

Nikolay Ivanov Kolev

Multiphase Flow Dynamics

3 THERMAL
INTERACTIONS

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Nikolay Ivanov Kolev

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Thermal Interactions

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To Iva, Rali and Sonja with love!



Morning, July. 2004, Nikolay Ivanov Kolev, 36×48cm oil on linen



Nikolay Ivanov Kolev, PhD, DrSc
Born 1.8.1951, Gabrowo, Bulgaria

Summary

This monograph contains theory, methods and practical experience for describing complex transient multiphase processes in arbitrary geometrical configurations. It is intended to help applied scientists and practicing engineers to understand better natural and industrial processes containing dynamic evolutions of complex multiphase flows. The book is also intended to be a useful source of information for students in the high semesters and in PhD programs.

This monograph consists of five volumes:

Vol. 1 Fundamentals, 4th edn, (14 Chapters and 2 Appendices), 782 pages;

Vol. 2 Mechanical Interactions, 4th edn, (11 Chapters), 364 pages;

Vol. 3 Thermal Interactions, 4th edn, (16 Chapters), 678 pages;

Vol. 4 Turbulence, Gas Absorption and Release by Liquid, Diesel Fuel Properties, 2nd edn, (13 Chapters), 328 pages;

Vol. 5 Nuclear Thermal Hydraulics, 2nd edn, (17 Chapters), 848 pages.

In Volume 1 the concept of three-fluid modeling is presented in detail “from the origin to the applications”. This includes derivation of local volume- and time-averaged equations and their working forms, development of methods for their numerical integration and finally finding a variety of solutions for different problems of practical interest.

Special attention is paid in Volume 1 to the link between the partial differential equations and the constitutive relations called closure laws without providing any information on the closure laws.

Volumes 2 and 3 are devoted to these important constitutive relations for the mathematical description of the mechanical and thermal interactions. The structure of the volumes is in fact a state-of-the-art review and selection of the best available approaches for describing interfacial transfer processes. In many cases the original contribution of the author is incorporated in the overall presentation. The most important aspects of the presentation are that they stem from the author’s long years of experience developing computer codes. The emphasis is on the practical use of these relationships: either as stand-alone estimation methods or within a framework of computer codes.

Volume 4 is devoted to the turbulence in multiphase flows.

The nuclear thermal hydraulic is the science providing knowledge about the physical processes occurring during the transferring the fission heat released in structural materials due to nuclear reactions into its environment. Along its way to

the environment the thermal energy is organized to provide useful mechanical work or useful heat or both. Volume 5 is devoted to the nuclear thermal hydraulics. In a way this is the most essential application of the multiphase fluid dynamics in analyzing steady and transient processes in nuclear power plants.

In particular, Volume 3 contains information on how to describe the flow patterns and the specific thermal interactions between the velocity fields in flight.

Chapter 1 presents nucleation in liquids. Chapter 2 presents different aspects of the bubble growth in superheated liquid and the connection to computational system models. Condensation of pure steam bubbles is considered in Chapter 3.

Chapter 4 considering the bubble departure mechanism on heated walls is updated with new information. The theory is extended to subcooled liquid.

Chapter 5 presents a solution of the coupled problem of transient bubble growth or collapse and relates it to the state-of-the-art. A comparison with experimental data is given. Finally, a discussion is provided on how to couple such low-scale physics with large-scale physics in multiphase flow computer codes.

Chapter 6 considering nucleate boiling is updated. Additional information coming from boiling of fluids with nanoparticles confirms the sound physical basics of the author's method. Additional information is provided for nucleation site density at high pressure.

An interesting result of the theory presented in these chapters is the prediction of a critical heat flux without an empirical correlation for critical heat flux as a result of the mutual bubble interaction for increasing wall superheating. Applying the theory for the inverted problem of the flashing of superheated water in pipes as given in Chapter 7, surprisingly supported the validity of the new approach.

The state-of-the-art in boiling theory is presented in Chapters 8 to 11 where boiling in subcooled liquid, natural convection film boiling, critical heat flux, forced convection film boiling, and film boiling on vertical plates and spheres is presented. The emphasis is on the elaboration of all coupling terms between the fluids, and between the wall and fluid required for closure of the overall description. Chapter 9 considering boiling of subcooled liquid is updated. Chapter 20 considering forced convection boiling is updated. The 2005 look-up table by *Groeneveld et al.* is demonstrated to be an excellent scaling base for critical heat flux in bundles for variety of geometries and conditions.

Chapter 12 provides information on all heat- and mass-transfer processes across a droplet interface starting with the nucleation theory, and going through the droplet growth, self-condensation stop, heat transfer across a droplet interface without mass transfer, direct contact condensation of pure steam on a subcooled droplet, spontaneous flushing of a superheated droplet, evaporation of a saturated droplet in superheated gas, and droplet evaporation in a gas mixture. A similar approach is applied to the description of the interface processes at a film/gas interface in Chapter 13 with a careful treatment of the influence of the turbulent pulsation on the interfacial heat and mass transfer. A set of updated empirical methods for prediction of condensation on cooled walls with and without a noncondensable

is presented in Chapter 14. Test examples are provided for demonstration of the application of the theory.

Chapter 15 provides information on the implementation of the discrete ordinate method for radiation transport in multiphase computer codes. In this chapter the dimensions of the problem, the differences between micro- and macrointeractions and the radiation transport equation are discussed. Then, the finite-volume representation of the radiation transport is given and different aspects of the numerical integration are discussed. The computation of some material properties is discussed. Then three specific radiation transport cases of importance for the melt–water interaction are discussed in detail: a spherical cavity of gas inside a molten material; concentric spheres of water droplets, surrounded by vapor surrounded by molten material; clouds of spherical particles of radiating material surrounded by a layer of vapor surrounded by water. For the last case the useful Lanzenberger’s solution is presented and its importance is demonstrated in two practical cases.

