## A.30 Computationally efficient 25-term expressions for the density of seawater in terms of $\Theta$ and $\theta$

Ocean models to date have treated their salinity and temperature variables as being Practical Salinity $S_P$ and potential temperature $\theta$. As the full implications of TEOS-10 are incorporated into ocean models they will need to carry Preformed Salinity $S_*$ and Conservative Temperature $\Theta$ as conservative variables (as discussed in appendices A.20 and A.21), and a computationally efficient expression for density in terms of Absolute Salinity $S_A$ and Conservative Temperature $\Theta$ will be needed.

Following the work of McDougall *et al*. (2003) and Jackett *et al*. (2006), the TEOS-10 density $\rho$ has been approximated by a rational function of the same form as in those papers. The fitted expression is the ratio of two polynomials of $(S_A, \Theta, p)$

$$\rho \approx \rho^{25} = P_{\text{num}}^{\rho 25} \big/ P_{\text{denom}}^{\rho 25}. \tag{A.30.1}$$

The density data has been fitted in a "funnel" of data points in $(S_A, t, p)$ space which is described in more detail in McDougall *et al.* (2010b). The "funnel" extends to a pressure of $8000\ \text{dbar}$. At the sea surface the "funnel" covers the full range of temperature and salinity while for pressures greater than 5500 dbar, the maximum temperature of the fitted data is 12°C and the minimum Absolute Salinity is $u_{PS}30\ \text{g kg}^{-1}$. That is, the fit has been performed over a region of parameter space which includes water that is approximately 10°C warmer and $5\ \text{g kg}^{-1}$ fresher in the deep ocean than exists in the present ocean (see Figure 1 of Jackett *et al*. (2006)). Table K.1 of appendix K contains the 25 coefficients of the expression (A.30.1) for density in terms of $(S_A, \Theta, p)$.

As outlined in appendix K, this 25-term rational-function expression for $\rho$ yields the thermal expansion and haline contraction coefficients, $\alpha^\Theta$ and $\beta^\Theta$, that are essentially as accurate as those derived from the full TEOS-10 Gibbs function for data in the "oceanographic funnel". The same cannot be claimed for the sound speed derived by differentiating Eqn. (A.30.1) with respect to pressure; this sound speed has an rms error in the "funnel" of almost $0.25\ \text{m s}^{-1}$ whereas TEOS-10 fits the available sound speed data with an rms error of only $0.035\ \text{m s}^{-1}$.

In dynamical oceanography it is the thermal expansion and haline contraction coefficients $\alpha^\Theta$ and $\beta^\Theta$ which are the most important aspects of the equation of state since the "thermal wind" is proportional to $\alpha^\Theta \nabla_p \Theta - \beta^\Theta \nabla_p S_A$ and the vertical static stability is given in terms of the buoyancy frequency $N$ by $g^{-1}N^2 = \alpha^\Theta \Theta_z - \beta^\Theta (S_A)_z$. Hence for dynamical oceanography we may take the 25-term rational function expression for density, Eqn. (A.30.1), as essentially reflecting the full accuracy of TEOS-10. This is confirmed in Fig. A.30.1 where the error in using the 25-term expression for density to calculate the isobaric northward density gradient is shown. The vertical axis on this figure is the magnitude of the difference in the northward isobaric density gradient in the world ocean below $1000\,\text{m}$ when evaluated using Eqn. (A.30.1) versus using the full TEOS-10 Gibbs function. The scales of the axes of this figure have been chosen to be the same as those of Fig. A.5.1 of appendix A.5 so that the smallness of the errors associated with using the 25-term density expression can be appreciated. The errors represented in Fig. A.30.1 represent perhaps half of the remaining uncertainty in our knowledge of seawater properties, and by comparing Figs. A.30.1 and A.5.1 it is clear that the much more important issue is to properly represent the effects of seawater composition on seawater density. The rms value of the vertical axis in Fig. A.30.1 is 11.4% of that of Fig. A.5.1.

