THE CLASSICAL MULTICOMPONENT NUCLEATION THEORY FOR CAVITATION IN WATER WITH DISSOLVED GASES

Tomáš Němec *
Department of Thermodynamics
Institute of Thermomechanics ASCR, v. v. i.
Dolejškova 5, 18200 Praha 8, Czech Republic
Email: nemec@it.cas.cz

František Maršík
Department of Thermodynamics
Institute of Thermomechanics ASCR, v. v. i.
Dolejškova 5, 18200 Praha 8, Czech Republic
Email: marsik@it.cas.cz

ABSTRACT

The Classical Nucleation Theory (CNT) in its multicomponent form is presented as a reliable tool for the investigation of homogeneous nucleation in cavitation processes in aqueous systems. Several cases are considered, starting form the most simple case of a void cavity emerging at negative pressure, then treating the case of a bubble composed of water vapor only, and finally investigating the influence of various gases dissolved in water on the nucleation rate and the composition of the critical cluster. Aqueous systems related to cavitation in hydraulic machinery and to cavitation in carbonated beverages are discussed.

INTRODUCTION

The CNT has already proven its strength in dealing with condensation processes of various aqueous systems [1]. The early works in the nucleation theory [2] treated the simple pure-water condensation process, later [3] the theory was extended to binary systems treating various important aqueous mixtures [4–6]. Today, although the theory still suffers from many flaws, a commonly accepted theoretical apparatus exists [7] that describes the nucleation process in a general multi-component condensing system. The nucleation theory was also applied to cavitation processes in the past [8–10]. In the case of cavitation, however, the usage of the CNT led to the conclusion that large negative pressures of the order of hundreds of MPa are required to make the homogeneous nucleation process in water possible [11, 12]. Cavitation processes in water that are observed at positive pressures are considered as being caused by inhomogeneities present in water.

In this paper, we show that the CNT predicts the nucleation properties accurately in pure water and also in more complex aqueous systems. We review the theory and show its proper usage in the various cases, i.e. empty cavity, pure water (unary) cavitation, and cavitation in water with dissolved gases (binary and ternary). We focus on the proper evaluation of the critical nucleation work and discuss our results in connection with cavitation in hydraulic machinery and cavitation in carbonated beverages.

CLASSICAL NUCLEATION THEORY

The main goal of the CNT is the evaluation of the nucleation rate J, i.e. the number of newly created clusters per unit time and unit volume inside the metastable thermodynamic system. CNT shows that the nucleation rate is exponentially proportional to the critical nucleation work $W^\star$, $J = J_0 \exp(-W^\star/kT)$. It is the nucleation work W that needs to be properly evaluated for the respective cavitating system under investigation in order to get accurate results. In general, the nucleation work for a cluster of a given size and composition is evaluated as an increase of a suitable thermodynamic potential. In the case of cavitation, the grand thermodynamic potential Ω whose total differential reads

$$d\Omega = -SdT - pdV - \sum_i n_i d\mu_i + \sigma dA \tag{1}$$
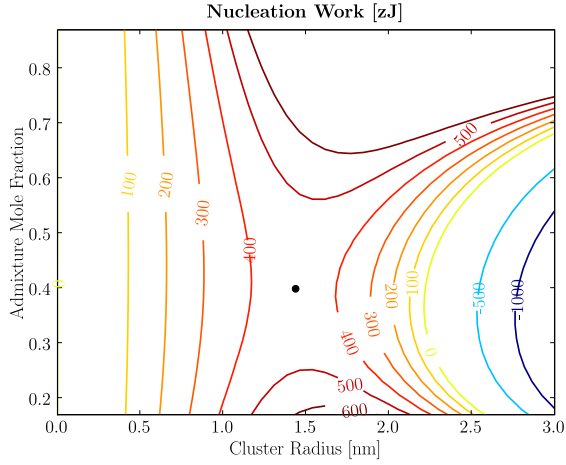
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*Address all correspondence to this author.

Figure 1. Saddle-shaped nucleation work surface of a model binary system of water–dissolved gas as a function of cluster size and mole fraction of admixture; the black dot shows the saddle point or, in other words, the size and composition of the critical cluster.

is a good choice. That is because the independent variables (temperature T, volume V, chemical potential (or composition respectively) μ_i, and surface area A) are usually prescribed and the remaining dependent variables (entropy S, pressure p, numbers of molecules n_i, and surface tension σ) are known functions of the independent ones. We are therefore able to integrate the total differential (1) from the initial thermodynamic state of the cavitating mixture to the final thermodynamic state of a given cluster inside the mixture yielding the nucleation work

$$W = A\sigma + Vp + \sum_{i=1}^{N} n_i \Delta\mu_i \qquad (2)$$

where N is the number of components of the cluster (N=0 in the case of a void cavity at negative pressure, N=1 in the case of unary (pure-water) nucleation, N=2 in the binary case of water with a dissolved gas etc.).