The book ends with Chapter 16, which provides information on how to verify multiphase flow models by comparing them with experimental data and analytical solutions. First, Section 16.2 contains a quick look of the IVA computer code with several interesting demonstration of the power of the technology described in this four Volumes work. A list of references is provided in Sections 16.3 and 16.4 documenting the IVA-code development and validation. The complexity of the problems is gradually increased from very simple ones to problems with very complex melt–water interaction multifluid flows with dynamic fragmentation and coalescence and strong thermal and mechanical interactions. In particular the following cases are described and compared with the prediction using the basics presented in different chapters of this book: material relocation – gravitational waves (2D), U-tube benchmarks such as adiabatic oscillations, single-phase natural convection in a uniformly heated vertical part of a U-tube, single-phase natural convection in a uniformly heated inclined part of a U-tube, single-phase natural convection in a U-tube with an inclined part heated by steam condensation, steady-state single-phase nozzle flow, pressure waves in single-phase flow, 2D gas explosion in a space filled previously with gas, 2D gas explosion in space with internals previously filled with liquid, film entrainment in pipe flow, water flashing in nozzle flow, pipe blow-down with flashing, single-pipe transients, complex pipe network transients, boiling in pipes and rod bundles, critical heat flux, post-critical heat flux heat transfer, film boiling, behavior of clouds of cold and very hot spheres in water, experiments with dynamic fragmentation and coalescence like the FARO L14, 20, 24, 28, 31 experiments, PREMIX 13, 15, 17, 18 experiment, RIT and IKE experiment. Chapter 16 also contains some additional experiments and movies documenting the performance of the method for fast pressure wave propagation in 2D geometry and interesting acoustical problems of melt-water interaction. Review of the state-of-the-art of the instability analyses of boiling systems is provided and interesting comparison of the modern IVA predictions with large-scale AREVA- experiments is provided in Section 16.6.3. Powerful

demonstration of the methods for analyzing pressure-wave propagations in single- and two-phase systems is given by comparison with the Interatome experiments from 1983 performed on simple and complex pipe networks, Section 16.8.3. Section 16.15 contains comparison with 333 experiments for variety of bundles, flow regimes including dry out, steady state and transients. It clearly demonstrates the power of the method and its well-defined uncertainty to simulate boiling processes in complex geometry. In addition an application of a powerful method for investigation of the propagation of input and model uncertainties on the final results by using the Monte Carlo method and regression analysis is demonstrated for the prediction of nonexplosive melt-water interactions. Benchmarks for testing the 3D capabilities of computer codes are provided for the rigid-body steady-rotation problem, pure radial symmetric flow, radial-azimuthal symmetric flow. Examples of very complex 3D flows are also given such as small break loss of coolant, asymmetric steam–water interaction in a vessel, and melt relocation in a pressure vessel. And finally, Section 16.21 contains the discussion regarding: Is it possible to design a universal multiphase flow analyzer? It contains my personal vision for future development of the multiphase fluid dynamics.

Chapter 16 of this volume together with Chapter 14 of Volume 1 are available from the WEB site of Springer. In addition many animated sequences (movies) are presented there. HTML documents are then executed using any Web browser available on the local computer of the reader.

29.12.2010
Herzogenaurach

Nikolay Ivanov Kolev

Table of Contents

1	Nucleation in liquids.....	1
1.1	Introduction.....	1
1.2	Nucleation energy, equation of <i>Kelvin</i> and <i>Laplace</i>	2
1.3	Nucleus capable of growth.....	3
1.4	Some useful forms of the <i>Clausius–Clapeyron</i> equation, measures of superheating.....	5
1.5	Nucleation kinetics.....	8
1.5.1	Homogeneous nucleation.....	8
1.5.2	Heterogeneous nucleation.....	9
1.6	Maximum superheat.....	15
1.7	Critical mass flow rate in short pipes, orifices and nozzles.....	18
1.8	Nucleation in the presence of noncondensable gases.....	19
1.9	Activated nucleation-site density – state-of-the-art.....	20
1.10.	Conclusions and recommendations.....	28
	Nomenclature.....	28
	References.....	31
2	Bubble growth in superheated liquid.....	35
2.1	Introduction	35
2.2	The thermally controlled bubble growth	36
2.3	The <i>Mikic</i> solution.....	39
2.4	How to compute the mass source terms for the averaged conservation equations?	47
2.4.1	Nonaveraged mass source terms	47
2.4.2	The averaged mass source terms.....	49
2.5	Superheated steam.....	54
2.6	Diffusion-controlled evaporation into mixture of gases inside the bubble.....	55
2.7	Conclusions	56
	Appendix 2.1 Radius of a single bubble in a superheated liquid as a function of time.....	56
	Nomenclature.....	62
	References.....	65

3	Condensation of a pure steam bubble in a subcooled liquid	67
3.1	Introduction	67
3.2	Stagnant bubble	67
3.3	Moving bubble	69
3.4	Nonaveraged source terms	74
3.5	Averaged source terms	75
3.6	Change of the bubble number density due to condensation	76
3.7	Pure steam bubble drifting in turbulent continuous liquid	77
3.8	Condensation from a gas mixture in bubbles surrounded by subcooled liquid.....	79
3.8.1	Thermally controlled collapse.....	80
3.8.2	Diffusion-controlled collapse.....	80
	Nomenclature.....	81
	References.....	85
4	Bubble departure diameter	87
4.1	How accurately can we predict bubble departure diameter for boiling?.....	87
4.2	Model development.....	90
4.3	Comparison with experimental data.....	95
4.4	Significance.....	100
4.5	Summary and conclusions.....	100
4.6	Extension of the theory to subcooled liquids	100
4.7	Influence of the wall material.....	103
	Nomenclature.....	104
	References.....	106
5	Bubble dynamics in single-component fluid	109
5.1	Introduction	109
5.2	The system of PDEs describing the problem.....	109
5.3	Numerical solution method	112
5.4	Validation of the method.....	113
5.4.1	Bubble collapse.....	113
5.4.2	Bubble growth.....	118
5.5	Use in computer codes operating with large computational cells	121
5.6	Comparison with the state-of-the-art.....	122
Appendix 5.1	The Raleigh–Plesset equation.....	129
Appendix 5.2	The liquid energy-conservation equation	134
Appendix 5.3	Pressure equation for the bubble.....	136
Appendix 5.4	Bubble energy conservation	138
	Nomenclature.....	138
	References.....	140

