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Quantification of Data Needs, Data Collection and Characterization to Support Validation and Calibration of Subcooled Flow Boiling Model

Anh Bui
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March 2013

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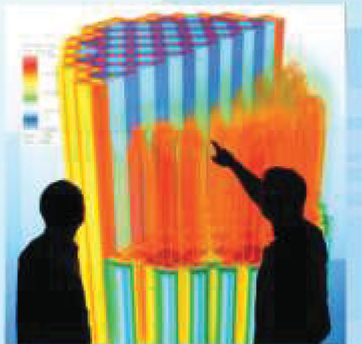

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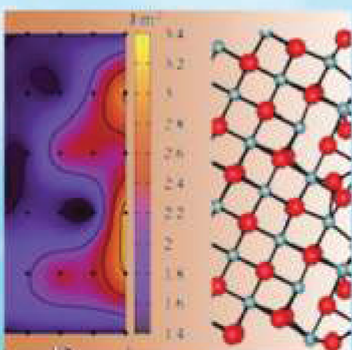

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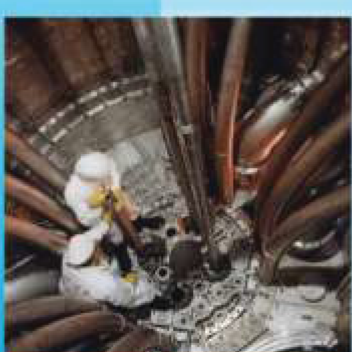

Plant operational data

CASL
Consortium for Advanced Simulation of LWRs

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ABSTRACT

Further to the development of a model analysis framework suitable for calibration and validation of complex multivariate multiphysics models detailed in [1], this report presents an approach to data collection and characterization which can work in parallel with the above-mentioned model analysis framework and support the calibration and validation of the case-study subcooled flow boiling model presented in [1].

This work presents a step forward in the development and realization of the "CIPS Validation Data Plan" [2][3] at the Consortium for Advanced Simulation of LWRs (CASL) to enable quantitative assessment of the CASL modeling of Crud-Induced Power Shift (CIPS) phenomenon, in particular, and the CASL advanced predictive capabilities, in general.

Advanced modeling of LWR systems normally involves a range of physic-chemical models describing multiple interacting phenomena, such as thermal hydraulics, reactor physics, coolant chemistry, etc., which are usually constrained by the lack of data suitable for model validation and calibration. The necessary employment of different modeling approaches in the advanced LWR modeling practice further complicates the situation, since each modeling approach has a unique requirement of validation data. The development and validation of closure model of wall heat transfer process employed in the subcooled flow boiling modeling, for instance, may require data of microscopic physics, i.e. wall heat flux partitioning, bubble nucleation, growth and detachment dynamics, etc. [4], which can hardly be obtained for reactor-prototypical conditions.

Although the model analysis framework proposed in [1] is designed to be robust enough to deal with a wide range of measurement data of different quality and availability, a strategy for data collection, data validation and data characterization is still needed which has been detailed in [3]. This work presents an implementation of that strategy for a case-study calibration/validation of a subcooled flow boiling model. The lesson learnt and implication to CIPS modeling and the overall CASL VUQ effort will also be discussed.

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

EXECUTIVE SUMMARY

This milestone supports a case study on development, testing and application of a strategy, methods and associated infrastructure for validation data support that enables assessment of CASL-developed predictive capability for Crud-Induced Power Shift (CIPS) challenge problem as formulated in a previous report for CASL.VUQ.VVDA.P4.02 [3]. Subcooled flow boiling (SFB) prediction is selected as a capability for which data collection, characterization and integration (model calibration) be performed, with the objective to develop recommendations on a CASL-wide Validation Data Process.

This milestone focuses on quantification of data needs, data collection and characterization, preparing the ground for the SFB model calibration and validation. The selected test case (simulation of subcooled flow boiling) is an important capability for CIPS prediction, whose development has been hampered by validation data challenges. Specifically, a model calibration/validation approach based on Bayesian inference is used in the analysis of a subcooled boiling flow model. The approach implements the "total data-model integration" concept to allow integration of different datasets obtained from different types of experiments and measurements.

For subcooled flow boiling, which is a relatively simple multiphysics problem, a vast quantity of legacy data are identified, which are reviewed and classified into either *integral effect data*, i.e. distributions of phase volume fraction, temperature, etc., and *separate effect data*, i.e. measurements and observations of nucleation, bubble dynamics, wall heat flux, etc. These data, however, are very different in their origin, relevancy and scalability to reactor-prototypical conditions, and uncertainty. Consequently, data validation and characterization are necessary before they can be effectively used in calibration and validation and uncertainty quantification (VUQ) of reactor modeling codes. A guideline for collection and characterization of validation data have been derived and outlined in this work. The guideline proposes the use of physics-dependent representative dimensionless groups to access the relevancy and scalability of data, and measurement error to access data uncertainty. A different (from current practice) and more comprehensive approach to improved assessment of measurement error has been suggested, which would provide more information for model calibration and VUQ (proposed to be based on statistical model analysis and Bayesian inference).

A systematic quantification of data needs, availability, and quality is crucial for CASL mission. It is suggested that the future effort be streamlined with a CASL Data Center that provides a standardized process and infrastructure for validation data warehousing and effectively interfacing with simulation and VUQ software.

CONTENTS

ACRONYMS

	Description
1D/2D/3D	One-/Two-/Three-Dimensional
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
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)
GTRF	Grid To Rod Fretting
IET	Integral Effect Test
MCMC	Markov Chain Monte Carlo sampling
MET	Multiple Effect Test
MIT	Massachusetts Institute of Technology
ONB	Onset of Nucleate Boiling
OSV	Onset of Significant Void
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

Bo	Boiling number
D_h	Hydraulic diameter
G	Mass flux
h	Enthalpy
p	Pressure
q,Q	Heat flux
x_{eq}	Equilibrium quality
We	Weber number

Greek letters

α	Volume fraction
ρ	Density
σ	Surface tension

Superscripts

Subscripts

cr	critical
f	fluid
fg	Transition from fluid to gas
g	vapor
w	wall

1. INTRODUCTION

Advanced Modeling and Simulation (AMS), which plays an increasingly important role in analysis, design and licensing of nuclear energy systems, is the focus of the Consortium for Advanced Simulations of LWRs (CASL) multi-year multi-institutional research program funded by the U.S. Department of Energy. In parallel with the CASL effort directed at the development of advanced modeling capabilities capable of high-resolution high-fidelity predictions of multi-scale multiphysics problems is an equal effort to verify and validate these predictive capabilities via a comprehensive strategy for model validation and uncertainty quantification (VUQ) [2][3].

Central to the CASL VUQ strategy is the Validation Data Plan (VDP) which has been developed and described in details in [3]. Recognizing the needs for holistic validation of advanced multiphysics modeling capabilities and the reality of validation data heterogeneity and inadequacy, the study suggested a pragmatic (application-oriented) and holistic (communication) approach to validation and validation data which brings together

- "Data realism" concept which employs advanced data strategies and VUQ tools to allow the extraction of more value from available data regardless of their origins, types, and qualities; and
- Application-oriented total data-model integration which simultaneously assimilates data at different scale and physics levels for uncertainty reduction.

Preliminary development of a statistical VUQ framework based on Bayesian inference for the case study modeling of subcooled flow boiling (SFB) is delineated in [1] and [5]. Subcooled flow boiling is an example of multiphysics systems and is one crucial phenomenon in the CASL Crud-Induced Power Shift (CIPS) challenge problem (Figure 1.1). SFB involves a range of physics occurring at different scales that include near-wall micro-/meso-scopic nucleation, bubble growth and bubble detachment and larger-scale interactions of flow and deforming interfaces (Figure 2.1). Even for this relatively simple multiphysics phenomenon, a range of modeling approaches are employed which include high-fidelity conservation laws-based description of the heat and mass transports by flow and evidences-based constitutive description of various wall-flow and phase-phase interactions. The VUQ framework proposed in [1] and [5] for calibration and VUQ of the SFB (and other multiphysics) model(s) is potentially able to

- represent the complex hierarchy of coupled multiphysics models;
- account for model form inadequacy and biases;
- account for data relevancy, scalability and uncertainty ;
- assimilate heterogeneous data available at different levels of model hierarchy;
- not be rendered unworkable when validation data are not available for some constitutive models.

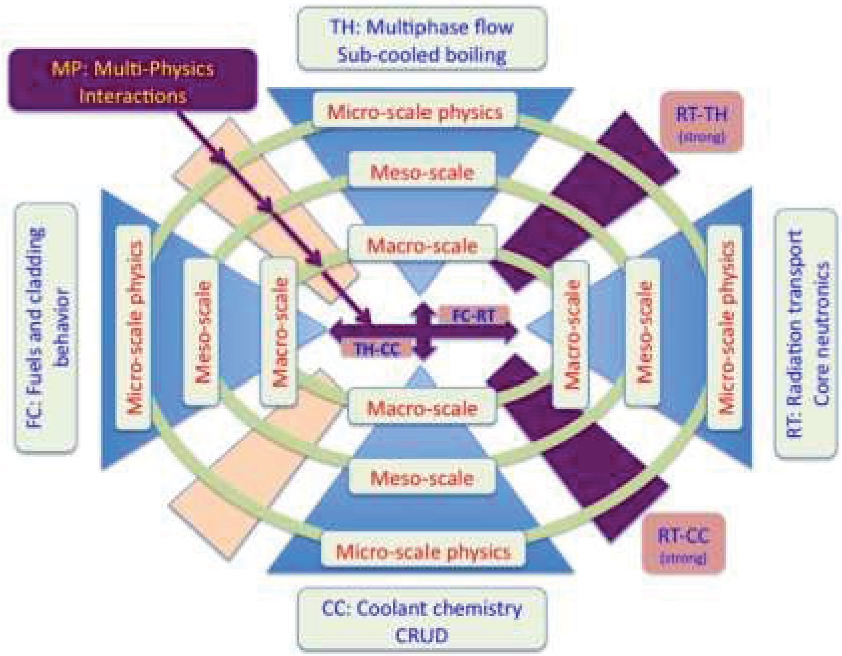

Figure 1.1. CIPS and Subcooled Flow Boiling (SFB) [3].

A wide range of data on subcooled flow boiling is available which includes:

- Integral effect data (obtained from integral effect tests or IETs), e.g. [6][7][8];
- Data on fundamental mechanisms of boiling heat transfer (obtained from separate effect tests or SETs), e.g. [9][10][11][12][13][14][15];
- Plant observations and measurements (PMOs) provided by, for instance, plant monitoring systems.

The values of the above data to calibration and VUQ of AMS codes are different depending on data quality, the level of software sophistication, and the scenarios/applications they are used for. For instance, calibration and VUQ of less sophisticated system analysis codes, such as RELAP5, TRACE, etc., only require integral effect data on 1D velocity, temperature, and void fraction distributions and some SET data on wall heat flux partitioning, while more complex CMFD codes would need/use 2D/3D distributions of flow characteristics and detailed measurement of wall evaporation mechanisms, e.g. nucleation, bubble growth, bubble detachment, etc., in their calibration and VUQ.

Data quality is an important factor which defines data value. As described in [3], data quality is characterized by not only data *uncertainty*, which is related to measurement error, but also by *relevancy* and *scalability*, which quantify the similarity between experimental and reactor-prototypical conditions and the applicability of codes calibrated/validated with use of these data in simulation of particular realistic scenarios/processes. For example, detailed measurements of wall evaporation phenomena, commonly conducted under significantly different from reactor-prototypical conditions (i.e. low pressure, simple geometry, low heat flux, etc.), are valuable for calibration and VUQ of sophisticated CMFD codes. However, such assessments will not necessarily reduce model prediction uncertainty, when the codes are used in simulations of real reactor/plant scenarios/ applications.

It is worth noting that many micro-/macro-scopic physics are stochastic in nature, which prevents them to be measured, analyzed, and modeled in a deterministic manner (see nucleation example in SFB [9]). The "averaging" introduced to enable the collection and quantification of stochastic data, while necessary, would bring about additional uncertainty which need to be quantified (and accounted for when data are used).

In multiphysics modeling, physical couplings are themselves described by closure models, e.g. wall heat transfer models used in conjugate heat transfer between fuel/heating rods and subcooled boiling flows, and interactions of turbulence and interfaces in two-phase flows. Calibration and validation of these coupling models require data, which, unfortunately, are difficult to obtain and often lacking.

Each multiphysics simulation software, therefore, has specific needs in validation data which need to be quantified. The change of the predominant physics from one plant scenario/process to another would make these validation data needs and characterization application-dependent. The issues concerning quantification of validation data needs, collection and characterization of data will be investigated in this study in the example of subcooled flow boiling modeling. The lesson learnt, implications and recommendation for the CASL validation data plan will also be discussed.

