Comparative study of scaling models related to thermodynamic properties of H$_2$O in the critical region

E E Ustyuzhanin$^1$, V F Ochkov$^1$, S V Rykov$^2$, V A Rykov$^2$, B E Znamensky$^1$, Aung Thu Ya Tun$^1$

$^1$Moscow Power Engineering Institute (Technical University), Krasnokazarmennaya 14, Moscow, 111250, Russia
$^2$Saint-Petersburg State University of Information Technologies, Mechahics and Optics, Kronverskii 49, Saint-Petersburg, 197101, Russia

E-mail: evgust@gmail.com

Abstract. An analysis of some literary sources is made in the report. They contain data on thermodynamic properties (the liquid density ($\rho_l$), the gas density ($\rho_g$), the mean diameter, ($f_d$), the pressure ($P$) on the saturation line) of H$_2$O. We have considered also scaling models, $\rho_g(\tau,D,C)$, $\rho_l(\tau,D,C)$ (Anisimov et al, 1990), here $\tau$ is the relative temperature, $D = (\alpha,\beta,T_c,...)$ are critical characteristics, $(\alpha, \beta)$ are critical indices, C are adjustable coefficients. A scaling model, $P(\tau,D,C)$, (Abdulagatov, 2007) is taken in account. These models meet the scaling theory of critical phenomena (ST) and work in the interval, $\tau = (0.002−0.012)$.

We have paid attention to a model, $f_d(\tau,D,C)$, (Anisimov et al, 1990). It describes $f_d$, includes the leading component with $(1−\alpha)$ index and is adapted to H$_2$O. Another type of $f_d(\tau,D,C)$ is developed in this work. Our model is different from $f_d(\tau,D,C)$ (Anisimov et al, 1990). Its structure is combined and contains the leading component with 2$\beta$ index. Similar combined scaling models have been developed too for properties (the order parameter, $f_s$, $\rho_l$, $\rho_g$, $P$).

There are got numerical estimates of parameters those are related to functions ($f_d(\tau,D,C)$, $\rho_g(\tau,D,C)$, $P(\tau,D,C)$ et al.) and based on ($\rho_l$, $\rho_g$, $P$, $T$) data, which are placed in the interval $3 \times 10^{-3} < \tau < 0.33$ and related to the formulation IAPWS-IF 97 of H$_2$O. The set of equations let us determine ($\rho_l$, $\rho_g$, $P$, $T$) values in the interval $10^{-5} < \tau < 10^{-2}$ including the extrapolation region. A comparative study is performed: we have compared our numerical values with ($\rho_l$, $\rho_g$, $P$, $T$) data those are determined on the basis of the equation of state (the formulation IAPWS–IF 95). The difference between two data sets is analyzed.

1. Introduction

We have considered several sources, which describe the liquid density ($\rho_l$), the gas density ($\rho_g$) and the pressure ($P$) related to the saturation line near the critical point of H$_2$O. In our analysis of the sources, there are analytical forms:

- the equation of state (EOS), which is named as EOS (IF-95) and included in the formulation (IF-95) [1];
- scaling equations ($\rho_l(\tau,D,C)$, $\rho_g(\tau,D,C)$), which are related to the densities and follow the scaling theory of critical phenomena (ST); among these equations, there are Anisimov models [2];
ρ equations. Several groups of scaling models are selected to analyze them. The first one (group X) includes

2. Analyses of some scaling models

analyses of some scaling models. The first one (group X) includes equations (\(f_d(\tau, D, C)\), \(f_s(\tau, D, C)\), \(P(\tau, D, B_p)\)) named as combined scaling models [8–11].

Anisimov models [2] is written in the form

\[
\begin{align*}
\rho_s &= B_{s0}^{1-\alpha_1} + B_{s1}\tau^{\beta_1}, \\
\rho_d &= B_{d0}\tau^{1-\alpha_1} + B_{d1}\tau,
\end{align*}
\]

where \(\rho_s = (\rho_l - \rho_g)/(2\rho_c)^{-1}\) is the order parameter, \(\alpha_1 = 0.11, \beta_1 = 0.325, \Delta = 0.5\) is the correction related to the first non asymptotic member [7], \(C = (B_s, B_d)\) are the coefficients got by a statistical treatment of the input \((\rho_l, \rho_g, P, T)\) data published before 1985, \(\rho_c, T_c\) are the critical parameters taken as literature data.