6	How accurately can we predict nucleate boiling?	143
6.1	Introduction	143
6.2	New phenomenological model for nucleate pool boiling.....	154
6.2.1	Basic assumptions	154
6.2.2	Proposed model.....	156
6.3	Data comparison	158
6.3.1	Nucleation-site density at high pressures	161
6.4	Systematic inspection of all the used hypotheses	162
6.5	Significance	163
6.6	Conclusions	164
6.7	Extension to forced convection with nucleate boiling.....	165
	Appendix 6.1 State-of-the-art of nucleate pool boiling modeling	167
	Nomenclature	173
	References.....	175
7	Heterogeneous nucleation and flashing in adiabatic pipes	179
7.1	Introduction	179
7.2	Bubbles generated due to nucleation at the wall	180
7.3	Bubble growth in the bulk	181
7.4	Bubble fragmentation and coalescence	181
7.5	Film flashing bubble generation in adiabatic pipe flow	183
7.6	Verification of the model.....	184
7.7	Significance and conclusions.....	189
	Nomenclature	190
	References.....	192
8	Boiling of subcooled liquid.....	195
8.1	Introduction	195
8.2	Initiation of visible boiling on the heated surface	195
8.3	Local evaporation and condensation	198
8.3.1	Relaxation theory	198
8.3.2	Boundary-layer treatment	200
	Nomenclature	203
	References.....	204
9	Natural convection film boiling.....	207
9.1	Minimum film boiling temperature	207
9.2	Film boiling in horizontal upwards-oriented plates.....	208
9.3	Horizontal cylinder.....	209
9.4	Sphere.....	210
	Nomenclature	211
	References.....	212

10	Forced convection boiling	213
10.1	Convective boiling of saturated liquid	213
10.2	Forced-convection film boiling	217
10.2.1	Tubes.....	219
10.2.2	Annular channel	222
10.2.3	Tubes and annular channels	222
10.2.4	Vertical flow around rod bundles	223
10.3	Transition boiling	223
10.4	Critical heat flux	225
10.4.1	The hydrodynamic stability theory of free-convection DNB	226
10.4.2	Forced-convection DNB and DO correlations	229
10.4.3	The 1995 and 2005 look-up tables.....	232
	Nomenclature	238
	References.....	241
11	Film boiling on vertical plates and spheres	245
11.1	Plate.....	245
11.1.1	Introduction.....	245
11.1.2	State-of-the-art	246
11.1.3	Problem definition	247
11.1.4	Simplifying assumptions.....	248
11.1.5	Energy balance at the vapor/liquid interface, vapor film thickness, average heat-transfer coefficient.....	251
11.1.6	Energy balance of the liquid boundary layer, layer thickness ratio	254
11.1.7	Averaged heat fluxes	257
11.1.8	Effect of the interfacial disturbances	258
11.1.9	Comparison of the theory with the results of other authors	259
11.1.10	Verification using the experimental data	261
11.1.11	Conclusions.....	262
11.1.12	Practical significance	263
11.2	Sphere.....	263
11.2.1	Introduction.....	263
11.2.2	Problem definition	263
11.2.3	Solution method.....	263
11.2.4	Model.....	264
11.2.5	Data comparison	272
11.2.6	Conclusions.....	276
	Appendix 11.1 Natural convection at vertical plate	276
	Appendix 11.2 Predominant forced convection only at vertical plate.....	276
	Nomenclature	277
	References.....	281

12	Liquid droplets	283
12.1	Spontaneous condensation of pure subcooled steam – nucleation	283
12.1.1	Critical nucleation size	284
12.1.2	Nucleation kinetics, homogeneous nucleation	286
12.1.3	Droplet growth	288
12.1.4	Self-condensation stop	290
12.2	Heat transfer across droplet interface without mass transfer	291
12.3	Direct contact condensation of pure steam on subcooled droplet ...	297
12.4	Spontaneous flashing of superheated droplet	299
12.5	Evaporation of saturated droplets in superheated gas.....	303
12.6	Droplet evaporation in gas mixture	306
	Nomenclature	312
	References.....	315
13	Heat and mass transfer at the film/gas interface.....	319
13.1	Geometrical film–gas characteristics.....	319
13.2	Convective heat transfer	321
13.2.1	Gas-side heat transfer	321
13.2.2	Liquid-side heat transfer due to conduction.....	325
13.2.3	Liquid-side heat conduction due to turbulence	326
13.3	Spontaneous flashing of superheated film.....	333
13.4	Evaporation of saturated film in superheated gas.....	334
13.5	Condensation of pure steam on subcooled film.....	335
13.6	Evaporation or condensation in presence of noncondensable gases	336
13.6.1	Useful definitions for describing the diffusion mass transfer.....	336
13.6.2	Modification of the velocity profile in the boundary layer due to diffusion mass transfer, <i>Ackerman's</i> multiplier	338
13.6.3	<i>Stefan's</i> theory of diffusion mass transport.....	342
13.6.4	Energy transport into or from the bulk flow due to the diffusion mass flow rate	346
13.6.5	Modification of the temperature boundary layer due to the diffusion mass flow rate	347
13.6.6	Some practical recipes	349
	Nomenclature	353
	References.....	356
14	Condensation at cooled walls	359
14.1	Pure steam condensation	359
14.1.1	Onset of the condensation	359
14.1.2	Gravitation films on plates	359
14.1.3	Gravitation films on pipes.....	368

14.2	Condensation from forced-convection two-phase flow at liquid film	369
14.2.1	Down-flow of vapor across horizontal tubes	369
14.2.2	The <i>Collier</i> correlation.....	369
14.2.3	The <i>Boyko</i> and <i>Krujilin</i> approach	370
14.2.4	The <i>Shah</i> modification of the <i>Boyko</i> and <i>Krujilin</i> approach.....	371
14.2.5	Flow regime associated models	371
14.3	Steam condensation from mixture containing noncondensing gases	373
14.3.1	Computation of the mass-transfer coefficient	375
	Nomenclature	377
	References.....	380
15	Discrete ordinate method for radiation transport in multiphase computer codes.....	383
15.1	Introduction	383
15.1.1	Dimensions of the problem.....	383
15.1.2	Micro- versus macrointeractions.....	384
15.1.3	The radiation-transport equation (RTE).....	384
15.2	Discrete ordinate method.....	385
15.2.1	Discretization of the computational domain for the description of the flow.....	387
15.2.2	Finite-volume representation of the radiation-transport equation	388
15.2.3	Boundary conditions	393
15.3	Material properties	395
15.3.1	Source terms – emission from hot surfaces with known temperature	395
15.3.2	Spectral absorption coefficient of water	396
15.3.3	Spectral absorption coefficient of water vapor and other gases.....	400
15.4	Averaged properties for some particular cases occurring in melt–water interaction.....	400
15.4.1	Spherical cavity of gas inside a molten material.....	401
15.4.2	Concentric spheres of water droplets, surrounded by vapor, surrounded by molten material.....	402
15.4.3	Clouds of spherical particles of radiating material surrounded by a layer of vapor surrounded by water – <i>Lanzenberger's</i> solution	406
15.4.4	Chain of infinite number of <i>Wigner</i> cells.....	419
15.4.5	Application of <i>Lanzenbergers's</i> solution.....	420
	Nomenclature	422
	References.....	423