2. OVERVIEW OF SUBCOOLED FLOW BOILING MODEL VALIDATION AND CALIBRATION

Advanced modeling of multiphysics problems, in general, and subcooled flow boiling, in particular, involves a lot of uncertainty related to:

- inadequacy of equation form - although model equation form is based on universal conservation laws and represented using mathematically rigorous ensemble-averaged PDEs, the averaging method, the chosen number of representative fields, the assumptions used in derivation of field equations (regarding field pressure, interfacial morphology and geometry, phase separation, etc.) would impose a constraint on the equation form adequacy. This depends also on the specifics of the considered problem, i.e. whether it involves flow regime change, crisis of heat transfer, critical flow conditions, etc.
- incorrect/improper application of closure laws – a range of small scale physics can not be directly modeled due to a lack of physical understandings or limited of computational resources, which are represented by various closure laws (or models). They are empirically or semi-empirically based and, therefore, much less universal and scalable compared to the conservation laws-based models. They are derived from certain set(s) of experimental data and can only be applicable in certain ranges of conditions (pressure, temperature, wall heat flux, system size/geometry, etc.). Extensive calibration of those models is required whenever they are applied to different problems with different conditions;
- limitation of numerical methods and computational resources in solving extremely large systems of non-linear and differently coupled model equations;
- uncertainty in specifying initial and boundary conditions of complex physical systems which vary greatly from scenario to scenario.

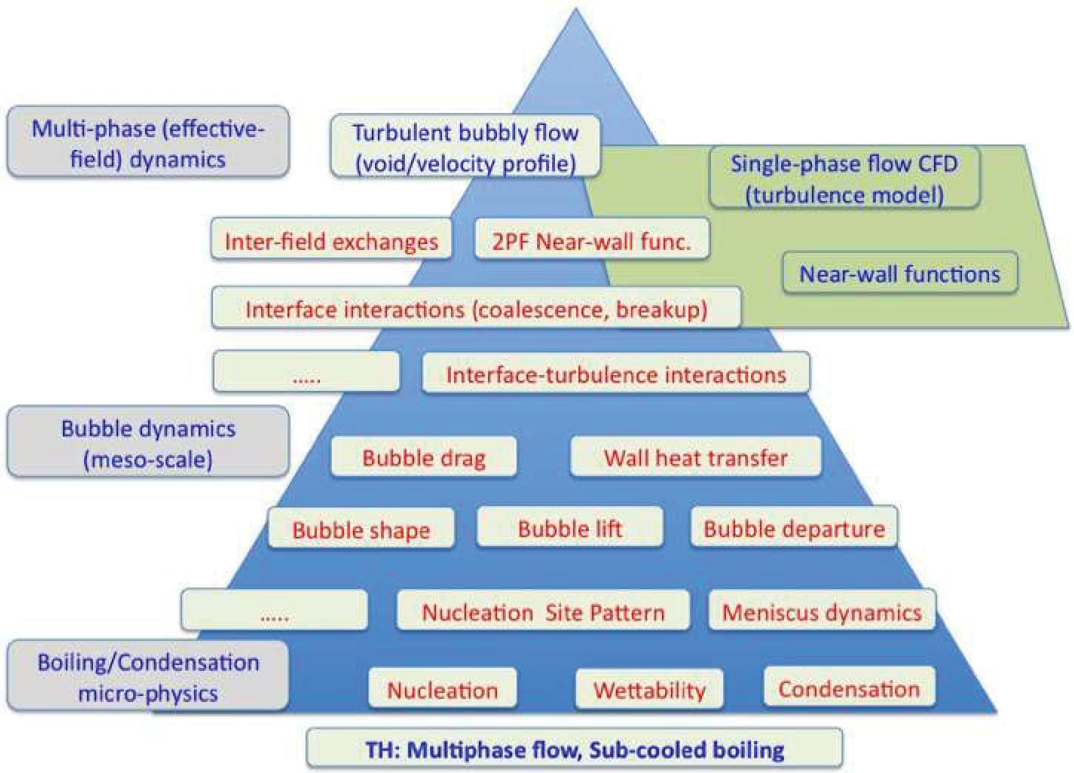

Figure 2.1. The pyramid of the subcooled boiling flow phenomenology [3].

The subcooled flow boiling model describes the physics schematically represented by the phenomenology pyramid in Figure 2.1. At the top of the pyramid, multiphase modeling techniques employing multiple inter-penetrating continuums (fluids) form a backbone of subcooled flow boiling model [4][16][17]. The equation system given in [4][16][17] (and Appendix A) is very similar in form to the Navier-Stokes equations derived for single-phase flows, and it is equally applicable to any flow dimensionality.

Different equation forms can be obtained based on the number of fluids employed and the assumptions about their interdependence. The drift-flux model, for instance, can be obtained from the more complex and complete multifluid model with an assumption about relative velocity between dispersed and continuous phases introduced [18]. Assumption about steam being at saturation condition would eliminate the need for steam energy equation. The multifluid model itself can be simplified by assuming a single pressure field for all phases. The usage of such assumptions would change the equation form of the whole model, add uncertainty to the modeling, and, in some cases, even complicate the solution process (e.g. by rendering the equation system non-hyperbolic or ill-posed).

The choice of model equation form also concerns the choice of model dimensionality (1D/2D/3D) and temporal/spatial resolutions, which can be succinctly termed as model fidelity. Model fidelity determines the “scale” of physics which can be resolved by a given model equation form and the associated discretization technique. It also affects the choice of averaging method, commonly employed to approximate unresolved physics and derive continuum approximation of discreet physics, and the formulations of many closure laws. There should be an agreement between model equation form/fidelity choice and validation data needs, since many physical processes are associated with multi-dimensional transport/distribution of the involved characteristics. 2D/3D vapor transport models, for instance, can hardly be calibrated or validated using only 1D axial measurement of vapor distribution.

Near the base of the phenomenology pyramid, a range of small-scale physics which can not be described by the model conservation laws-based equations, have to be approximated and represented by empirical or semi-empirical closure laws. For subcooled flow boiling, these include important physics of convective and boiling heat transfer on walls, involving nucleation, bubble growth and departure, and heat-mass interactions between phases and phase-turbulence (see Table 2.1).

The use of experimental observations and data in their derivation reduces the versatileness and robustness of whole model and necessitate model calibration before it can be applied to the analysis of particular plant conditions. It is notable that experimental data can hardly be obtained for such small-scale physics under high-pressure, high-flow rate, and high-heat flux plant conditions to calibrate closure models and, thus, huge uncertainty is introduced into the modeling of subcooled flow boiling in nuclear power systems associated with the use of such closure laws. Furthermore, these closure laws change with the change of flow regime which depends not only on system geometry and configuration (e.g. flow orientation and inclination), but also pressure, flow rate, heat flux, etc., expanding the number of used closure laws and calibration requirement.

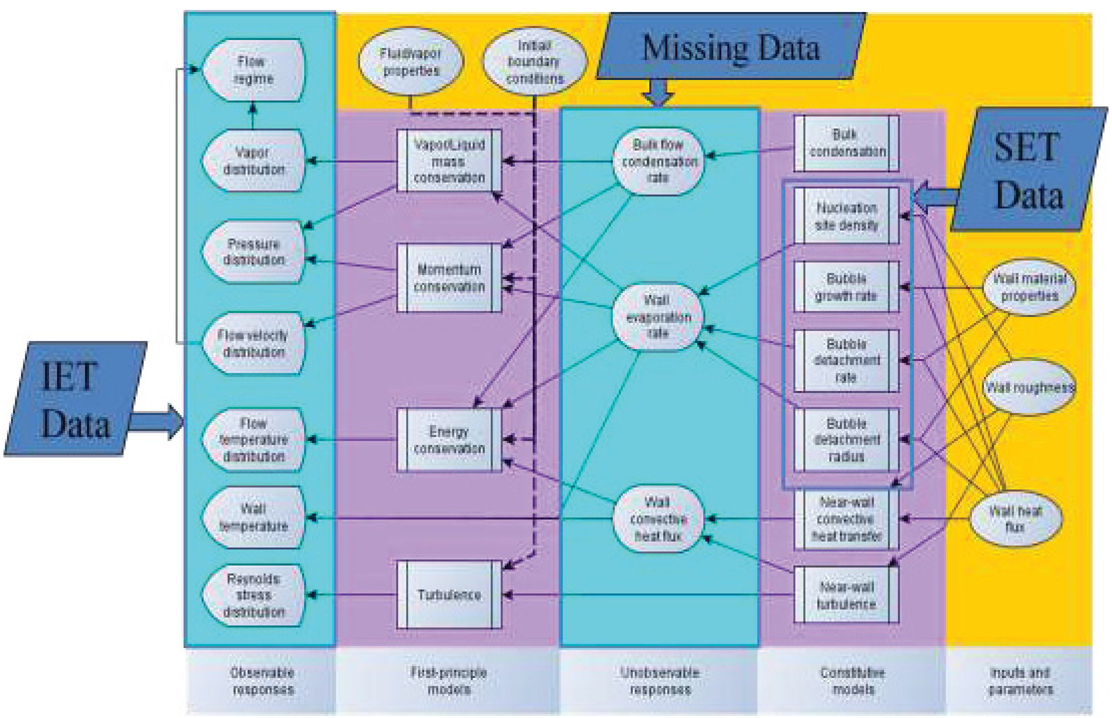

Figure 2.2. Hierarchy of subcooled boiling flow model [3].

In multiphysics systems, interactions between participating physics greatly complicate the validation and calibration tasks, since the models of physical couplings themselves also require calibration and validation. For the considered subcooled flow boiling, thermal coupling between heat generation/conduction inside fuel rods and coolant flows at walls is an example of such interactions which involves a number of closure laws and models to represent it.

The fact that closure models are mostly "locally" formulated and, therefore, dimensionality-independent allows them to be universally employed in either 1D, 2D, or 3D CMFD models, where the resolution/fidelity of the models is not sufficient to resolve the related physics with model equations.

Table 2.1. Incomplete list of closure models used in a drift-flux two-phase model of subcooled flow boiling [1].

Model description	Reference	Comments
Drift velocity	[18]	Flow regime dependent
Mixture-wall friction factor	[18]	Flow regime dependent
Wall boiling – heat flux partitioning	[19][20]	Flow regime dependent
Wall boiling - nucleation density	[21][12][22]	Nucleation boiling mode
Wall boiling - bubble detachment frequency	[21][14]	Nucleation boiling mode
Wall boiling- bubble detachment size	[21][15]	Nucleation boiling mode
Bulk flow condensation	[21][23][24]	
Flow regime transition model	[4][21]	
Critical Heat Flux (CHF) or Departure from Nucleate Boiling (DNB)	[25][21]	Flow regime dependent

In defining the characteristics and thermal-hydrodynamic physics of two-phase flows, there is no other more important parameter than flow regime. The flow regime is entirely defined by interfacial morphology, as seen in Figure 2.3, and, in modeling of subcooled flow boiling, the choice of important hydrodynamic and heat transfer closure laws depends on the identification of flow regime (see Table 2.1). Uncertainty in identification of flow regime is, therefore, a major contributor to uncertainty in modeling of two-phase flows and subcooled flow boiling, which is relying heavily on these closure laws. Due to this intertwining of flow regime transition, boiling mode and other closure models, reduction of uncertainty of two-phase model predictions as a whole can not simply be realized via validation and/or calibration of closure models separately, but a "total data-model integration" strategy would be needed [1].

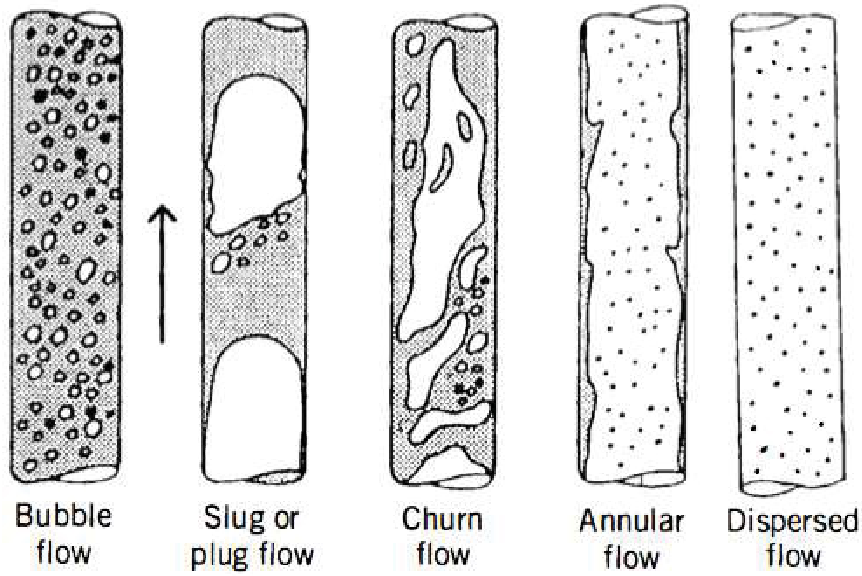

Figure 2.3. Interfacial morphology and flow patterns in vertical two-phase flows [25].

In system modeling of two-phase flows, identification of flow pattern (or flow regime) is based on flow regime maps, which define the boundaries of transition between flow patterns based on few local parameters, such as superficial phase velocities of vapor and liquid, and/or local void fraction (Figure 2.4).