McDougall *et al*. (2010b) have also provided a 25-term rational-function expression for density in terms of $(S_A, \theta, p)$. The 25 coefficients can be found in Table K.2 of appendix K. As an approximation to density, this 25-term rational function is approximately as accurate as the one described above in terms of $(S_A, \Theta, p)$. It must be emphasized though

that an ocean model that treated potential temperature as a conservative variable would make errors in its treatment of heat fluxes, as described in appendices A.13, A.14 and A.17, and as illustrated in Figures A.13.1, A.14.1 and A.17.1.
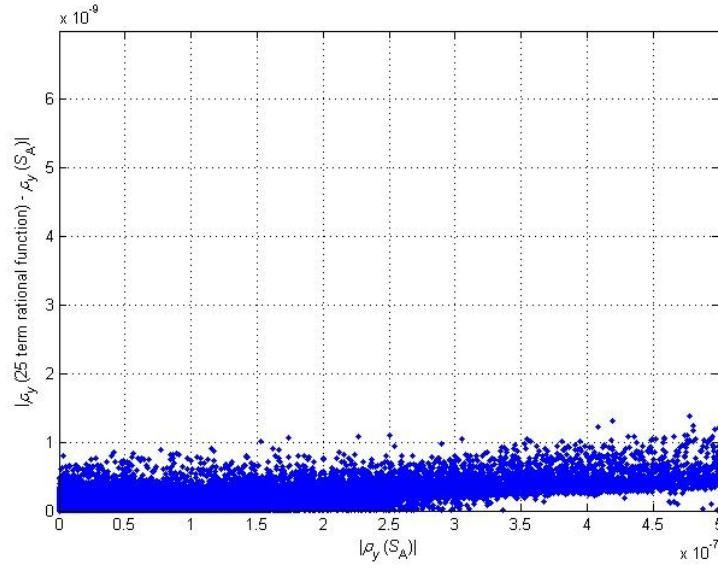


**Figure A.30.1.** The northward density gradient at constant pressure (the horizontal axis) for data in the world ocean atlas of Gouretski and Koltermann (2004) for $p > 1000$ dbar . The vertical axis is the magnitude of the difference between evaluating the density gradient using the 25-term expression Eqn. (A.30.1) instead of using the full TEOS-10 expression, using Absolute Salinity $S_A$ as the salinity argument in both cases.

Appendix P describes how an expression for the enthalpy of seawater in terms of Conservative Temperature, specifically the functional form $\hat{h}(S_A, \Theta, p)$, together with an expression for entropy in the form $\hat{\eta}(S_A, \Theta)$, can be used as an alternative thermodynamic potential to the Gibbs function $g(S_A, t, p)$. The need for the functional form $\hat{h}(S_A, \Theta, p)$ also arises in section 3.32 and in Eqns. (3.26.3) and (3.29.1). The 25-term expression, Eqn. (A.30.1), for $\rho^{25} = \hat{\rho}^{25}(S_A, \Theta, p)$ can be used to find a closed expression for $\hat{h}(S_A, \Theta, p)$ by integrating the reciprocal of $\hat{\rho}^{25}(S_A, \Theta, p)$ with respect to pressure (in Pa), since $\hat{h}_P = v = \rho^{-1}$ (see Eqn. (2.8.3)).

The 25-term expression for specific volume, Eqn. (A.30.1), is first written explicitly as the ratio of two polynomials in sea pressure $p$ (in dbar) as

$$\hat{v}^{25} = \frac{1}{\hat{\rho}^{25}} = \frac{a_0 + a_1 p + a_2 p^2 + a_3 p^3}{b_0 + 2b_1 p + b_2 p^2}, \tag{A.30.2}$$

where the coefficients $a_0$ to $a_3$ and $b_0$ to $b_2$ are the following functions of $S_A$ and $\Theta$

$$a_0 = 1 + c_{14}\Theta + c_{15}\Theta^2 + c_{16}\Theta^3 + c_{17}\Theta^4 + c_{18}S_A + c_{19}S_A\Theta + c_{20}S_A\Theta^3 + c_{21}(S_A)^{1.5} + c_{22}(S_A)^{1.5}\Theta^2,$$

$$a_1 = c_{23},$$

$$a_2 = c_{24}\Theta^3,$$

$$a_3 = c_{25}\Theta,$$

$$b_0 = c_1 + c_2\Theta + c_3\Theta^2 + c_4\Theta^3 + c_5 S_A + c_6 S_A\Theta + c_7(S_A)^2,$$

$$b_1 = 0.5(c_8 + c_9\Theta^2 + c_{10}S_A),$$

$$b_2 = c_{11} + c_{12}\Theta^2,$$

and the numbered coefficients $c_1$ to $c_{25}$ are so identified in Table K.1 (note that $c_{13} = 1$).