16 Validation of multiphase flow models.....	425
16.1 Introduction.....	426
16.2 Quick look at IVA computer code	427
16.3 References documenting the IVA-code development	435
16.4 IVA-validation database.....	444
16.5 References of data sources and references documenting the validation of IVA.....	450
16.6 Material relocation: gravitational waves (1D, 2D), density waves in boiling and condensing systems	459
16.6.1 Flow through straight microchannel with constant cross-section	459
16.6.2 Critical gas flow through nozzles and pipes with constant cross-section.....	460
16.6.3 U-tube benchmarks.....	462
16.6.4 Flow boiling stability.....	467
Conclusions.....	473
16.6.5 Flow condensation stability	473
16.6.6 Gravitational 2D waves	480
References.....	481
16.7 Steady-state single-phase nozzle flow	485
References.....	486
16.8 Pressure waves – single phase	487
16.8.1 Gas in a shock tube.....	488
16.8.2 Water in a shock tube	491
16.8.3 The 1983 Interatome experiments	493
16.8.4 Pressure-wave propagation in a cylindrical vessel with free surface (2D).....	507
References.....	511
16.9 2D: N₂ explosion in space filled previously with air.....	513
References.....	515
16.10 2D: N₂ explosion in space with internals filled previously with water	517
References.....	521
16.11 Film entrainment in pipe flow.....	523
References.....	525

16.12 Water flashing in nozzle flow	527
References.....	530
16.13 Pipe blow-down with flashing	533
16.13.1 Single pipe	533
16.13.2 Complex pipe network.....	537
References.....	537
16.14 1D boiling, critical heat flux, postcritical heat flux heat transfer	539
References.....	551
16.15 Flow boiling in bundles: 333 experiments for variety of bundles, flow regimes including dry out, steady state and transients.....	553
16.15.1 Introduction	554
16.15.2 Steady-state boiling	554
16.15.3 Transient boiling.....	579
16.15.4 Steady-state critical heat flux	584
16.15.5 Outlook – towards the fine-resolution analysis	599
16.15.6 Conclusions	600
Appendix 16.15.1 Some relevant constitutive relationship addressed in this analysis	601
Nomenclature.....	602
References.....	603
16.16 Film boiling.....	607
References.....	609
16.17 Behavior of clouds of cold and very hot spheres in water	611
References.....	615
16.18 Experiments with dynamic fragmentation and coalescence.....	617
16.18.1 L14 experiment	617
16.18.2 L20 and L24 experiments.....	621
16.18.3 Uncertainty in the prediction of nonexplosive melt–water interactions	622
16.18.4 Conclusions	623
16.18.5 L28, L31 experiment.....	624
16.18.6 PREMIX-13 experiment.....	628
16.18.7 PREMIX 17 and 18 experiments.....	635
16.18.8 RIT and IKE experiments.....	648
References.....	649
16.19 Assessment for detonation analysis.....	651
References.....	652

16.20 Other examples of 3D capabilities	653
16.20.1 Case 1. Rigid-body steady-rotation problem	653
16.20.2 Case 2. Pure radial symmetric flow	654
16.20.3 Case 3. Radial-azimuthal symmetric flow	656
16.20.4 Case 4. Small-break loss of coolant.....	658
16.20.5 Case 5. Asymmetric steam–water interaction in a vessel	659
16.20.6 Case 6. Melt relocation in a pressure vessel	664
References.....	666
16.21 General conclusions: Is it possible to design a universal multiphase flow analyzer?	667
16.21.1 The idea of multiple velocity fields.....	668
16.21.2 Do we have adequate mathematical reflection of the conservation laws based on averaging?.....	668
16.21.3 Coexisting fields	669
16.21.4 Geometry definition.....	669
16.21.5 Solvers	669
16.21.6 Summary of the ideas	670
16.21.7 Is there any chance to overcome the overwhelming complexity and design algorithms that are of practical use?	670
Conclusions	671
Appendix 1 Knowledge data base required to design a universal multiphase flow analyzer.....	671
References.....	672
Index.....	675

1. Nucleation in liquids

After reviewing the literature for description of the nucleation in superheated liquids the following conclusions and recommendations have been drawn. The maximum superheating in technical systems is a function of the depressurization velocity and of the produced turbulence. The maximum superheating can be predicted by the Algimir and Lienhard and by the Bartak correlations within an error band of 48.5%. Flashing in short pipes and nozzles leads to critical flows driven by the pressure difference equal to the entrance pressure minus the flashing inception pressure. For the prediction of the maximum achievable superheating, which represents the spinoidal line the Skripov correlation is recommended. The wetting angle is an important property of the polished surface characterizing its capability to activate nucleation sites. For the prediction of the activated nucleation sites the correlation obtained by Wang and Dhir is recommended. The establishing of a vapor film around a heated surface having temperature larger than the minimum film boiling temperature takes a finite time. The availability of small bubbles of noncondensing gases reduces the superheating required to initiate evaporation. Evaporation at lower than the saturation temperature is possible.

1.1 Introduction

Liquids having temperature above the saturation temperature corresponding to the local pressure are called superheated liquids. Superheated liquids are unstable and start to disintegrate. This process is in generally called *flashing*. The process of rupturing a *continuous* liquid by decrease in pressure at roughly constant liquid temperature is often called *cavitation* – a word proposed by *Froude*. The process of rupturing a *continuous* liquid by increase the temperature at roughly constant pressure is often called *boiling*. The fluctuation of molecules having energy larger than that characteristic of a stable state causes the formation of clusters of molecules, which after reaching some critical size are called nuclei. The theory of the nucleation provides us with information about the generation of nuclei per unit time and unit volume of the liquid as a function of the local parameter.

