PHYSICS OF LIQUIDS AND LIQUID SYSTEMS, BIOPHYSICS AND MEDICAL PHYSICS

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ANALYTIC CALCULATION OF THE CRITICAL TEMPERATURE AND ESTIMATION OF THE CRITICAL REGION SIZE FOR A FLUID MODEL

An analytic procedure for calculating the critical temperature and estimating the size of the critical region for a cell fluid model is developed. Our numerical calculations are illustrated by the case of the Morse potential parameters characterizing the alkali metals (sodium and potassium). The critical temperatures found for liquid sodium and potassium as solutions of the resulting quadratic equation agree with experimental data. The expression for the relative temperature determining the critical region size is obtained proceeding from the condition for the critical regime existence. In the cases of sodium and potassium, the value of this temperature is of the order of a few hundredths.

K e y w o r d s: cell fluid model, Morse interaction potential, grand partition function, recurrence relations, critical temperature, critical region.

1. Introduction

Critical phenomena in simple and multicomponent liquid systems have been the subject of many theoretical and experimental studies during the past decades (see, for example, [1–11]). These systems are of great practical importance, as well as very interesting from theoretical point of view. Experimental work is the basis for having a database of the properties of pure fluids and mixtures, and theoretical models can provide a large amount of information about a fluid in a rapid, clean, and cheap manner.

This paper supplements our previous study [12] based on a cell fluid model. The interaction in the system is chosen in the form of the Morse potential possessing the Fourier transform. Despite the great successes in the investigation of Morse fluids made by means of various methods (for example, the NpT plus test particle method [13], the grand-canonical transition matrix Monte Carlo method [14], the approach using integral equations [15], molecular dynamics simulations in a canonical ensemble [16]), the statistical description of the behavior of the mentioned fluids near the critical point on the microscopic level without any general assumptions are still of interest.

In [12], the cell fluid model is used for studying the behavior of a simple Morse fluid in the immediate vicinity of the liquid–gas critical point. The parameters of the Morse interaction potential used for calculations are inherent to alkali metals (sodium and potassium). The values of the critical temperature

and the size of the critical region are given in [12] without describing the method for obtaining them. In the present paper, we describe an analytic procedure for calculating the critical temperature and estimating the critical region size for a fluid model.

2. Model for Describing a Fluid System

The volume of the system V composed of N interacting particles is conventionally divided into N_v cells, each of volume $v = V/N_v = c^3$ (c is the linear size of a cubic cell) [12, 17, 18]. Note that, in contrast to a cell gas model (where it is assumed that a cell may contain only one particle or does not contain any particle) [19, 20], a cell within our approach may contain more than one particle [21, 22].

The grand partition function of the cell fluid model within the framework of the grand canonical ensemble has the form [12, 17, 18]

$$\Xi = \sum_{N=0}^{\infty} \frac{(z)^N}{N!} \int_V (dx)^N \exp\left[-\frac{\beta}{2} \sum_{\mathbf{l}_1,\mathbf{l}_2 \in \Lambda} \tilde{U}_{l_{12}} \rho_{\mathbf{l}_1}(\eta)\rho_{\mathbf{l}_2}(\eta)\right], \tag{1}$$

where $z = e^{\beta\mu}$ is the activity, $\beta = 1/(kT)$ is the inverse temperature, and μ is the chemical potential. Integration with respect to the coordinates of all particles $x_i = (x_i^{(1)}, x_i^{(2)}, x_i^{(3)})$ is noted as $\int_V (dx)^N = \int_V dx_1 \cdots \int_V dx_N$, and $\eta = \{x_1, ..., x_N\}$ is the set of coordinates. The interaction potential $\tilde{U}_{l_{12}}$ is a function of the distance $l_{12} = |\mathbf{l}_1 - \mathbf{l}_2|$ between cells. Each vector $\mathbf{l}_i$ belongs to the set

$$\Lambda = \Big\{\mathbf{l} = (l_1, l_2, l_3)|l_i = cm_i;\ m_i = 1, 2, ..., N_a;$$
$$i = 1, 2, 3;\ N_v = N_a^3\Big\}. \tag{2}$$

