Onset of Flash Boiling Under Rapid Depressurization Conditions Across Positive and Negative Pressure Ranges – A Theoretical Model

Omry Magen*[1], Yoram Kozak[1], Laura Di Lucchio[2], Marco Marengo[2], Tali Bar-Kohany[1,3]
[1]School of Mechanical Engineering, Tel Aviv University, Tel Aviv, Israel
[2]Department of Civil Engineering and Architecture, University of Pavia, Pavia, Italy
[3]Department of Mechanical Engineering, NRCN, Israel
*Corresponding author: omrymagen1@tauex.tau.ac.il

Introduction

Flash boiling atomization occurs when a liquid undergoes rapid depressurization below its saturation pressure, resulting in the formation of a fine spray characterized by wider spray angles and reduced penetration depth [1, 2]. This phenomenon is critical in various engineering applications, including fuel injection systems, cryogenic spray technologies, and carbon capture processes. Understanding the onset of nucleate boiling (ONB) [3] under rapid depressurization is essential for optimizing such systems, yet predicting nucleation conditions remains challenging due to the complex thermodynamic processes involved. [1]

The rate at which pressure decreases plays a crucial role in determining whether nucleation occurs through heterogeneous sites or if the liquid can penetrate deeper into the metastable region, potentially reaching spinodal conditions where spontaneous phase transition becomes inevitable [4].

This work presents an analytical thermodynamic model capable of predicting the ONB across both positive and negative pressure conditions. By leveraging classical nucleation theory (CNT) and introducing normalized thermodynamic parameters, the model establishes a universal correlation applicable to various fluids over a wide temperature range ($0.6 < T_r < 0.98$). The model addresses two fundamental questions: (1) What is the minimal depressurization rate required to reach spinodal conditions? (2) For a given depressurization rate and initial conditions, at what pressure does nucleation occur?

Theoretical Framework and Model Development

The classical nucleation theory provides a phenomenological approach to estimate nucleation rates by examining the energy barrier that must be overcome to form stable nuclei. For heterogeneous nucleation at solid-liquid interfaces, the nucleation flux is expressed as:

$$J = J_0 B \exp(-Gb\phi) \tag{1}$$

The Gibbs number, Gb, characterizes this barrier by comparing the minimal work required to form a critical nucleus with the thermal energy of the system:

$$Gb = \frac{W_{min}}{k_B T_c} = \frac{16\pi\sigma^3}{3k_B T(1 - v_l/v_v)^2 \Delta p_{ONB}^2} \tag{2}$$

where W_{min} is the critical work, k_B is Boltzmann's constant, T_c is the critical temperature, σ is surface tension, v_l and v_v are specific volumes of liquid and vapor phases. Δp_{ONB} represents the pressure difference between saturation and ONB [3] conditions. ϕ is the heterogeneity factor accounting for deviations from homogeneous conditions, and the pre-exponential factor is:

$$J_0 = \left(\frac{N_A}{v_l}\right)^{2/3}; \quad B = \frac{k_B T}{h_p} \tag{3}$$

with N_A being Avogadro's number and h_p Planck's constant.
At high degrees of superheating, curvature effects on surface tension become significant, which in turn, influences the nucleation flux predicted by the CNT [5]. The Tolman correction length is thus used to realize such dependency. Following [6], the following relationship is acquired:

$$\sigma(r,T) = \sigma_\infty - \delta\left(1 - \frac{v_l}{v_v}\right)\Delta p_{ONB} \tag{4}$$

where δ is the Tolman length, which varies with temperature according following [7] with fluid-specific constants which are determined through calibration with experimental data [6].
The Jakob number, representing the ratio of sensible to latent heat, can be reformulated using a linearized Clausius-Clapeyron relation:

$$Ja = \frac{\rho_l C_{p,l} T_{sat} \Delta p_{ONB}}{(\rho_v h_{fg})^2} \tag{5}$$

By normalizing the Jakob number relative to its maximum value at spinodal conditions, one obtains [6]:

$$Ja_r = \frac{Ja_{ONB}}{Ja_{sp}} = \frac{\Delta p_{ONB}}{\Delta p_{sp}} \tag{6}$$