1.2 Nucleation energy, equation of Kelvin and Laplace

Let us abstract from a superheated *nonstable liquid a spherical volume*, having an initial radius R_{10} , a volume $\frac{4}{3}\pi R_{10}^3$, pressure p , temperature T_2 and density $\rho_2 = \rho_2(p, T_2)$. After some time the selected sphere liquid volume increases due to *evaporation* to the radius R_1 (respectively to the volume $\frac{4}{3}\pi R_1^3$) and reaches a pressure $p'(T_2)$. The pressure inside the bubble is assumed to be uniform because of the small bubble size. The density of the evaporated steam inside the sphere is $\rho'' = \rho''[p'(T_2)] = \rho''(T_2)$. The *initial* and the *end spheres have the same mass* per definition, therefore

$$\left(\frac{R_{10}}{R_1}\right)^3 = \frac{\rho''}{\rho_2}. \quad (1.1)$$

Consequently, the initial volume of the sphere is changed by

$$\frac{4}{3}\pi(R_1^3 - R_{10}^3) = \frac{4}{3}\pi R_1^3 \left(1 - \frac{\rho''}{\rho_2}\right). \quad (1.2)$$

During this expansion a *mechanical work*

$$\begin{aligned} 4\pi \int_{R_{10}}^{R_1} [p'(T_2) - p] r^2 dr &\approx \frac{4}{3}\pi (R_1^3 - R_{10}^3) [p'(T_2) - p] \\ &= \frac{4}{3}\pi R_1^3 \left(1 - \frac{\rho''}{\rho_2}\right) [p'(T_2) - p] \end{aligned} \quad (1.3)$$

is performed and transferred into total kinetic energy of the surrounding liquid Skripov et al. (1980). In other words, this work is introduced into the liquid. For the creation of a sphere with a free surface, additional work

$$\int_0^{R_1} \frac{2\sigma}{r} 4\pi r^2 dr = 4\pi R_1^2 \sigma \quad (1.4)$$

is needed. The surface tension of water in N/m, σ , in contact with its vapor is given in Lienhard (1976) with great accuracy by

$$\sigma = 0.2358 \left[1 - \frac{T'(p)}{T_c}\right]^{1.256} \left\{1 - 0.625 \left[1 - \frac{T'(p)}{T_c}\right]\right\}, \quad (1.5)$$

where the T_c is the thermodynamic critical temperature (for water $T_c = 647.2$ K). For the region of 366 to 566 K the above equation can be approximated by

$$\sigma = 0.14783(1 - T/T_c)^{1.053} \quad (1.6)$$

with an error of $\pm 1\%$. The surface tension is a function of the surface temperature, which can strongly vary in transients. The surface tension is usually measured at macroscopic surfaces. Whether the so-obtained information is valid for the microscopic metastable bubbles is not clear. Next, we assume that this relationship holds also for microscopic surfaces.

Thus, the work necessary to create a single bubble with radius R_1 is

$$\Delta E_1 = 4\pi R_1^2 \sigma - [p'(T_2) - p] \frac{4}{3} \pi R_1^3 \left(1 - \frac{\rho''}{\rho_2}\right) = 4\pi \sigma \left(R_1^2 - \frac{2}{3} \frac{R_1^3}{R_{1c}} \right), \quad p'(T_2) > p \quad (1.7)$$

We see that this work depends on the bubble radius and has a maximum

$$\Delta E_{1c} = \frac{16\pi\sigma^3}{3[p'(T_2) - p]^2 \left(1 - \frac{\rho''}{\rho_2}\right)^2} = \frac{4}{3} \pi \sigma R_{1c}^2 \approx \frac{4}{3} \pi \sigma \left[\frac{T'(p)}{T_2 - T'(p)} \frac{2\sigma}{\rho''(h'' - h')} \right]^2 \quad (1.8)$$

for

$$R_{1c}^2 = \frac{3\Delta E_{1c}}{\sigma 4\pi} = \left\{ \frac{2\sigma}{[p'(T_2) - p](1 - \rho''/\rho_2)} \right\}^2. \quad (1.9)$$

The corresponding bubble volume is then

$$V_{1c} = \frac{4}{3} \pi \left(\frac{3\Delta E_{1c}}{\sigma 4\pi} \right)^{3/2}. \quad (1.10)$$

The equation (1.9) is known as the *Laplace* and *Kelvin* equation. *Gibbs* (1878) noted that the expression for the maximum “... does not involve any geometrical magnitudes”.

1.3 Nucleus capable of growth

The above consideration did not lead to any conclusion whether a bubble with size R_{1c} will further grow or collapse. It says only that at that size the mechanical energy needed to create a bubble at the initial state $R_1 = 0$ and at the final state $R_{1\infty} > R_{1c}$ possesses a maximum at R_{1c} and no more. There are many papers in which this size is taken to represent the bubble size, at which the bubble is further capable to grow, which as we will show below is not true.

Next, we consider the conservation of the liquid mechanical energy in order to describe the bubble growth from the beginning through the critical radius. The mass-conservation equation of the liquid can be approximated by

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_2) \approx 0, \quad (1.11)$$

or integrating with the boundary condition

$$r = R_1, \quad u_2 = \frac{\partial R_1}{\partial \tau} \quad (1.12)$$

$$u_2 = \text{const} / r^2 = \frac{\partial R_1}{\partial \tau} (R_1 / r)^2. \quad (1.13)$$

This gives the liquid velocity as a function of the radius if the liquid is assumed to be incompressible during the bubble expansion. The total kinetic energy of the liquid environment estimated using the above equation is therefore

$$\begin{aligned} \int_{R_1}^{\infty} \frac{1}{2} \rho_2 u_2^2 dVol_2 &= \frac{1}{2} \rho_2 \left(\frac{\partial R_1}{\partial \tau} \right)^2 R_1^4 4\pi \int_{R_1}^{\infty} \frac{dr}{r^2} = 2\pi \rho_2 \left(\frac{\partial R_1}{\partial \tau} \right)^2 R_1^4 \int_{R_1}^{\infty} d \left(-\frac{1}{r} \right) \\ &= 2\pi \rho_2 \left(\frac{\partial R_1}{\partial \tau} \right)^2 R_1^3. \end{aligned} \quad (1.14)$$

During the bubble growth, the work performed by the bubble expansion is transferred in total kinetic energy of the liquid environment, i.e.,

$$2\pi \rho_2 \left(\frac{\partial R_1}{\partial \tau} \right)^2 R_1^3 = -4\pi \sigma \left(R_1^2 - \frac{2}{3} \frac{R_1^3}{R_{1c}} \right) \equiv \Delta E_1$$

or

$$\left(\frac{\partial R_1}{\partial \tau} \right)^2 = \frac{2\sigma}{\rho_2} \left(\frac{2}{3} \frac{1}{R_{1c}} - \frac{1}{R_1} \right). \quad (1.15)$$

The constant $2/3$ valid for bubble growth in a bulk liquid should be replaced by $\pi/7$ if a spherical bubble grows on a flat surface.

