Extrapolation of IAPWS-IF97 data: The liquid and gas densities on the saturation line near the critical point of H$_2$O

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Abstract. An analysis of some literary sources is made in the work. These sources describe the liquid density ($\rho_l$) and the gas density ($\rho_g$), which are related to the saturation line near the critical point of H$_2$O. In the analysis, we have considered analytical forms of (i) an equation of state (EOS) that is included in a formulation IF95 and recommended by IAPWS and (ii) $\rho_l(T)$ and $\rho_g(T)$ equations among them Anisimov models they are valid in a narrow temperature interval. We have analyzed $\rho_l$, $\rho_g$, $T$ data included in tables IF97. A combined scaling model is elaborated in the work. This model has a modern structure and meets the scaling theory of critical phenomena. We have got $\rho_l(T)$ and $\rho_g(T)$ equations on the basis of the combined scaling model. Our analysis shows that these equations satisfactorily reproduce $\rho_l$, $\rho_g$, $T$ data, which are related to tables IF97 and valid in a wide temperature interval. These equations have been used to generate $\rho_l$, $\rho_g$, $T$ data and to compare them with the results, which are determined the basis of analytical forms including EOS IF95. Numerical data are got in some extrapolation region near the critical temperature.

1. Introduction

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

- an equation of state (EOS) that is named as EOS IF95 and included in a formulation IF95 [1]; this EOS is recommended by the International Association for the Properties of Water and Steam (IAPWS) for scientific investigation;
- $\rho_l(\tau)$ and $\rho_g(\tau)$ equations including Anisimov models [2], where $\tau = (T_c - T)/T_c$ is a relative temperature.

We have analyzed tabulated $\rho_l$, $\rho_g$, $T$ data among them:

- data [3], which are included in tables IF97 and recommended by IAPWS;
- results presented in works of Anisimov et al [2] and Alexandrov et al [4, 5].
Table 1. The parameters of models (1) and (2).

| $\rho_l$, 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     |

EOS IF95 have an analytical form. So, at first, this EOS can satisfactorily reproduce $\rho_l$, $\rho_g$, $T$ data related to a regular part of the thermodynamic surface. At second, this EOS does not follow ST and has no opportunity to describe a singular behavior of row functions, for example, $d\rho_l/d\tau \to \infty$ when $\tau \to 0$, $df_d/d\tau \to \infty$ when $\tau \to 0$, here $f_d = (\rho_l + \rho_g)(2\rho_c)^{-1} - 1$ is the mean diameter. At third, this EOS allowed us to determine $\rho_l$, $\rho_g$, $T$ data in the interval $10^{-5} < \tau < 10^{-1}$ or in the critical region related to the phase transition from the liquid to the vapor. Our analysis has shown that the accuracy of these numerical data is lower than the accuracy of the data, which are calculated in the regular region.

This is an interesting problem to improve the accuracy of EOS in a wide range of temperatures and pressures, including the critical region. The problem of EOS designing has been considered in some works e.g. [1, 3, 6–13]. Authors of [6–9, 13] have elaborated EOSs, which are related to some metals. In the case, the critical points are located at high temperatures and high pressures. Authors of [11, 12] have considered a singular behavior, which is related to functions $[\rho_l(\tau), \rho_g(\tau), f_d(\tau), \ldots]$ and connected with EOS of Al, Cu and U near the critical point.

Anisimov models are related to functions $[\rho_l(\tau), \rho_g(\tau), f_d(\tau), \ldots]$ and have been developed in 1990 [2]. These models include critical indices ($\alpha_1 = 0.109$, $\beta_1 = 0.325$) and can be written in the form

$$f_s = B_{s0}\tau^{\beta_1} + B_{s1}\tau^{\beta_1+\Delta},$$

$$f_d = B_{d0}\tau^{1-\alpha_1} + B_{d1}\tau,$$

where $f_s = (\rho_l - \rho_g)(2\rho_c)^{-1}$ is the order parameter, $\Delta = 0.5$ is the correction included in the first non-asymptotic member [14], $C = (B_{si}, B_{di})$ are the coefficients got by a statistical treatment of the input $\rho_l$, $\rho_g$, $T$ data, $\rho_c$, $T_c$ are the critical parameters taken as literature data.