Being able to evaluate the nucleation work of every possible cluster within the mixture using (2), we can search for the critical nucleation work $W^\star$. As shown in Fig. 1, the nucleation work has the shape of a saddle, where the saddle point denotes the energetic barrier that needs to be overcome by the cluster to become a new, stably growing bubble. Once the saddle point $W^\star$ is found the nucleation rate J can be readily evaluated as mentioned above. The general CNT nucleation rate formula [13] is

$$J = \frac{c_0(1)|\lambda|}{\sqrt{2\pi kT \det D}} \exp\left(-\frac{W^\star}{kT}\right) \qquad (3)$$

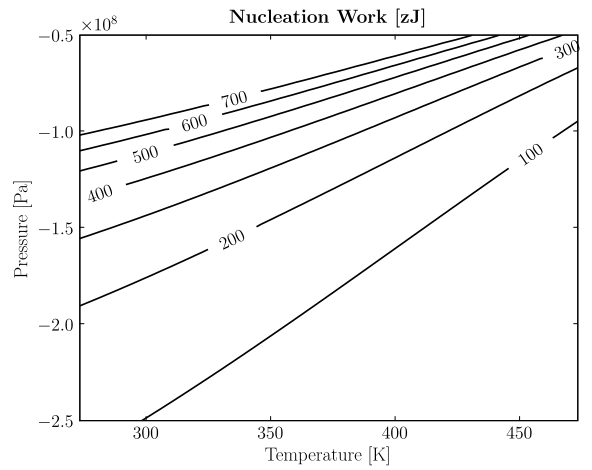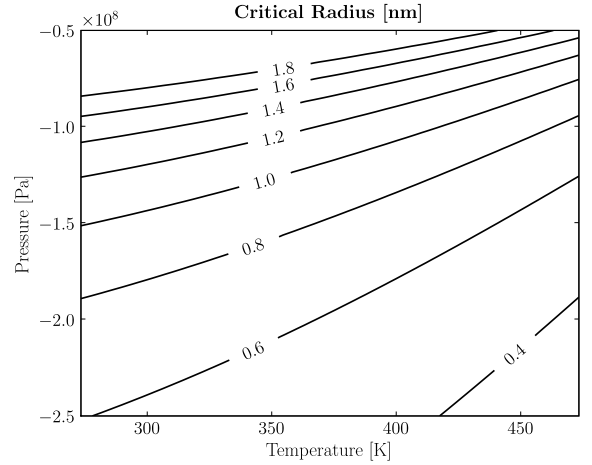We will not discuss the pre-exponential factor in (3) in more de-

Figure 2. Critical radius and critical nucleation work as functions of pressure and temperature calculated according to Eqs. (4) for pure water. The units of the nucleation work are zeptojoules 1 zJ = 10^{-21} J.

tail. Its influence on the calculated nucleation rates is far less important than the critical nucleation work in the exponential. The pre-exponential term is basically a slightly altered concentration of monomers in the mother liquid mixture $c_0(1)$. Let us therefore focus on the nucleation work and review its forms in the various cases of cavitating systems from the simplest one (void cavity) to a general N-component mixture.

EMPTY CAVITY

The simplest system that can be described with Eq. (2) is an empty cavity inside bulk liquid. In this case, the nucleation work consists of a volume part Vp needed to create an extra volume V in the liquid under pressure p, and a surface part necessary to create the new surface being a product of the surface tension σ and the cavity surface area A. No matter is transfered between
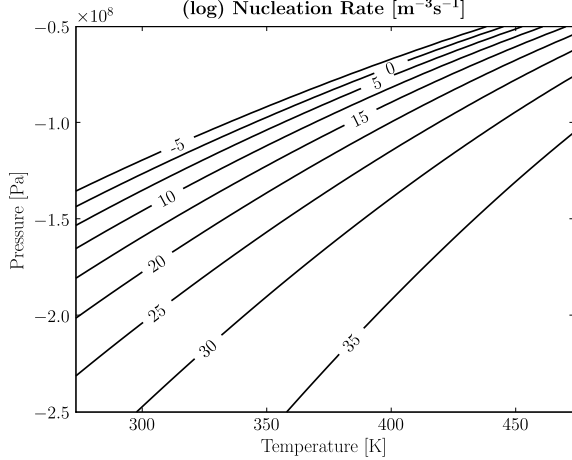
Figure 3. Nucleation rate according to Eq. (3) as a function of temperature and pressure during the void cavitation in water at negative pressures.
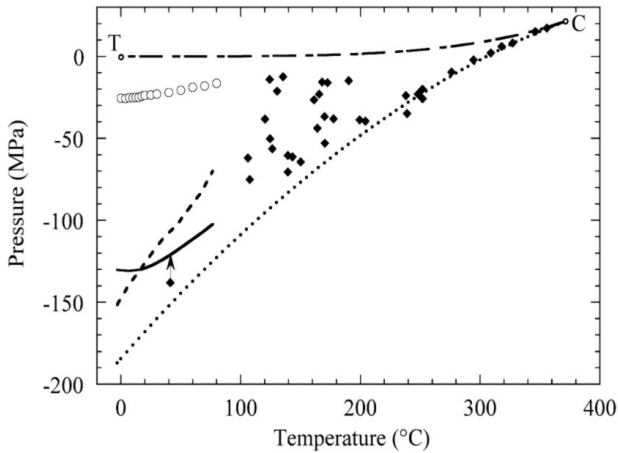

