

Appendix 2. Derivation of the coefficients of thermal expansion and compressibility for use in FEFLOW 5[®]

(Magri 2004)

In this appendix the coefficients of thermal expansion and compressibility appearing in the equation of state for the fluid density (Eq. (1.40 Appendix 1)) will be derived for a wide range of pressure and temperature $p_{Sat} < p \leq 100$ MPa and $0 \leq T \leq 350$ °C.

This is of big use for modelling heat transfer in geothermal reservoir such as the NEGB where high temperature and pressure are involved in the simulations. Indeed in thermohaline problems, the fluid density ρ^f varies with pressure p , temperature T and concentration of various components C^e (where C^e stands for the C^e 's of all components present in the fluid) according to relations called equations of state:

$$\rho^f = \rho^f(T, p, C^e) \quad (2.1)$$

From Eq.(2.1) it follows that:

$$\begin{aligned} d\rho^f &= \left. \frac{\partial \rho^f}{\partial T} \right|_{p, C^e} dT + \left. \frac{\partial \rho^f}{\partial p} \right|_{T, C^e} dp + \sum_e \left. \frac{\partial \rho^f}{\partial C^e} \right|_{p, T} dC^e \\ &= \rho^f (\beta dT + \gamma dp + \alpha^e dC^e) \end{aligned} \quad (2.2)$$

where

$$\beta \equiv \frac{1}{\rho^f} \left. \frac{\partial \rho^f}{\partial T} \right|_{p, C^e} \quad (2.3)$$

$$\gamma \equiv \frac{1}{\rho^f} \left. \frac{\partial \rho^f}{\partial p} \right|_{T, C^e} \quad (2.4)$$

$$\alpha^e \equiv \frac{1}{\rho^f} \left. \frac{\partial \rho^f}{\partial C^e} \right|_{p, T} \quad (2.5)$$

with:

β : coefficient of thermal expansion at constant pressure and concentration,

γ : coefficient of compressibility of the fluid at constant temperature and concentration,

α^e : introduces the effect of a density change due to the concentration of a e-component at constant temperature and pressure.

If, in certain ranges of p , T and C , the coefficients β , γ and α^e are constants or can be approximated as such for a given fluid, the equation of state (Eq.1) takes on the specific form

$$\begin{aligned}\rho^f &= \rho_0^f \exp\left[-\beta(T - T_0) + \gamma(p - p_0) + \sum_e \alpha^e (C^e - C_0^e)\right] \\ &\approx \rho_0^f \left(1 - \bar{\beta}(T - T_0) + \bar{\gamma}(p - p_0) + \sum_e \bar{\alpha}^e (C^e - C_0^e)\right)\end{aligned}\quad (2.6)$$

with

$$\bar{\beta} \equiv - \left. \frac{1}{\rho_0^f} \frac{\partial \rho^f}{\partial T} \right|_{p, C^e} \quad (2.7)$$

$$\bar{\gamma} \equiv \left. \frac{1}{\rho_0^f} \frac{\partial \rho^f}{\partial p} \right|_{T, C^e} \quad (2.8)$$

$$\bar{\alpha}^e \equiv \left. \frac{1}{\rho_0^f} \frac{\partial \rho^f}{\partial C^e} \right|_{T, p} \quad (2.9)$$

where $\rho^f = \rho_0^f$ when $T = T_0$, $p = p_0$ and $C^e = C_0^e$ that is when T , p and C^e are respectively equal to the reference temperature T_0 , reference pressure p_0 and reference concentration C_0^e .

Eq.(2.6) states that the density ρ^f can be approximated by a linear form.

In FEFLOW[®] 5 the following EOS for fluid density is implemented:

$$\rho^f = \rho_0^f \left(1 - \bar{\beta}(T - T_0) + \frac{\bar{\alpha}}{C_s - C_0} (C - C_0)\right) \quad (2.10)$$

with $\bar{\beta}$ defined in Eq.(2.7) and $\bar{\alpha}$, defined in Eq.(2.9), is normalized by the saturation concentration of the solute at saturation, C_s .

