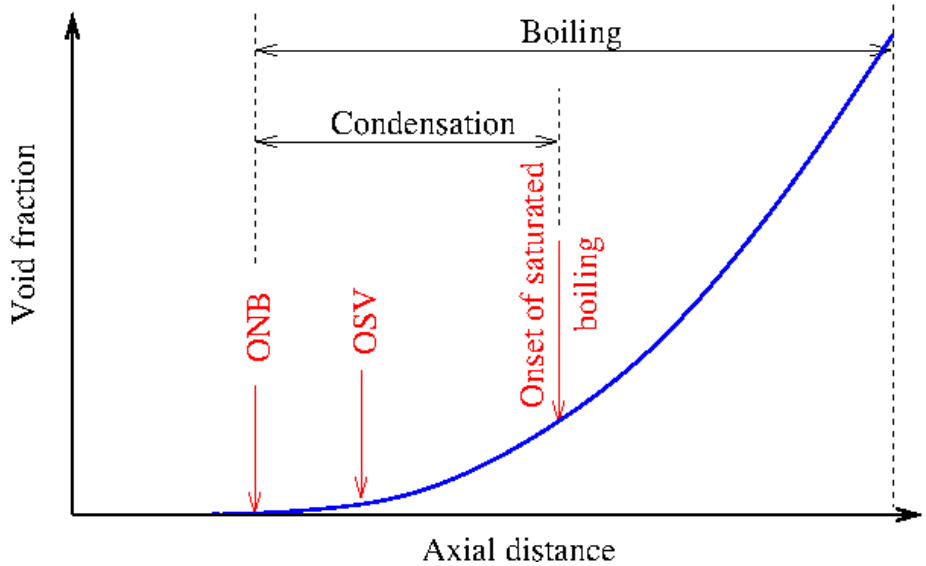
with h_{fd} being the fluid enthalpy at the bubble detachment threshold (or OSV) and defined by [**55**]

$$h_{fd} = h_{f,sat} - \frac{q_w D c_{p,f}}{0.0065\, k_f \max(Pe_f, 7 \times 10^4)}.$$

It is worth noting that the above Saha-Zuber's OSV correlation usually does not work well for high pressure, high flow rate, or large Peclet number (over 400,000).

Model parameters which may be subjected to calibration include: (i) boiling thresholds ONB and OSV; (ii) boiling heat transfer coefficient h_{NB}; and (iii) evaporation suppression factor.

Using the knowledge about the physics of subcooled boiling flows, a simplified strategy for sequential (hierarchical) model calibration and/or "manual" dimensionality reduction can be implemented. For instance, the variation of axial void fraction distribution in the saturated boiling region where no condensation occurs can be used to independently calibrate the boiling heat transfer coefficient correlation. Similarly, the ONB threshold can also be calibrated using only the data near the place where vapor starts to appear. However, all available data (void fraction, temperature, etc.) in the region from the ONB to the onset of saturated boiling are probably needed to calibrate the other factors and parameters. The onset of saturated boiling can approximately be estimated from the axial temperature distribution.



Appendix B

Bulk flow condensation model

When the fluid temperature is less than the boiling threshold, vapor bubbles generated at the wall can condense and collapse in the subcooled bulk flow, reducing the net vapor generation rate. By employing the interface heat transfer coefficient proposed by Ünal [**56**], the condensation rate is calculated as follows [**18**]:

$$\Gamma_{cond} = 0.9 C_{cond} \frac{C \cdot F \cdot (T_{sat} - T_f)}{\left(\frac{1}{\rho_g} - \frac{1}{\rho_f}\right)}$$

where

$$F = \begin{cases} 1 & \text{for } |u_f| \leq 0.61\ m/s \\ \left|\frac{u_f}{0.61}\right|^{0.47} & \text{otherwise} \end{cases}$$

$$C = \begin{cases} 65 - 6.36\,(p-1) & \text{for } p \leq 10\ bar \\ 203.208\ p^{-1.418} & \text{otherwise} \end{cases}$$

with C_{cond} being an empirical constant subjected to calibration.