Figure 4. Cavitation pressure [12] as a function of temperature and pressure according to the CNT (dotted line) and DFT (full line). The dash-dotted line shows the saturation pressure of water starting from the triple point (T) to the critical point (C). The other symbols shows various measurements of nucleation rates in water at negative pressures as summarized by Caupin and Herbert [12].

the liquid and the cavity and therefore Eq. (2) simplifies to

$$W = A\sigma + Vp = 4\pi\sigma r^2 + \frac{4}{3}\pi p r^3 \qquad (4)$$

where r is the radius of the newly created cavity. At given pressure and temperature Eq. (4) is a function of one parameter r only, and therefore the saddle point reduces to a maximum of a one-dimensional curve. The maximum can be evaluated analytically in this simple case by solving $\frac{dW}{dr} = 0$. And the critical parameters take the form

$$r^\star = -\frac{2\sigma}{p} \qquad W^\star = \frac{4\pi r^{\star 2}\sigma}{3} \qquad (5)$$

We see that this type of nucleation can occur at negative pressures only. At positive pressures the nucleation work W increases with increasing cluster radius having no maximum and therefore rendering the occurrence of a stable cavity impossible.

To illustrate the results of this simple empty-cavity nucleation model, we show in Fig. 2 the values of critical radius and critical nucleation work calculated according to Eqs. (5).

The nucleation rates corresponding to the critical nucleation work of Fig. 2 are shown in Fig. 3. We see that the negative pressures required to arrive at observable nucleation rates (higher than roughly $10^6 \text{ m}^{-3}\text{s}^{-1}$) reach hundreds of MPa's. This behavior was observed in many cavitation experiments. The review paper of Caupin and Herbert [12] summarizes the measurements as can be seen in Fig. 4 in terms of the so-called cavitation pressure. This is a little bit vaguely defined property giving us the pressure when the probability to cavitate reaches 0.5. However, by comparing the dotted line on Fig. 4 with our nucleation rates in Fig. 3 we see that the cavitation pressure corresponds to nucleation rates between roughly 10^5 and 10^{10} m^{-3}s^{-1} which effectively describes the onset of an observable cavitation process.

UNARY SYSTEM

The next step in developing the nucleation theory for use in cavitation processes is to account for the transfer of molecules between the liquid and gaseous phases. Apart from the volume and surface portion of the nucleation work, we will take into account the work needed to transfer certain amount of molecules n from the liquid phase to the gaseous phase. The liquid phase is characterized by the chemical potential μ_l and the gaseous phase inside the bubble by μ_g. Therefore, the nucleation work formula (4) needs to be extended by $n\Delta\mu$, where $\Delta\mu = \mu_g - \mu_l$, and it takes the form

$$W = A\sigma + Vp + n\Delta\mu =$$
$$= 4\pi\sigma r^2 + \frac{4}{3}\pi p r^3 + kTn\ln\frac{p}{p_{sat}} \qquad (6)$$