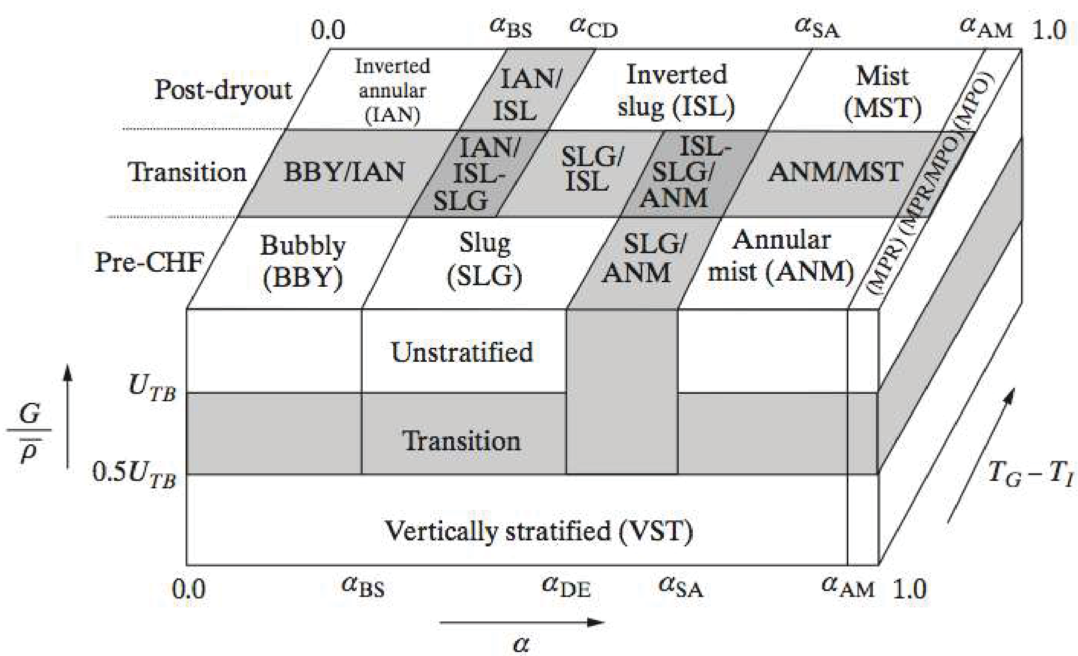

Figure 2.4. RELAP5-3D vertical flow regime map [21].

It is worth noting that different flow regime maps are needed for different flow configurations (flow orientation, inclination, geometry, fluid properties, etc.). Without exception, all flow regime maps are derived based experimental observations, and, for some flow configurations of importance to nuclear reactor thermal hydraulics, e.g. flows in tube bundles, experimental data are severely lacking. Clear-cut boundaries between flow regimes are not only unrealistic, but also introduce additional difficulties to numerical solution due to discontinuous switching of closure models at the boundaries.

Complex structure of the SFB model hierarchy (Figure 2.2) makes calibration and validation of the whole model difficult and intractable tasks. Simultaneous and effective use of validation data, available at different scale levels, for different physics, having different quality and relevancy, is not feasible during the processes.

The so-called "traditional" approach of multiphysics model calibration and validation is schematically shown in Figure 2.2 (left panel), which is known to have several shortcomings, e.g.

- 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.

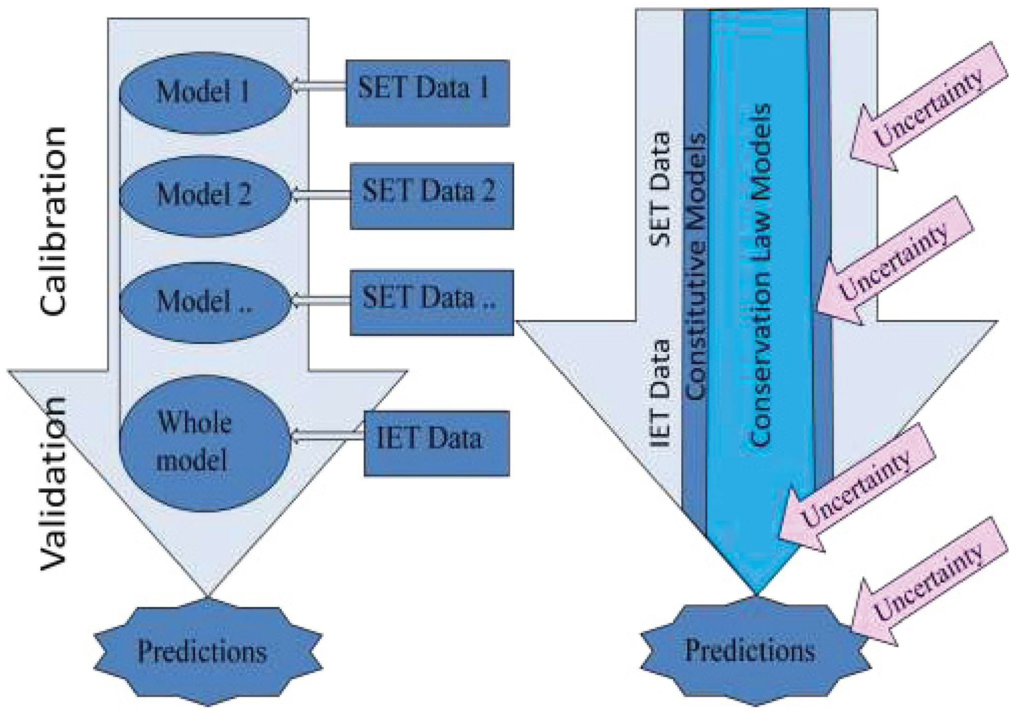

Figure 2.2. "Traditional" approach to multiphysics model calibration & validation (left) versus "total data-model integration" approach (right)[1].

Given the perpetual "imperfect" states of validation data and models, unaccounting for data and prediction uncertainties is not permissible in modern advanced simulation using complex models and software.

"Total data-model integration" approach based on Bayesian inference and data assimilation techniques has been proposed in [3] and [1] for complex multiphysics model calibration, validation, and uncertainty quantification (Figure 2.2 (right panel)), which is potentially able to:

- 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.

Technical implementation of the proposed "total data-model 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 [1] and [5], which employs a range of statistical modeling methods and techniques, e.g. 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. Calibration of the case-study 1D SFB model described in [1] and [5] has been successfully conducted with use of two one-dimensional (1D) datasets (one for void fraction and one for fluid temperature) with the results shown in Figures 2.3 and 2.4. It is noteworthy that, in this example, not only the closure model parameters have been calibrated, but also the model discrepancy, which indicates the adequacy of overall model form, has been evaluated.

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, which are to be discussed in the following sections.

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 multiphysics models and software.

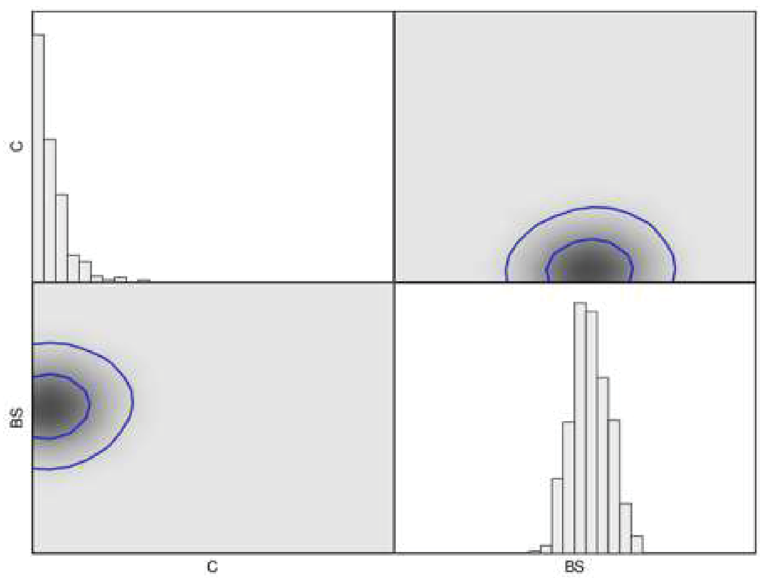

Figure 2.3. Posterior distributions of the condensation (C) and boiling suppression (BS) parameters [5].

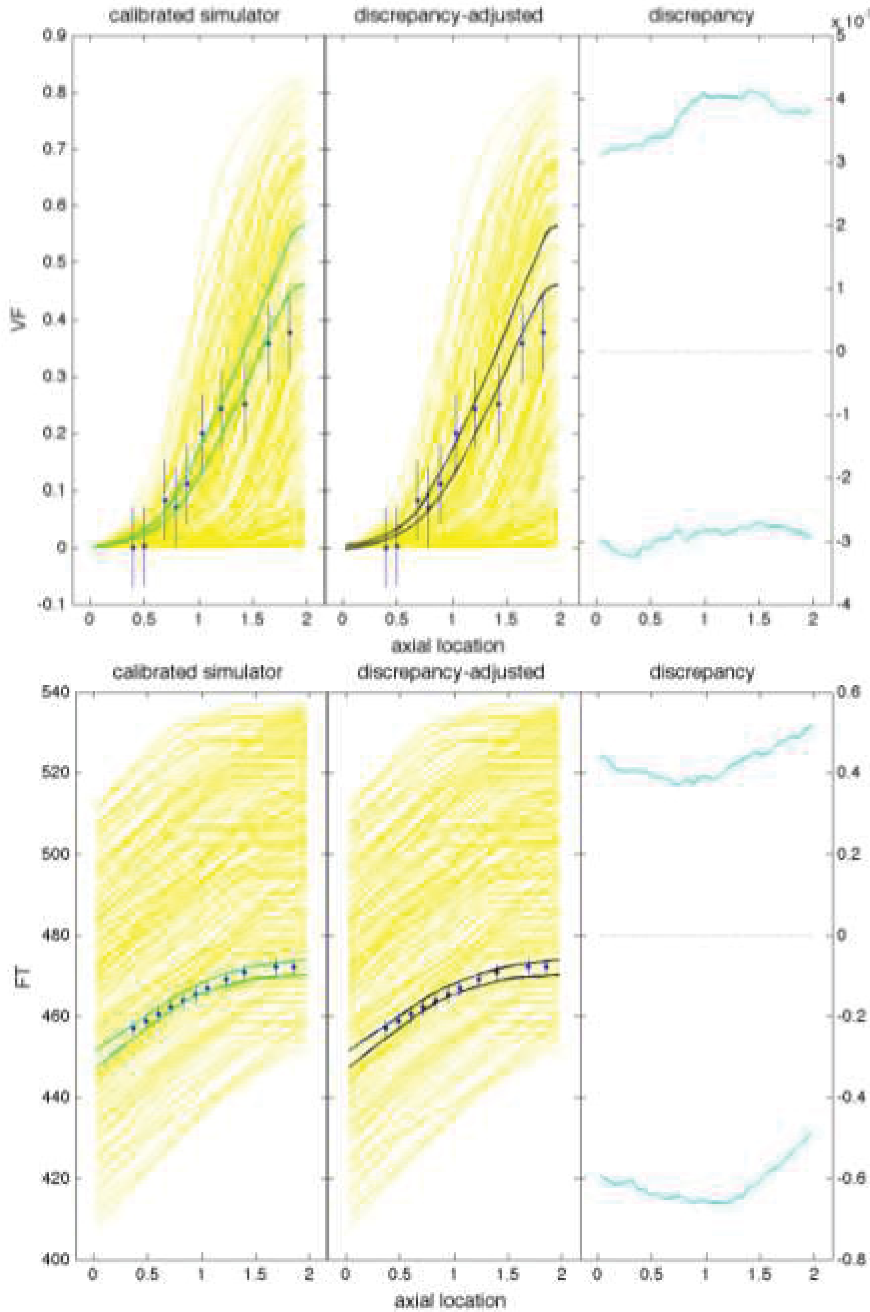

Figure 2.4. 90% pointwise probability intervals from calibrated model (green), discrepancy (cyan), and discrepancy-adjusted (black) posterior processes obtained for void fraction (left panel) and fluid temperature (right panel). Model simulations used for emulator construction are shown as yellow curves, while observed data are shown as blue dots with $\pm(1\sigma)$ *error bars. Bartolomej's void fraction (VF) data* [6] *and artificially generated (from simulation result) fluid temperature (FT) data were used* [5].