Equations (1) and (2) include a linear component and scaling components with indices $\alpha_1$ and $\beta_1$. These models follow to the scaling theory of critical phenomena (ST) and are characterized by the fact that they comprise singular components, for example, $B_{s0}\tau^{\beta_1}$; it means that the derivative $df_s/d\tau$ is singular ($df_s/d\tau \approx B_{s0}\tau^{\beta_1-1} \to \infty$ when $\tau \to 0$). These models are based on the density data accumulated up to 1980 in the interval $\tau = 0.002$–0.03. Their parameters are placed in table 1.

We have planned in the investigation to elaborate a combined scaling model that follow some border conditions:

(i) the model is connected with properties ($\rho_l$, $\rho_g$, $f_d$, $f_s$) and includes critical characteristics $D = (T_c, \rho_c, \alpha, \beta \ldots)$ and coefficients $C = (B_{si}, B_{di})$;

(ii) its structure is modern, correlated with ST and contains scaling components;

(iii) there are regular components in this model; they allow us to increase the applicability area up to $\tau \approx 0.1$ in a comparison with the area of models (1) and (2);

(iv) $D$ characteristics and $C$ coefficients are calculated on the basis of a statistical treatment that include reliable $\rho_l$, $\rho_g$, $T$ data in the area $10^{-3} < \tau < 0.1$. 


2. A choice of scaling models for $f_d$ and $f_s$

An improvement of models (1) and (2) has been made in several steps. The first one is related to Anisimov models [15] those have been developed in 2007 and written in the form

$$ f_s = B_{d0}\tau^{\beta_1} + B_{s1}\tau^{\beta_1+\Delta}, $$

$$ f_d = B_{d0}\tau^{1-\alpha_1} + B_{d1}\tau + B_{d2}\tau^{2\beta_1}. $$

Equation (4) meets the following conditions:

- it involves an additional singular component in a comparison with a structure of (2);
- the indices $D = (\alpha_1, \beta_1)$ follow the inequality: $1 > 1 - \alpha_1 > 2\beta_1$;
- the second singular component is dominant over other components in some temperature region, $0 < \tau < \tau_A$.

In the interval $0 < \tau < \tau_A$ equations (3), (4) can be written as

$$ f_s = B_{d0}\tau^{\beta_1}, \quad f_d = B_{d2}\tau^{2\beta_1}. $$

Equations (4), (5) are characterized by a fact that $df_d/d\tau$ is singular ($df_d/d\tau \approx B_{d2}\tau^{2\beta_1-1}$, when $\tau \rightarrow 0$).

Models (4), (5) contain an additional scaling component $B_{d2}\tau^{2\beta_1}$ that is discussed since 2003 in few studies including [11, 12, 15–18]. Authors of [18] have got models, which work in the asymptotic region of $T_c$ and have a form

$$ f_s = B_{d0}\tau^{\beta_3}, \quad f_d = B_{d0}\tau^{2\beta_3}, $$

where $2\beta_3 = 1 - v < 1$.

It is shown in [18] that models (6) follow such criteria as

- $B_{d0} > 0$, $B_{s0} > 0$;
- $f_d$ includes a linear component if $v = 0$;
- $f_d$ includes a singular component, $B_{d0}\tau^{2\beta_3}$, and does not contain a linear member, if the condition $0 < v < 1$ takes place, for example, $\beta_3 = 1/3$ if $v = 1/3$.

Numerical data on parameters ($B_{di}$) (4) are obtained in [15] for multiple substances including SF$_6$ and N$_2$ in the range, $1 \times 10^{-4} < \tau < 6 \times 10^{-2}$; it can be seen that

- the value of $B_{d2}$ depends on substances and can be positive (SF$_6$ etc) and negative (N$_2$ etc);
- $B_{d0}, B_{d2}$ coefficients have the opposite signs;
- the authors of [15] have attracted the input $\rho_1, \rho_0, T$ data to estimate values of ($B_{d1}, B_{s1}$); some information on the heat capacity, $C_v$, and the saturation pressure, $P$, are also used;
- values of $D = (\rho_c, T_c)$ are selected as the data taken from the literature.