A structure of (1), (2) includes: scaling components with \((\alpha_1, \beta_1)\) indices and a linear component. The leading components of (1) and (2) have the forms: \(B_{s0}\tau^{\alpha_1-1}\) with \((1-\alpha_1)\) index and \(B_{s0}\tau^{\beta_1}\) with \(\beta_1\) index. These models follow to ST and are characterized by the fact that they comprise singular components, for example, \(B_{s0}\tau^{\beta_1}\). It means that the derivative, \(d\rho_s/d\tau\), is singular \((d\rho_s/d\tau \approx B_{s0}\tau^{\beta_1-1} \to \infty)\). If we use \(\rho_l = (f_d + f_s + 1)\rho_c\), then it is seen: \(d\rho_l/d\tau \to \infty\) when \(\tau \to 0\). Parameters of (1), (2) are placed in (table 1) and on the bases of \((\rho_l, \rho_g, T)\) data accumulated up to 1985 in the interval \(0.002 < \tau < 0.03\).

| \(\rho_c\), kg/m\(^3\) | \(T_c\), K | \(\alpha\) | \(\beta\) | \(\Delta\) | \(B_{s0}\) | \(B_{s1}\) | \(B_{d0}\) | \(B_{d1}\) |
|---|---|---|---|---|---|---|---|---|
| 322.778 | 647.067 | 0.11 | 0.325 | 0.5 | 1.975 | 0.59 | -1.48 | 4.3 |

We have planned to elaborate a combined scaling model that is connected with a property \((\rho_l, \rho_g, f_d, P, \ldots)\); for example, \(\rho_l(\tau, D, C)\) has to describe \(\rho_l\) and includes critical characteristics \(D = (T_c, \rho_c, \alpha, \beta, \ldots)\) and coefficients \(C = (B_s, B_d)\). The model follows some border conditions:

(i) The structure of \(\rho_l(\tau, D, C)\) correlates with ST, is valid in in the interval \(0.002 < \tau < 0.3\) and contains scaling and regular components.

(ii) \(D\) characteristics and \(C\) coefficients have to be calculated on the basis of a statistical treatment, which includes reliable \((\rho_l, \rho_g, P, T)\) data in the area, \(10^{-3} < \tau < 0.3\).

2. Analyses of some scaling models

Several groups of scaling models are selected to analyze them. The first one (group X) includes
These equations have the forms
\[ f_s = B_{s0}\tau^{\beta_1} + B_{s1}\tau^{\beta_1+\Delta} + B_{s2}\tau^{\beta_1+2\Delta} + B_{s3}\tau^2 + B_{s4}\tau^3, \]  
\[ f_d = B_{d0}\tau^{-\alpha_1} + B_{d1}\tau^{-\alpha_1+\Delta} + B_{d2}\tau^{-\alpha_1+2\Delta} + B_{d3}\tau^2 + B_{d4}\tau^3, \]  
\[ \ln(P/P_c) = B_p\tau^{2-\alpha_1} + B_{p1}\tau^{-\alpha_1+\Delta} + B_{p2}\tau^{-\alpha_1+2\Delta} + B_{p3}\tau + B_{p4}\tau^5 + B_{p5}\tau^7 + B_{p6}\tau^9, \]

where \( C = (B_{si}, B_{di}), \) \( B_p = (B_{pi}) \) are coefficients.