It is important to notice that the EOS for the fluid density coded in the present version of FEFLOW[®] 5 (Eq.10) is valid only in a range of 0-100°C. Moreover it does **not** take in account the coefficient of compressibility $\bar{\gamma}$ and only **one** component can be considered in the effect of a density change due to its concentration. The following empirical relationship is given for $\bar{\alpha}$

$$\bar{\alpha} = \frac{\rho^f(C_s) - \rho_0^f}{\rho_0^f} \quad (2.11)$$

While the above linear approximation for $\bar{\alpha}$ is normally sufficient for the most practical needs, wide ranges of pressure and temperature require variable thermal fluid expansion $\bar{\beta}$ Eq.(2.7) and fluid compressibility $\bar{\gamma}$ Eq.(2.8) within the state equation of density Eq.(2.10).

Figure 1 shows the well-known pressure-temperature diagram of water. The phase of interest is the liquid phase in a range of 0-350 °C for the temperature and less or equal than 100 Mpa for the pressure. Therefore the area of study in the pressure-temperature diagram is **region 1**, bounded by $p_{Sat} < p \leq 100 \text{ MPa}$ and $0 \leq T \leq 350 \text{ °C}$, where p_{Sat} is the saturation pressure of water.

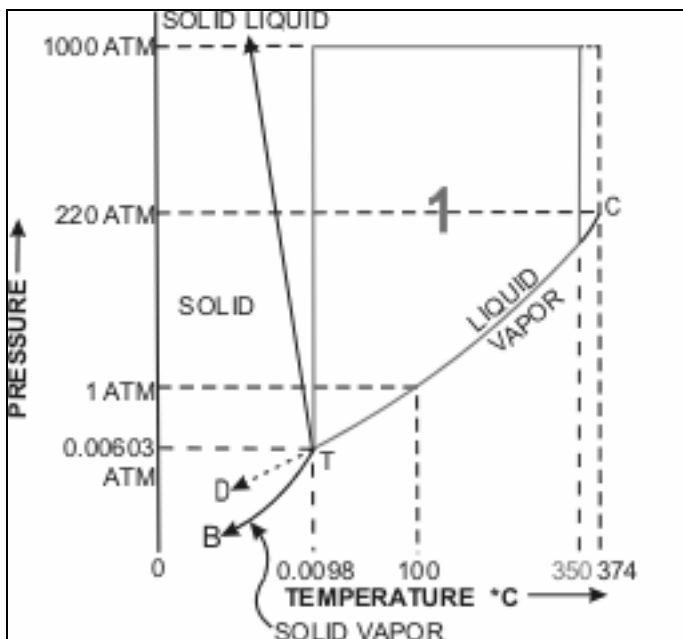


Fig 1. Pressure-temperature diagram of water. Our domain of interest is region 1, which boundaries are $p_{sat} < p \leq 100 \text{ MPa}$ and $0 \leq T \leq 350 \text{ °C}$

The first step for calculating the coefficients of thermal expansion and compressibility is to derive a polynomial fitting which accurately reproduces the fresh water density as a function of pressure and temperature. For this purpose, the industrial standard IAPWS-IF97 data (Bernhard Spang 1997; Wagner 2000) have been fitted by use of Surfer 8[®].

The following expression provides a good approximation with an accuracy of 0.5% for ρ^f in region 1 (figure 1).

$$\rho^f(T, p) = a(p) + b(p)T + c(p)T^2 + d(p)T^3 + e(p)T^4 + f(p)T^5 + g(p)T^6 \quad \text{in } [\text{kg/m}^3]$$

$0 \leq T \leq 350$ and $p_{sat} < p \leq 100$

where

$$a(p) = a_0 + a_1p + a_2p^2$$

$$b(p) = b_0 + b_1p + b_2p^2$$

.....

$$g(p) = g_0 + g_1p + g_2p^2$$

} (2.12)

with temperature T in °C and the pressure p in kPa. The coefficients of the derived polynomial fitting are:

a₀	9.99792877961606E+02
a₁	5.07605113140940E-04
a₂	-5.28425478164183E-10
b₀	5.13864847162196E-02
b₁	-3.61991396354483E-06
b₂	7.97204102509724E-12
c₀	-7.53557031774437E-03
c₁	6.32712093275576E-08
c₂	-1.66203631393248E-13

d₀	4.60380647957350E-05
d₁	-5.61299059722121E-10
d₂	1.80924436489400E-15
e₀	-2.26651454175013E-07
e₁	3.36874416675978E-12
e₂	-1.30352149261326E-17
f₀	6.14889851856743E-10
f₁	-1.06165223196756E-14
f₂	4.75014903737416E-20

g₀	-7.39221950969522E-13
g₁	1.42790422913922E-17
g₂	-7.13130230531541E-23

Table 2-1. Coefficients of the polynomial surface fitting of freshwater density $\rho^f(p, T)$ in region 1 as expressed in Eq.(6)

The coefficients have been derived for freshwater conditions, so the surface given by Eq.(2.12) is related to a reference concentration $C_0=0$. Fig.2 illustrates the fresh water density ρ^f as a function of pressure and temperature in region 1.