Authors of [17] have proposed models, which operate in an asymptotic region of $T_c$ for SF$_6$ and written as

$$ f_s = B_{d0}\tau^{\beta_4} + B_{s1}\tau^{\beta_4+\Delta}, \quad f_{d \text{ opt}} = B_{d0}\tau^{1-\alpha_4} + B_{d \text{ exp}}\tau^{2\beta_4}, $$

where $D = (T_c, \rho_c, \alpha_4, \beta_4, B_{d0}, B_{d0}, B_{d \text{ exp}})$ are the characteristics determined on a basis of the experimental $\rho_1, \rho_0, T$ data placed in the interval $2 \times 10^{-4} < \tau < 0.01$, $\alpha_4 = 0.1099, \beta_4 = 0.3474, B_{d0} = 0.4695, B_{d \text{ exp}} = 0.0518$.

The second step of the modernization is connected with combined scaling models [19] written in the forms

$$ f_s = B_{d0}\tau^{\beta_4} + B_{s1}\tau^{\beta_4+\Delta} + B_{d0}\tau^{\beta_4+2\Delta} + B_{s3}\tau^2 + B_{s4}\tau^3, $$

$$ f_d = B_{d0}\tau^{1-\alpha_4} + B_{d1}\tau^{1-\alpha_4+\Delta} + B_{d2}\tau^{1-\alpha_4+2\Delta} + B_{d3}\tau^2 + B_{d4}\tau^3, $$

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where $D = (T_c, \rho_c, \alpha_4, \beta_4, B_{d0}, B_{d0}, B_{d \text{ exp}})$ are the characteristics determined on a basis of the experimental $\rho_1, \rho_0, T$ data placed in the interval $2 \times 10^{-4} < \tau < 0.01$, $\alpha_4 = 0.1099, \beta_4 = 0.3474, B_{d0} = 0.4695, B_{d \text{ exp}} = 0.0518$.

The second step of the modernization is connected with combined scaling models [19] written in the forms

$$ f_s = B_{d0}\tau^{\beta_4} + B_{s1}\tau^{\beta_4+\Delta} + B_{d0}\tau^{\beta_4+2\Delta} + B_{s3}\tau^2 + B_{s4}\tau^3, $$

$$ f_d = B_{d0}\tau^{1-\alpha_4} + B_{d1}\tau^{1-\alpha_4+\Delta} + B_{d2}\tau^{1-\alpha_4+2\Delta} + B_{d3}\tau^2 + B_{d4}\tau^3, $$

where $2\beta_3 = 1 - v < 1$.
where \((B_{si}, B_{di}; i = 0, 1, 2)\) are the coefficients related to \(F_{\text{scale}}\) part of the models, \((B_{si}, B_{di}; i = 3, 4)\) are the coefficients related to \(F_{\text{reg}}\) part.

\(F_{\text{scale}}\) meets ST. Models (8) and (9) include \(D = (T_c, \rho_c, \alpha_4, \beta_4, \ldots)\) characteristics and \(C = (B_{si}, B_{di})\) coefficients, which are determined on a basis of statistical treatment of experimental \(\rho_t, \rho_g, T\) data. The treatment is a nonlinear least squares method (NRMS) that is used in [17–19]. Numerical results [17–19] show that models (8) and (9) are adopted to a group of substances. In the case, an approximation error, \(\delta f_d\), is in a satisfactory agreement with the error, \(\delta f_{d\text{tab}}\), of the input points in the temperature range from \(\tau_{ow} = 10^{-4}\) to the relative temperature that is close to the triple point, \(\tau_{tr}\). Parameters of equations (8) and (9) are given in [19] for \(H_2O\) including \(D\) values: \(\alpha_4 = 0.1324, \beta_4 = 0.34594, T_c = 647.18\) K, \(\rho_c = 321.915\) kg/m\(^3\), \(B_{s0} = 2.2234, B_{d0} = 1.2095\).