Due conditions i, ii, equations (3), (4), (5) consist of scaling parts \( (F_{\text{scale}}) \) and regular parts \( (F_{\text{reg}}): F_{\text{scale}} \) parts meet ST. It is shown in [8,9] that equation (4) should not contain the linear member in comparison with (4). Characteristics, \( D = (T_c, \rho_c, \alpha_1, \beta_1, \ldots) \), of (3), (4) have to be calculated together with the coefficients \( C = (B_{di}, B_{si}) \) on the basis of statistical processing of input \( (\rho_l, \rho_g, T) \) data. This treatment is a nonlinear least squares approximation (NRMS) and is used in [8,9].

It is shown in [8] and [10] that \( B_{p0} > 0 \). Characteristics, \( D = (P_c, B_{p0}, \ldots) \), of (5) have to be calculated together with the coefficients \( B_p \) on the basis of NRMS [8,10,11] of input \( (P, T) \) data. Characteristics, \( D = (T_c, \alpha_1) \) are accepted as general parameters of (3), (4), (5).

Group \( Y \) includes equations, \( f_d(\tau, D, C) \), which are elaborated in [12–15]
\[ f_d = B_{d0}\tau^{1-\alpha_1} + B_{d1}\tau + B_{d2}\tau^{2\beta_1}, \]  
\[ f_d = B_{d0}\tau^{1-\alpha_1} + B_{d1}\tau^{2\beta_1} + B_{d2}\tau^{1-\alpha_1+\Delta} + B_{d3}\tau^2 + B_{d4}\tau^3. \]  

It is seen from equations (6), (7) that their structures contain leading components with 2\( \beta \) indices \( (B_{d2}\tau^{2\beta_1}, B_{d2}\tau^{2\beta_1}) \). In the asymptotic region \( 0 < \tau < \tau_{as} \), equation (6) (7) have the forms \( f_d = B_{d\text{exp}}\tau^{2\beta_1}, f_d = B_{d2}\tau^{2\beta_1} \) which are significantly different from form leading component \( B_{d0}\tau^{\alpha_1-1} \).

It is an interesting task to prepare \( Z \) group, which includes equations (3), (5), (7). We have investigated some border conditions to group \( Z \). Authors of [13] have studied a scaling part related to (4), (7) and written as
\[ f_s = B_{s0}\tau^{\beta_1} + B_{s1}\tau^{\beta_1+\Delta}, \quad f_d = B_{d0}\tau^{1-\alpha_1} + B_{d\text{exp}}\tau^{2\beta_1}. \]

It is shown in [13] that equations (8) meet the conditions:

(iii) \( B_{d0} > 0, B_{s0} > 0, B_{d\text{exp}} > 0. \)

There are some numerical data in [13]: \( \alpha_1 = 0.1099, \beta_1 = 0.3474, B_{d0} = 0.4695, B_{d0} = 0.0518, B_{s0} = 1.4563. \) These values are determined on the basis of the experimental \( (\rho_l, \rho_g, T) \) data of SF6 placed in the interval \( 2 \times 10^{-4} < \tau < 0.01. \) The error, \( \delta\rho_{\text{imp}} \), of these input \( (\rho_l, \rho_g, T) \) data is determined as \( \delta\rho_{\text{imp}} = 0.1\%. \)

We’re interested in the sign of \( f_d \). To decide the question, let us consider a substance in a vertical cylinder, which has a volume \( V \). In state 1, this substance has a mass \( M \) and parameters \( (\rho = \rho_c, \) and the temperature \( T_1 = T_c) \). We place the virtual plane perpendicular to the axis of the cylinder and select the upper and lower parts, which have the volume as \( V/2 \). Let’s move the substance to state 2, and the isochoric conditions are considered: (a) \( \rho = \rho_c = \text{const} \) and (b) \( T_2 = T_c - \Delta T, \) here \( \Delta T > 0. \) As a result of this isochoric process, a condensation occurs and the mass \( M/2 \) is reduced by \( \Delta M > 0 \) in the upper part. The virtual plane moves to the phase boundary. The phase densities can be written as \( \rho_g = \rho_c + \Delta\rho_g\rho_c \) and \( \rho_l = \rho_c + \Delta\rho_l\rho_c, \) here \( \Delta\rho_l = (\rho_l - \rho_c)/\rho_c, \Delta\rho_g = (\rho_g - \rho_c)/\rho_c. \)

