Method for calculating the equilibrium properties of individual substances within the framework of scale theory

Rykov V.A.^{1,@}, Kudryavtseva I.V.¹, Ustyuzhanin E.E.², Rykov S.V.¹, Rykov V.A.¹, Kudryavtseva I.V.¹, Ustyuzhanin E.E.² and Rykov S.V.¹

¹ ITMO University, Kronvergskiy 49, Saint-Petersburg, 197101, None

² National Research University Moscow Power Engineering Institute,

Krasnokazarmennaya 14, Moscow, 111250, None

[@] togg1@yandex.ru

The phenomenological theory of the critical point [1] is used, based on the method of pseudo-critical points and Benedek's hypothesis [2]. The proposed method for calculating the equilibrium properties of individual substances is based on the expression for entropy:

$$\Delta S \cdot X_i^{(1-\alpha)/\phi_i} = \varphi_0 + \varphi_2 \cdot m^2, m = \Delta \rho \cdot X_i^{\beta/\phi_i}.$$
 (1)

Here $\Delta S = (\rho T_c/p_c)[S(\rho, T) - S_0(\rho, T)]$; p_c is the critical pressure; T_c is the critical temperature; $S_0(\rho, T)$ is the regular function; $\Delta \rho = \rho/\rho_c - 1$; ρ_c is the critical density; φ_0 and φ_2 are constants; the function X_i successively takes on the values of isochoric heat capacity $(X_1 = C_v, \phi_1 = \alpha)$, isothermal compressibility coefficient $(X_2 = K_T, \phi_2 = \gamma)$ and isobaric heat capacity $(X_3 = C_p, \phi_3 = \gamma);\alpha$, β and γ are critical indices.

Using known thermodynamic equalities based on (refm1), a unified fundamental equation of state (UEoS) in the form of Helmholtz free energy has been developed. The proposed UEoS in the asymptotic vicinity of the critical point satisfies all the requirements of the largescale theory.

- [1] Kudryavtseva I V and Rykov S V 2024 Russ. J. Phys. Chem. A 98 2461–2474
- Benedek G B 1968 Polarization Matiere et Rayonnement, Livre de Jubile en l'Honneur du Professeur A. Kastler 71