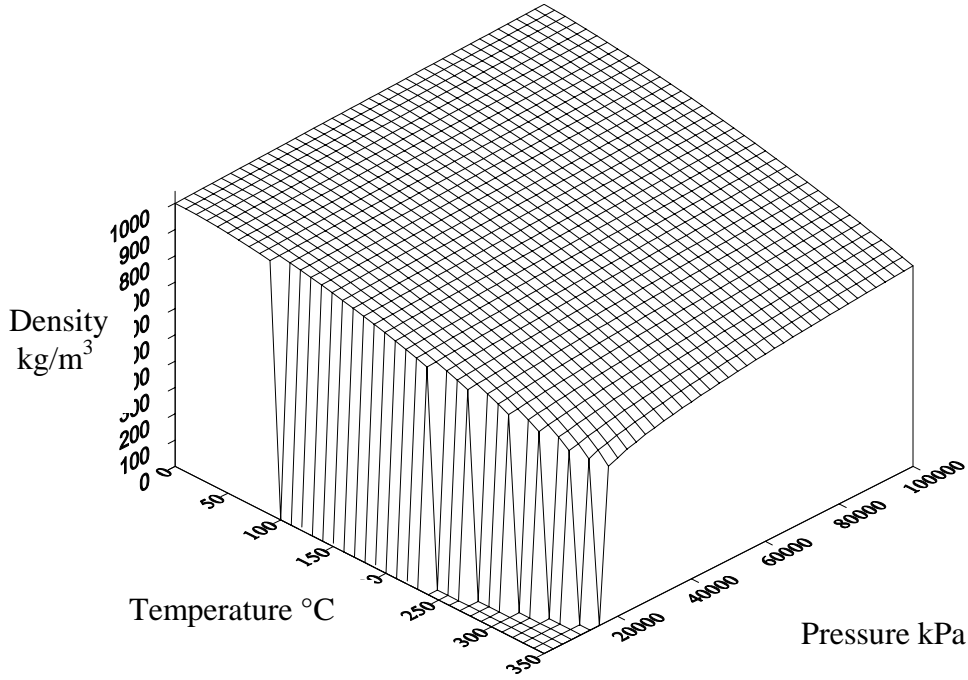


Figure 2 Fresh water density ρ^f as a function of pressure and temperature in region 1. For pictorial clarity, ρ^f is set to zero outside region 1.

The reference fluid density ρ_0^f can be derived by introducing in Eq.(2.12) the reference temperature T_0 and the reference pressure p_0 leading to:

$$\begin{aligned} \rho_0^f(T_0, C_0, p_0) = & a(p_0)|_{C_0} + b(p_0)|_{C_0} T_0 + c(p_0)|_{C_0} T_0^2 + d(p_0)|_{C_0} T_0^3 + e(p_0)|_{C_0} T_0^4 \\ & + f(p_0)|_{C_0} T_0^5 + g(p_0)|_{C_0} T_0^6 \end{aligned} \quad (2.13)$$

For instance, taking the atmospheric pressure ($p_0=100$ kPa) and $T_0=0$ °C as the reference pressure and temperature respectively, from Eq.(2.13) and Eq.(2.12) it follows:

$$\rho_0^f(T_0, C_0, p_0) = a(p_0) = a_0 + a_1 p_0 + a_2 p_0^2 = 998.8396 \text{ [g/l]} \quad (2.14)$$

The goal is to find the thermally variable fluid density $\bar{\beta}(p, T)$ and the variable fluid compressibility $\bar{\gamma}(p, T)$ of the fluid density function

$$\rho^f = \rho_0^f \left[1 + \underbrace{\bar{\gamma}(T, p)}_{\text{variable expansion}} (p - p_0) - \underbrace{\bar{\beta}(T, p)}_{\text{variable expansion}} (T - T_0) \right] \quad (2.15)$$

in order to implement them in FEFLOW[®] 5. No effects from concentration of a component are taken in account in the fluid density since these are already included in FEFLOW as shown in Eq.(2.10)