It is not difficult to rearrange Eqn. (A.30.2) into the form

$$\hat{v}^{25} = \hat{v}^{25}\left(S_A, \Theta, p\right) = \left(\frac{a_2}{b_2} - \frac{2a_3 b_1}{b_2^2}\right) + \frac{a_3}{b_2}p + \frac{N + Mp}{b_0 + 2b_1 p + b_2 p^2}, \qquad (A.30.3)$$

where $N$ and $M$ are given by

$$N = a_0 + \frac{2a_3 b_0 b_1}{b_2^2} - \frac{a_2 b_0}{b_2}. \qquad \text{and} \qquad M = a_1 + \frac{4a_3 b_1^2}{b_2^2} - \frac{a_3 b_0}{b_2} - \frac{2a_2 b_1}{b_2}. \qquad (A.30.4)$$

The pressure integral of the last term in Eqn. (A.30.3) is well known (see for example section 2.103 of Gradshteyn and Ryzhik (1980)) and is dependent on the sign of the discriminant of the denominator. In our case it can be shown that $b_1^2 > b_0 b_2$ over the domain of the "funnel" and also that both $b_0$ and $b_1$ are positive, while $b_2$ is negative and bounded away from zero. The indefinite integral, with respect to sea pressure measured in Pa, of the last term in Eqn. (A.30.3) is (with $N^* = 10^4 N$ and $M^* = 10^4 M$)

$$\int \frac{N + Mp}{b_0 + 2b_1 p + b_2 p^2}\,dP' = \frac{M^*}{2b_2}\ln\left|b_0 + 2b_1 p + b_2 p^2\right| + \frac{N^* b_2 - M^* b_1}{2b_2\sqrt{b_1^2 - b_0 b_2}}\ln\left|\frac{b_2 p + b_1 - \sqrt{b_1^2 - b_0 b_2}}{b_2 p + b_1 + \sqrt{b_1^2 - b_0 b_2}}\right|, \qquad (A.30.5)$$

The enthalpy $\hat{h}^{25}\left(S_A, \Theta, p\right)$ is the definite integral of Eqn. (A.30.3) from $P_0$ to $P$, plus $c_p^0 \Theta$, being the value of enthalpy at $P_0$ (i. e. at $p = 0$ dbar). Hence the full expression for $\hat{h}^{25}\left(S_A, \Theta, p\right)$ is (with $A = b_1 - \sqrt{b_1^2 - b_0 b_2}$ and $B = b_1 + \sqrt{b_1^2 - b_0 b_2}$)

$$\begin{aligned}
\hat{h}^{25}\left(S_A, \Theta, p\right) = {} & c_p^0 \Theta + 10^4\left(\frac{a_2}{b_2} - \frac{2a_3 b_1}{b_2^2}\right)p + 10^4 \frac{a_3}{2b_2}p^2 \\[2mm]
& + \frac{M^*}{2b_2}\ln\left(1 + \frac{2b_1}{b_0}p + \frac{b_2}{b_0}p^2\right) + \frac{N^* - \frac{b_1}{b_2}M^*}{(B - A)}\ln\left(1 + p\frac{b_2\,(B - A)}{A\,(B + b_2 p)}\right).
\end{aligned} \qquad (A.30.6)$$

The factor of $10^4$ that appears here and in $N^*$ and $M^*$ effectively serves to convert the units of the integration variable from dbar to Pa so that $\hat{h}^{25}\left(S_A, \Theta, p\right)$ has units of J kg$^{-1}$. In these equations $S_A$ is in g kg$^{-1}$, $\Theta$ in °C and $p$ is in dbar. The arguments of the two natural logarithms in Eqn. (A.30.6) are always greater than 1, and in fact they are between 1 and 1.2 even for $p$ as large as $10^4$ dbar (note that both $b_2$ and $A$ are negative). Also, when the enthalpy difference at the same values of $S_A$ and $\Theta$ but at different pressures (see Eqn. (3.32.2)) is evaluated using Eqn. (A.30.6), the expression can also be arranged to contain only two logarithm terms.