3. DATA COLLECTION AND CHARACTERIZATION TO SUPPORT SFB MODEL VALIDATION AND CALIBRATION

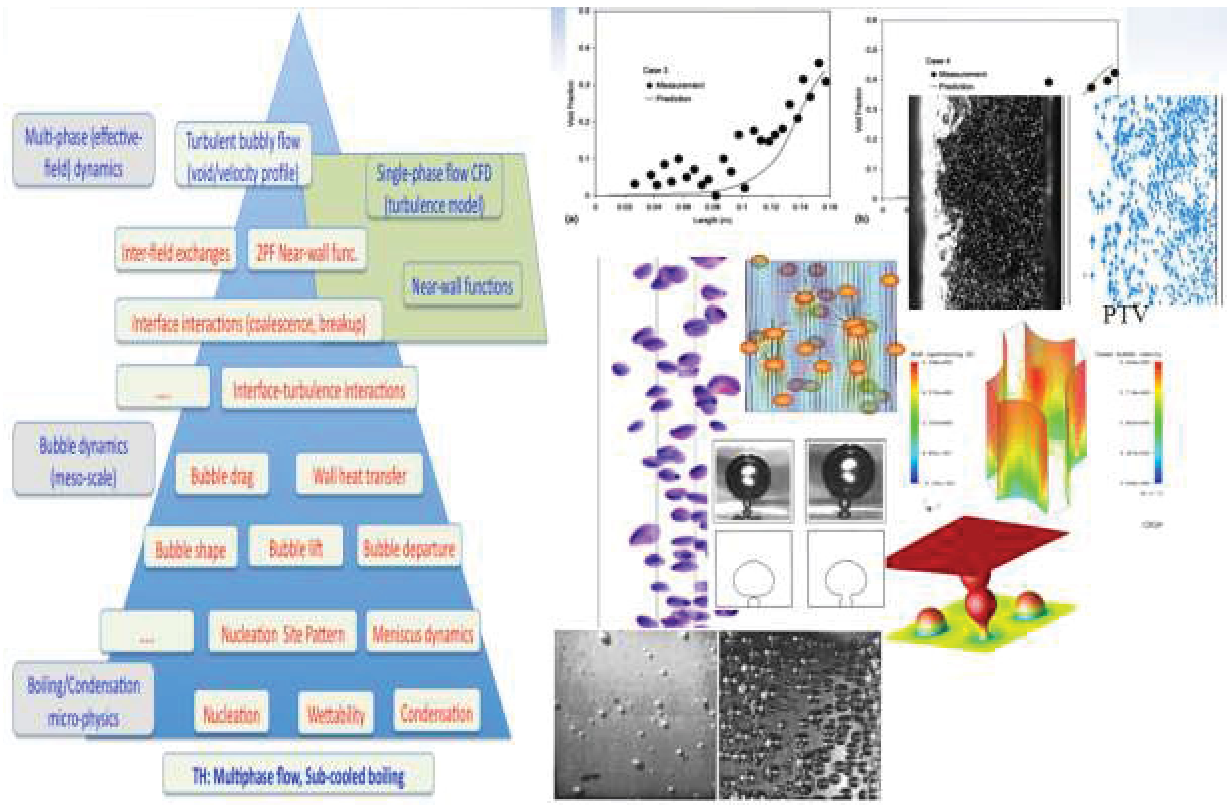

Figure 3.1. Subcooled flow boiling phenomenology and data sources.

3.1. Overview of the state-of-the art of (boiling) multiphase flow experimentation

Multiphase flow measurement is highly complicated due to:

- presence of multiple interacting phases with significantly different properties and high concentration of interfaces which obscures the flows and leads to difficulty in using optical measurement methods
- inter-dependence of flow characteristics/physics and interface morphology which varies significantly and, sometimes, abruptly with the change of flow regime
- strong influence of pressure, flow rate and heat flux on flow regime change which decreases scalability of data
- wide range of involved physical scales, from small scale, e.g. wall nucleation, bubble dynamics, etc., to large scale flow pattern change
- high speed, high frequency physics, e.g. bubble nucleation and growth, which can be hard to measure or observe
- presence of some important physics which can not be directly measured, observed or even known (e.g. partitioning of wall heat flux, heat transfer coefficient, etc.) and can only be indirectly deduced from others.

Measurement techniques are chosen depending on the considered physics:

- scale – large, small, microscopic, mesoscopic;
- flow conditions – pressure, temperature, flow rate;
- experiment type - SET or IET;
- flow characteristics of interest;
- fluid properties, etc.

Measurement of flows of subcooled boiling light water, which is used in LWRs as coolant, is greatly different from measurement of other multiphase flows which involve, for instance, oil, other liquids, or solid particles. The flow orientation (which defines the flow regime map) is mostly vertical.

The parameters which are measured in subcooled flow boiling experiments include [26]: (i) mass flow and velocity; (ii) temperature; (iii) void fraction; (iv) flow regimes; (v) wall shear stress and turbulence; (vi) critical heat flux (CHF); (vii) liquid level and film thickness; etc. Different techniques may be required for measurement of the above flow characteristics.

The transparency of water allows the use of optical or optical-based measurement methods, such as Particle Image Velocimetry (PIV), Ultrasonic/ Laser Doppler Anemometry (LDA), high-speed photography/videography, etc., which are used to study local characteristics of interfaces, e.g. bubble dynamics, bubble merge or breakup, flow regime transition, etc. These measurement techniques are commonly employed in small-scale separate effect tests (SETs) or experiments [11]. As seen in Table 3.1.1, such SETs are normally conducted under conditions with low pressure (mostly near atmospheric condition), low heat flux, low flow rate, and simplified flow geometry, which are much different from LWR-prototypical conditions.

In addition to optical-based methods and visual observations, non-intrusive methods such as (multi-beam) gamma-ray densitometry, X-ray tomography, X-ray attenuation, acoustic attenuation, gamma-ray/neutron scattering, etc., can be used to measure distributions of void fraction and variation of flow pattern [6][27].

Local flow characteristics can also be measured with intrusive methods using hot-film/wire anemometer probe, Pitot tube, microthermocouple [10], etc., in local velocity and temperature measurements, and fiber-optical probe, impedance void metering [28], double-sensor conductivity probe [29][30], capacitive sensor, etc., in local phase characteristic measurements.

Table 3.1.1. Some SFB experiments using optical-based measurement methods [11].

Publications	Euh et al. (2010)	Situ et al. (2004, 2008)	Basu et al. (2002)		Thorncroft et al. (1998)	Del Valle and Kenning (1985)
Reference No.	2	3, 4	5		6	7
Fluid	Water	Water	Water	Water	FC-87	Water
Flow Channel Geometry	Annulus	Annulus	almost square	3x3 rod bundle	Rectangular	Rectangular
Flow Directions	Upflow	Upflow	Upflow	Upflow	Upflow and Downflow	Upflow
Flow Area (cm^2)	8.54	8.54	16.33	9.66 (flow channel area - rods)	1.59	0.6
Heater Geometry	Cylindrical cartridge heater	Cylindrical cartridge heater	flat	nine-rod bundle zircalloy tubes (1.429 cm-pitch, 1.11 cm-OD)	Heating strip adhered to channel wall	flat rectangular strip
Heater Dimensions (length/ diameter)	1.91cm dia., 448cm length (284.5cm heated)	1.91cm dia., 267cm length (173cm heated)	30.5 cm length, 3.175 cm wide	91 cm - length 1.11 cm - tube dia. 0.015 cm -wall thickness	30cm long, 1.27cm wide, 0.015cm thick	0.08-0.2mm thickness
Heater Material	Stainless Steel	Stainless Steel	copper on one side of the channel	zircalloy-4 cladding	Nichrome	Stainless Steel
Heated Perimeter (cm)	6	6	3.175	9 rods x 3.49cm perimeter/rod	1.27	-
Heat Flux, kW/m^2	61-238	54.0-206	2.5-96.3	1.6-14.3	1.3-14.6	7500
Pressure, kPa	167-346	103	101.3	101.3	101	116.7
Saturation Temp (T_{sat})	~115-139°C	~100°C	~100°C	~100°C	38.4-42.3°C	104
Mass Flux (G), kg/m^2s	214-1869	466-900	124-886	186-631	190-666	up to 2000
Reynolds Number (Re)	1.75e4-1.78e6	-	-	-	3.3e3-11.5e3	V=1.7 m/s
Subcooling, K	7.5-23.4	80-98.5 (Inlet Temp.)	6.6 - 52.5	1.7 - 46	1.0-5.0	84
Contact Angle	-	-	30-90	57	-	-
Measurement Instrument	High-Speed Camera	CCD Camera	CCD Camera	CCD Camera	Digital High-Speed Camera	High speed cine films
Measured Parameters						
Bubble Depature Size	No	Yes	No	No	Yes	yes
Bubble Departure Frequency	Yes	Yes	No	No	Yes	no
Nucleation Site Density	No	No	Yes	Yes	No	Yes
Heat Flux at Onset of Nucleate Boiling	No	No	Yes	Yes	No	Yes
Bubble Growth Rate	No	Yes	No	No	Yes	Yes
Heat Transfer Coefficient	No	No	No	No	No	No
Bubble Velocity	No	Yes	No	No	No	No
Liquid Velocity	No	Yes	No	No	No	No
Void Fraction	No	No	No	No	No	No

Due to its importance in two-phase flow modeling, special interest has been devoted to flow pattern identification and flow regime map construction. Flow pattern identification can be based on a variety of measurement techniques and signals, which are classified as follows [26]:

- Direct observation using
    - Visual and high-speed photography/videography
    - X-ray attenuation imaging
    - Electrical contact probes
    - Gamma-ray densitometry
- Indirect determination from
    - Static pressure oscillation analysis
    - X-ray attenuation fluctuation analysis
    - Thermal neutron scattering "noise" analysis
    - Drag-disk signal analysis.

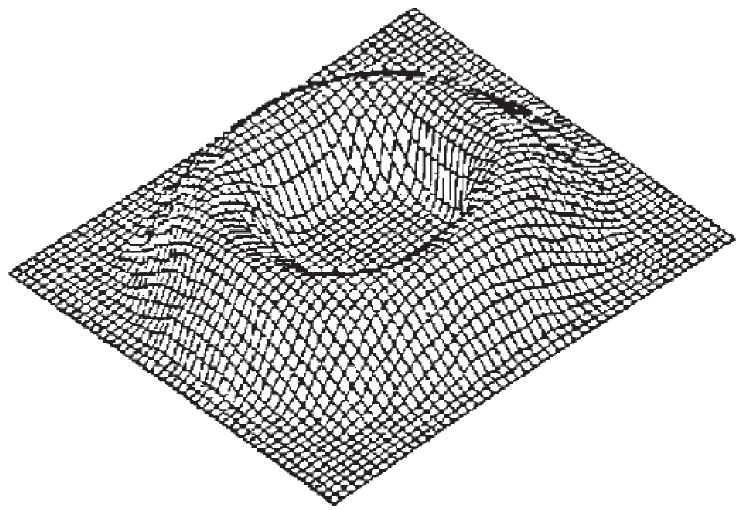

Figure 3.1.1. Void fraction distribution in a concentric annulus measured by Lahey, 1988, using gamma-ray scattering technique [27].

These techniques vary greatly in accuracy, intrusiveness, and working range limitations (concerning pressure, temperature, flow rate, etc.). Since the flow pattern can not directly be measured, interpretation of measurement data and observations and construction of flow regime maps have to rely on sophisticated "models" which reflect current understandings about the involved physics [26]. For instance, a model of attenuation of gamma rays of different energies in two-phase vapor-fluid medium and wall material is needed to determine void fraction from the ray intensity measurements using gamma-densitometry technique [27]. The employment of such "models", however, introduces extra "epistemic" uncertainty to flow regime map modeling.

Regarding measurement errors, high measurement accuracy is generally expected for small-scale laboratory tests using non-intrusive measurement methods and, conversely, lower accuracy is expected for plant observations and intrusive measurements. As noted earlier, each measurement technique has its own rangeability, sensitivity, response time, accuracy and reliability specifics, which have to be taken into account in determining measurement errors and associated data uncertainty. In nuclear industrial applications, the reliability is an important characteristic of measurement instruments/sensors used in long-term plant monitoring and their accuracy degradation or drifting caused by long exposure to adverse conditions should be accounted for in measurement error calculation.

Uncertainty arises when a parameter is deduced from several measured parameters leading to *error propagation* [27]. For instance, error in the mixture density estimate can be very high at high void fraction, when it is calculated using measurements of vapor and fluid densities and volume fractions (Figure 3.1.2).

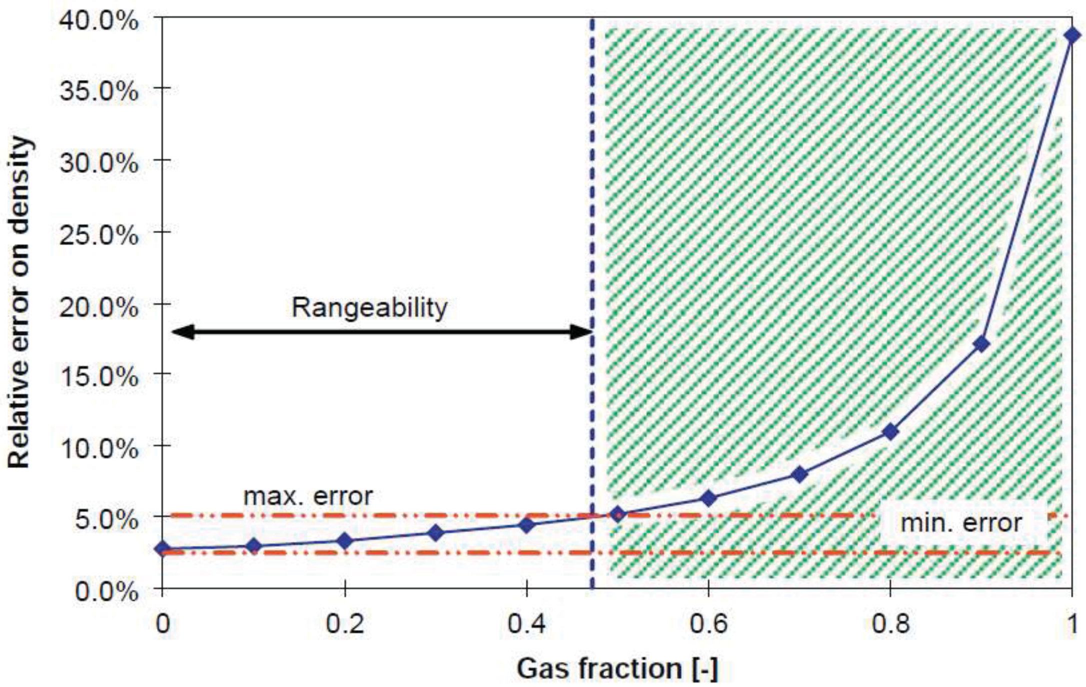

Figure 3.1.2. Relative error for the mixture density defined as a function of void and fluid fractions and densities [27].