This normalization reveals a fundamental relationship between the degree of superheating and the depressurization rate. It was shown in [8, 6] that by integrating J with respect to time while assuming a maximal bubble density on the solid wall surface (Z), the following simple expression can be acquired:

$$Z = \frac{J \Delta p_{ONB}}{\Sigma'} \tag{7}$$

where Σ' is the depressurization rate within the metastable region.
The relatively acquired depressurization rate ,$\Sigma'/\Sigma_{min,sp}$, is the experimental pressure drop rate normalized by the minimal required depressurization rate to reach the spinodal, $\Sigma_{min,sp}$. Inserting Eq. 7 into this definition reveals the proportion of superheating once again. Thus, the following statement can be formulated:

$$\frac{Ja}{Ja_{sp}} = F\left(\frac{\Sigma'}{\Sigma_{min,sp}}\right) \tag{8}$$

Results and Discussion

The model was validated against expansion tube experiments conducted on water, carbon dioxide, and R22 over an initial relative temperature range of $0.6 < T_r < 0.98$. Figure 1 presents the normalized Jakob number as a function of the normalized depressurization rate, demonstrating excellent collapse of data from different fluids and experimental conditions onto a single universal curve.
A semi-empirical correlation for the heterogeneity factor was developed based on the entire experimental database [6]:

$$\phi = 10^{(19.5T_r - 18.4)(1 - 0.4\Sigma_r^{0.8})} \tag{9}$$

This correlation successfully captures experimental results across the range $0.61 \leq T_r \leq 0.947$ and $10^{-9} \leq \Sigma_r \leq 0.99$ and is presented in Figure 2.
The successful collapse of experimental data from different fluids onto a single universal curve validates the theoretical framework and demonstrates the applicability of the normalized approach. The model's ability to predict nucleation across both positive and negative pressure regions represents a significant advance in understanding flash boiling dynamics.

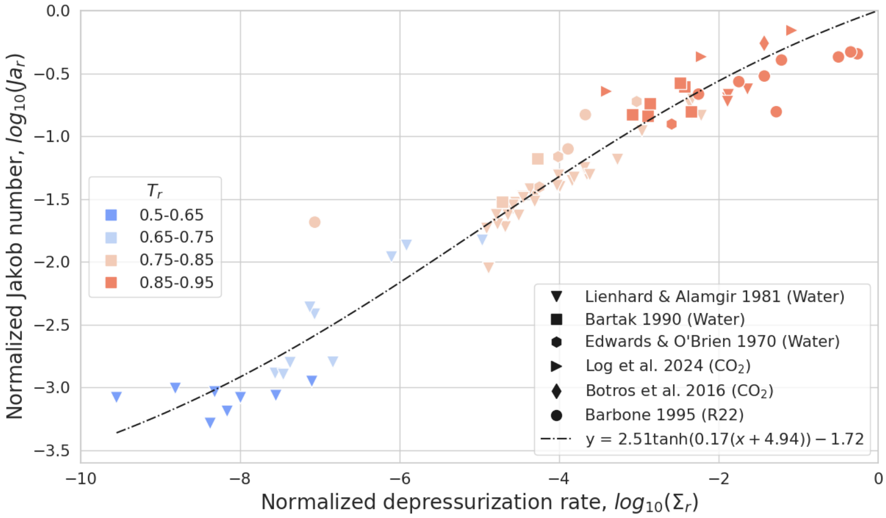

Figure 1. Normalized Jakob number vs. normalized depressurization rate showing universal behavior across different fluids: water (circles, stars, pentagons), CO_2 (crosses, plus signs), and R22 (triangles). The solid line represents the theoretical prediction. Adopted from Magen et al. [6]

The role of surface tension at high superheating levels is crucial for accurate predictions. Without accounting for curvature effects through the Tolman length correction, nucleation flux predictions would be orders of magnitude lower than physically realistic values, especially near the critical point.

The model provides practical tools for engineering applications in two ways: (1) as a standalone analytical method for quick predictions of ONB conditions, and (2) as a sub-model for implementation in computational fluid dynamics (CFD) simulations where the nucleation flux serves as a source term for bubble generation.

Conclusions

An analytical thermodynamic model has been developed to predict the onset of flash boiling under rapid depressurization conditions across positive and negative pressure ranges. The key findings include:

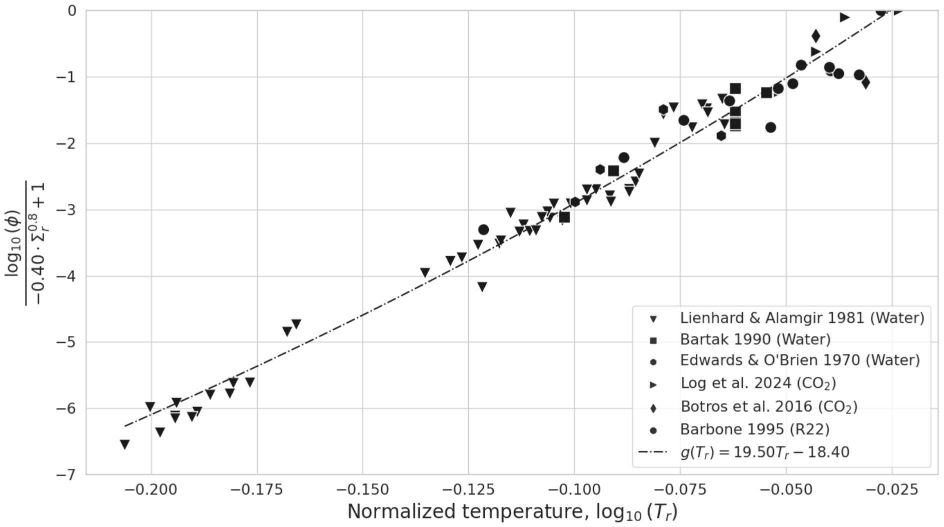

Figure 2. Heterogeneity factor function correlation using experimental data available: water (circles, stars, pentagons), CO_2 (crosses, plus signs), and R22 (triangles). The solid line represents the theoretical prediction. Adopted from Magen et al. [6]

The minimal depressurization rate required to reach spinodal conditions ($\Sigma_{min,sp}$) exhibits universal behavior across different fluids when properly normalized. The model successfully predicts nucleation pressures for given depressurization rates and initial conditions over a wide range ($0.4 < T_r \leq 0.98$, $10^{-9} \leq \Sigma_r \leq 1$). A new correlation for the heterogeneity factor extends applicability across diverse experimental conditions. The normalized Jakob number demonstrates a universal relationship with normalized depressurization rate, collapsing experimental data from water, CO_2, and R22 onto a single curve.Surface tension corrections accounting for curvature effects are essential for physically meaningful predictions at high superheating levels.

Nomenclature

B	Molecular collision frequency [s^{-1}]
C_p	Specific heat capacity [J/kg·K]
Gb	Gibbs number [-]
h_{fg}	Latent heat [J/kg]
h_P	Planck's constant [J·s]
J	Nucleation flux [m^{-2}s^{-1}]
Ja	Jakob number [-]
k_B	Boltzmann's constant [J/K]
N_A	Avogadro's number [mol^{-1}]
p	Pressure [Pa]
r	Radius [m]
T	Temperature [K]
v	Specific volume [m^3/kg]
W	Work [J]
Z	Nuclei density [m^{-2}]

Greek symbols

δ	Tolman length [m]
ϕ	Heterogeneity factor [-]
ρ	Density [kg/m^3]
Σ'	Depressurization rate [Pa/s]
σ	Surface tension [N/m]

Subscripts

c	Critical
l	Liquid
min	Minimal
ONB	Onset of Nucleate Boiling
r	Reduced/relative
sat	Saturation
sp	Spinodal
v	Vapor
∞	Low curvature reference

References

[1] E. Sher, T. Bar-Kohany, and A. Rashkovan, “Flash-boiling atomization,” *Progress in energy and combustion science*, vol. 34, no. 4, pp. 417–439, 2008.

[2] T. Bar-Kohany, M. Arogeti, A. Malka, and E. Sher, “Advances in liquid atomization via flash boiling—a global overview,” *Energies*, vol. 16, no. 19, p. 6763, 2023.

[3] T. Bar-Kohany, “Minimal heating rate for isobaric nucleation at the spinodal in liquids,” *International Journal of Heat and Mass Transfer*, vol. 165, p. 120636, 2021.

[4] S. V.P, “Metastable liquids,” 1974.

[5] M. E. M. Azouzi, C. Ramboz, J.-F. Lenain, and F. Caupin, “A coherent picture of water at extreme negative pressure,” *Nature Physics*, vol. 9, no. 1, pp. 38–41, 2013.

[6] O. Magen, Y. Kozak, L. Di Lucchio, M. Marengo, and T. Bar-Kohany, “Predicting nucleation pressure under rapid depressurization: Bridging positive and negative pressure regions,” *International Journal of Heat and Mass Transfer*, vol. 251, p. 127309, 2025.

[7] S. Gong, Z. Hu, L. Dong, and P. Cheng, “Temperature-and curvature-dependent surface tensions and tolman lengths for real fluids: a mesoscopic investigation,” *Physics of Fluids*, vol. 35, no. 7, 2023.

[8] M. Alamgir and J. Lienhard, “Correlation of pressure undershoot during hot-water depressurization,” *Journal of Heat Transfer*, vol. 103, no. 1, pp. 52–55, 1981.