Following Young (2010), the difference between specific enthalpy and $c_p^0 \Theta$ may be called "dynamic enthalpy" and can be readily calculated from Eqn. (A.30.6), recognizing that this equation is based on the computationally efficient 25-term expression for density of McDougall *et al.* (2010b) rather than being evaluated from the full TEOS-10 Gibbs function. Similarly, the partial derivatives of $\hat{h}^{25}\left(S_A, \Theta, p\right)$ with respect to Absolute Salinity $S_A$ and with respect to Conservative Temperature $\Theta$ can be calculated either by algebraic differentiation of Eqn. (A.30.6) or by first algebraically differentiating Eqn. (A.30.1) and then numerically integrating this expression with respect to pressure (this second procedure is motivated by taking the appropriate $S_A$ or $\Theta$ derivatives of Eqn. (3.2.1); see Eqns. (A.18.4) and (A.18.5)).

An expression $\tilde{h}^{25}\left(S_A, \theta, p\right)$ for enthalpy as a function of potential temperature $\theta$ can be found in a similar manner to that outlined above, but with the coefficients of the 25-term rational-function expression for density now being taken from Table K.2, and with the first term being expressed as the exact polynomial expression for $\tilde{h}\left(S_A, \theta, 0\right)$ instead of as $c_p^0 \Theta$.

# Appendix K: Coefficients of 25-term expressions for the density of seawater in terms of $\Theta$ and of $\theta$

The TEOS-10 Gibbs function of seawater $g\left(S_A, t, p\right)$ is written as a polynomial in terms of in situ temperature $t$, while for ocean models, density needs to be expressed as a computationally efficient expression in terms of either Conservative Temperature $\Theta$ or potential temperature $\theta$ (referenced to $p_r = 0$ dbar). McDougall *et al*. (2010b) have fitted the TEOS-10 values of density $\rho$ to $S_A$, $\Theta$ and $p$ in a "funnel" of data points in $\left(S_A, t, p\right)$ space. The fitted expression is in the form of a rational function, being the ratio of two polynomials of $\left(S_A, \Theta, p\right)$

$$\rho = P_{\text{num}}^{\rho 25} / P_{\text{denom}}^{\rho 25} . \tag{K.1}$$

The "funnel" of data points in $\left(S_A, t, p\right)$ space is described in more detail in McDougall *et al*. (2010b); at the sea surface it covers the full range of temperature and salinity while for pressure greater than 5500 dbar, the maximum temperature of the fitted data is 12°C and the minimum Absolute Salinity is $u_{PS} 30$ g kg$^{-1}$. The maximum pressure of the "funnel" is 8000 dbar. Table K.1 contains the 25 coefficients of the expression (K.1) for density in terms of $\left(S_A, \Theta, p\right)$. The coefficients $c_1 - c_{12}$ in this table have units of kg m$^{-3}$ and the coefficients $c_{13} - c_{25}$ are dimensionless, and the normalizing values of $S_A$, $\Theta$ and $p$ are taken to be 1 g kg$^{-1}$, 1 K and 1 dbar respectively.

The rms error of this 25-term approximation to the TEOS-10 density is less than 0.0015 kg m$^{-3}$ over the "funnel"; this can be compared with the rms uncertainty of 0.004 kg m$^{-3}$ of the underlying laboratory density data to which the TEOS-10 Gibbs function was fitted (see the first two rows of Table O.1 of appendix O). Similarly, the appropriate thermal expansion coefficient,

$$\alpha^{\Theta} = -\frac{1}{\rho} \frac{\partial \rho}{\partial \Theta}\bigg|_{S_A, p} , \tag{K.2}$$

of the 25-term equation of state is different from the same thermal expansion coefficient evaluated from TEOS-10 with an rms error in the "funnel" of less than $0.3 x 10^{-6}$ K$^{-1}$, compared with the rms error of the thermal expansion coefficient of the laboratory data to which the Feistel (2008) Gibbs function was fitted of $0.6 x 10^{-6}$ K$^{-1}$ (see row six of Table O.1 of appendix O). In terms of the evaluation of density gradients, the haline contraction coefficient evaluated from Eqn. (K.1) is more accurate than the thermal expansion coefficient. Hence we may consider the 25-term rational function expression for density, Eqn. (K.1), to be equally as accurate as the full TEOS-10 expressions for density, the thermal expansion coefficient and the saline contraction coefficient for data that reside inside the "oceanographic funnel".