The estimates of accuracy and measurement errors of a typical boiling experiment using gamma-ray densitometry are shown in Tables 3.1.2 and 3.1.3.

Table 3.1.2. Estimated accuracy of NUPEC measurements [31].

Quantity	Accuracy
Process parameters	
Pressure	1 %
Flow	1.5%
Power	1 %
Fluid temperature	1 Celsius
Void fraction measurement	
CT measurement	
Gamma-ray beam width	1 mm
Subchannel averaged (steady-state)	3% void
Spatial resolution of one pixel	0.5 mm
Chordal measurement	
Gamma-ray beam width (center)	3 mm
Gamma-ray beam width (side)	2 mm
Sub-channel averaged (steady-state)	4% void
Sub-channel averaged (transient)	5% void

Table 3.1.3. Estimates of error sources in NUPEC void measurements [31].

Error source		Chordal Averaged		CT Averaged
		Steady-state	Transient	
γ-ray measurement	Effect of surrounding condition (magnetic-field and temperature) on measurement system	0.1%	0.1%	0.1%
	Randomness of γ-ray source decay	0.02%	0.2%	0.1%
	Correction error due to back ground	0.0%	0.0%	0.0%
	Correction error due to counting loss	<0.5%	<0.5%	<0.1%
	Calibration error	0.1%	0.1%	0.1%
	Correction error due to attenuation by surrounding water	0.0%	0.0%	-
	Correction error due to scattering from multi γ-rays	<0.2%	<0.2%	-
	Total	<0.55%	<0.6%	<0.2%
Sub-channel density	Transfer to density	<9 kg/m^3	<10 kg/m^3	<15 kg/m^3
	Distribution error to Sub-channel	<5 kg/m^3	<5 kg/m^3	-
Correlation error from Chordal averaged to CT averaged		<6 kg/m^3	<6 kg/m^3	-
Sub-channel density		<20 kg/m^3	<21 kg/m^3	<15 kg/m^3
Sub-channel void*		0.040	0.042	0.030
Uncertainty (1σ)		4 %	5 %	3 %

Recommendation: To be useful in model calibration and validation, measurement data should be accompanied with information about measurement technique, history of measurement sensor calibration, error estimates of the relevant measured parameters and the formulations (or models) used to derive the data of interest from raw measurements. Such information is needed to independently assess data uncertainty.

3.2. Review of experimental and DNS data relevant to subcooled flow boiling

The purpose of experimental studies into subcooled flow boiling conducted in the past were mostly to acquire better knowledge and understanding about phenomenology and (local) mechanisms, which were needed in the development of analytical models used in various engineering practices (not restricted to nuclear engineering). Tables 3.2.1 and 3.2.2 list some of those experiments, most of them can be classified as integral effect tests (IETs) as the primary objectives of these measurements were distributions of void fraction, fluid temperature, and, in some cases, phase velocities and/or pressure drop. All the experiments in the tables used water as working fluid, and few experiments were conducted under the pressure range comparable to that of either BWRs (~7 MPa) or PWRs (15-16 MPa). It is worth to note modern experiments, which employed refrigerants as working fluid, such as DEBORA tests [32], whose conditions after scaling were comparable to those of high-pressure water tests.

Table 3.2.1. Low-pressure subcooled flow boiling experiments [33].

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

Table 3.2.2. High-pressure subcooled flow boiling experiments [33].

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

Table 3.2.3. Experiments to determine bubble departure size [33].

Author	Geometry (m) D or Dh	Pressure (kPa)	Heat flux (MW m^{-2})	Mass flux (kg m^{-2} s^{-1})	Measurement instrument
Fritz (1935)[a]	–	–	–	–	–
Gunther (1951)	Rectangular 0.0017	101–1100	–	1400–10 760	High-speed photography
Koumoutsos et al. (1968)	Rectangular 0.0476	101	–	34–340	High-speed cinematography
Al-Hayes and Winterton (1981)	Circular 0.019	–	–	–	–
Bibeau and Salcudean (1994a,b)	Annular 0.0093	105	0.1–1.2	79–790	High-speed cinematography
Zeitoun and Shoukri (1997)	Annular 0.0127	117–168	0.29–0.71	150–410	High-speed photography, video
Thorncroft (1998)	Rectangular 0.0127	101	0.0013–0.0146	190–670	High-speed video
Bartel et al. (1999)	Annular 0.019	101	0.024–0.14	400–750	High-speed photography

Many separate effect experiments (SETs) were also conducted to investigate particular phenomena, which govern subcooled flow boiling, in particular

- Boiling curve [34][10];
- Wall heat flux partitioning [13][20];
- Onset of Nucleate Boiling (ONB) and Significant Void (OSV) [35][12][10];
- Departure from Nucleate Boiling (DNB) and Critical boiling Heat Flux (CHF) [10];
- Nucleation site density [9][22][12][36];
- Interfacial area density [33][10][37];
- Bubble growth and departure dynamics [38][33][14][36] (Table 3.2.3);
- In-flow bubble dynamics [39][40][37];
- Boiling crisis - DNB and CHF [41][42][43][44][45].

Being conducted under laboratorial (controlled), atmospheric/low pressure conditions, the above SETs (mostly employing optical methods) could provide data on small-scale phenomena with low measurement error (unless the stochastic nature of some phenomena makes “deterministic” measurement intractable.

These data were used in the development of phenomenological analytical models as described in [19][46], which can be used in CMFD codes as closure models.

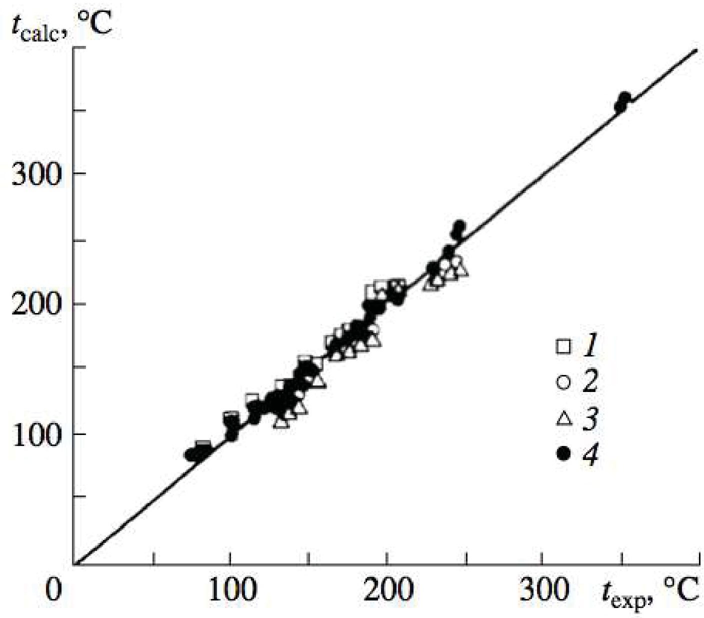

Figure 3.2.1. Wall temperature measurements [19] *– p = 0.6-17 MPa, q = 0.5-6 MW/m^2.*

	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 3.2.2. Experimental data on the ONB [12] *– 0.1-13.75 MPa, velocity = 0-17 m/s.*

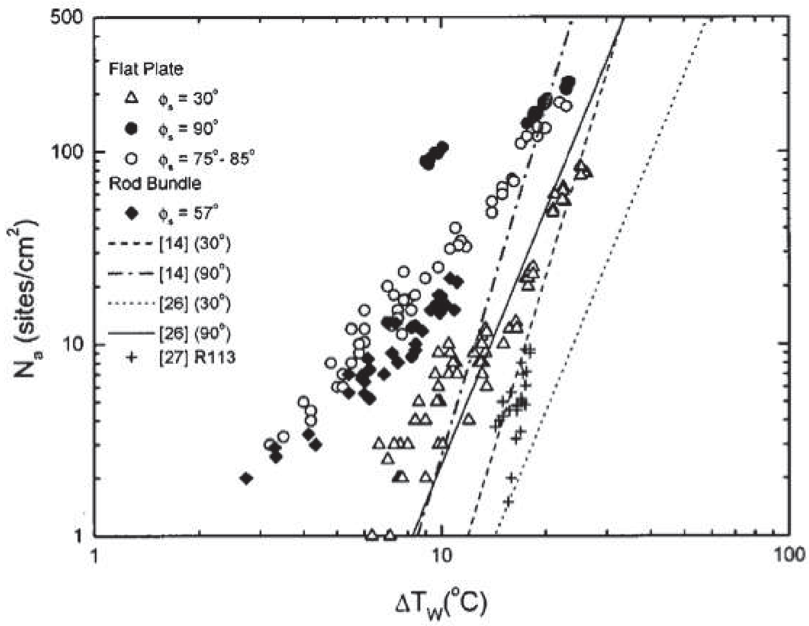

Figure 3.2.3. Measured nucleate site density [12] *– 0.1-13.75 MPa, velocity = 0-17 m/s. Note a large uncertainty in characterization of foundational processes in boiling.*

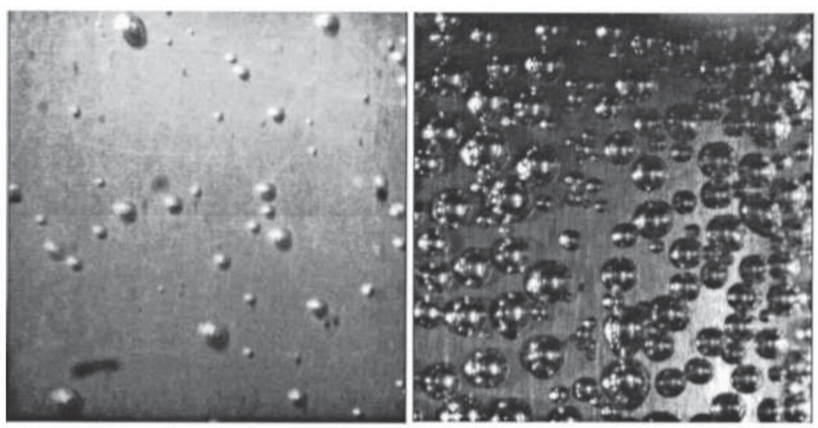

Figure 3.2.4. Observations of the boiling surface [12] *– (a) contact angle of 30^o; (b) contact angle of 90^o. Note a significant dependence on surface characteristics (a diffeernt physics).*

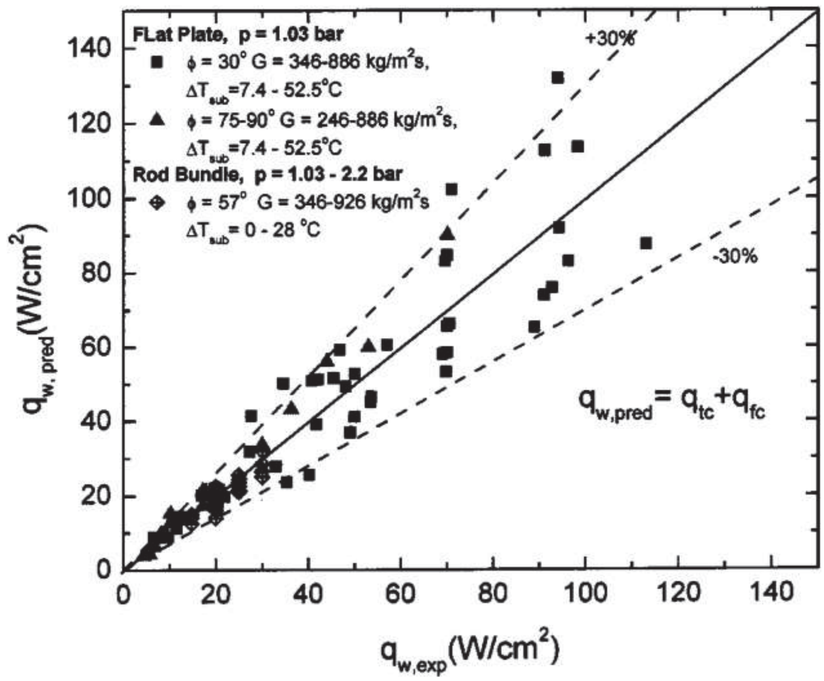

Figure 3.2.5. Wall heat flux [20] – *p=0.1-0.22 MPa. Note the low pressure and relatively low mass flux range of data.*

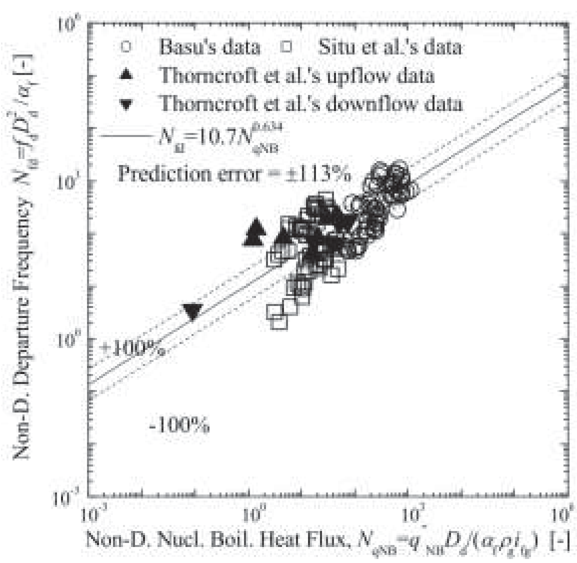

Figure 3.2.6. Comparison between predicted and measured dimensionless bubble departure frequencies [14] – *atmospheric pressure. Note a large uncertainty in characterization of fundamental mechanisms/processes.*