We write \( V \) as a function of the arguments \( (\Delta M, \Delta\rho_g, \Delta\rho_l) \) in the form
\[ V = \left( \frac{M}{2} - \Delta M \right) \frac{1}{\rho_c + \Delta\rho_g\rho_c} + \left( \frac{M}{2} + \Delta M \right) \frac{1}{\rho_c + \Delta\rho_l\rho_c}. \]
It is possible to express a $\Delta M/M$ function from (9) as

$$\frac{\Delta M}{M} = \left(\frac{\Delta \rho_l + \Delta \rho_g}{2} + \Delta \rho_l \Delta \rho_g\right) \frac{1}{\Delta \rho_g - \Delta \rho_l}.$$ \hspace{1cm} (10)

We introduce the known functions $f_d = (\Delta \rho_l + \Delta \rho_g)/2$, $f_s = (\Delta \rho_l - \Delta \rho_g)/2$ in (10) and note the equalities $(\Delta \rho_g - \Delta \rho_l = -2f_s$, $\Delta \rho_g \Delta \rho_l = f_d^2 - f_s^2)$. After some transformations, we obtain

$$\frac{\Delta M}{M} = \frac{f_s}{2} - \frac{f_d}{2} = \frac{f_d^2}{2f_s}.$$ \hspace{1cm} (11)

The change $\Delta V_g$ in the volume of the upper part is represented as

$$\Delta V_g = \left(\frac{M}{2} - \Delta M\right) \frac{1}{\rho_c + \Delta \rho_g \rho_c} - \frac{V}{2}.$$ \hspace{1cm} (12)

The relative change, $\Delta V_g/V$, of the gas volume can be written in the form

$$\frac{\Delta V_g}{V} = \left(\frac{\rho_c}{2} - \frac{\Delta M}{M}\rho_c\right) \frac{1}{\rho_c (1 + \Delta \rho_g)} - \frac{1}{2} \simeq \left(\frac{1}{2} - \frac{\Delta M}{M}\right) (1 - \Delta \rho_g) - \frac{1}{2}.$$ \hspace{1cm} (13)

Note that there is equality $\Delta \rho_g = f_d - f_s$. After the substitution of (11) in (13) and some algebraic transformations, we obtain $\Delta V_g/V$ in the form

$$\frac{\Delta V_g}{V} = \frac{(f_d + f_d^2 - f_s^2)(1 + f_s - f_d)}{2f_s} - \frac{f_d - f_s}{2}.$$ \hspace{1cm} (14)

Using (14), we can write $\Delta V_g/V$ in the first approximation as

$$\frac{\Delta V_g}{V} = \frac{f_d}{f_s} \left(1 + \frac{f_d f_s}{2} + \frac{f_d f_s^2}{2} + \ldots\right).$$ \hspace{1cm} (15)

Let us consider the following conditions ($\Delta V_g/V > 0$, $f_s > 0$), that is the volume of the upper part increases in this isochoric process. Under these conditions in the asymptotic temperature range ($\Delta > 0$ is a small value) it is possible to conclude from (15)

$$f_d > 0.$$ \hspace{1cm} (16)

Inequality (16) supports condition iii connected with a positive value of leading component, $B_{d_{exp}}^{2\beta_0}$, and the inequality, $B_{d_{exp}} > 0$. Let us underline, that $B_{d_0}^{\alpha_1}$ component of (2) is negative.

It is accepted that equations (3), (7) of Z group have to meet conditions i, ii, iii.

3. Numerical parameters of combined scaling models and some comparison results

It is an interesting task to search for the parameters of equations (3), (7). In this case, we have used the input orthobaric $(\rho_l, \rho_g, T)$ data related to formulation (IF-97) [16] and placed at $3 \times 10^{-3} < \tau < 0.3$. The number of these points is $N = 228$, among them 32 points are added to simulate the scattering data in the error corridor $\delta \rho_{\text{sim}} = \pm 0.2\%$, at $3 \times 10^{-3} < \tau < 3 \times 10^{-2}$. An error of the input $(\rho_l, \rho_g, T)$ data is accepted as $\delta \rho_{\text{imp}} = 0.2\%$ at $3 \times 10^{-3} < \tau < 3 \times 10^{-2}$. Characteristics, $D$, and coefficients, $C$, of (3), (7) (table 2) are calculated with the usage of NRMS [8,9] and input $(\rho_l, \rho_g, T)$ data.