The sound speed evaluated from the 25-term rational function Eqn. (K.1), has an rms error over the "funnel" of almost 0.25 m s$^{-1}$ which is approximately five times the rms error of the underlying sound speed data that was incorporated into the Feistel (2008) Gibbs function (see rows 7 to 9 of Table O.1 of appendix O). Hence, the 25-term expression for density is not a particularly accurate expression for the sound speed in seawater, even in the "funnel". But for dynamical oceanography where $\alpha^{\Theta}$ and $\beta^{\Theta}$ are the aspects of the equation of state that, together with spatial gradients of $S_A$ and $\Theta$ drive ocean currents and affect the calculation of the buoyancy frequency, we may take the 25-term rational-function expression for density, Eqn. (K.1), as essentially reflecting the full accuracy of TEOS-10.

| | $P_{\text{num}}^{\rho 25}$ | Coefficients | | $P_{\text{denom}}^{\rho 25}$ | Coefficients |
|---|---|---|---|---|---|
| $c_1$ | | $9.998\,438\,029\,070\,821\,4 \times 10^2$ | $c_{13}$ | | $1.0$ |
| $c_2$ | $\Theta$ | $7.118\,809\,067\,894\,091\,0 \times 10^0$ | $c_{14}$ | $\Theta$ | $7.054\,768\,189\,607\,157\,6 \times 10^{-3}$ |
| $c_3$ | $\Theta^2$ | $-1.945\,992\,251\,337\,968\,7 \times 10^{-2}$ | $c_{15}$ | $\Theta^2$ | $-1.175\,369\,560\,585\,864\,7 \times 10^{-5}$ |
| $c_4$ | $\Theta^3$ | $6.174\,840\,445\,587\,464\,1 \times 10^{-4}$ | $c_{16}$ | $\Theta^3$ | $5.921\,980\,948\,827\,490\,3 \times 10^{-7}$ |
| $c_5$ | $S_A$ | $2.892\,573\,154\,127\,765\,3 \times 10^0$ | $c_{17}$ | $\Theta^4$ | $3.488\,790\,222\,801\,251\,9 \times 10^{-10}$ |
| $c_6$ | $S_A\Theta$ | $2.147\,149\,549\,326\,832\,4 \times 10^{-3}$ | $c_{18}$ | $S_A$ | $2.077\,771\,608\,561\,845\,8 \times 10^{-3}$ |
| $c_7$ | $(S_A)^2$ | $1.945\,753\,175\,118\,305\,9 \times 10^{-3}$ | $c_{19}$ | $S_A\Theta$ | $-2.221\,085\,729\,372\,299\,8 \times 10^{-8}$ |
| $c_8$ | $p$ | $1.193\,068\,181\,853\,174\,8 \times 10^{-2}$ | $c_{20}$ | $S_A\Theta^3$ | $-3.662\,814\,106\,789\,528\,2 \times 10^{-10}$ |
| $c_9$ | $p\Theta^2$ | $2.696\,914\,801\,183\,075\,8 \times 10^{-7}$ | $c_{21}$ | $(S_A)^{1.5}$ | $3.468\,821\,075\,791\,734\,0 \times 10^{-6}$ |
| $c_{10}$ | $pS_A$ | $5.935\,568\,592\,503\,565\,3 \times 10^{-6}$ | $c_{22}$ | $(S_A)^{1.5}\Theta^2$ | $8.019\,054\,152\,807\,065\,5 \times 10^{-10}$ |
| $c_{11}$ | $p^2$ | $-2.594\,338\,980\,742\,903\,9 \times 10^{-8}$ | $c_{23}$ | $p$ | $6.831\,462\,955\,412\,332\,4 \times 10^{-6}$ |
| $c_{12}$ | $p^2\Theta^2$ | $-7.273\,411\,171\,282\,270\,7 \times 10^{-12}$ | $c_{24}$ | $p^2\Theta^3$ | $-8.529\,479\,483\,448\,544\,6 \times 10^{-17}$ |
| | | | $c_{25}$ | $p^3\Theta$ | $-9.227\,532\,514\,503\,807\,0 \times 10^{-18}$ |

**TABLE K.1  Coefficients of the polynomials $P_{\text{num}}^{\rho 25}(S_A, \Theta, p)$ and $P_{\text{denom}}^{\rho 25}(S_A, \Theta, p)$ that define the 25-term rational-function Eqn. (K.1) for density.**