The third step is related to integrating \(B_{d\text{exp}}\tau^{2\beta_4}\) component in (9). We have considered a form

\[
\delta f_d = B_{d0}\tau^{1-\alpha_4} + B_{d\text{exp}}\tau^{2\beta_4} + B_{d1}\tau^{1-\alpha_4+\Delta} + B_{d3}\tau^2 + B_{d4}\tau^3. \tag{10}
\]

It is planned in the work to determine \(D\) characteristics and \(C\) coefficients of equations (8) and (10) with the usage of the input \(\rho_t, \rho_g, T\) data related to tables IF97 [3]. We have to underline that equations (8) and (10) are a new variant of combined scaling models. First of all, it meets the criterion of “complete scaling” that is described by Fisher M. in his pioneer work [16]. Equation (10) is aimed to improve the traditional structure of \(f_d\) model and to increase an accuracy of \(f_d\) model in a wide temperature interval including the critical region. The equation reflects current trends of ST.

In the asymptotic region, equation (10) has a form \(f_d = B_{d\text{exp}}\tau^{2\beta_4}\) and correlates with equation (6). It is shown in [18] that \(f_d\) can include a linear component if \(\beta_3 = 0.5\). In our case (see below), \(\beta_4 = 0.34593\). We have considered an option of equation (10) that has included a linear component. In the case, the approximation error, \(\delta f_d\), has been significantly higher than the error, \(\delta f_{d\text{tab}}\) which depends on the error of the \(\rho_t, \rho_g, T\) data [3].

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

Searching for the parameters of equations (8) and (10), it has adopted a number of restrictions including the conditions (i) and (ii) formulated on page 2. Characteristics, \(D\), and coefficients, \(C\), of (8) and (10) (table 2) are calculated together on the basis of NRMS [17–19] and input \(\rho_t, \rho_g, T\) data [3]. The array is located in both regular and critical areas in the interval \(\tau = 3 \times 10^{-3} – 0.335\). The number of input points of the array is \(N = 228\), among them 32 points are added to simulate the scattering data in a corridor, \(\delta \rho_{\text{sim}} = \pm 0.2\%\), at relative temperatures \(\tau = 3 \times 10^{-3} to 3 \times 10^{-2}\) (figure 1).

Initial approximations of \(C\) and \(D\) are taken in this method according to results [17,19]; the values of \(D_0 = (T_c, \rho_c, \alpha_4, \beta_4, B_{s0}, B_{d0})_0\) are shown above; \(B_{d\text{exp}0}\) is selected as \(B_{d\text{exp}0} = 0.05\) on the recommendation of [17].

Combined equations \((\rho_t(\tau), \rho_g(\tau))\) are built with an usage of (1) and (2), (8) and (10). The analysis shows that these models satisfactorily reproduce input \(\rho_t, \rho_g, T\) data [3]; thus, deviations, \(\delta \rho_t = 100(\rho_{t\text{exp}} - \rho_{t\text{calc}})/\rho_{t\text{exp}}\), are placed in the range from \(-0.4\%\) to \(0.2\%\) at relative temperatures, \(3 \times 10^{-3} < \tau < 0.33\), and the deviations, \(\delta \rho_g\), lie in the range from \(-0.4\%\) to \(0.3\%\) at temperatures \(3 \times 10^{-3} < \tau < 0.30\) (figure 1). A standard RMS deviation, \(S_t\), is determined as \(S_t = 0.19\%\) for input data on the liquid density at these temperatures. The same deviation, \(S_g\), is determined as \(S_g = 0.21\%\) for the input data on the density at these temperatures. Characteristics \(D = (T_c, \rho_c)\) (table 2) are in a good agreement with \(T_c = 647.096\) K, \(\rho_c = 321.957\) kg/m\(^3\) recommended in [3] (within the error of the latter).