Appendix C

Sample of relevant experimental data

1. IETs

Low pressure experiments [**28**]

Authors	Geometry (m) D or Dh	Pressure (kPa)	Heat flux (MW m^{-2})	Mass flux (kg m^{-2} s^{-1})	Measurement instrument
Ferell (1964)[a]	Circular 0.0118	410	0.36	540–1060	–
Costa (1967)[a]	Rectangular 0.0038–0.0066 Circular 0.006	174–499	1.0-4.2	3000–7500	–
Staub (1968)[a]	Rectangular 0.0139	110–300	0.31–0.79	320–2800	Gamma-ray
Whittle and Forgan (1967)	Rectangular 0.0026–0.0057 Circular 0.0064	117–172	0.42–3.50	816–11200	Differential pressure
Evangelisti and Lupoli (1969)	Annular 0.006	113	0.44–0.89	608–1420	Gamma-ray
Sekoguchi et al. (1974)	Circular 0.0136–0.0158	127–407	0.017–0.046	290–1950	Conductivity probe
Edelman and Elias (1981)	Circular 0.0113	103	0.015–0.096	28–190	Gamma-ray
McLeod (1986)	Annular 0.0089–0.0169	155	0.6–1.19	66–456	Gamma-ray
Rogers et al. (1987)	Annular 0.0089	155	0.32–1.20	67–440	Gamma-ray
Dougherty et al. (1990a,b)	Circular 0.0091-0.028	240-450	1.25-3.16	1300-9400	Differential pressure
Bibeau and Salcudean (1994a,b)	Annular 0.0091	155	0.30-0.98	210-440	Gamma-ray
Zeitoun and Shoukri (1997)	Annular 0.0127	145–165	0.2–0.6	160–400	Gamma-ray
Bartel et al. (1999)	Annular 0.0195	101.3	0.01–0.193	480–1900	Conductivity probe, video

High pressure experiments [**28**] [**19**]

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

2. SETs

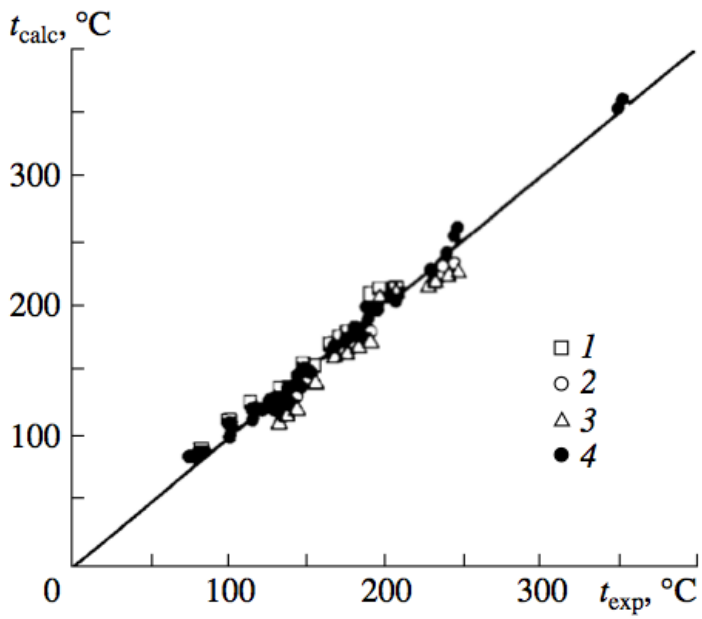


Figure C.1. Wall temperature measurements [**11**] *– p = 0.6-17 MPa, q = 0.5-6 MW/m^2.*

	G (kg/m^{2}s)	ϕ_s (deg)	ΔT_{sub} (°C)	$q_{w,ONB}$ (W/cm^2)	$\Delta T_{w,ONB}$ (°C)	Bergles and Rohsenow Eq. (4) $\Delta T_{w,ONB}$ (°C)	Sato and Matsumara Eq. (5) $\Delta T_{w,ONB}$ (°C)	Davis and Anderson Eq. (6) $\Delta T_{w,ONB}$ (°C)
Flat Plate	124	30	50.3	21.3	10	6.5	6.3	8.7
	346	30	26.5	17.4	9.1	5.9	5.8	7.9
	346	30	50.3	26.0	10.0	7.1	7.1	9.6
	868	30	26.5	57	17	10.4	10.6	14.5
	886	30	52.5	70	16	11.3	11.6	15.8
Rod Bundle	186	57	2.2	3.2	2.7	2.7	2.5	3.1
	336	57	9.6	8.0	4.0	4.1	3.9	4.9
	336	57	38.6	13.3	4	5.2	5.0	6.3
	596	57	1.7	5.4	3.3	3.4	3.2	4.0