Here, N_a is the number of cells along each axis. The occupation numbers of cells appearing in Eq. (1) are defined as

$$\rho_{\mathbf{l}}(\eta) = \sum_{x \in \eta} I_{\Delta_{\mathbf{l}}(x)}, \tag{3}$$

where $I_{\Delta_{\mathbf{l}}(x)}$ is the indicators of cubic cells $\Delta_{\mathbf{l}} = (-c/2, c/2]^3 \subset \mathbb{R}^3$, that is, $I_{\Delta_{\mathbf{l}}(x)} = 1$ if $x \in \Delta_{\mathbf{l}}$ and $I_{\Delta_{\mathbf{l}}(x)} = 0$ otherwise. The role of the interaction potential $\tilde{U}_{l_{12}}$ is played by the Morse potential:

$$\tilde{U}_{l_{12}} = \Psi_{l_{12}} - U_{l_{12}};$$
$$\Psi_{l_{12}} = De^{-2(l_{12}-1)/\alpha_R},$$
$$U_{l_{12}} = 2De^{-(l_{12}-1)/\alpha_R}. \tag{4}$$

Here, $\Psi_{l_{12}}$ and $U_{l_{12}}$ are the repulsive and attractive parts of the potential, respectively, and $\alpha_R = \alpha/R_0$ (α is the effective interaction radius). The parameter R_0 corresponds to the minimum of the function $\tilde{U}_{l_{12}}$, and D determines the depth of a potential well. Note that the R_0-units are used for the length measuring in terms of convenience. As a result, R_0- and R_0^3-units are used for the linear size of each cell c and volume v, respectively.

3. Grand Partition Function, Recurrence Relations and Their Solutions

When calculating the grand partition function, we use the method of "layer-by-layer" integration with respect to the collective variables (CV) $\rho_{\mathbf{k}}$ proposed by Yukhnovskii for magnetic systems [23–27]. This procedure has already been represented for the simpler ρ^4 model in [17]. As a result of the step-by-step calculation of the grand partition function, the number of integration variables in the expression for this quantity decreases gradually. The grand partition function of the cell fluid is then represented as a product of the partial partition functions of individual layers and the integral of the "smoothed" effective measure density:

$$\Xi = 2^{(N_{n+1}-1)/2} G_\mu (Q(r_0))^{N_v} Q_1 ... Q_n [Q(P_n)]^{N_{n+1}} \times$$

$$\times \int W_{n+1}(\rho)(d\rho)^{N_{n+1}}. \tag{5}$$

The quantities G_μ and $Q(r_0)$ are given in [17], n is the layer number in the CV phase space, $N_{n+1} = N_v s^{-3(n+1)}$, s is the parameter of division of the CV phase space into layers. The partial partition function of the nth layer

$$Q_n = [Q(P_{n-1})Q(d_n)]^{N_n} \tag{6}$$

is expressed by the quantities

$$Q(d_n) = (2\pi)^{1/2} \left(\frac{3}{a_4^{(n)}}\right)^{1/4} \exp\left(\frac{x_n^2}{4}\right) U(0, x_n),$$
$$Q(P_n) = (2\pi)^{-1/2} \left(\frac{a_4^{(n)}}{\varphi(x_n)}\right)^{1/4} s^{3/4} \exp\left(\frac{y_n^2}{4}\right) U(0, y_n). \tag{7}$$

The variable $y_n = s^{3/2}U(x_n)(3/\varphi(x_n))^{1/2}$ is a function of the variable $x_n = g_n(B_{n+1}, B_n)(3/a_4^{(n)})^{1/2}$. The variable x_n is determined by the coefficients

$g_n(k)$ and $a_4^{(n)}$ appearing in the expression for the non-Gaussian quartic density of measure of the nth layer. The special functions

$$U(x_n) = U(1, x_n)/U(0, x_n) \qquad (8)$$

and

$$\varphi(x_n) = 3U^2(x_n) + 2x_n U(x_n) - 2 \qquad (9)$$

are combinations of the parabolic cylinder functions

$$U(a, t) = \frac{2}{\Gamma(a + \frac{1}{2})} e^{-t^2/4} \int_0^\infty x^{2a} \exp\left(-tx^2 - \frac{1}{2}x^4\right) dx. \qquad (10)$$