The same procedure has been used by McDougall *et al.* (2010b) to fit a rational function of the form of Eqn. (K.1) but where the polynomials in the numerator and denominator are functions of $(S_A, \theta, p)$ rather than of $(S_A, \Theta, p)$. This form of the 25-term rational function expression for density is of approximately the same accuracy as that described above, and the 25 coefficients of this expression are given in Table K.2. The coefficients $c_1 - c_{12}$ in this table have units of kg m$^{-3}$ and the coefficients $c_{13} - c_{25}$ are dimensionless, and the normalizing values of $S_A, \theta$ and $p$ are taken to be $1\,\text{g kg}^{-1}$, $1\,\text{K}$ and $1\,\text{dbar}$ respectively.

| | $P_{\text{num}}^{\rho 25}$ | Coefficients | | $P_{\text{denom}}^{\rho 25}$ | Coefficients |
|---|---|---|---|---|---|
| $c_1$ | | $9.998\ 427\ 704\ 040\ 868\ 8 \times 10^2$ | $c_{13}$ | | $1.0$ |
| $c_2$ | $\theta$ | $7.353\ 990\ 725\ 780\ 200\ 0 \times 10^0$ | $c_{14}$ | $\theta$ | $7.288\ 277\ 317\ 994\ 539\ 7 \times 10^{-3}$ |
| $c_3$ | $\theta^2$ | $-5.272\ 502\ 484\ 658\ 053\ 7 \times 10^{-2}$ | $c_{15}$ | $\theta^2$ | $-4.427\ 042\ 357\ 570\ 579\ 5 \times 10^{-5}$ |
| $c_4$ | $\theta^3$ | $5.105\ 140\ 542\ 790\ 050\ 1 \times 10^{-4}$ | $c_{16}$ | $\theta^3$ | $4.821\ 816\ 757\ 416\ 573\ 2 \times 10^{-7}$ |
| $c_5$ | $S_A$ | $2.837\ 207\ 495\ 416\ 299\ 4 \times 10^0$ | $c_{17}$ | $\theta^4$ | $1.966\ 643\ 777\ 649\ 954\ 1 \times 10^{-10}$ |
| $c_6$ | $S_A\theta$ | $-5.746\ 287\ 373\ 866\ 898\ 5 \times 10^{-3}$ | $c_{18}$ | $S_A$ | $2.019\ 220\ 131\ 573\ 115\ 6 \times 10^{-3}$ |
| $c_7$ | $(S_A)^2$ | $2.016\ 582\ 840\ 401\ 100\ 5 \times 10^{-3}$ | $c_{19}$ | $S_A\theta$ | $-7.838\ 666\ 741\ 074\ 767\ 1 \times 10^{-6}$ |
| $c_8$ | $p$ | $1.150\ 668\ 012\ 876\ 069\ 5 \times 10^{-2}$ | $c_{20}$ | $S_A\theta^3$ | $-2.749\ 397\ 117\ 121\ 584\ 4 \times 10^{-10}$ |
| $c_9$ | $p\theta^2$ | $1.202\ 602\ 702\ 900\ 458\ 1 \times 10^{-7}$ | $c_{21}$ | $(S_A)^{1.5}$ | $4.661\ 419\ 029\ 016\ 429\ 3 \times 10^{-6}$ |
| $c_{10}$ | $pS_A$ | $5.536\ 190\ 936\ 504\ 846\ 6 \times 10^{-6}$ | $c_{22}$ | $(S_A)^{1.5}\theta^2$ | $1.518\ 271\ 263\ 728\ 829\ 5 \times 10^{-9}$ |
| $c_{11}$ | $p^2$ | $-2.756\ 315\ 640\ 465\ 192\ 8 \times 10^{-8}$ | $c_{23}$ | $p$ | $6.414\ 629\ 356\ 742\ 288\ 6 \times 10^{-6}$ |
| $c_{12}$ | $p^2\theta^2$ | $-5.883\ 476\ 945\ 993\ 336\ 4 \times 10^{-12}$ | $c_{24}$ | $p^2\theta^3$ | $-9.536\ 284\ 588\ 639\ 736\ 0 \times 10^{-17}$ |
| | | | $c_{25}$ | $p^3\theta$ | $-9.623\ 745\ 548\ 627\ 732\ 0 \times 10^{-18}$ |

TABLE K.2  Coefficients of the polynomials $P_{\text{num}}^{\rho 25}(S_A, \theta, p)$ and $P_{\text{denom}}^{\rho 25}(S_A, \theta, p)$ that define the 25-term rational-function Eqn. (K.1) for density.