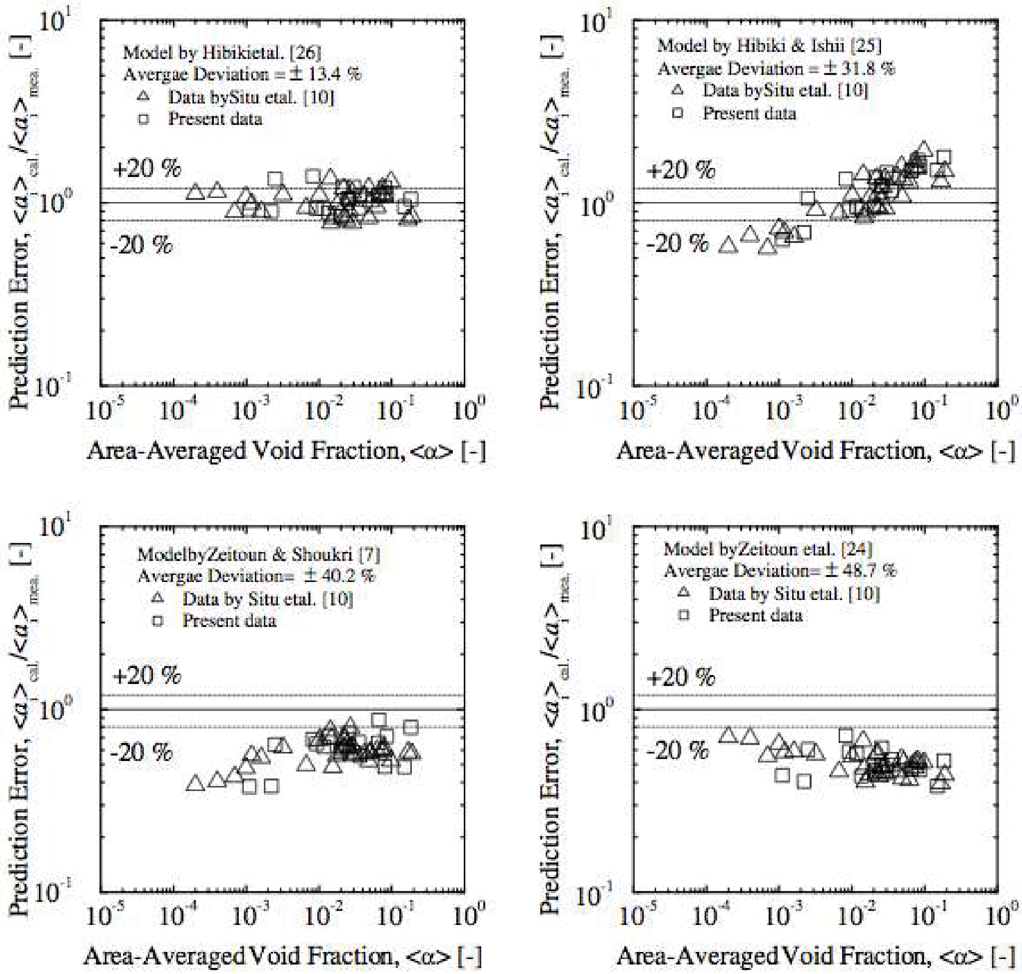

Figure 3.2.7. Measurement and prediction of average interfacial area [37] *– low pressure conditions. (Note: integral quantities are characterized with lower, still large, uncertainty).*

Plant measurements and observations (PMOs) are mostly at the large scale, integral-physics level. They can be provided, for instance, by various plant online monitoring systems and system/component maintenance logs. Such data are very plant-dependent and mostly proprietary information. Although having good relevancy and scalability (for a particular plant/system), such data may be of poor quality, since measurement error/uncertainty is usually not controlled. For some plant conditions, e.g. during severe accident progression, these data are the only information, which is available for comparison with model predictions.

Direct Numerical Simulations (DNS) based on high-fidelity first-principle modeling of two-phase flows and related interfacial phenomena [15][47] can also provide "data" for calibration and VUQ of computer models of lower precision. The accuracy of data can be determined from estimates of numerical error and model-form/model-assumption inadequacy. Numerical experiments based on DNS have an advantage that they can provide detailed data of almost any temporal and spatial resolutions, which are only restricted by available computational resources.

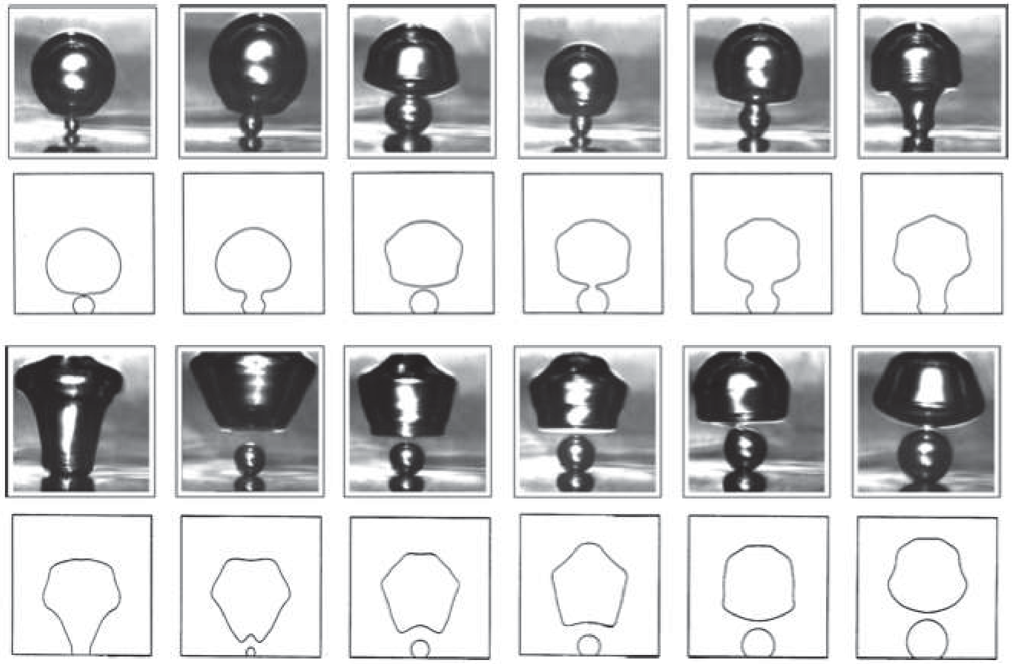

Figure 3.2.8. Bubble dynamics – experimental data and ITM-DNS results [15] *– atmospheric pressure. Note: multi-dimensional data (images), both experimental and computational, require a different approach to validation.*

New experiments have been planned and conducted for CASL validation of CMFD and ITM capabilities [48][49]; all of them have been extensively employing optical-based measurement methods, e.g. high-speed videography, IR thermography, PIV, etc. The MIT experiments [49] seem to be most comprehensive and providing a wide range of data on mechanisms of subcooled flow boiling including subcooled boiling curves, heat transfer coefficient, nucleate site density, bubble departure frequency/diameter, and bubble sliding. The data have been processed to develop models for bubble departure diameter, microlayer heat transfer, and bubble condensation, which can be used as closure models in CMFD codes to determine wall heat flux partitioning and evaporation rate. It is worth noting that the MIT experiments have employed water as working fluid and been conducted under near atmospheric pressure condition (see Table 3.2.4). Consequently, care must be exercised in applying these data for calibration of models to be used for predicting SFB and DNB under the PWR reactor conditions.

Table 3.2.4. Comparison of experimental conditions and scaling parameters [49].

Parameter:	Sugrue et al. (MIT)	Situ et al.	DEBORA	PWR hot channel
Fluid	Water	Water	Refrigerant R12	Water
Orientation	0°, 30°, 45°, 60°, 90°, 180°	Vertical upflow	Vertical upflow	Vertical upflow
Channel	Rect., D_e=16.7mm	Annular, D_e=19.1mm	Pipe, D_e=19.2mm	Rod Bundle, D_e=11.8mm
Mass Flux [kg/m²s]	250 – 400	466 – 900	2000 – 3000	~3700
Heat Flux [kW/m²]	50, 100	54 – 206	73, 76	1000-1400
Subcooling [°C]	10°, 20°	2 – 20°	13 – 29°	10 – 30°
Pressure [kPa]	101, 202, 505	101	1460 – 2620	1550
Reynolds #	11800 – 34500	2.9×10^4 - 5.7×10^4	3.05×10^5 – 4.47×10^5	~5.3×10^5
Froude #	0.42 – 1.06	6.2 – 12.5	22 – 54	~199
Typical Bubble Size:	0.23 – 1.0 mm	0.15 – 0.61 mm	0.3 – 0.6 mm	~0.1 mm
Contact Angles:	α = 91°, β = 8°	α = 55° β = 35°	None measured	α^2 = 30-50° β^2 = 5-15°
Boiling #	1.11×10^{-7} – 8.49×10^{-5}	2.66×10^{-8} – 1.96×10^{-7}	3.23×10^{-4} – 4.36×10^{-4}	2.80×10^{-7}
Jakob #	0.0056 – 0.00934	0.0056 – 0.0187	0.976 – 1.33	0.0465
Eotvos #	0.008 – 0.159	0.003 – 0.059	2.3 – 4.6	0.0103
Morton #	3.91×10^{-13}	3.91×10^{-13}	2.6×10^{-11} – 1×10^{-10}	5.95×10^{-12}
Weber #	0.255 – 2.834	0.577 – 8.75	0.73×10^3 – 2.18×10^3	495

3.3. Strategy for quantification of data needs, data collection, validation, and characterization

With the model calibration, validation and uncertainty quantification proposed as above, 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 are broadly outlined by Nam Dinh in [2] and [3], which can be based on the factors, such as:

- Scope of involved physics and strength of their couplings – turbulence, boiling, heat transfer mode, convection mode, etc.; single physics (SETs) or multiphysics (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.;

Parameters, such as Reactor Prototypicality Parameter (RPP) and Experimental Measurement Uncertainty (EMU) have been introduced in [3] to quantify the above characteristics of data. While EMU can be derived from data errors as briefly described in section 3.1, RPP, which quantifies data scalability, is not simply defined as the ratio of scaling parameters $[Sc_{Mod\_K}]_{EXP}$ /$[Sc_{Mod\_K}]_{APP}$ as in [3]. The reason is that the involved physics are not linearly or similarly scaled up or down based on system size or any of parameters of interest such as pressure, temperature, material properties, etc. Consequently, scalings based on size, material properties, pressure, temperature, etc. may have different weights, which contribute differently to the overall scalability of a dataset. The RPP, therefore, is worth to decompose into a number of sub-parameters which represent the scalabilities of every parameters of significance in defining the similarity between the experiment and the considered reactor conditions.

Traditionally, many dimensionless numbers/groups have been derived and used to "homogenize" or generalize experimental data, e.g. Reynolds, Re, Prandtl, Pr, Nusselt, Nu, Raleigh, Ra, Biot, Bi, Peclet, Pe, Strouhal, St, etc., numbers in general thermal fluid dynamics, and Weber number, We, boiling number, Bo, bubble Reynolds number, Re_b, Jacob number, Ja, Eötvös number, Eo, Martinelli parameter, X, etc., in systems involving evaporation, condensation and bubble formation/transport. These dimensionless numbers and groups can be useful in our classification and characterization of subcooled flow boiling data for the purpose of scalability assessment. Examples of data scaling shown in Figures 3.3.1-3.3.2 demonstrate the use of dimensionless groups and numbers to reveal the relevancy of data obtained from small-scale low-pressure tests using fluids of different properties to what happening under LWR-prototypical conditions/scenarios.

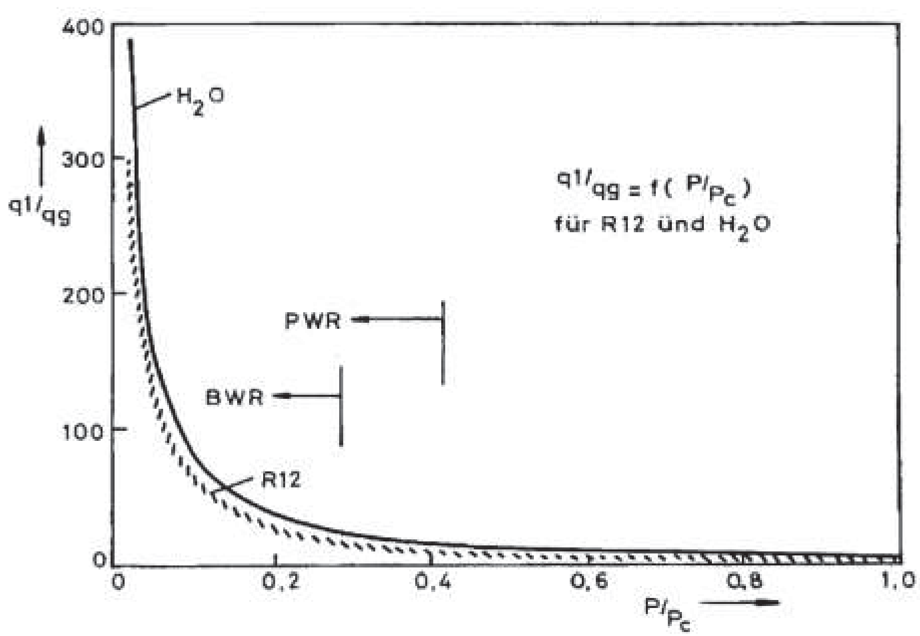

Figure 3.3.1. Similarity of liquid-vapor density ratio of water and Freon 12 as a function of dimensionless (p/p_{cr}) (p_{cr} - critical pressure) [50] .