The argument t may be the main variable x_n or the intermediate variable y_n. The effective quartic measure density $W_{n+1}(\rho)$ appearing in Eq. (5) has the form

$$W_{n_p+1}(\rho) = \exp\left[a_1^{(n+1)}\sqrt{N_{n+1}}\rho_0 - \right.$$

$$- \frac{1}{2}\sum_{\mathbf{k} \in \mathcal{B}_{n+1}} g_{n+1}(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} -$$

$$\left. - \frac{a_4^{(n+1)}}{4!}\frac{1}{N_{n+1}}\sum_{\substack{\mathbf{k}_1, \ldots, \mathbf{k}_4 \\ \mathbf{k}_i \in \mathcal{B}_{n+1}}} \rho_{\mathbf{k}_1}\cdots\rho_{\mathbf{k}_4}\delta_{\mathbf{k}_1 + \cdots + \mathbf{k}_4}\right], \qquad (11)$$

where $\delta_{\mathbf{k}_1 + \cdots + \mathbf{k}_4}$ is the Kronecker symbol, and the region of wave vectors $\mathbf{k}$ is defined as

$$\mathcal{B}_{n+1} = \left\{\mathbf{k} = (k_1, k_2, k_3) | k_i = -\frac{\pi}{c_{n+1}} + \frac{2\pi}{c_{n+1}}\frac{n_i}{N_{n+1,i}}; \right.$$

$$\left. n_i = 1, 2, \ldots, N_{n+1,i}; \quad i = 1, 2, 3; N_{n+1} = N_{n+1,1}^3\right\}. \qquad (12)$$

The coefficients in the exponent of the quartic measure densities of the $(n+1)$th and nth layers are connected through the general recurrence relations (RR) [17]

$$w_{n+1} = s^{\frac{d+2}{2}}w_n,$$
$$r_{n+1} = s^2[-q + (r_n + q)N(x_n)], \qquad (13)$$
$$u_{n+1} = s^{4-d}u_n E(x_n).$$

with the initial conditions

$$w_0 = M(\beta W(0))^{1/2}, \quad r_0 = 1 - \beta W(0)\tilde{a}_2,$$

$$u_0 = a_4(\beta W(0))^2. \qquad (14)$$

Here,

$$w_{n+1} = s^{(n+1)}a_1^{(n+1)},$$
$$r_{n+1} = s^{2(n+1)}g_{n+1}(0), \qquad (15)$$
$$u_{n+1} = s^{4(n+1)}a_4^{(n+1)}.$$

The quantity q is associated with the averaging of the wave vector square, $d = 3$ is the space dimension. The functions $N(x_n)$ and $E(x_n)$ satisfy the expressions

$$N(x_n) = \frac{y_n U(y_n)}{x_n U(x_n)}, \quad E(x_n) = s^{2d}\frac{\varphi(y_n)}{\varphi(x_n)}. \qquad (16)$$

The quantity M is expressed by the chemical potential, $W(0)$ is the Fourier transform of the effective interaction potential at the zero value of the wave vector, $\tilde{a}_2$ and a_4 are the coefficients in the initial expression for the grand partition function (see [17]).

The coordinates of the fixed point (w^*, r^*, u^*) can be found from the conditions

$$w_n = w_{n+1} = w^*, \ r_n = r_{n+1} = r^*, \ u_n = u_{n+1} = u^*. \qquad (17)$$

For w^*, we have $w^* = 0$, since $s > 1$. The third equation for u_{n+1} [see Eqs. (13)] yields the relation

$$sE(x^*) = 1, \qquad (18)$$

which juxtaposes the own x^* to every s. Our calculations are performed for some fixed value of the parameter $s = s^* = 3.5977$. For such a preferred value of s nullifying the variable $x_n = (r_n + q)(3/u_n)^{1/2}$ at the fixed point ($x^* = 0$), the mathematical description becomes less complicated. Using the second equation for r_{n+1} [see Eqs. (13)], we arrive at the following expression:

$$(u^*)^{1/2} = q(1 - s^{-2})\sqrt{3}U(x^*)/(y^*U(y^*)). \qquad (19)$$

Thus, the fixed point coordinates are $w^* = 0$, $r^* = -q$, and u^* is determined from Eq. (19). Note that the variable y_n takes large values. Taking this into account, we obtain the expressions

$$w_{n+1} = s^{\frac{d+2}{2}}w_n,$$

$$r_{n+1} = s^2\left[-q + \frac{\sqrt{u_n}}{\sqrt{3}}\frac{1}{U(x_n)} - \frac{1}{2s^3}\frac{\sqrt{u_n}}{\sqrt{3}}\frac{\varphi(x_n)}{U^3(x_n)}\right], \qquad (20)$$

$$u_{n+1} = su_n\frac{\varphi(x_n)}{3U^4(x_n)}\left[1 - \frac{7}{2}s^{-3}\frac{\varphi(x_n)}{U^2(x_n)}\right]$$

and

$$(u^*)^{1/2} = q(1 - s^{-2})\sqrt{3}U(x^*)\left[1 + \frac{3}{2}(y^*)^{-2}\right] \quad (21)$$

corresponding to relations (13) and (19), respectively. The quantity q does not depend on the temperature, so r^* and u^* are also not functions of the temperature. They depend on $\alpha_R = \alpha/R_0$.