On the basis of numerical \(f_d\) data (10) (figure 2), we have fulfilled some comparisons.
Figure 1. Deviations of the input density data from values obtained on the basis of models (8) and (10): 1—deviations of $\rho_l$, $T$ data; 2—deviations of $\rho_g$, $T$ data.

Table 2. The parameters of equations (8) and (10).

| $\rho_c$, kg/m$^3$ | $T_c$, K | $\alpha_4$ | $\beta_4$ | $B_{s0}$ | $B_{s1}$ | $B_{s2}$ |
|------------------|---------|-----------|-----------|----------|--------|--------|
| 321.71           | 647.068 | 0.1145    | 0.34593   | 2.2721   | 0.029978 | -0.093563 |
| $B_{s3}$         | $B_{s4}$ | $B_{d0}$  | $B_{d\exp}$ | $B_{d1}$  | $B_{d2}$ | $B_{d3}$ |
| -0.876712        | 1.148671 | 0.8911   | 0.1145    | -0.21952 | 0.802212 | -1.184982 |

It is shown in figure 2:

- $f_d$ values (10), which are in a satisfactory agreement with values of $f_{d\text{tab}}$ at an interval of temperatures $3 \times 10^{-3} < \tau < 0.33$;
- $B_{d0}\tau^{1-\alpha_4}$ component of (10), it is positive and placed lower than $f_{d\text{tab}}$ at the interval;
- $B_{d\exp}\tau^{2\beta_4}$ component of (10), it is positive and placed lower than $B_{d0}\tau^{1-\alpha_4}$ at the interval.

In figure 3 with an usage of logarithmic coordinates, we have demonstrated a linear behavior of $f_d$ (10) and its scaling components ($B_{d0}\tau^{1-\alpha_4}$, $B_{d\exp}\tau^{2\beta_4}$) at temperatures $3 \times 10^{-3} < \tau < 0.01$. Our analyses allowed us to conclude:

- in the logarithmic scale of coordinates $f_d$ and its scaling components are linear functions; there is determined a relative temperature, $\tau_A \approx 10^{-5}$; an equality, $B_{d0}\tau^{1-\alpha_4} = B_{d\exp}\tau^{2\beta_4} = 0.4 \times 10^{-3}$, is realized at this temperature; an inequality, $(B_{d\exp}\tau^{2\beta_4} > B_{d0}\tau^{1-\alpha_4})$, is satisfied at $\tau < \tau_A$; this interval is a region where $B_{d\exp}\tau^{2\beta_4}$ plays a leading role of $f_d$ (10);
- it is possible to use $f_d$ (10) in an extrapolation region, $10^{-5} < \tau < 3 \times 10^{-3}$.

Numerical data for $f_s$ (10) and some comparisons allow us to find out that $f_s$ (10) is in a satisfactory agreement with $f_{s\text{tab}}$ values built on a basis of input $\rho_l$, $\rho_g$, $T$ data [3] at the range of temperatures $3 \times 10^{-3} < \tau < 0.33$. 

\[ \]
Figure 2. Diameter, \( f_d \) and its components: 1—\( f_{d\text{tab}} \) built on the basis of input \( \rho_l, \rho_g, T \) data; 2—a border, \( f_{d \text{ high}} \); 3—a border, \( f_{d \text{ low}} \); 4—\( f_d(10) \); 5—\( B_d 0 \tau_{1-\alpha} \); 6—\( B_d \exp \tau \beta_4 \).

Figure 4 shows a distribution of deviations, \( \Delta f_s = f_{s\text{tab}} - f_s \), for \( f_s \). Our analyses allowed us to estimate:

- \( f_s \) (8) and the component, \( B_d 0 \tau^{2\beta} \), have a linear form in logarithmic coordinates in the range of temperatures \( 3 \times 10^{-3} < \tau < 0.01 \);
- it is possible to use \( f_s \) (8) in an extrapolation region, \( 10^{-5} < \tau < 3 \times 10^{-3} \).