Combined models, $p_l(\tau, D, C)$, $\rho_g(\tau, D, C)$, are built with an usage of models (3), (7) and equations ($p_l = (f_d + f_s + 1)\rho_c$, $\rho_g = (f_d - f_s + 1)\rho_c$). It is important to note: due to NRMS, we have used some standard relative root mean square deviation (RMS, $S\%$); among them

$$S_g = \left[\frac{\sum (100 (\rho_{g_{\text{exp}} - \rho_g(\tau, D, C)}/\rho_{g}(\tau, D, C))^2}{N_g}\right]^{0.5},$$ \hspace{1cm} (17)
Table 2. The parameters of equations (3), (7).

| $\rho_c$, kg/m$^3$ | $T_c$, K | $\alpha_4$ | $\beta_4$ | $B_{s0}$ | $B_{s1}$ | $B_{s2}$ | $B_{s3}$ | $B_{s4}$ |
|-------------------|----------|------------|------------|----------|----------|----------|----------|----------|
| 321.71            | 647.068  | 0.13211    | 0.34593    | 2.27105  | -0.169248| 0.126731 |
| $B_{s3}$          | $B_{s4}$ | $B_{d0}$   | $B_{d\exp}$| $B_{d2}$ | $B_{d3}$ | $B_{d4}$ |
| -1.55352          | 1.811386 | 0.89475    | 0.11449    | 0.653311 | -1.429225| 0.912035 |

where $N_g$ is a number of points at temperatures $\Delta \tau_{\text{scale}}$ in the gas phase,

$$S_l = \left[ \frac{\sum (100 (\rho_{\exp} - \rho_l(\tau, D, C))/\rho_l(\tau, D, C))^2}{N_l} \right]^{0.5},$$

(18)

where $N_l$ is a number of points in the whole temperature area up to $\tau = 0.3$ in the liquid phase,

$$S_1 = \left( \frac{S_g^2 + S_l^2}{2} \right)^{0.5}.$$  

(19)

Similar RMS deviations are considered, if we use $F_{\text{scale}}$ part of models (3), (7) and involve RMS deviations $(S_g, S_l, S_2)$, which are related to $(\rho_l, \rho_g, T)$ data from the interval, $\Delta \tau_{\text{scale}}$. $S_2$ has the form

$$S_2 = \left( \frac{S_g^2 + S_l^2}{2} \right)^{0.5},$$

(20)

where $(S_g, S_l)$ are RMS deviations, which are written as formulas (17), (18) with numbers $(N_l, N_g)$ related to $\Delta \tau_{\text{scale}}$.

NRMS can be used in variant I, when we determine $(D, C)$ values of models (3), (7) and optimize the criterion $S_1$. As a result we get in the case: $S_1 = S_{1\min}$ and $(D_I, C_I)$ values. NRMS can be used in variant II, when we determine $(D, C)$ values of $F_{\text{scale}}$ part and optimize the criterion $S_2$. As a result we get in the case: $S_2 = S_{2\min}$ and $(D_{II}, C_{II})$ values. Our tests have shown:

- $S_{1\min}$ does not coincide with $S_{2\min}$
- $D_I$ values do not coincide with $D_{II}$ values
- $C_I$ values do not coincide with $C_{II}$ values

NRMS can be used in variant III, when we determine $(D, C)$ values of models (3), (7) and optimize a compromise criterion $S_c$, which has the form

$$S_c = \left( \frac{S_1^2 + S_2^2}{2} \right)^{0.5}.$$  

(21)