Here, we have evaluated the chemical-potential difference $\Delta\mu$ in the ideal-gas and ideal-liquid approximation $\Delta\mu = kT\ln(p/p_{sat})$. Formula (6) is again a function of one parameter, the bubble radius r namely. The critical nucleation work, however, can not be in a general case calculated analytically as was
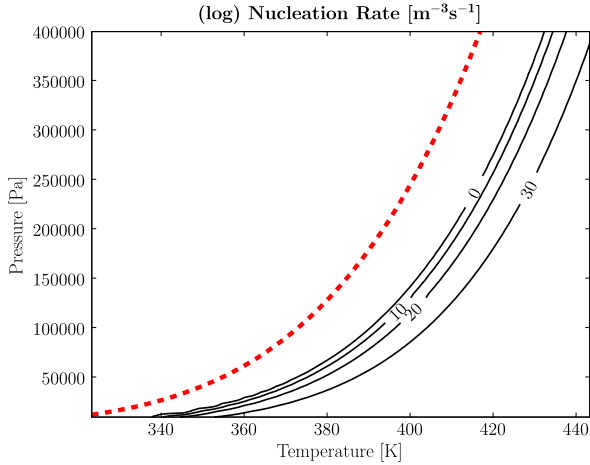
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Figure 5. Nucleation rate of cavitation in pure water calculated according to the unary model of the nucleation work (6). The red dashed line shows (here, and in all subsequent figures) the saturation pressure of water.
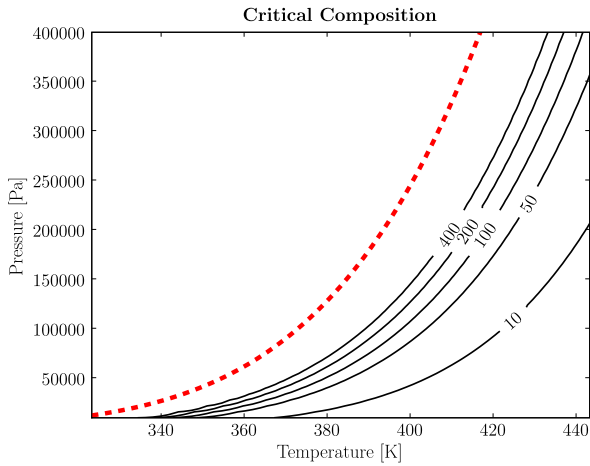

Figure 6. The number of water molecules in the critical cluster calculated according in the unary nucleation model and corresponding to the nucleation rates shown in Fig. 5.

the previous case of empty cavity. This is due to the fact that the number of cluster molecules n is a function of cluster density ρ_g

$$ n = \frac{\rho_g V N_A}{M} \tag{7} $$

The density ρ_g, in terms of the equation of state, depends on the pressure inside the bubble p_g which in turn is a function of cluster radius r due to the Laplace equation $p_g = p + 2\sigma/r$. As the functional dependence $\rho_g = \rho_g(p_g)$ given by a certain equation
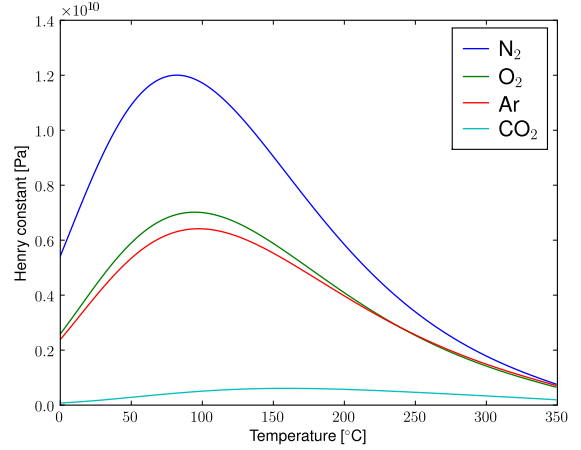

Figure 7. Henry constant k_{Hi} [15] of atmospheric gases dissolved in water as functions of temperature.

of state[1] might be quite complex it is not guaranteed that we are able to perform the derivative $\frac{dW}{dr} = 0$ analytically and arrive at equations analogous to (5). In such a case a numerical iterative procedure needs to be employed to find the maximum $W^\star$ of the nucleation work (6).

We have performed such a calculation for the case of pure water cavitation where all the thermophysical properties required by Eq. (6) are available. The resulting nucleation rate is shown in Fig. 5 as function of temperature and pressure. There is a crucial difference from the previous case. We see that we no longer need negative pressures to induce nucleation which is caused by fact that the last term in Eq. (6) reaches negative values when the system pressure drops below the saturation pressure of water. The nucleation process starts slightly below the vapor-liquid equilibrium plotted in Fig. 5 as the saturation pressure of water. For example, at 100 °C when the system pressure drops below roughly 0.5 bar the nucleation process occurs. Or, from another point of view, at 1 bar water needs to be superheated by roughly 20 °C to reach an observable nucleation rate. This result suggests that if water had to nucleate homogeneously we would observe boiling at roughly 120 °C .