The solutions of RR in the vicinity of the fixed point (w^*, r^*, u^*) can be written through the eigenvalues of the matrix $\mathcal{R}$ of the linear transformation

$$\begin{pmatrix} w_{n+1} - w^* \\ r_{n+1} - r^* \\ u_{n+1} - u^* \end{pmatrix} = \mathcal{R}\begin{pmatrix} w_n - w^* \\ r_n - r^* \\ u_n - u^* \end{pmatrix}. \quad (22)$$

They assume the form [17]

$$w_n = w_0 E_1^n,$$
$$r_n = r^* + c_1 E_2^n + c_2 R E_3^n, \quad (23)$$
$$u_n = u^* + c_1 R_1 E_2^n + c_2 E_3^n,$$

where E_l are the eigenvalues of the matrix $\mathcal{R}$. The coefficients

$$c_1 = [r_0 - r^* + (u^* - u_0)R]\mathcal{D}^{-1},$$
$$c_2 = [u_0 - u^* + (r^* - r_0)R_1]\mathcal{D}^{-1} \quad (24)$$

are determined by the eigenvalues and elements of the renormalization group linear transformation matrix, coordinates of the fixed point, and initial coefficients $\tilde{a}_2$, a_4. The quantities R, R_1, and $\mathcal{D}$ appearing in Eqs. (23) and (24) satisfy the expressions

$$R = R^{(0)}(u^*)^{-1/2}, \quad R^{(0)} = \frac{R_{23}^{(0)}}{E_3 - R_{22}},$$
$$R_1 = R_1^{(0)}(u^*)^{1/2}, \quad R_1^{(0)} = \frac{E_2 - R_{22}}{R_{23}^{(0)}}, \quad (25)$$
$$\mathcal{D} = \frac{E_2 - E_3}{R_{22} - E_3}.$$

In the case where $s = s^*$, we get the following numerical values:

$$E_1 = s^{\frac{d+2}{2}} = 24.551, \quad E_2 = 8.308, \quad E_3 = 0.374,$$
$$R^{(0)} = -0.530, \quad R_1^{(0)} = 0.162, \quad \mathcal{D} = 1.086. \quad (26)$$

Let us represent $c_1(T)$ and $c_2(T)$ from Eqs. (24) as expansions in powers of the relative temperature $\tau = (T - T_c)/T_c$ (T_c is the critical temperature). Using

expressions (14) for r_0 and u_0 and taking into account that the coordinates of the fixed point of RR (13) are not functions of the temperature, we can write

$$c_1 = c_{10} + c_{11}\tau + c_{12}\tau^2,$$
$$c_2 = c_{20} + c_{21}\tau + c_{22}\tau^2. \quad (27)$$

Here, $c_{10} = 0$ because of the equation $c_1(T_c) = 0$, which, actually, is used to determine the critical temperature. Other coefficients in the expression for c_1 are defined as

$$c_{11} = \beta_c W(0)\mathcal{D}^{-1}\left[\tilde{a}_2 + 2R^{(0)}\beta_c W(0)a_4(u^*)^{-1/2}\right],$$
$$c_{12} = -\beta_c W(0)\mathcal{D}^{-1}\left[\tilde{a}_2 + 3R^{(0)}\beta_c W(0)a_4(u^*)^{-1/2}\right]. \quad (28)$$

For the coefficients $c_{2l}(l = 0, 1, 2)$, we find

$$c_{20} = \mathcal{D}^{-1}\Big[-u^* - R_1^{(0)}\sqrt{u^*}(1 + q) +$$
$$+ R_1^{(0)}\sqrt{u^*}\tilde{a}_2\beta_c W(0) + a_4(\beta_c W(0))^2\Big],$$
$$c_{21} = -\mathcal{D}^{-1}\Big[R_1^{(0)}\sqrt{u^*}\tilde{a}_2\beta_c W(0) + 2a_4(\beta_c W(0))^2\Big], \quad (29)$$
$$c_{22} = \mathcal{D}^{-1}\Big[R_1^{(0)}\sqrt{u^*}\tilde{a}_2\beta_c W(0) + 3a_4(\beta_c W(0))^2\Big].$$

Let us now proceed to the calculation of the critical temperature and the estimation of the size of the critical region.