As a result we get in the case: $S_c = S_{c\min}$ and $(D_{III}, C_{III})$ values. Our tests have shown:

- a criterion $S_{c\min}$ is intermediate between criteria $S_{1\min}$ and $S_{2\min}$
- $(D_{III}, C_{III})$ values are the same for models (3), (7) and $F_{\text{scale}}$ part
- models $(\rho_l(\tau, D_{III}, C_{III}), \rho_g(\tau, D_{III}, C_{III}))$ satisfactorily reproduce input $(\rho_l, \rho_g, T)$ data
- $(D_{III}, C_{III})$ values are placed in table 2.
In NRMS, initial approximations of $C$ and $D$ are taken in this method according to results [13], which include:

\[
\alpha_4 = 0.1321, \quad \beta_4 = 0.34593, \quad B_{a0} = 2.2721, \quad B_{d0} = 0.8911, \quad B_{d,exp0} = 0.1145.
\]

Values of $T_0$ and $\rho_0$ are chosen as ($T_c = 647.096$ K, $\rho_c = 321.957$ kg/m$^3$) recommended in [16].

If we use relations ($\rho_l = (f_s + f_d + 1)\rho_c$, $\rho_g = (f_d - f_s + 1)\rho_c$) and equations (3), (7), then we can get combined equations, $\rho_l(\tau, D, C)$, $\rho_g(\tau, D, C)$. Our analysis shows that these models satisfactorily reproduce input ($\rho_l$, $\rho_g$, $T$) data; thus

- deviations, $\delta \rho_l = 100(\rho_{l,inp} - \rho_{l,calc})/\rho_{l,inp}$, are placed in the range from $-0.4\%$ to $0.2\%$ at relative temperatures, $3 \times 10^{-3} < \tau < 0.3$;
- deviations, $\delta \rho_g$, lie in the range from $-0.4\%$ to $0.3\%$ at temperatures $3 \times 10^{-3} < \tau < 0.3$ (figure 1).

A standard RMS deviation, $S_l$, is determined as $S_l = 0.19\%$ for liquid densities at these temperatures. A deviation, $S_g$, is determined as $S_g = 0.21\%$ for gas densities at these temperatures. Characteristics, $D = (T_c, \rho_c)$, (table 2) are in good agreement with $T_c = 647.096$ K, $\rho_c = 321.957$ kg/m$^3$ recommended in [16] (within the error of the latter).

Models ($\rho_l(\tau, D, C)$, $\rho_g(\tau, D, C)$) let us obtained ($\rho_l$, $\rho_g$, $T$)$_{calc}$ data in the interval $1 \times 10^{-5} < \tau < 0.03$ including an extrapolation region. These values follow to ST. A similar property is got with a help of models (1), (2) [2] in the interval $1 \times 10^{-5} < \tau < 0.03$. Local deviations ($\%$) are determined in the form, $\delta \rho_l = 100(\rho_l[2] - \rho_{l,calc})/\rho_{l,calc}$, for the liquid phase and $\delta \rho_g = 100(\rho_g[2] - \rho_{g,calc})/\rho_{g,calc}$ for the gas phase. The deviations have the following character:

- $\delta \rho_l = (-0.35 - 0.25)\%$ when $1 \times 10^{-3} < \tau < 0.03$; $\delta \rho_l$ reaches $-0.65\%$ at $1 \times 10^{-5} < \tau < 1 \times 10^{-3}$;

![Figure 1](image.png)  
*Figure 1.* Function $F_d$ and its components: 1—function $F_d$ related to (7), 2—function $F_d$ related to (2), 3—$B_{d1} \tau \rho_c$ related to (2), 4—$B_{d0} \tau^{1-\alpha_4} \rho_c$ related to (7), 5—$B_{d,exp} \tau^{\beta_4} \rho_c$ related to (7).
• $\delta \rho_g = (0.5 - 0.6)\%$ at $1 \times 10^{-3} < \tau < 0.03$, $\delta \rho_g$ reaches 7% when $1 \times 10^{-5} < \tau < 1 \times 10^{-3}$.