In Fig. 6 the number of water molecules in the critical cluster is shown that corresponds to the nucleation rates in Fig. 5.

MULTI-COMPONENT SYSTEM

The extension of the above mentioned theoretical treatment to multi-component systems is straightforward. In the case of N components taking part on the nucleation process, the formula for the nucleation work takes the general form of Eq. (2). Similarly to the previous case, the chemical-potential difference

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[1]In our case of pure water the IAPWS-95 [14] equation of state was used.

Table 1. The composition of the atmosphere according to the definition of the *US standard atmosphere* [16] at 101325 Pa and 15 °C . For the 4 most abundant atmospheric gases we show their volume fraction in air x_v, partial pressure p_i, Henry constant in water k_H [15], and the corresponding mole fraction of the respective gas dissolved in water x_l.

i	x_v	p_i [Pa]	k_H [GPa]	x_l
N_2	0.78084	79118.61	7.34546	1.07711×10^{-5}
O_2	0.20948	21225.16	3.65143	5.81283×10^{-6}
Ar	0.00934	946.3755	3.33221	2.84008×10^{-7}
CO_2	0.00031	31.81605	0.12544	2.53635×10^{-7}

between the liquid and gaseous phase of the water component can be expressed as $\Delta\mu_1 = kT\ln(x_{g1}p/p_{sat}) - kT\ln(x_{l1})$, again adopting the ideal gas and ideal mixture assumptions.

The form of the chemical-potential difference of the other components in the mixture depends on the availability of their vapor-liquid equilibrium data. For admixtures whose pure-component saturation pressure data is available, the same expression as in the case of water can be used. For dissolved gases, however, it is more convenient to use the Henry constant data. The Henry constant for a gas dissolved in water is defined as

$$k_{Hi} = \lim_{x_{li} \to 0} \frac{f_{gi}}{x_{li}} \qquad (8)$$

where f_{gi} is the fugacity of the gas, often approximated by partial pressure p_{gi}. The Henry constant can be used to evaluate the chemical-potential difference as $\Delta\mu_i = kT\ln(x_{gi}p/k_{Hi}) - kT\ln(x_{li})$ in the case of a dissolved-gas component i. Henry constants of the most abundant atmospheric gases are plotted in Fig. 7 as functions of temperature. We see that CO_2 has a very low Henry constant resulting in high solubility in water and therefore it could be suspected to enhance the nucleation process more than the other gases. Its low concentration in atmosphere, on the other hand may lower its effects.

More information regarding the Henry constant is given in Tab. 1. Based on the amount of the respective gases in atmosphere and their Henry constant the mole concentration of the gas dissolved in water is evaluated at 15 °C . The high solubility of CO_2 is illustrated – the concentration of O_2 in atmosphere is roughly 3 orders of magnitude higher than CO_2 while the CO_2 concentration in water is just one order of magnitude lower than O_2. Indeed, among the atmospheric gases it is the carbon dioxide that, according to our calculations, shows the highest influence on the nucleation process.

The final form of the nucleation work (2) in the case of a N-component liquid mixture of water with dissolved gases takes
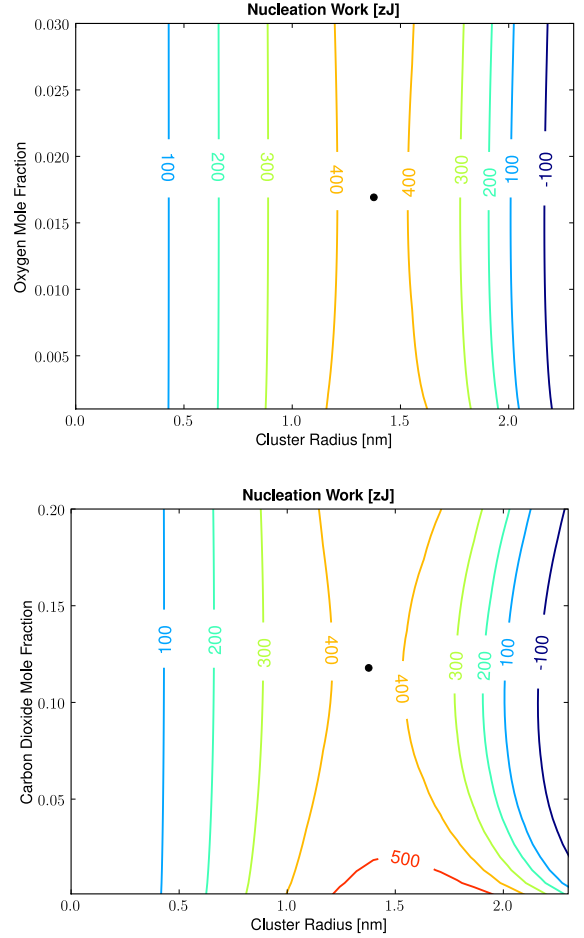