4. Critical Temperature and Critical Region Size

There is a temperature $T = T_c$ at which

$$c_1(T_c) = 0. \quad (30)$$

When $M = 0$ and $T = T_c$, all three quantities w_n, r_n, and u_n from Eqs. (23) go to their fixed values at $n \to \infty$. With regard for the expression for c_1 [see Eqs. (24)], we can rewrite Eq. (30) for the critical temperature T_c in the following form:

$$1 - \tilde{a}_2\beta_c W(0) - r^* - R(a_4(\beta_c W(0))^2 - u^*) = 0. \quad (31)$$

Since $r^* = -q$, we obtain the equation

$$1 + q + R^{(0)}\sqrt{u^*} - \tilde{a}_2\beta_c W(0) - R^{(0)}\frac{a_4}{\sqrt{u^*}}(\beta_c W(0))^2 = 0, \quad (32)$$

where $\beta_c = 1/(kT_c)$, and the value of $R^{(0)}$ is given in Eqs. (26). This equation allows us to find the critical

temperature in the fluid model as a function of the microscopic parameters of the interaction potential and the coordinates of the fixed point of RR. The calculations in this paper are performed for the parameters of the Morse interaction potential taken from [17,18], which correspond to the data for sodium and potassium [14]. We have $R_0/\alpha = 2.9544$ for sodium (Na) and $R_0/\alpha = 3.0564$ for potassium (K).

The quantities included in Eq. (32) and the critical temperatures obtained for liquid metals (Na and K) from this equation are given in Table 1. Numerical values of the critical temperature represented in the form of reduced dimensionless units are obtained in different ways: from our present researches on the basis of the cell fluid model (see kT_c/D in Table 1), from Monte Carlo simulation results for the continuous system with the Morse potential in the grand canonical ensemble (see kT_c/D [14]), and from experiment (see kT_c/D [28]).

As can be seen from Table 1, our estimates of the critical temperature for Na and K agree better with the experimental data [28] than the numerical results [14] obtained by Monte Carlo simulations.

The renormalization group symmetry that occurs in the system indicates a change in the temperature behavior of the thermodynamic functions, when the temperature approaches T_c. The absence of the region of the critical regime means that the system will be described by a Gaussian regime of fluctuations, which leads to the classical values of critical exponents. From the point of view of the theoretical description of the phase transition at the microscopic level, the critical exponents are completely determined by the critical regime region. The transition of the classical critical exponents (the region of Gaussian fluctuations of the order parameter) to non-classical ones is determined by the quantity τ^* and takes place, only if there is the critical regime of fluctuations. This quantity determines the size of the critical region.

The size of the critical region is an important element of each theoretical scheme describing the phase transition. The Ginzburg criterion for determining the size of the critical region of temperatures is well known (see, for example, [29,30] and references cited herein). In this paper, an alternative option is described.

Let us estimate the order of magnitude of τ^*. The solutions of the renormalization group type (23) cor-

Table 1. **The quantities appearing in Eq. (32) for the critical temperature and the values of the dimensionless critical temperature for liquid alkali metals (Na and K). The constant D is the energy parameter for the Morse potential ($D = 0.9241 \times 10^{-13}$ ergs for Na and $D = 0.8530 \times 10^{-13}$ ergs for K [14])**

Metal	q	u^*	$\tilde{a}_2$	a_4	$W(0)/D$	kT_c/D	kT_c/D [14]	kT_c/D [28]
Na	1.236	3.626	0.324	0.038	17.769	4.028	5.874	3.713
K	0.880	1.839	0.313	0.039	16.072	3.304	5.050	3.690

Table 2. **The coefficients c_{11}, c_{20}, and c_{21} appearing in Eqs. (35) and (36) and the values of the relative temperatures τ_1^*, τ_2^*, and τ^* obtained for Na and K**

Metal	c_{11}	c_{20}	c_{21}	τ_1^*	τ_2^*	τ^*
Na	0.942	−2.894	−1.755	0.039	−0.352	0.04
K	0.735	−0.910	−2.020	0.023	−0.162	0.02

respond to the region of the critical regime. In these solutions, the terms proportional to E_3^n describe the entry to the critical regime, and the terms proportional to E_2^n describe the exit from the critical regime. The condition for the critical regime existence is that the exit from the critical regime for $n \to 1$ should not prevail over the entry to this regime. Using solutions (23) and this condition, we can determine the temperature range $\tau < \tau^*$ in which the critical regime occurs. The temperature τ^* will be equal to the magnitude (the absolute value) of the smallest root (τ_1^* or τ_2^*) of the two equations

$$c_1(\tau_1^*)E_2 = c_2(\tau_1^*)RE_3,$$
$$c_1(\tau_2^*)R_1E_2 = c_2(\tau_2^*)E_3. \tag{33}$$