Equation (1.15) is a very important result. We see that real bubble growth is possible *if and only if*

$$R_1 > \frac{3}{2} R_{1c}. \quad (1.16)$$

For the case of $R_1 \gg R_{1c}$ Eq. (1.15) transforms into

$$\left(\frac{\partial R_1}{\partial \tau}\right)^2 = \frac{4}{3} \frac{\sigma}{\rho_2 R_{1c}}. \quad (1.17)$$

This mechanism of bubble growth is called *inertially controlled bubble growth*. For low pressure where the assumption $\rho''/\rho_2 = 0$ is reasonable the above equation reduces to one obtained for the first time by *Besand* (1859) and in a more elegant way by *Rayleigh* (1917). This mechanism controls the bubble growth within the first 10^{-8} s of the life of the stable bubble.

It follows from the above consideration that for the creation of a bubble with a critical unstable diameter $3/2 R_{1c}$, a surplus of internal energy of the liquid is needed greater than E_{1c} , and for creation of bubble that is capable to grow, a surplus of internal energy of the liquid – greater than $(9/4) E_{1c}$.

1.4 Some useful forms of the *Clausius–Clapeyron* equation, measures of superheating

Usually, the liquid superheating is expressed by the temperature difference $T_2 - T'(p)$. Sometimes, the pressure difference $\Delta p = p'(T_2) - p$ corresponding to the superheating of the liquid with respect to the saturation temperature $T_2 - T'(p)$ is also used as a measure for the liquid superheating. Using the *Clausius–Clapeyron* equation

$$\frac{dT}{dp} = \frac{v'' - v'}{s'' - s'} = \frac{\rho' - \rho''}{s'' - s'} \frac{1}{\rho' \rho''} = T'(p) \frac{\rho' - \rho''}{h'' - h'} \frac{1}{\rho' \rho''} \quad (1.18)$$

integrated between the initial state $[p, T'(p)]$ and the final state $[p'(T_2), T_2]$ for

$$\frac{\rho' - \rho''}{h'' - h'} \frac{1}{\rho' \rho''} \approx \text{const} \quad (1.19)$$

one obtains

$$p'(T_2) - p = (h'' - h') \frac{\rho' \rho''}{\rho' - \rho''} \ln \left[1 + \frac{T_2 - T'(p)}{T'(p)} \right]. \quad (1.20)$$

With this result the critical bubbles size can be approximated by

$$R_{1c} \approx 2\sigma / \left\{ (h'' - h') \rho' \ln \left[1 + \frac{T_2 - T'(p)}{T'(p)} \right] \right\}. \quad (1.22)$$

For $T_2 - T'(p) \ll T'(p)$ we have for the tensile pressure difference

$$p'(T_2) - p = (h'' - h') \frac{\rho' \rho''}{\rho' - \rho''} \frac{T_2 - T'(p)}{T'(p)}, \quad (1.23)$$

and for the critical bubble size

$$R_{1c} \approx \frac{T'(p)}{T_2 - T'(p)} \frac{2\sigma}{\rho''(h'' - h')}. \quad (1.24)$$

Thus, one can use as a measure of liquid superheating either the *tension pressure difference* $p'(T_2) - p$ or the *liquid superheat* $T_2 - T'(p)$.

Equation (1.23) makes it possible to compute the liquid superheating corresponding to the radius R_{1c} from Eq. (1.9)

$$[T_2 - T'(p)]/T'(p) = \frac{2\sigma}{R_{1c}} \frac{(\rho' - \rho'')\rho_2}{(\rho_2 - \rho'')\rho'\rho''} \frac{1}{h'' - h'} \approx 2 \frac{\sigma}{R_{1c}} \frac{1}{\rho''(h'' - h')} \quad (1.25)$$

or corresponding to $3 R_{1c}/2$

$$[T_2 - T'(p)]/T'(p) = \frac{4}{3} \frac{\sigma}{R_{1c}} \frac{(\rho' - \rho'')\rho_2}{(\rho_2 - \rho'')\rho'\rho''} \frac{1}{h'' - h'} \approx \frac{4}{3} \frac{\sigma}{R_{1c}} \frac{1}{\rho''(h'' - h')}. \quad (1.26)$$

For the atmospheric pressure Eq. (1.23) gives

$$T_2 - T'(p) = 6.4197 \times 10^{-5} / D_{1c}. \quad (1.27)$$

This linearization is valid for very small deviations from the saturation. In general, the participating properties are not a linear function of temperature. A nonlinear expression is obtained also for low pressure for which the density difference between liquid and vapor is very large. In this case Eq. (1.18) simplifies to $dT/dp = v''/(T\Delta h)$. This equation has been known since 1828 in France as the *August* equation. Assuming the vapor behave as a perfect gas results in $dp/p = (\Delta h/R) dT/T^2$, where R is the vapor gas constant for the specific substance. Integrating between an initial state $[p, T'(p)]$ and a final state $[p'(T_2), T_2]$ and rearranging results in useful expression for computing the relation between *tension pressure difference* $p'(T_2) - p$ and the *liquid superheat* $T_2 - T'(p)$ of metastable liquid,

$$\frac{p'(T_2) - p}{p} = \exp \left[\frac{\Delta h}{RT_2} \frac{T_2 - T'(p)}{T'(p)} \right] - 1. \quad (1.28)$$

With this result the *Laplace* and *Kelvin* equation reads

$$R_{1c} \approx \frac{2\sigma}{\left\{ \exp \left[\frac{\Delta h}{RT_2} \frac{T_2 - T'(p)}{T'(p)} \right] - 1 \right\} p (1 - \rho''/\rho_2)}. \quad (1.29)$$

One should carefully use the approximations of the *Laplace* and *Kelvin* equation. At low pressure the approximations are good as shown in Fig.1.1. In this case at higher superheat Eq. (1.29) is much closer to the accurate equation.