Figure 8. Saddle point in 4D of the nucleation work of the ternary water–oxygen–carbon dioxide mixture. The mole fractions of the components of the cavitating liquid mixture are x_{l,H_2O}=0.9972, x_{l,O_2}=0.00277, and x_{l,CO_2}=0.0000807. The mixture is cavitating at 115 °C and 101325 Pa. The critical nucleus (r_c=1.377 nm, x_{g,O_2}=0.0169 a x_{g,CO_2}=0.1178) is shown in two projections of the nucleation work surface. The upper graph shows the nucleation work in the vicinity of the critical nucleus for the critical carbon dioxide concentration x_{g,CO_2}=0.1178 as function of cluster diameter and oxygen concentration. Similarly, the lower graph shows the nucleation work for the critical oxygen concentration x_{g,O_2}=0.0169 as function of cluster radius and carbon dioxide concentration. In both these projections a 3D saddle point can be observed which gives us the saddle in 4D.

the form

$$W = 4\pi\sigma r^2 + \frac{4}{3}\pi p r^3 +$$
$$+ kTn_1 \ln\frac{x_{g1}p}{p_{sat}x_{l1}} + kT\sum_{i=2}^{N} n_i \ln\frac{x_{gi}p}{k_{Hi}x_{li}} \qquad (9)$$

Table 2. Nucleation parameters of the binary water – dissolved gas cavitating systems at 30 °C and 1200 Pa. Concentrations of the gas in water are given by the last column of Tab. 1. The nucleation rate in pure water is $1723980 \ \mathrm{m^{-3}s^{-1}}$ at these conditions. The size of the critical cluster is in all cases roughly 1.06 nm.

i	$n_{g,\mathrm{H_2O}}$	$n_{g,i}$	$W^\star$ [zJ]	J [$\mathrm{m^{-3}s^{-1}}$]
$\mathrm{N_2}$	127.2369	3.76×10^{-6}	331.29424	1720225
$\mathrm{O_2}$	127.2364	4.02×10^{-5}	331.29409	1720287
$\mathrm{CO_2}$	124.8678	0.6143	328.69566	3200576

where the numbers of molecules in the cluster n_i depend on the cluster concentrations as follows

$$ n_i = \frac{x_{gi} V N_A}{\sum_{i=1}^{N} \frac{x_{gi} M_i}{\rho_{gi}}} \qquad (10) $$

To find the critical cluster, i.e. the critical radius $r^\star$ and critical concentrations of admixtures $x_{g2}^\star, \ldots, x_{gN}^\star$, one needs to find the saddle point of the N-dimensional function (9). We use a numerical least-increase-type saddle-search algorithm to achieve this goal. The result of a model calculation of a three-component mixture is shown in Fig. 8. It is plotted as a pair of two 3D projections of the 4D nucleation work surface[2]. In every projection one admixture concentration is fixed at its critical value and the other admixture concentration and the cluster radius are varied around their critical values. In both projections, we see the saddle-shaped nucleation work producing the saddle in 4D.

Let us discuss the influence of various gases mentioned above. In the binary case, i.e. considering only one dissolved gas in water, we studied three systems, water–nitrogen, water–oxygen, water–carbon dioxide. The concentrations of gases in the liquid phase were taken according to Tab. 1 which means that they correspond to their natural concentrations in water. The results show that oxygen and nitrogen have no real influence on the nucleation process; the calculated nucleation rates are the same as in the case of pure water. Only carbon dioxide shows a slight increase in the nucleation rate, although less than one order of magnitude which is negligible. Tab. 2 shows the calculated nucleation rates at 30 °C and 1200 Pa for the three above-mentioned binary mixtures. The critical nuclei are composed almost entirely of water, the nucleation rates are close to the pure-water nucleation rates. Carbon dioxide is able to lower the critical nucleation work slightly resulting in double the nucleation rates when compared to the pure-water case.