Equations (33) accurate to within τ^* assume the following form:

$$c_{11}\tau_1^*E_2 = (c_{20} + c_{21}\tau_1^*)\frac{R^{(0)}}{\sqrt{u^*}}E_3,$$
$$c_{11}\tau_2^*R_1^{(0)}\sqrt{u^*}E_2 = (c_{20} + c_{21}\tau_2^*)E_3. \tag{34}$$

The first and second equations (34) have the solutions

$$\tau_1^* = \frac{c_{20}\frac{R^{(0)}}{\sqrt{u^*}}E_3}{c_{11}E_2 - c_{21}\frac{R^{(0)}}{\sqrt{u^*}}E_3} \tag{35}$$

and

$$\tau_2^* = \frac{c_{20}E_3}{c_{11}R_1^{(0)}\sqrt{u^*}E_2 - c_{21}E_3}, \qquad (36)$$

respectively. The quantities $R^{(0)}$, $R_1^{(0)}$, E_2, and E_3 are presented in Eqs. (25) and (26). The values of the fixed point coordinate u^* for Na and K are given in Table 1. Table 2 contains numerical estimates for c_{11}, c_{20}, and c_{21}, as well as for τ_1^*, τ_2^*, and τ^*. Thus, we obtain $\tau^* = \tau_1^* \approx 0.04$ (in the case of liquid sodium) and $\tau^* = \tau_1^* \approx 0.02$ (in the case of potassium).

5. Conclusions

A calculation technique for estimating the critical temperature and the size of the critical region for a fluid system is elaborated within the cell fluid model framework. For this purpose, we use expressions (23) for solutions of recurrence relations between the coefficients of the effective measure densities. Solutions (23) have the general form of the renormalization group solutions obtained by Wilson (see, for example, [31]) and differ from them by explicit expressions for c_1 and c_2.

In this paper, the calculations are performed for the Morse potential parameters characterizing real substances (sodium and potassium metals).

The equation for the critical temperature is obtained. The critical temperature is calculated and not introduced into the Hamiltonian of the system phenomenologically, as is done in the field theory approach or in the Landau theory. In the Landau theory, the quantity $T - T_c$ is included in the coefficient of the second power of the order parameter.

Our values of the critical temperature for liquid alkali metals (Na and K) agree more closely with the experimental data [28] than the Monte Carlo simulation results from [14].

Expression (35) makes it possible to find the value of the temperature τ^* at which the coordinate of the point of entry to the critical regime coincides with the coordinate of the point of exit from it. This means that there is no region of the critical regime for the temperature range $\tau > \tau^*$, but such a region exists for the temperature range $\tau < \tau^*$. The value of the temperature τ^* determining the critical region size is of the order of a few hundredths ($\tau^* = 0.04$ in the case of liquid sodium and $\tau^* = 0.02$ for potassium). The region of interest for most applications of supercritical fluids covers this temperature value (usually $1 < T/T_c < 1.1$ (or $0 < \tau < 0.1$) [32]).

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АНАЛІТИЧНИЙ РОЗРАХУНОК КРИТИЧНОЇ ТЕМПЕРАТУРИ ТА ОЦІНКА ВЕЛИЧИНИ КРИТИЧНОЇ ОБЛАСТІ ДЛЯ МОДЕЛІ ПЛИНУ

Розроблено аналітичну процедуру розрахунку критичної температури та оцінки розміру критичної області для коміркової моделі плину. Наші числові розрахунки проілюстровано на прикладі параметрів потенціалу Морзе, що характеризують лужні метали (натрій і калій). Критичні температури, знайдені для рідких натрію та калію як розв'язки отриманого квадратного рівняння, узгоджуються з експериментальними даними. Виходячи з умови існування критичного режиму, одержано вираз для відносної температури, що визначає величину критичної області. У випадках натрію і калію значення цієї температури становить кілька сотих.

К л ю ч о в і с л о в а: коміркова модель плину, потенціал взаємодії Морзе, велика статистична сума, рекурентні співвідношення, критична температура, критична область.