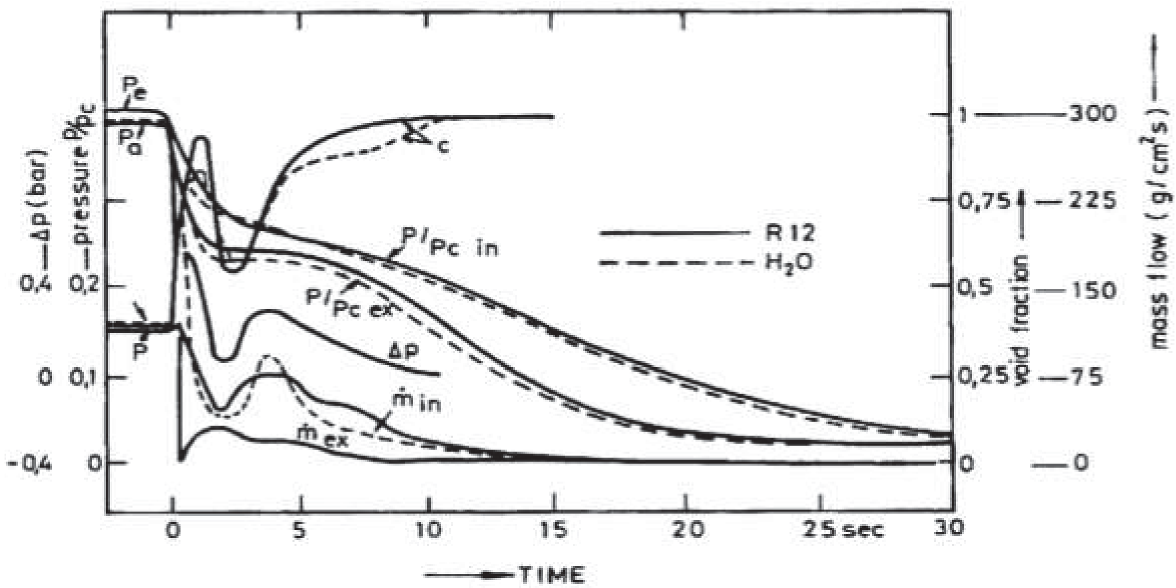

Figure 3.3.2. Comparison of water and Freon 12 measurements of blowdown during LOCA [50] .

Review of scaling laws applicable to two-phase flows and boiling heat transfer can be found in the study by Mayinger [50]. A few important conclusions were drawn as follows:

- Scaling law applicability is more restricted in two-phase flows as compared to single-phase flows: scaling laws can be applied simultaneously to hydrodynamics and heat transfer in single-phase flows, while, in two-phase flows, each scaling law or number is only valid for a single specific phenomenon.
- The above restriction/limitation of scaling in two-phase flows is caused by the involvement of more interacting physics/ phenomena, which makes it necessary to use more physics-dependent scaling laws/groups which may have different “weights” in defining overall scalability.
- Testing and validation of scaling laws can be done with use of advanced modeling software (which is based on the universally applicable (regardless of the scale) conservation laws and other thermodynamic fundamentals).

The last conclusion is especially interesting, as it points to the potential use of CFD and even less advanced system thermal hydraulic codes like RELAP5, TRACE, etc., in scalability and relevancy assessment of experimental data.

The employment of multiple physics-dependent scaling laws and groups necessitates a deep understanding of each involved physical phenomenon and its significance in the considered scenario/application. For instance, the physics of evaporation at heating walls is of paramount importance in subcooled flow boiling and scaling groups concerning heat transfer near the walls (wall heat flux partitioning, nucleation, bubble growth/departure dynamics, etc.) are going to have higher weights compared to the ones representing other physics. However, the “significance” of particular physics should be quantified. Decomposition of the SFB model hierarchy (Figure 2.2) and experimental and/or numerical sensitivity study of the involved physical models can provide information for this “significance” quantification. The approach outlined in [25] for phenomena importance ranking can also be applied in this respect.

An example of statistical analysis of the SFB sub-models (condensation with parameter *C* and evaporation with parameter *BS*) is presented in [5], which indicated the relative small significance of condensation of vapor in subcooled fluid in defining vapor and temperature distributions in a pipe (Figure 3.3.3).

Scaling analysis can be made application- or scenario-dependent as described in [25], in which scaling of a complex system/process/scenario with all participating physics is analyzed using a hierarchical two-tiered (bottom-up and top-down) scaling methodology. Such an analysis helps to determine relevant dimensionless groups and reveal the relative importance/significance of participating physics and/or system characteristics (size, material properties, etc.).

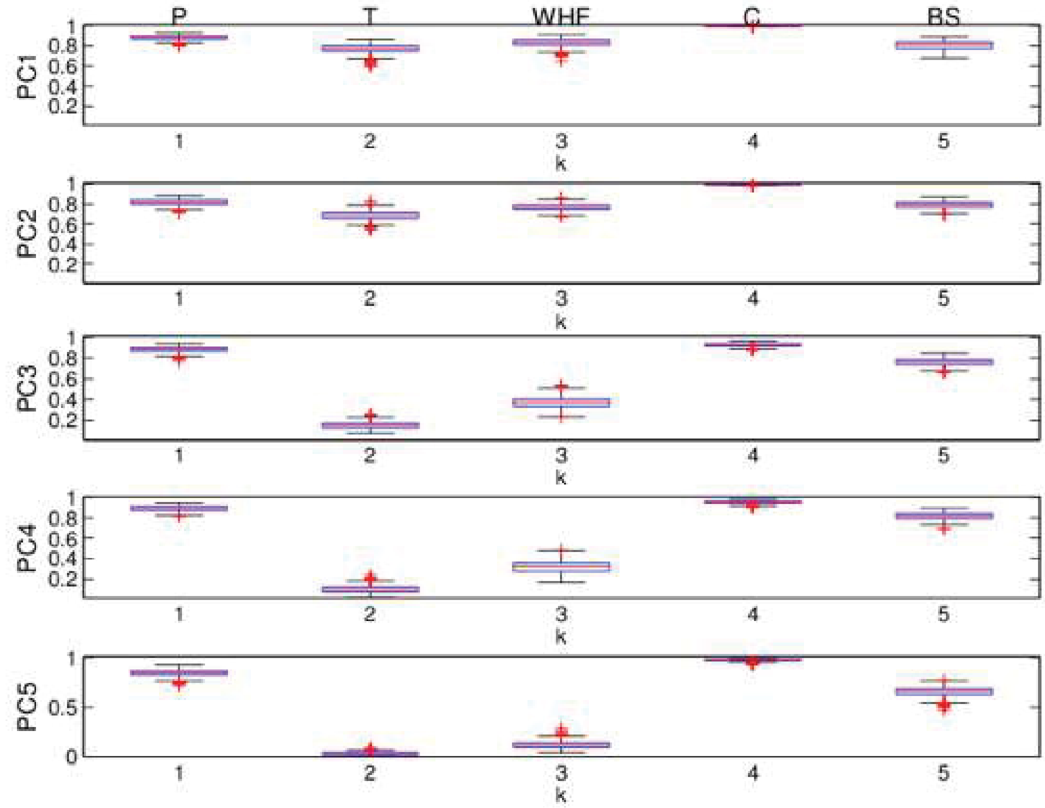

Figure 3.3.3. Boxplots of the marginal posterior distribution of parameter $\rho_{\omega i}$ (correlation length) of different principal components (PC) [5]. *Values for condensation parameter C are seen to concentrate near 1 indicating that C is an insensitive parameter.*

Data validation is important as it helps to detect and correct faulty data. As described in [51], faulty data can be detected with use of simple checks for the “outliers”, which are outside the range of either sensor or physical feasibility, gaps in the data, unphysical invariance or erratic change of data, which are indications of faulty sensors, etc. Faulty data can also be identified using more sophisticated physical or mathematical model based methods, which rely on statistical/correlation/inconsistency analyses, physical modeling and/or data mining technology [51]. Numerical analysis using advanced modeling tools can be added to this group and used to establish an envelope of data variation which helps to filter out faulty data.

When faulty data are found, they can either be eliminated altogether or corrected using interpolation, smoothing, and/or data reconciliation methods [51]. Sophisticated data mining technology can also be used to extract as much useful information as possible from a faulty dataset and/or to substitute faulty data with more probable values.

Based on the above discussions, a step-by-step guideline for validation data collection and characterization can be derived for a specific application/ scenario as follows:

1. Construction of the list of involved physics with graded significance. Conducting physics sensitivity study if needed;
2. Collection of data relevant to all prevailing participating physics and overall phenomenology;
3. Classification of data based on physics and associated significance;
4. Data validation using the methods delineated in [51];
5. Assessment of data uncertainty based on available measurement error information and scalability based on representative (corresponding to physics) dimensionless groups; construction of weighting factors based on this assessment;
6. Storing of validated data based on classification (defined in step 3) and weighting factors (derived in step 5);
7. Identification of additional data needed for validation of particular physical models and assessment of their significance.

3.4. Example of quantification of data needs, data classification and characterization to support SFB model validation and calibration

For the subcooled flow boiling phenomenon, the major involved physics are schematically shown in Figure 2.2 and also in Table 3.4.1 together with information about available data sources.

Table 3.4.1. Major physics involved in SFB and data sources.

Physics			Exp. data acquisition method	Data availability	
				Exp.	DNS
Two-phase fluid dynamics	Turbulence		Direct	●	●
	(Dispersed) phase transport		Direct	●	●
	Wall friction		Indirect	●	
	Mixing in the complex geometry of a LWR core		Indirect	●	●
	Two-phase flow instability		Direct	●	
	Mechanical interactions between phases	Drag, Lift, Virtual mass forces	Indirect	●	●
		Interfacial tension force - bubble breakup & coalescence	Direct	●	●
Two-phase heat-mass transfer	Convective heat transfer		Indirect	●	
	Wall heat flux partitioning		Indirect	●	
	Wall evaporation	ONB, OSV	Direct	●	
		Nucleation		●	
		Bubble growth dynamics		●	●
		Bubble detachment		●	●
		Boiling crisis (CHF)	Indirect	●	
	Thermal interactions between phases	Vapor condensation in bulk flow	Indirect	●	

ONB – Onset of Nucleate Boiling; OSV – Onset of Significant Void; CHF – Critical Heat Flux; Indirect – indirect determination; Direct – direct measurements and observations.

The significance of physics can be estimated based on the dominant factors which govern the process/scenario of interest. For SFB, heat-mass transfer is the dominant factor and, among many physics which defines heat-mass transfer, wall evaporation is found to be most important phenomenon. Wall evaporation, however, is driven by other processes, e.g. nucleation, bubble growth/detachment dynamics, etc. Consequently, it can only be indirectly determined from other measurements and observations, leading to high data uncertainty (caused by error propagation as described in section 3.1).

The sensitivity analysis presented in [5] helps to determine that wall evaporation is more important compared to condensation in SFB.

The physics listed in Table 3.1 are sometimes inter-dependent. Wall heat flux partitioning, for instance, is closely related to wall convective heat transfer and wall evaporation, and the rate of vapor condensation in subcooled bulk flow is dependent of vapor bubble transport from wall to flow core. Another example is the increase of boiling crisis threshold (CHF) due to the presence of mixing promotion devices in LWR core, i.e. mixing vanes.

Currently considered SFB model [1] is one-dimensional and relies on a closure model of wall boiling heat flux, which is an integral quantity related to both wall heat flux partitioning and wall evaporation. Direct measurement of wall boiling heat transfer is not possible and it has been indirectly derived from other models and measurements as described in [13][20], which include models of (i) ONB and OSV thresholds, (ii) nucleation site density, (ii) bubble growth and weighting times, (iii) bubble departure and lift-off, etc., and corresponding measurements [12] to verify these models. (The employment of such "sub-models" for data derivation would introduce additional uncertainty to data, since they are all based on current (not necessarily correct as pointed out in [3] – nucleation prediction example) understandings about underlying physics.)

With this relatively simple formulation of the SFB model and current implementation of calibration & validation technique, integral data on 1D axial vapor and fluid temperature distributions together with measurement error are needed. Although experimental data on vapor and fluid temperature distributions can be found in many references, e.g. [6][7][32][8], detailed information about measurement errors are hard to come by.