Figure C.2. Experimental data on the ONB [**13**] *– 0.1-13.75 MPa, velocity = 0-17 m/s.*

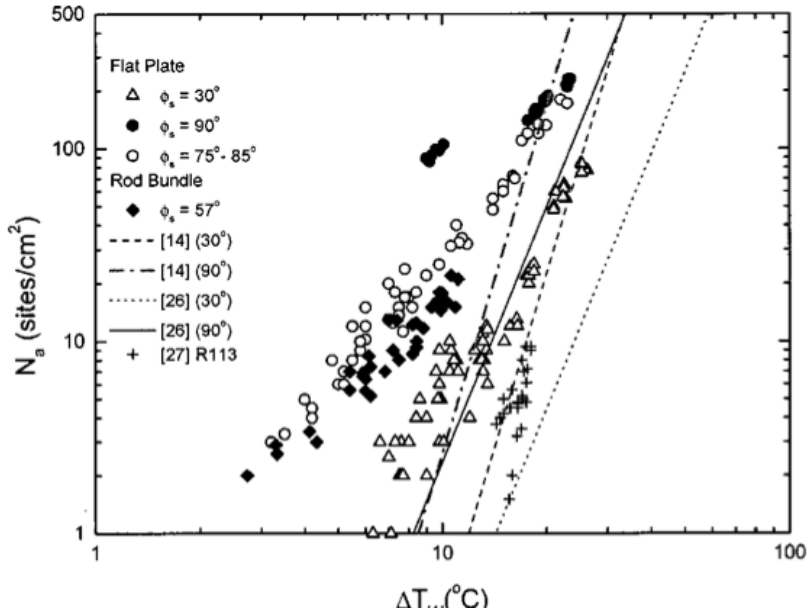


Figure C.3. Measured nucleate site density [**13**] *– 0.1-13.75 MPa, velocity = 0-17 m/s. Note a large uncertainty in characterization of foundational processes in boiling.*

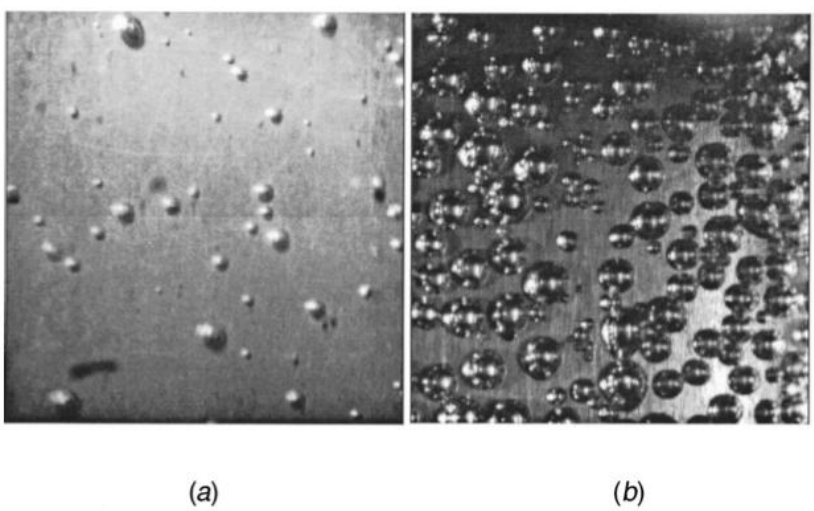


Figure C.4. Observations of the boiling surface [**13**] *– (a) contact angle of 30°; (b) contact angle of 90°. Note a significant dependence on surface characteristics (a diffeernt physics).*