These results are also illustrated in Fig. 9. The nucleation rates of pure water cavitation are plotted in the range of pres-

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[2] By 4D we mean that the function has three variables and therefore to plot its graph we need a 4-dimensional space.
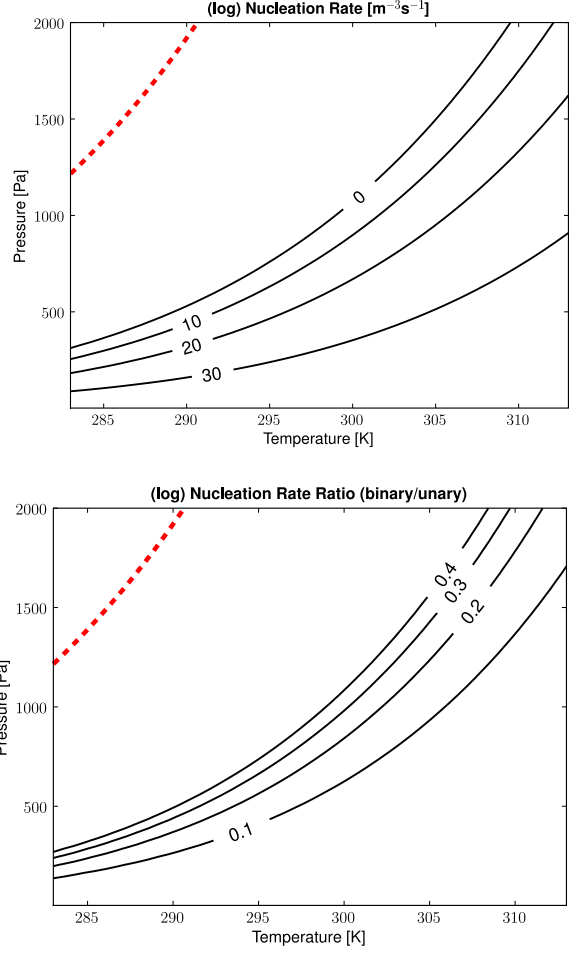

Figure 9. Nucleation rate in pure-water cavitation (upper graph) compared to the nucleation rate in the binary water–carbon dioxide system (lower graph). The mole fraction of carbon dioxide dissolved in water is 3×10^{-7}.

sures between 0 and 2 kPa and temperatures between 10 and 40 °C in the upper graph. The lower graph in Fig. 9 then compares the nucleation rates in the binary water–carbon dioxide cavitating system to the unary case. The binary nucleation rates are slightly higher, by a factor of roughly 2. This tiny increase in nucleation rates of binary systems of water with dissolved gas takes us to the conclusion that the presence of gases in water, in concentrations corresponding to their concentrations at normal atmospheric conditions, has no dramatic effect on the homogeneous nucleation process. And it is appropriate to neglect the presence of dissolved gases and use pure-water nucleation rates at these conditions, e.g. in the case of describing nucleation in hydrodynamic machinery like water pumps.

Although our numerical solver is able to calculate the nucleation parameters of a general N-component mixture, we will not
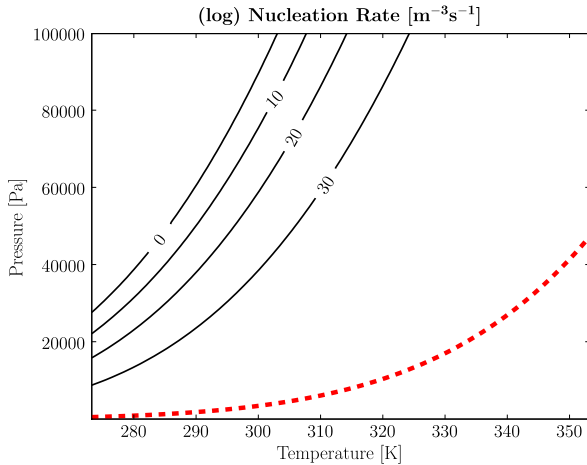
Figure 10. Nucleation rate in the binary water–carbon dioxide system with CO_2 mole fraction of 0.003 (originally saturated at 5 atm and 25 °C) as a function of temperature and pressure.

treat the more complicated three- and four-component mixtures of water with the various atmospheric gases which the proper description of the influence of dissolved air in water would require. Let us just state that the results are no different from the previous binary results. This is caused by the fact that the influence of various gases is independent, in other words, the presence of one gas does not influence the effects of others. And therefore the only decent effect of the dissolved air is caused by the presence of carbon dioxide increasing the nucleation rate by a factor of around 2 over the pure-water nucleation rates.

Finally, let us turn our attention to systems where the presence of dissolved gases is of higher importance. The carbonated beverages present a convenient example of such a system. Of course, our approximation of carbonated beverages is the binary system of water with dissolved carbon dioxide. Water is saturated with carbon dioxide at pressures of several atmospheres (usually around 5) which results in CO_2 mole fraction of tenths percent. Such a high gas concentration results, after exposing the mixture to normal atmospheric pressure (opening the bottle), in a quite fast nucleation process.