We have analyzed some results, which are got in [2] and related to \( f_d(2) \). It can be seen that the presence of a negative coefficient, \( B_d = -1.48 \), (table 1) leads to facts:

- the leading component, \( B_d \tau^{1-\alpha_1} \), is negative and \( df_d/d\tau \approx -B_d \tau^{-\alpha_1} \to \infty \) at \( \tau \to 0 \) (compare with \( f_{d\text{tab}} \) and \( B_d \tau^{1-\alpha_1} \), figures 2 and 3);
- there is a temperature, \( \tau = \tau_B = 1 \times 10^{-3} \); an equality \( (B_d \tau + B_d \tau^{1-\alpha_4} = 0, B_d = 4.3) \) is realized at this temperature; values of \( f_d(2) \) become negative in the interval, \( 0 < \tau < \tau_B \); it is an abnormal region of \( f_d \) in the case of \( \text{H}_2\text{O} \).

These is the following anomalous behavior: values of \( f_d(2) \) increase when approaching \( T_c \) in a region, \( 0 < \tau < \tau_B \). Note, that \( f_{d\text{tab}} \) is reduced steadily when decreases in the investigated interval \( 3 \times 10^{-3} < \tau < 0.3 \) (see \( f_{d\text{tab}} \), figure 2).

Results for \((\rho_l, \rho_g, T)\) \( \text{calc} \) have been obtained with a help of models (8) and (10). A similar massive is got with a help of models (1) and (2) [2] in the interval \( 1 \times 10^{-5} < \tau < 0.03 \). Local deviations (%) are determined in the form, \( \delta \rho_l = 100(\rho_l(2) - \rho_{l\text{calc}})/\rho_{l\text{calc}} \) for the liquid phase and \( \delta \rho_g = 100(\rho_g(2) - \rho_{g\text{calc}})/\rho_{g\text{calc}} \) for the gas phase. The deviations have the following character:
Figure 3. A behavior of $f_d$ (10) and its components in the interval $0.001 < \tau < 0.1$: 1—$f_d$ (10); 2—a border, $f_d$ high; 3—a border, $f_d$ low; 4—$B_d\alpha\tau^{-1-\alpha_1}$; 5—$B_{d\exp}\tau^{2\beta_4}$.

Figure 4. Deviations of $f_{\text{stab}}$ built on the basis of input $\rho_l$, $\rho_g$, $T$ data from values of $f_s$ (8).

- $\delta\rho_l = -0.35$ to $0.25\%$, when $1 \times 10^{-3} < \tau < 0.03$; $\delta\rho_l$ reaches $-6.5\%$ at $1 \times 10^{-5} < \tau < 1 \times 10^{-3}$;
- $\delta\rho_g = -0.5$ to $0.6\%$ 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 data for $\rho_l$, $\rho_g$, $T$ with a help of the EOS IF95 in an extrapolation region. Our comparison has shown:

- deviations, $\delta\rho_l = 100(\rho_{l[i]} - \rho_{l\text{calc}})/\rho_{l\text{calc}}$, 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 \(10^{-5}\).

4. Conclusion

Combined scaling models (8) and (10) allow describing \( f_d \) and \( f_s \) in a wide temperature interval including the critical region. A structure of model (10) has \( B_d \exp(\tau^{2\beta_4}) \) component and meets ST. It is got a satisfactory agreement of our calculated \((\rho_l, \rho_g, T)\text{calc}\) data with the input points related to tables IF97 in the critical region. There is a good correlation:

- between \((T_c, \rho_c)\) values and the data recommended in [2];
- between \((\alpha_4, \beta_4)\) indexes and parameters \((\alpha_1, \beta_1)\); the discrepancy between these data lies in the interval \(\pm(1-3)\%\);
- between \((f_s, f_d)\) values (8) and (10) and appropriate values those are built on a base of input \(\rho_l, \rho_g, T\) data [2] at relative temperatures, \(0.003 < \tau < 0.33\).

Equations (8) and (10) can be used in the extrapolation region down to \(\tau = 1 \times 10^{-5}\). We have got \((\rho_l, \rho_g, T)\text{calc}\) data related to models (8) and (10) in this interval. These data can be considered as the first numerical information in the extrapolation region.

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