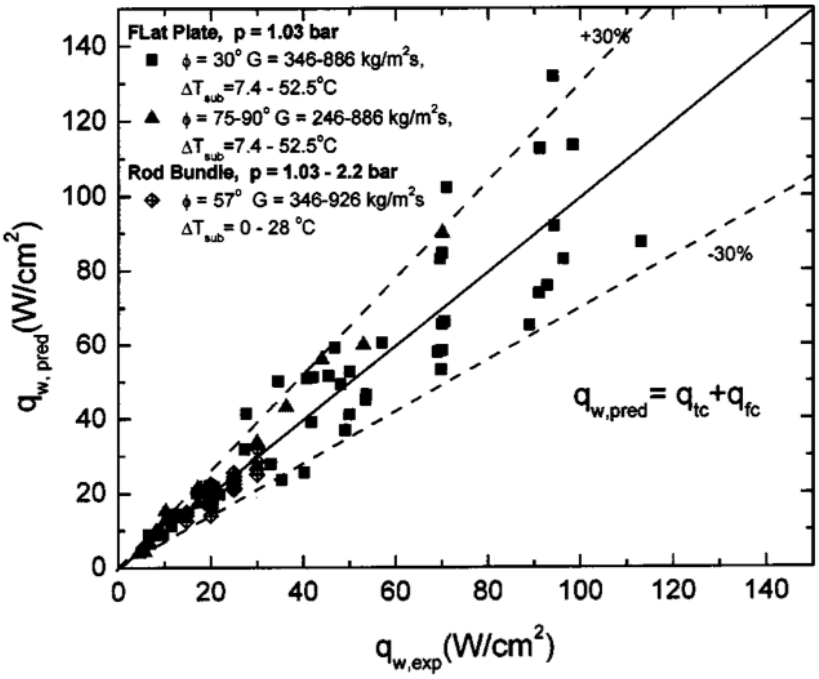


Figure C.5. Wall heat flux [**12**] *– p=0.1-0.22 MPa. Note the low pressure and relatively low mass flux range of data.*

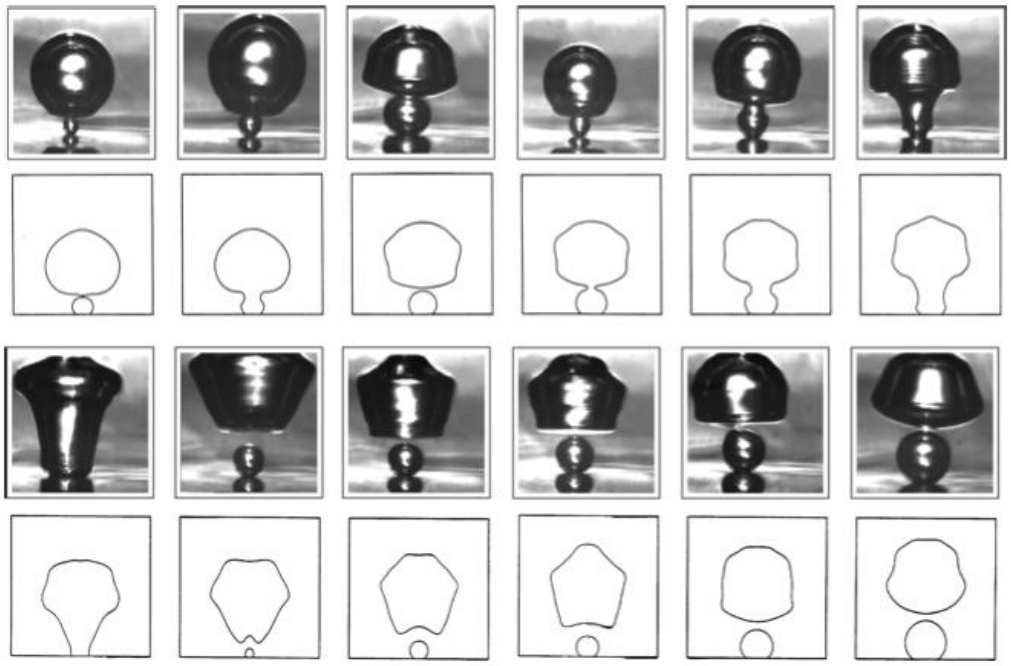


Figure C.6. Bubble dynamics – experimental data and ITM-DNS results [**16**] *– atmospheric pressure. Note: multi-dimensional data (images), both experimental and computational, require a different approach to validation.*