Let's consider a Taylor series expansion for the fluid density $\rho^f(T, p)$ around T_0 and p_0 where a 6th order approximation is used for the temperature T and a 2nd order approximation is used for the pressure dependence, viz.,

$$\begin{aligned} \rho^f(T, p) = & \rho^f(T_0, p_0) + (\rho^f)^{(1,0)} \Big|_{T_0, p_0} (T - T_0) + \frac{1}{2} (\rho^f)^{(2,0)} \Big|_{T_0, p_0} (T - T_0)^2 + \\ & \frac{1}{3!} (\rho^f)^{(3,0)} \Big|_{T_0, p_0} (T - T_0)^3 + \frac{1}{4!} (\rho^f)^{(4,0)} \Big|_{T_0, p_0} (T - T_0)^4 + \frac{1}{5!} (\rho^f)^{(5,0)} \Big|_{T_0, p_0} (T - T_0)^5 + \\ & \frac{1}{6!} (\rho^f)^{(6,0)} \Big|_{T_0, p_0} (T - T_0)^6 + (p - p_0) \left[(\rho^f)^{(0,1)} \Big|_{p_0, T_0} + (\rho^f)^{(1,1)} \Big|_{T_0, p_0} (T - T_0) + \right. \\ & \frac{1}{2} (\rho^f)^{(2,1)} \Big|_{T_0, p_0} (T - T_0)^2 + \frac{1}{3!} (\rho^f)^{(1,3)} \Big|_{T_0, p_0} (T - T_0)^3 + \frac{1}{4!} (\rho^f)^{(4,1)} \Big|_{T_0, p_0} (T - T_0)^4 + \\ & \left. \frac{1}{5!} (\rho^f)^{(5,1)} \Big|_{T_0, p_0} (T - T_0)^5 + \frac{1}{6!} (\rho^f)^{(6,1)} \Big|_{T_0, p_0} (T - T_0)^6 \right] + (p - p_0)^2 \left[\frac{1}{2} (\rho^f)^{(0,2)} \Big|_{T_0, p_0} + \right. \\ & \frac{1}{2} (\rho^f)^{(1,2)} \Big|_{T_0, p_0} (T - T_0) + \frac{1}{4} (\rho^f)^{(2,2)} \Big|_{T_0, p_0} (T - T_0)^2 + \frac{1}{12} (\rho^f)^{(3,2)} \Big|_{T_0, p_0} (T - T_0)^3 + \\ & \left. \frac{1}{48} (\rho^f)^{(4,2)} \Big|_{T_0, p_0} (T - T_0)^4 + \frac{1}{240} (\rho^f)^{(5,2)} \Big|_{T_0, p_0} (T - T_0)^5 + \frac{1}{1440} (\rho^f)^{(6,2)} \Big|_{T_0, p_0} (T - T_0)^6 \right] \end{aligned} \quad (2.16)$$

where

$$(\rho^f)^{(i,j)} \Big|_{T_0, p_0} \equiv \frac{\partial^{i+j} \rho^f(T, p)}{\partial T^i \partial p^j} \Big|_{T_0, p_0} \quad (2.17)$$

By utilizing Eq.(2.12), the above derivatives (Eq.(2.17)) can be calculated at p_0 and T_0 leading to the following equation:

$$\begin{aligned}
\rho^f(T, p) = & a_0 + p_0 a_1 + p_0^2 a_2 + T_0(b_0 + p_0 b_1 + p_0^2 b_2) + T_0^2(c_0 + p_0 c_1 + p_0^2 c_2) + T_0^3(d_0 + p_0 d_1 + p_0^2 d_2) + \left. \vphantom{\rho^f(T, p)} \right\} \rho_0^f \\
& T_0^4(e_0 + p_0 e_1 + p_0^2 e_2) + T_0^5(f_0 + p_0 f_1 + p_0^2 f_2) + T_0^6(g_0 + p_0 g_1 + p_0^2 g_2) + \\
& (T - T_0)^6(g_0 + p_0 g_1 + p_0^2 g_2) + (T - T_0)^5(f_0 + p_0 f_1 + p_0^2 f_2 + 6T_0(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (T - T_0)^4(e_0 + p_0 e_1 + p_0^2 e_2 + 5T_0(f_0 + p_0 f_1 + p_0^2 f_2) + 15T_0^2(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (T - T_0)^3(d_0 + p_0 d_1 + p_0^2 d_2 + 4T_0(e_0 + p_0 e_1 + p_0^2 e_2) + 10T_0^2(f_0 + p_0 f_1 + p_0^2 f_2) + 20T_0^3(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (T - T_0)^2(c_0 + p_0 c_1 + p_0^2 c_2 + 3T_0(d_0 + p_0 d_1 + p_0^2 d_2) + 6T_0^2(e_0 + p_0 e_1 + p_0^2 e_2) + 10T_0^3(f_0 + p_0 f_1 + p_0^2 f_2) + \\
& 15T_0^4(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (T - T_0)(b_0 + p_0 b_1 + p_0^2 b_2 + 2T_0(c_0 + p_0 c_1 + p_0^2 c_2) + 3T_0^2(d_0 + p_0 d_1 + p_0^2 d_2) + 4T_0^3(e_0 + p_0 e_1 + p_0^2 e_2) + \\
& 5T_0^4(f_0 + p_0 f_1 + p_0^2 f_2) + 6T_0^5(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (p - p_0)^2(a_2 + T_0 b_2 + T_0^2 c_2 + T_0^3 d_2 + T_0^4 e_2 + T_0^5 f_2 + T_0^6 g_2 + (T - T_0)^6 g_2 + (T - T_0)^5(f_2 + 6T_0 g_2) + \\
& (T - T_0)^4(e_2 + 5T_0 f_2 + 15T_0^2 g_2) + (T - T_0)^3(d_2 + 4T_0 e_2 + 10T_0^2 f_2 + 20T_0^3 g_2) + \\
& (T - T_0)^2(c_2 + 3T_0 d_2 + 6T_0^2 e_2 + 10T_0^3 f_2 + 15T_0^4 g_2) + \\
& (T - T_0)(b_2 + 2T_0 c_2 + 3T_0^2 d_2 + 4T_0^3 e_2 + 5T_0^4 f_2 + 6T_0^5 g_2)) + \\
& (p - p_0) \left[a_1 + 2p_0 a_2 + T_0(b_1 + 2p_0 b_2) + T_0^2(c_1 + 2p_0 c_2) + T_0^3(d_1 + 2p_0 d_2) + T_0^4(e_1 + 2p_0 e_2) + \right. \\
& T_0^5(f_1 + 2p_0 f_2) + T_0^6(g_1 + 2p_0 g_2) + (T - T_0)^6(g_1 + 2p_0 g_2) + (T - T_0)^5(f_1 + 2p_0 f_2 + 6T_0(g_1 + 2p_0 g_2)) + \\
& (T - T_0)^4(e_1 + 2p_0 e_2 + 5T_0(f_1 + 2p_0 f_2) + 15T_0^2(g_1 + 2p_0 g_2)) + \\
& (T - T_0)^3(d_1 + 2p_0 d_2 + 4T_0(e_1 + 2p_0 e_2) + 10T_0^2(f_1 + 2p_0 f_2) + 20T_0^3(g_1 + 2p_0 g_2)) + \\
& (T - T_0)^2(c_1 + 2p_0 c_2 + 3T_0(d_1 + 2p_0 d_2) + 6T_0^2(e_1 + 2p_0 e_2) + 10T_0^3(f_1 + 2p_0 f_2) + 15T_0^4(g_1 + 2p_0 g_2)) + \\
& (T - T_0)(b_1 + 2p_0 b_2 + 2T_0(c_1 + 2p_0 c_2) + 3T_0^2(d_1 + 2p_0 d_2) + 4T_0^3(e_1 + 2p_0 e_2) + \\
& \left. 5T_0^4(f_1 + 2p_0 f_2) + 6T_0^5(g_1 + 2p_0 g_2)) \right] \tag{2.18}
\end{aligned}$$

Comparing the above equation with the EOS for the fluid density Eq.(2.15) the expression for the coefficient of thermal expansion and the coefficient of compressibility are obtained, viz.