As an example, let us consider a mole fraction of carbon dioxide in water 0.003 which corresponds to saturating the water under 5 atmospheres of CO_2 at 25 °C . Our calculated nucleation rate of this binary system is shown in Fig. 10 as a function of temperature and pressure. The pressures span from 0 to 1 atm and the temperatures go from 0 to 80 °C . At the atmospheric pressure, we see that the nucleation rate of $1 \ \mathrm{m^{-3}s^{-1}}$ is reached at roughly 30 °C , and by increasing the temperature by only 5 °C the nucleation rate grows immensely to $10^{10} \ \mathrm{m^{-3}s^{-1}}$. We also notice that the nucleation process starts considerably above the vapor-liquid equilibrium of pure water (shown by the red dashed
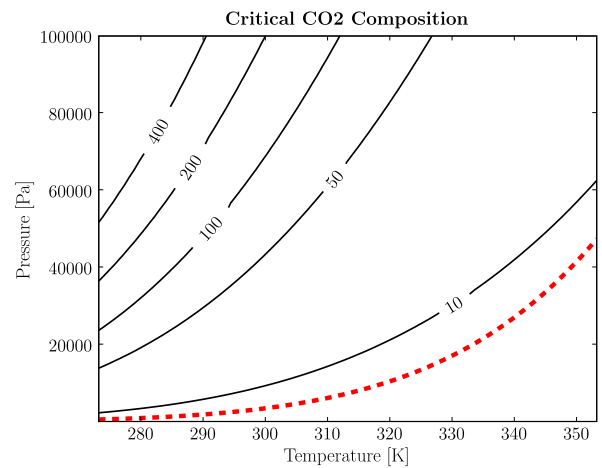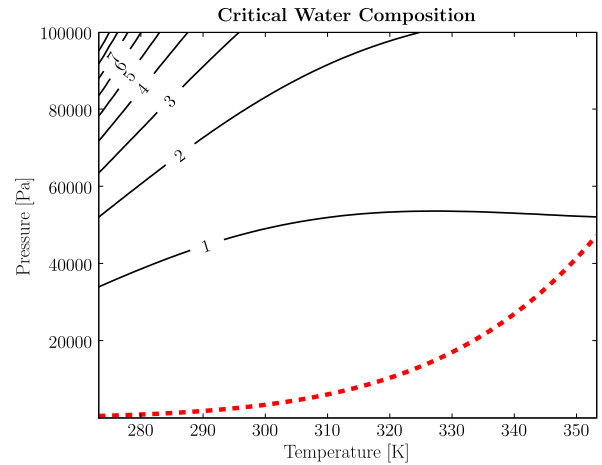

Figure 11. Numbers of water molecules (upper graph) and carbon dioxide molecules (lower graph) in the critical cluster corresponding to the nucleation rate shown in Fig. 10.

line in Fig. 10). On the contrary to the previously studied cases of water with considerably lower concentrations of dissolved gases, it is the carbon dioxide here which is the main component driving the nucleation process. This is illustrated in Fig. 11. We see that the critical clusters are composed mainly of carbon dioxide molecules.

CONCLUSION

We have studied the application of the Classical Nucleation Theory to homogeneous cavitation processes in water and aqueous systems. We have focused on the proper evaluation of the nucleation work which is the crucial property when calculating the nucleation rate.

The results of our calculations of aqueous cavitating systems (i.e. pure water, water with dissolved atmospheric gases)

are presented as starting points for the discussion about the influence of dissolved air on the nucleation process in water. Our conclusion is that the nucleation process at the temperatures and pressures relevant to hydraulic machinery (water pumps) is being enhanced by the presence of dissolved atmospheric gases in an almost negligible way due to their low concentration. The multicomponent nucleation rates are hardly twice as large when compared to the nucleation rates in pure water, and it is therefore plausible to neglect the presence of air and to consider the pure-water nucleation only during the cavitation processes in hydraulic machinery. An other question is, of course, whether the nucleation processes in hydraulic machinery cavitation can be modelled as homogeneous. If this is not the case, the influence of the inhomogeneity should be investigated in more detail, as it might considerably enhance the nucleation process over the homogeneous one.

We also studied the nucleation in aqueous systems with high concentration of a dissolved gas. The highly saturated, binary water – carbon dioxide system was used to approximate the cavitating behavior of a carbonated beverage. At atmospheric pressure our calculations predict the nucleation process to start at room temperature which complies with our everyday experience with carbonated beverages. The above-mentioned remark questioning the homogeneity of the nucleation processes applies also here. Moreover, the other components of the beverage could have some influence on certain physical properties of water, e.g. the surface tension, altering the nucleation rates as well.

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