We have got $(\rho_l, \rho_g, T)$ data with a help of EOS (IF-95) [1] in an extrapolation region. Our comparison has shown:

- deviations, $\delta \rho_l = 100(\rho_l[1] - \rho_l\text{ calc})/\rho_l\text{ calc}$, are increasing from 0.05% to 3.2% if $\tau$ decreases from $10^{-3}$ to $10^{-5}$;
- deviations, $\delta \rho_g = 100(\rho_g[1] - \rho_g\text{ calc})/\rho_g\text{ calc}$, are decreasing from −0.05% to −3.7% if $\tau$ decreases from $10^{-3}$ to $10^{-5}$.

An analysis of $f_s$ (3) and $f_d$ (7) is fulfilled. We have compared $f_s$ (3) and $f_d$ (7): (a) with ($f_{d\text{ imp}}$, $f_{s\text{ imp}}$) values and (b) the literary equivalents of ($f_s$, $f_d$) [2,16]. It is established that there is a good agreement between our values with the literary equivalents of ($f_s$, $f_d$) [16] at temperatures $3 \times 10^{-3} < \tau < 0.3$.

It interesting to study a behavior of $F_d$ function, which is based on $f_d$ (7) and written as $F_d = (\rho_g + \rho_l)/2 - \rho_c = \rho_c f_d$. These values of $F_d$, kg/m³, and its components are shown in figure 1 at extrapolation temperatures, $10^{-5} < \tau < 3 \times 10^{-3}$. It is possible to see positive components $B_{d0}\tau^{1-\alpha_1}\rho_c$ and $B_{d\text{ exp}}\tau^{2\beta_1}\rho_c$ of $F_d$ function related to (7). It is possible to see a behavior of $F_d$ function related to (2).

When searching for the parameters of equation (5), it has been adopted a number of restrictions including: (a) $B_{p0} > 0$ [8]; at the condition, the second derivative, $d^2 P/dT^2$, meets ST and has a scaling-type, $d^2 P/dT^2 \approx A_\tau T^{-\alpha}$, in the asymptotic region, (b) characteristics, $D = (\alpha = \alpha_4 = 0.1321, T_c = 647.068 K)$, are general for equations (3), (5), (7).

Parameters $D$ and $B_{p}$ of (5) (table 3) are calculated together on the basis of NRMS [8,11] and input ($P$, $T$) data [16]. This input array is located in both regular and critical areas of the interval $0.002 < \tau < 0.5$. Initial approximations, $D_0$ and $B_{p0}$ are taken according to results [11].

Table 3. Parameters of equation (5).

| $P_c$, MPa | $B_{p0}$  | $B_{p1}$  | $B_{p2}$  | $B_{p3}$  | $B_{p4}$  | $B_{p5}$  | $B_{p6}$  |
|------------|----------|----------|----------|----------|----------|----------|----------|
| 22.057     | 1.915    | −15.964407 | 1.147928 | −7.741428 | −37.438954 | 15.745531 | −71.674113 |

RMS deviation, $S_p$, of input ($P$, $T$) data from equation (5) is determined as $S_p = 0.0062\%$.

A value of $P_c$ (table 3) are in good agreement with $P_c = 22.057$ MPa recommended in [16] (within the error of the latter). Local deviations (%) are determined in the form, $\delta P = 100(P_{\text{imp}} - P_{\text{calc}})/P_{\text{calc}}$; these deviations are placed are within the error, $\delta P_{\text{imp}}$, is determined as $\delta P_{\text{imp}} = (0.01 - 0.03)\%$ in the interval $= 3 \times 10^{-3} - 0.5$.

We have got ($P_{\text{calc}}$, $T$) data on the basis of (7) and ($P$, $T$) data with a help of EOS (IF-95) [1] in an extrapolation region. Our comparison has shown: deviations, $\delta P = 100(P[1] - P_{\text{calc}})/P_{\text{calc}}$, are increasing from −0.02 to 0.03% if $\tau$ decreases from $10^{-3}$ to $10^{-5}$.