$$\begin{aligned}
\bar{\beta}(T, p) = & -\frac{1}{\rho_0^f} \left[(T - T_0)^5(g_0 + p_0 g_1 + p_0^2 g_2) + (T - T_0)^4(f_0 + p_0 f_1 + p_0^2 f_2 + 6T_0(g_0 + p_0 g_1 + p_0^2 g_2)) + \right. \\
& (T - T_0)^3(e_0 + p_0 e_1 + p_0^2 e_2 + 5T_0(f_0 + p_0 f_1 + p_0^2 f_2) + 15T_0^2(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (T - T_0)^2(d_0 + p_0 d_1 + p_0^2 d_2 + 4T_0(e_0 + p_0 e_1 + p_0^2 e_2) + 10T_0^2(f_0 + p_0 f_1 + p_0^2 f_2) + 20T_0^3(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (T - T_0)(c_0 + p_0 c_1 + p_0^2 c_2 + 3T_0(d_0 + p_0 d_1 + p_0^2 d_2) + 6T_0^2(e_0 + p_0 e_1 + p_0^2 e_2) + 10T_0^3(f_0 + p_0 f_1 + p_0^2 f_2) + \\
& 15T_0^4(g_0 + p_0 g_1 + p_0^2 g_2)) + \\
& (b_0 + p_0 b_1 + p_0^2 b_2 + 2T_0(c_0 + p_0 c_1 + p_0^2 c_2) + 3T_0^2(d_0 + p_0 d_1 + p_0^2 d_2) + 4T_0^3(e_0 + p_0 e_1 + p_0^2 e_2) + \\
& \left. 5T_0^4(f_0 + p_0 f_1 + p_0^2 f_2) + 6T_0^5(g_0 + p_0 g_1 + p_0^2 g_2)) \right] \tag{2.19}
\end{aligned}$$

and

$$\begin{aligned}
\bar{\gamma}(\mathbf{T}, \mathbf{p}) = & \frac{1}{\rho_0^f} \left\{ (p - p_0) \left(a_2 + T_0 b_2 + T_0^2 c_2 + T_0^3 d_2 + T_0^4 e_2 + T_0^5 f_2 + T_0^6 g_2 + (T - T_0)^6 g_2 + (T - T_0)^5 (f_2 + 6T_0 g_2) + \right. \right. \\
& (T - T_0)^4 (e_2 + 5T_0 f_2 + 15T_0^2 g_2) + (T - T_0)^3 (d_2 + 4T_0 e_2 + 10T_0^2 f_2 + 20T_0^3 g_2) + \\
& (T - T_0)^2 (c_2 + 3T_0 d_2 + 6T_0^2 e_2 + 10T_0^3 f_2 + 15T_0^4 g_2) + \\
& \left. (T - T_0) (b_2 + 2T_0 c_2 + 3T_0^2 d_2 + 4T_0^3 e_2 + 5T_0^4 f_2 + 6T_0^5 g_2) \right) + \\
& \left[a_1 + 2p_0 a_2 + T_0 (b_1 + 2p_0 b_2) + T_0^2 (c_1 + 2p_0 c_2) + T_0^3 (d_1 + 2p_0 d_2) + T_0^4 (e_1 + 2p_0 e_2) + \right. \\
& T_0^5 (f_1 + 2p_0 f_2) + T_0^6 (g_1 + 2p_0 g_2) + (T - T_0)^6 (g_1 + 2p_0 g_2) + (T - T_0)^5 (f_1 + 2p_0 f_2 + 6T_0 (g_1 + 2p_0 g_2)) + \\
& (T - T_0)^4 (e_1 + 2p_0 e_2 + 5T_0 (f_1 + 2p_0 f_2) + 15T_0^2 (g_1 + 2p_0 g_2)) + \\
& (T - T_0)^3 (d_1 + 2p_0 d_2 + 4T_0 (e_1 + 2p_0 e_2) + 10T_0^2 (f_1 + 2p_0 f_2) + 20T_0^3 (g_1 + 2p_0 g_2)) + \\
& (T - T_0)^2 (c_1 + 2p_0 c_2 + 3T_0 (d_1 + 2p_0 d_2) + 6T_0^2 (e_1 + 2p_0 e_2) + 10T_0^3 (f_1 + 2p_0 f_2) + 15T_0^4 (g_1 + 2p_0 g_2)) + \\
& (T - T_0) (b_1 + 2p_0 b_2 + 2T_0 (c_1 + 2p_0 c_2) + 3T_0^2 (d_1 + 2p_0 d_2) + 4T_0^3 (e_1 + 2p_0 e_2) + \\
& \left. \left. 5T_0^4 (f_1 + 2p_0 f_2) + 6T_0^5 (g_1 + 2p_0 g_2) \right) \right] \left. \right\} \tag{2.20}
\end{aligned}$$

with ρ_0^f computed from Eq.(2.14) and the coefficients $(a_k, b_k, c_k, d_k, e_k, f_k, g_k)_{k=0,1,2}$ are given in Table 2-1.

These two expressions can be implemented in FEFLOW by the use of the interface manager (IFM) as shown in Appendix 3.