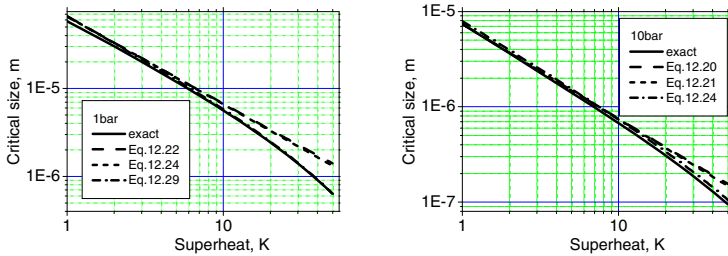


Fig. 1.1 Critical bubbles size at low pressure as a function of the liquid superheat

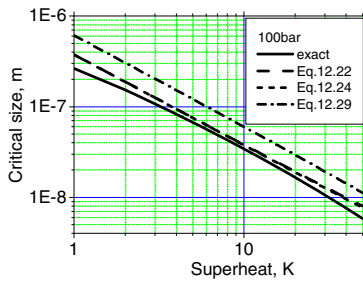


Fig. 1.2 Critical bubbles size at high pressure as a function of the liquid superheat

At high pressure the approximations may deviate substantially from the exact solution as shown in Fig. 1.2.

The dimensionless number constructed as follows

$$Gb_2 = \frac{\Delta E_{1c}}{kT_2} = \frac{\Delta S_{1c}}{k} = \frac{16\pi\sigma^3}{kT_2 3 [p'(T_2) - p]^2 (1 - \rho''(T_2) / \rho_2)^2} \quad (1.30)$$

is called the *Gibbs* number. Here, $k = 13.805 \times 10^{-24}$ J/K is the *Boltzmann* constant. The *Gibbs* number is frequently used as a dimensionless measure of superheating. The greater the superheating the smaller the *Gibbs* number. Gb_2 converging to infinity means no superheating. For $T_2 = T_c$, $\sigma = 0$ and $Gb_2 = 0$.

However, it should be noted that neither of the measures discussed above tells us at what ΔT liquid starts boiling or flashing.

1.5 Nucleation kinetics

1.5.1 Homogeneous nucleation

Now we discuss the dependence between liquid superheating and production rates of bubbles with critical size called nuclei. Consider a continuous liquid characterized by average state parameters p and T_2 . An observer measures a long time $\Delta\tau$ the time $\Delta\tau_n$ in which a mass Δm_{2c} of the continuum departs from the normal, average, state. The entropy change necessary for this fluctuation is $\Delta m_{2c} \Delta s_{2c} = \Delta S_{2c}$. *Volmer* (1939) p. 81 following *Boltzmann* and *Einstein* assumed that

$$\Delta\tau_n / \Delta\tau \approx \text{const } e^{-\Delta S_{2c}/k} = \text{const } e^{-Gb_2} \quad (1.31)$$

where k is the *Boltzmann* constant. This means that the smaller the needed entropy change for the fluctuation the higher the probability of this fluctuation. This is the leading idea for describing such processes. It did not change with the years. Actually it is known from experimental observations that the greater the superheating the greater the probability of initiation of bubbles with critical size. The probability of initiation of a single bubble is defined as

$$\text{probability of initiation of single bubble} = \frac{\text{nucleation events}}{\text{molecular colisions}}. \quad (1.32)$$

Thus,

$$\frac{\text{nucleation events}}{\text{molecular colisions}} = \exp(-Gb_2) \quad (1.33)$$

Obviously for $T_2 = T_c$ and $\sigma_2 = 0$, the probability of initiation of a single bubble $\exp(-Gb_2) = 1$. Nuclei with critical size can originate in the bulk liquid. This phenomenon is called *homogeneous* nucleation. Nuclei with critical size can originate also at the wall. This phenomenon is called *heterogeneous* nucleation. The theories modeling the nucleation in the bulk liquid are called homogeneous nucleation theories. The theories modeling the nucleation at surfaces are called heterogeneous nucleation theories. Next, we give the main result of the homogeneous nucleation theory.

Kaishew and *Stranski* computed in 1934 the number of the created nuclei per unit time in unit volume of the liquid as follows

$$\begin{aligned} \dot{n}_{1cin} &= N_2 \left\{ \frac{6\sigma}{[2 + p/p'(T_2)]\pi m_2} \right\}^{1/2} \exp(-Gb_2) \\ &= \exp \left\{ \ln \left[\rho_2 \left(\frac{N_A}{m_\mu} \right)^{3/2} \left\{ \frac{6\sigma}{[2 + p/p'(T_2)]\pi m_2} \right\}^{1/2} \right] - Gb_2 \right\}. \end{aligned} \quad (1.34)$$

Here, $N_2 = \rho_2/m_2 = \rho_2 N_A/m_\mu$ ($\approx 3.3\text{--}10^{28}$ for water) is the number of the molecules in one cubic meter, $m_2 = m_\mu/N_A$ is the mass of a single molecule, m_μ is the kg-mole mass (18 kg for water), $N_A = 6.02 \times 10^{26}$ (1/kg-mole) is the number of molecules in one kilogram-mole mass, the *Avogadro* number, and

$$\left\{ \frac{6\sigma}{[2 + p/p'(T_2)]\pi m_2} \right\}^{1/2} \quad (1.35)$$

is the frequency with which each single liquid molecule interacts with its neighbors. The logarithmic expression is not very sensitive with respect to p and T_2 and ranges over

$$\ln \left[\rho_2 \left(\frac{N_A}{m_\mu} \right)^{3/2} \left\{ \frac{6\sigma}{[2 + p/p'(T_2)]\pi m_2} \right\}^{1/2} \right] \approx 80 \text{ to } 83 \quad (1.36)$$

for water.