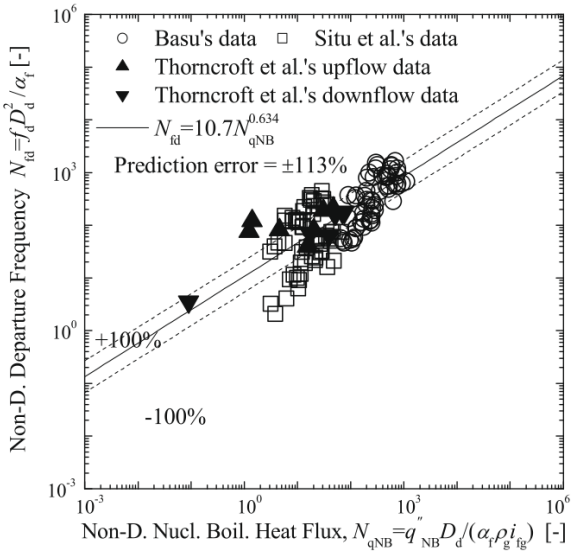


Figure C.7. Comparison between predicted and measured dimensionless bubble departure frequencies [**15**] *– atmospheric pressure. Note a large uncertainty in characterization of fundamental mechanisms/processes.*

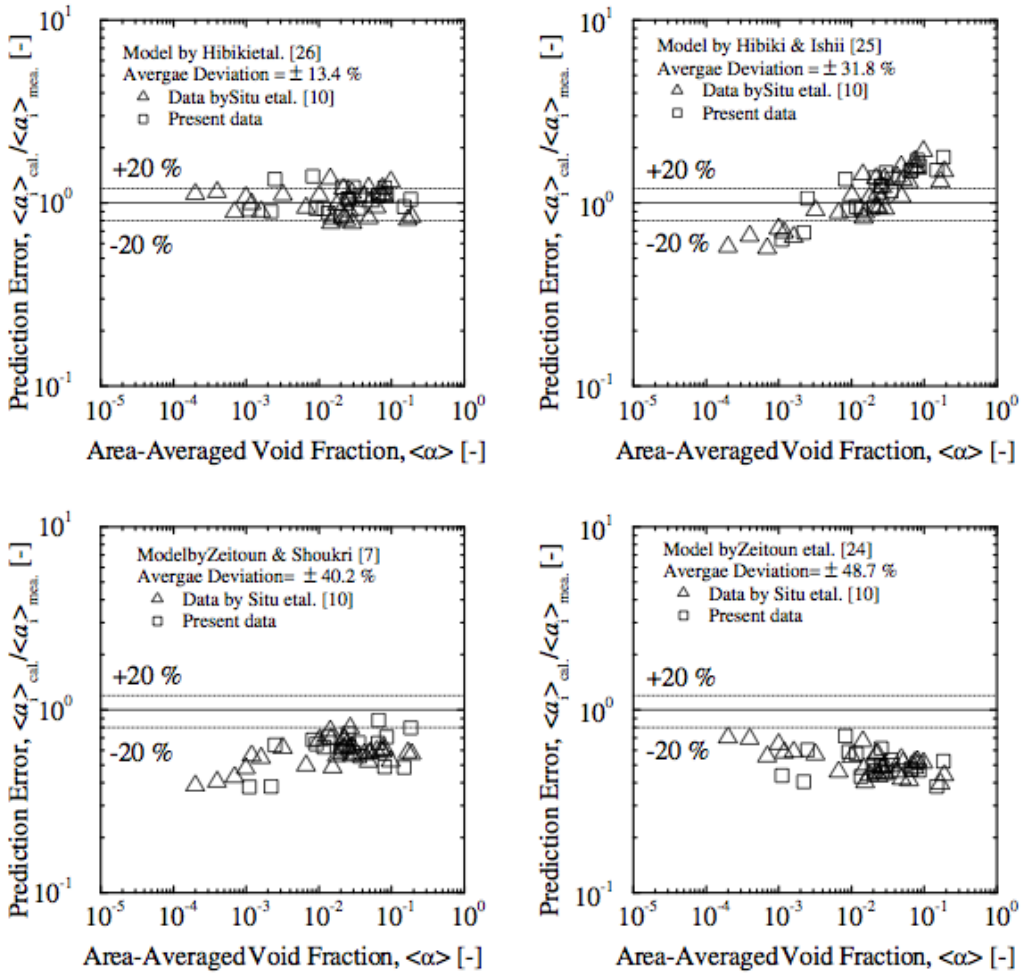


Figure C.8. Measurement and prediction of average interfacial area [**27**] *– low pressure conditions. (Note: integral quantities are characterized with lower, still large, uncertainty).*