Following Delhaye et al. [52], the following scaling factors are used here in subcooled boiling flow data characterization:

- Pressure scale, p/p_{cr};
- Geometric scale, $D_h/D_{h,RPP}$;
- Vapor/liquid density ratio, i.e. ρ_g / ρ_f;
- Weber number, which quantifies the similarity in mass flux, i.e. We = $G^2 D_h/(\sigma \rho_f)$;
- Boiling number, which quantifies the similarity in evaporation, i.e. Bo = $q_w/(G h_{fg})$;
- Inlet equilibrium quality, which quantifies the similarity in inlet fluid subcooling, i.e. $x_{eq,in} = (h_{f,in} - h_f)/h_{fg}$.

A scaling factor that quantifies the effects of LWR core geometric "complexity", i.e. rod/gap sizes, spacer positions, mixing vane presence, etc., may also be needed in a more comprehensive characterization of validation data for LWR applications.

If bubble transport model is the objective of calibration and validation, other scaling factors, such as bubble Reynolds number, Eötvös number, and Morton number, should be taken into account. Here, the so-called "application-oriented" approach to validation data characterization is again demonstrated.

Table 3.4.2: Operating conditions of typical LWRs [45]

Condition	PWR	BWR	VVER
Pressure (MPa)	~15.7	~7.2	~15.7
Average mass flux ($kg/m^2 s$)	~4000	~3000	~4000
Core exit temperature (^oC)	~315	Saturation temperature	~315÷320
Fuel rod diameter (mm)	~9.5	~12.3	9.1
Pitch to diameter ratio	~1.3	~1.3	~1.4
Fuel lattice configuration	Square	Square	Hexagonal

Table 3.4.3: Estimates of scaling factors of Bartolomej et al's [6][7] and DEBORA [28][53] experiments compared to the PWR conditions.

Scaling factor	Bartolomej et al.'s experiments	DEBORA experiments	PWR conditions
p/p_{cr}	0.136-0.682	0.353-0.633	0.712
$D_h/D_{h,PWR}$	1.1	1.745	1.0
ρ_g / ρ_f	0.053÷0.161	0.072÷0.169	0.176
We, 10^3	0.151÷17.107	0.73÷2.18	3.32
Bo, 10^{-4}	1.9÷13.3	3.23÷4.36	3.56
$x_{eq,in}$	-(0.455÷0.156)	-(0.126÷0.059)	-0.357

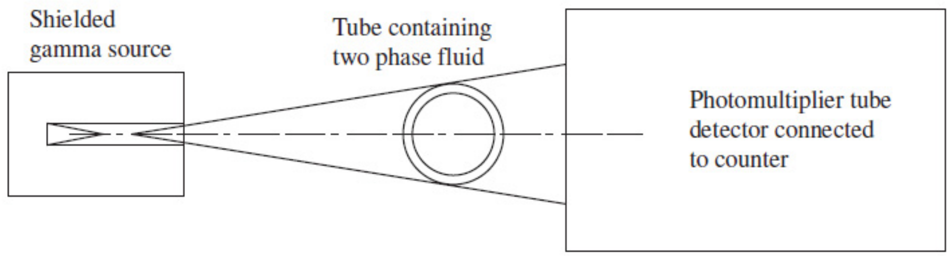

Figure 3.4.1: The principle of "broad-beam" gamma densitometry used in Bartolomej et al. [6][7] *experiments (illustration from* [27]*).*

Two experiment series are compared here in terms of data characterization: the high-pressure Bartolomej et al's [6][7], which employed water as working fluid, and the low-pressure DEBORA, which used Freon 12 (R-12) [54]. Axial gas volume fraction was measured by means of moving "broad-beam" gamma densitometry (Figure 3.4.1) in Bartolomej et al's experiments, while radial profile of gas volume fraction at the end of the heating section was obtained using a two-sensors optical probe in DEBORA experiments. Some measurements of radial profile of fluid temperature in Bartolemej et al's experiments and axial profile of fluid temperature in DEBORA experiments were also reported.

As seen in Table 3.3, experimental data obtained in Bartolomej et al's [6][7] and DEBORA experiments are scaled relatively well compared to the PWR conditions using the scaling parameters shown in the table. The value of these data in calibration and validation of computer models which are going to be used in PWR simulations can be judged based on these scaling parameters. In this limited study, the scaling parameters were determined for whole experiment series. It is, however, recommended that each dataset (obtained from a separate experiment) is accompanied with such information. An overall scalability grading factor can be derived based on these parameters and *a sensitivity analysis*, which defines the weight of each parameter.

In measurement of void fraction in [6][7], a maximum relative error of 1% was reported. However, since void fraction was not directly measured, but determined from the resulted beam intensity which changes as a result of absorption in accordance with the following correlation [24]

$$I = I_0 \exp(-\mu_w l_w) \exp(-\mu_f l_f),$$

where I_0 is the initial beam intensity, $\mu_{w,f}$ are the linear absorption coefficients in wall and fluid, and $l_{w,f}$ are the path lengths though wall and fluid, the measurement error may vary greatly as a result of "error propagation" (see section 3.1), and additional uncertainty is introduced from errors in estimating above parameters. Complicating the matter further, in the plane shown in Figure 3.4.1, the portions of gamma beam absorbed in walls and in fluid vary greatly depending on the direction of each beam path and it is difficult to precisely determine the average (over channel cross-section) void/fluid volume fraction based on the integral measurement of beam intensity provided by the detector. As fluid density and correspondingly fluid gamma absorption coefficient change with pressure, measurement calibration is necessary for each new experimental pressure setting. The measurement error may also depend on the flow pattern change, which can not be determined from this integral measurement alone. The resulted measurement error, therefore, may vary along the measurement length, and this *local* measurement error (instead of the normally provided *global* measurement error estimate [7][8]) can be used in the chosen calibration and validation technique [5].

Uncertainty in direct measurement of local (radial) void fraction by means of optical probe as in DEBORA experiments [28][32] can be resulted from the inference of void fraction from the frequency of (discrete) gas and fluid phase passage (respective residence times) and possible disturbance of flow and phase transport by the probe. In the DEBORA experiments [32], a global uncertainty of ±0.01 for void fraction measurement was estimated. However, there were several assumptions used in data treatment which might affect this estimate which included

- The flow regime was bubbly and the bubbles were spherical;
- The gas velocity was constant for every bubble regardless of its size;
- The effect of sensor intrusion on bubble shape, velocity and trajectory was negligible;
- Small bubbles which could not be detected by the sensor(s) had insignificant effect on void fraction.

Since the local phase velocity was not measured, information about flow pattern could only be defined indirectly using a model of gas velocity, which added significant uncertainty to this estimation. In early stage of subcooled flow boiling, bubbles are small, concentrate near the heating wall, and are mostly stationary, which make the void fraction measurement using this intrusive method highly questionable.

Recommendation: A set of scaling factors, which is specific to a considered application/problem, is useful in defining the relevancy and scalability values of data. More rigorous and comprehensive estimations of measurement uncertainty are still needed for the above-considered (and other) experiments and data. Measurement error is normally provided globally, but it, in fact, can change from dataset to dataset and time-/location-dependent. The proposed VUQ approach [1][5] allows to take the advantage of the local measurement error if it can be determined.

3.5. Recommendations for CASL validation data center

Validation data support for all CASL VERA developers, researchers, and users can be effectively realized by mean of a CASL data center (CDC) as proposed in [3].

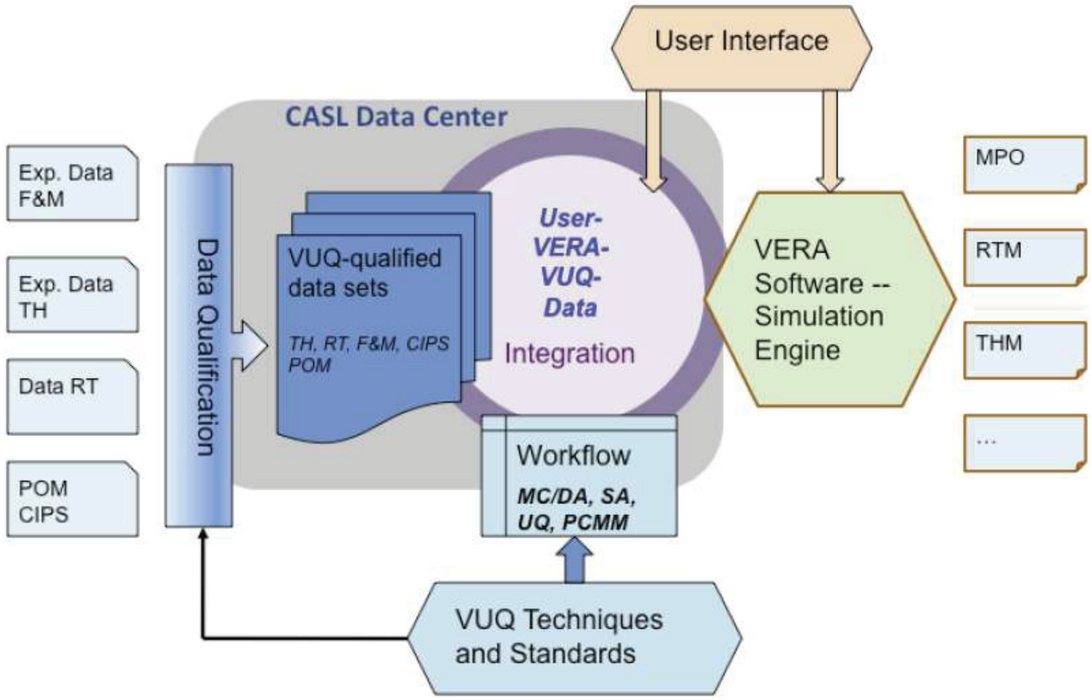

Figure 3.5: CDC in support of the development and VUQ of CASL advanced modeling capabilities [3].

Based on the above review of validation data and recommended VUQ approach, a validation center suitable for multiphysics model analysis should be able to accommodate

- Data of different formats, e.g. tables, plots, pictures, photos, etc.
- Data digitalization and conversion facilities;
- Data of greatly different dimensionality (including multidimensional transient DNS prediction results);
- Analytical models derived directly/indirectly from experimental data together with information regarding their past validation;
- (Locally defined) measurement errors and/or information needed for their evaluation;
- Data validation capability;
- Data quantification capability;
- A data sorting and searching system based on types (IET, SET, PMO, DNS), involved physics, and data quality (relevancy, scalability, and uncertainty), list of possible applications, etc.;
- Flexible interface with simulation and VUQ codes/software;

Many of above features are already available in the Nuclear Energy – Knowledge base for Advanced Modeling and Simulation (NE-KAMS), which is being developed at the Idaho National Laboratory in conjunction with Bettis Laboratory, SNL, ANL, ORNL, Utah State University, and others [55][56]. The knowledge base leverages on the database software and expertise from:

- Gen IV Materials Handbook Database System from the ORNL;
- Generalized Environment for Modeling Systems (GEMS) from the INL;
- VELO – A collaborative knowledge management framework for simulation and modeling from the PNNL.

4. CONCLUSIONS AND RECOMMENDATIONS

The strategy and procedure for SFB validation data collection and characterization outlined in this work can be equally applicable to other CASL multiphysics challenge problems including DNB, CIPS [3], GTRF [57], etc., and CASL advanced modeling capabilities.

Following this "application-oriented" validation data strategy, collection of validation data and their characterization need be based on:

- Decomposition of the considered multiphysics model and quantification of sensitivity and uncertainty of every submodels;
- Model characteristics, i.e. fidelity, dimensionality, etc., which also dictate the needs and characteristics of validation data;
- Quantification of validation data needs based on the above *model analysis* as well as considered *problem/scenario specifics* which define the significance of each involved physical phenomenon and epistemic uncertainty related to its deficient/incomplete understanding.

For subcooled flow boiling, which is a relatively simple multiphysics problem, a vast quantity of legacy data are available, which can mostly be classified into either *integral effect data*, i.e. distributions of phase volume fraction, temperature, etc., and *separate effect data*, i.e. measurements and observations of nucleation, bubble dynamics, wall heat flux, CHF, etc. These data, however, are very different in their origin, relevancy and scalability to reactor-prototypical conditions, and uncertainty. Consequently, data validation and characterization are necessary before they can be effectively used in calibration and VUQ of reactor modeling codes.

A guideline for collection and characterization of validation data have been derived and outlined in section 3.3, which is applicable to not only subcooled flow boiling problem, but to other CASL case study problems as well. The guideline basically proposes the use of physics-dependent representative dimensionless groups to access the relevancy and scalability of data, and measurement error to access data uncertainty. A different (from current practice) and more comprehensive approach to improved assessment of measurement error has been suggested, which would provide more information for model calibration and VUQ (proposed to be based on statistical model analysis and Bayesian inference).

The proposed "application-oriented" validation data strategy will help to quantify the application/model-dependent needs for validation data and to identify the validation data "gaps", thus, assisting the development and design of new experiments to fill these gaps. The scalability analysis based on dimensionless groups also helps in this experiment design. New data are desirably to be accompanied with better assessments of measurement error which eases the post-experiment data uncertainty evaluation.

Quantification of validation data needs and availabilities becomes crucial now given the rapidly increasing capability and complexity of CASL advanced modeling. A facility for validation data warehousing and effectively interfacing (with modeling and VUQ softwares), which has some built-in data validation and characterization capabilities, (i.e. a realization of CASL Data Center) is essential for CASL effort on advanced modeling capability VUQ. The development of such a facility is suggested to leverage on the experience and insight gained from the Nuclear Energy – Knowledge base for Advanced Modeling and Simulation (NE-KAMS) development.

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