1.5.2 Heterogeneous nucleation

1.5.2.1 Characteristics of the surfaces and of the liquid/surface contact

Technical surfaces possess roughness as a result of the manufacturing procedure. The structure of the roughness is an important characteristic of the nucleation processes at the surface. Another important characteristic is the molecular interaction between the surface and the liquid. It is usually characterized by the so-called contact angle. The angle between the tangent to the interface and the wall θ is called the contact angle. Hydrophobic surfaces, $\theta > 0$, cause heterogeneous nucleation at much reduced pressure difference (tensile strength). In this section, we give some examples of the characteristics of surfaces influencing the heterogeneous nucleation kinetics.

At real surfaces there are several cavities. For ordinary machined surfaces the cavities have sizes from 2 to 6 μm with density in the range of

$$n_w'' \approx (10 \text{ to } 250) \times 10^4 \text{ m}^{-2} \quad (1.37)$$

For mirror finished copper surfaces as described in *Wang and Dhir* (1993) physically existing cavities have been found to have surface densities depending on the equivalent cavity size in the range

$$n_w'' \approx 9 \times 10^{-9} / D_{\text{cav}}^2 \quad \text{for } D_{\text{cav}} \geq 5.8 \times 10^{-6} \text{ m} \quad (1.38)$$

$$n_w'' \approx 10.3 \times 10^4 + 1.5 \times 10^{-25.2} / D_{\text{cav}}^{5.2} \quad \text{for } 3.5 \times 10^{-6} \leq D_{\text{cav}} \leq 5.8 \times 10^{-6} \text{ m} \quad (1.39)$$

$$n_w'' \approx 2.2135 \times 10^7 + 3.981 \times 10^{-26.4} / D_{cav}^{5.4} \text{ for } D_{cav} \leq 3.5 \times 10^{-6} \text{ m}. \quad (1.40)$$

These are surface properties, which depend on the surface manufacturing only. The authors discovered that only cavities having a nearly spherical form and mouth angle less than the static contact angle serve as nucleation sites. The mouth angle is the angle between the boiling surface and the internal surface of the cavity forming the mouth. The region of changing the heat flux covers the entire nucleate boiling region.

The following tables give some information on how the contact angle can change for different wall materials and different surface preparation procedures.

Table 1.1 Static contact angles θ for distilled water at polished surfaces.

Steel	$\pi/3.7$	<i>Siegel and Keshock (1964)</i>
Steel, Nickel	$\pi/4.74$	<i>Bergles and Rohsenow (1964)</i>
Nickel	$\pi/4.76$ to $\pi/3.83$	<i>Tolubinsky and Ostrovsky (1966)</i>
Nickel	$\pi/4.74$ to $\pi/3.83$	<i>Siegel and Keshock (1964)</i>
Chrome-Nickel Steel	$\pi/3.7$	<i>Arefeva and Aladev (1958)</i>
Silver	$\pi/6$ to $\pi/4.5$	<i>Labuntsov (1963)</i> for $p = 1$ to 150 bar
Zinc	$\pi/3.4$	<i>Arefeva and Aladev (1958)</i>
Bronze	$\pi/3.2$	<i>Arefeva and Aladev (1958)</i>
Zr-4	$\pi/3.16$	<i>Basu, et al. (2002)</i>
Note the contradictory data for copper in the literature		
Copper	$\pi/4$	<i>Arefeva and Aladev (1958)</i>
Copper	$\pi/3$	<i>Gaertner and Westwater (1960)</i>
Copper	$\pi/2$	<i>Wang and Dhir (1993)</i>
Stainless steel 304 (25 °C)	$\theta_{25} \approx \pi/2.25$	<i>Hirose et al. (2006)</i>
Zircaloy (25 °C)	$\theta_{25} \approx \pi/2.46$	<i>Hirose et al. (2006)</i>
Aluminum (25 °C)	$\theta_{25} \approx \pi/2$	<i>Hirose et al. (2006)</i>

Table 1.2 Static contact angle θ for distilled water at thermally or chemically treated polished surfaces

Copper heated to 525 K and exposed to air one hour:	$\pi/5.14$	<i>Wang and Dhir (1993)</i>
Copper heated to 525 K and exposed to air two hour:	$\pi/10$	<i>Wang and Dhir (1993)</i>
Chrome-Nickel Steel chemically treated:	$\pi/2.9$	<i>Arefeva and Aladev (1958)</i>

Hirose et al. (2006) found that the wetting angle is a function of the wall temperature. He correlated measurements within $\pm 12.5\%$ uncertainty band for nitrogen and argon and water–stainless steel 304, water–zircaloy and water–aluminum for pressures 1 to 151 bar and temperatures 20 to 300 °C by the expression

$$\theta = \theta_{25} \tanh\left(2.55 \times T^{*1.72}\right) \text{ for } T^* > 0.3,$$

$$\theta = \theta_{25} \tanh\left(2.55 \times 0.3^{1.72}\right) \text{ for } T^* < 0.3,$$

where $T^* = \frac{T_{cr} - T_w}{T_{cr} - (273.15 + 25)}$, T_{cr} is the critical water temperature and T_w is the wall temperature and $\theta_{25} = \theta(25^\circ\text{C})$. Note that there is no zero wettability at the critical temperature. This is important finding. The work by *Hirose et al.* (2006) shows that measurements for wetting angles can be compared to each other if they are made at the same wall temperature.

In the case of nucleation at walls the segment of a bubble attached at the cavity possesses

$$\text{surface area} = \varphi 4\pi R_{1c}^2, \quad (1.41)$$

which is less than the nucleation surface by a factor of φ . Therefore, less energy is needed for the creation of bubbles at walls

$$\Delta E_{1c}^* = \varphi \Delta E_{1c}, \quad (1.42)$$

than inside the liquid. Consequently, the superheating that can be achieved in technical systems is much smaller than in spontaneous bulk nucleation systems. φ is frequently called the work-reduction factor in the literature.

Tolubinski (1980) computed the work-reduction factor, φ , for an idealized wall surface having *plane geometry* without cavities as follows

$$\varphi = \frac{1}{4}(1 + \cos \theta)^2 (1 - \cos \theta). \quad (1.43)$$

Using the values from Table 1.1 we have φ s in the range of 0.078 to 0.25.

The work-reduction factor for surface with cavities calculated by *Kottowski* (1973) is

$$\varphi = \frac{1}{4} \left[2 - 3 \sin(\theta - \Phi) + \sin^3(\theta - \Phi) \right]. \quad (1.44)$$

Here, Φ is the cavity angle if the cavity is idealized as a cone.