4. Conclusion
There have been studied combined scaling models (3), (7), which describe $f_d$ and $f_s$ in a wide temperature interval including the critical region. A structure of model (7) includes $B_{d\text{ exp}}\tau^{2\beta_1}$ as a leading component and meets ST. Numerical estimations of characteristics, $D = (T_c, \rho_c, \alpha_4, \beta_1, \ldots)$, and $C$ coefficients of these models are determined on the basis of a
statistical treatment of accurate ($\rho_l$, $\rho_g$, $T$) data [16]. Indeces ($\alpha_4$, $\beta_4$) coincide with parameters ($\alpha_1$, $\beta_1$) within (1–3)%.

There has been considered model $P(\tau, D, B)$ (5), which describes $P$ in a wide temperature interval including the critical region. Adjustable parameters of (5) are determined by fitting the model to input ($P$, $T$) data [16]. Values of ($T_c$, $P_c$, $\rho_c$) are in a satisfactory agreement with the data recommended in [16].

It is shown that equations (3), (5), (7) can be used in an extrapolation region up to $\tau = 1 \times 10^{-5}$. We have got some results in this region including:

- ($\rho_l$, $\rho_g$, $T$) data related to models (3), (7);
- ($\rho_l$, $\rho_g$, $T$) data related to Anisimov models [2];
- ($P$, $T$) data related to model (7);
- ($\rho_l$, $\rho_g$, $T$) data and ($P$, $T$) data calculated with the help of EOS–IF95 [1].

These data can be considered as the first numerical information, which is related to these thermodynamic properties of $\text{H}_2\text{O}$ in the extrapolation region. A comparative study is fulfilled of some sources containing these properties.

References

[1] Wagner W and Pruß A 2002 J. Phys. Chem. Ref. Data 31 387–535
[2] et al M A A 1990 Termodynamika kriticheskogo sostoyaniya individual’nykh veshchestv (Moscow: Energoizdat)
[3] Bazaev A R, Abdulagatov I M, Bazaev E A and Abdurashidova A 2007 J. Phys. Chem. Ref. Data 28 194–219
[4] Kudryavtseva I V, Rykov V A and Rykov S V 2008 Journal of IAR 2 36–39
[5] Apfelbaum E M and Vorob’ev V S 2015 J. Phys. Chem. B 119 8419
[6] Fortov V E, Khishchenko K V, Levashov P R and Lomonosov I V 1998 Nucl. Instr. Meth. Phys. Res. A 415 604–8
[7] Wegner C 1985 Int. J. Thermophys. 11 421
[8] Ustjuzhanin E E, Reutov B F, Utenkov V F and Rykov V A 2007 Soft Matter under Exogenic Impact. NATO Science Series II (Edit. S. Rzoska and V. Mazur) vol 242 (Springer) p 325
[9] Ustjuzhanin E E, Shishakov V V, Popov P V, Rykov V A and Frenkel M L 2011 Vestnik MEI 6 167–79
[10] Ustjuzhanin E E, Shishakov V V, Abdulagatov I M, Rykov V A and Popov P V 2012 Vestnik MEI 2 34–43
[11] Ustuzhanin E E, Ochkov V F, Shishakov V V and Rykov A V 2015 J. Phys.: Conf. Ser. 653 012109
[12] Wang J and Anisimov M A 2007 Phys. Rev. E E 75 061107
[13] Ochkov V F, Rykov V A, Rykov S V, Ustjuzhanin E E and Znamensky B E 2018 J. Phys.: Conf. Ser. 946 012119
[14] Vorob’ev V S, Rykov V A, Ustjuzhanin E E, Shishakov V V, Popov P V and Rykov S V 2016 J. Phys.: Conf. Ser. 774 012017
[15] Vorobev V S, Ochkov V F, Rykov V A, Rykov S V, Ustuzhanin E E and Pokholchenko V A 2019 J. Phys.: Conf. Ser. 1147 012016
[16] IAPWS 2012 IAPWS R7-97(2012) Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS. http://www.iapws.org)