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Summary

A self-consistent set of values have been computed for enthalpy, total specific heat at constant pressure, compressibility factor, viscosity, total thermal conductivity, and total Prandtl number of equilibrium air from 500 to 30 000 K over a pressure range of 10^{-4} to 10^{2} atm. Previous results for most of these properties are limited to a temperature of 15 000 K. The mixture values are calculated from the transport and thermodynamic properties of the individual species provided in a recent study by the present authors. The concentrations of the individual species, required in the mixture relations, are obtained from a free-energy-minimization calculation procedure. Calculations are based on an 11-species air model (O_2, N_2, O, N, NO, O^+, N^+, NO^+, O^{++}, N^{++}, and e^-). For pressures less than 10^{-2} atm and temperatures of about 15 000 K and greater, the concentrations of N^{++} and O^{++} become important, and consequently they are included in the calculations for determining the various properties. The differences in the computed values given herein and those obtained by other researchers (which are based on temperatures to 15 000 K) may be attributed to the differences in the properties employed for the individual species, mixing laws used for the mixture, and (to a lesser degree) the number of chemical species considered in the mixture. Finally, all the computed properties are curve fit as a function of temperature at a constant value of the pressure. These curve fits reproduce the computed values to within 5 percent for the entire temperature range considered at specific pressures and provide an efficient means for computing the flow-field properties of equilibrium air, provided the elemental composition remains constant at 0.24 for oxygen and 0.76 for nitrogen by mass.

Introduction

Equilibrium air chemistry calculations can be performed either by using the free-energy-minimization procedure (ref. 1) or by using the equilibrium constant method (refs. 2 and 3). Flow-field calculations based on either of these approaches (refs. 4 and 5) can be quite time consuming; however, the assumption of chemical equilibrium without elemental separation does allow the governing equations to be written in a form such that the individual species concentrations are not required explicitly. In this format, the specific heat at constant pressure C_p, the thermal conductivity K, and the Prandtl number N_{Pr} are defined as total properties (refs. 6, 7, and 8). Hansen (ref. 7) has provided these properties in a tabular form for temperatures up to 15 000 K and pressures from 10^{-4} to 10^{2} atm using a seven-species air model (N_2, O_2, N, O, N^+, O^+, and e^-). Peng and Pindroh (ref. 9) provide tabulated values of total thermal conductivity for a nine-species air model (N_2, O_2, N, O, NO, N^+, O^+, NO^+, and e^-); however, no values are given for the total specific heat or the Prandtl number. The tabulated values of reference 9 are for temperatures up to 15 000 K and pressures of 10^{-2} to 10^{2} atm. Both reference 7 and reference 9 have incorporated a lower order electron pressure correction (compared with the one used in ref. 8) in the transport properties of ionic species to obtain the mixture values for equilibrium air. The thermodynamic properties provided in these two references and in reference 10[1] are based on an equilibrium air model that did not include N^{++} and O^{++} among its constituent species. These two species are not significant at pressures of 10^{-4} to 10^{2} atm for temperatures less than 15 000 K. However, for higher temperatures (such as those considered in ref. 10), these two species (especially N^{++}) become quite significant. (See fig. 1.)

Since curve fits to the various properties permit efficient computation for flow-field analyses (ref. 11), it is desirable to have the curve fits in preference to the tabulated values. Further, for accurate calculations, it is imperative that these curve fits be obtained to values that are

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[1] Vinokur and his colleagues have recently included doubly ionized atomic species in their calculations of the thermodynamic properties. These results, however, have not been published.

computed in a self-consistent manner from the same set of data and other physical properties. Srinivasan et al. (refs. 12 and 13) recently obtained curve fits to the tabulated transport properties of reference 9 and the thermodynamic properties of reference 14. No curve fits are readily available for tabulated values of Hansen (ref. 7).

This report presents accurate curve fits for the computed values of enthalpy, total specific heat, compressibility factor, viscosity, and total values of thermal conductivity and Prandtl number of equilibrium air over a more extensive range of parameters than had been available. This has been accomplished by using both the thermodynamic and the transport properties of the individual species (in the form of curve fits) from reference 8 along with a free-energy-minimization procedure (ref. 1) for computing the equilibrium composition. Figure 1 shows the calculated composition of equilibrium air (used in the calculations of the properties obtained herein) as a function of temperature for pressures of 10^{-4}, 10^{0}, and 10^{2} atm. As shown in figure 1(b), the doubly ionized atomic species are dominant at a pressure of 10^{-4} atm for temperatures of about 15 000 K and greater. Their appearance and dominance are delayed to higher temperatures at higher pressures. (See figs. 1(d) and 1(f).) With the individual species composition and properties known, the mixture properties for an 11-species air model (N_2, O_2, NO, N, O, N^+, O^+, NO^+, N^{++}, O^{++}, and e^-) are then calculated. These computed mixture properties are curve fit for temperatures of 500 to 30 000 K and for specific pressures of 10^{-4} to 10^{2} atm. Calculations are limited to 25 000 K at 10^{-4} atm and 28 000 K at 10^{-3} atm to avoid the necessity of including contributions from triply ionized species. Tabulated values of these curve-fit coefficients are given herein and computer subroutines to evaluate the various properties using these coefficients are provided in reference 15. These values and codes may be obtained for a fee from the following:

COSMIC
Computer Services Annex
University of Georgia
Athens, GA 30602
(404) 542-3265

Request the code by the designation LAR 14760. This code is written in FORTRAN 77 for use on computers with a FORTRAN compiler.

Detailed comparisons of the curve-fit data with computed results are presented to demonstrate the accuracy of the obtained curve fits. Further, the presently computed values are compared with existing data in the literature. Comparisons are also included to show the effect of the number of species included in an air model on the equilibrium properties.

The curve fits provided herein can only be used for equilibrium air calculations without ablation or with or without air injection, that is, with constant elemental composition through the flow field. Values of 0.24 and 0.76 for the elemental composition by mass of oxygen and nitrogen, respectively, are employed in this work.

The properties are obtained herein under the assumption of charge neutrality for the ionized air. Therefore, the associated electric field effects are neglected. This assumption can generally be made for an ionized gas mixture in thermochemical equilibrium. Further, the transport properties are computed from the approximate formulas of references 8, 9, 16, 17, and 18 instead of the complete kinetic theory expressions of reference 19. These approximate formulas, although still somewhat complicated, are much simpler to use than the equations given by the first Chapman-Enskog approximation (ref. 19) and give results within a few percent of those of reference 19 for unionized air through temperatures of 8000 K (ref. 20). Since the accuracies of collision integrals $\overline{\Omega}_{ij}^{(1,1)}$ and $\overline{\Omega}_{ij}^{(2,2)}$ at high temperatures are known only to about 10 to

20 percent at best, the error introduced in our calculations by the use of approximate formulas in place of the complete Chapman-Enskog approximation may be, therefore, relatively insignificant. For more exact treatment, however, the formulas given in reference 8 (based on the relations developed by Yos, ref. 21) may be used to compute the mixture properties.

The accuracy of the basic calculations carried out herein for the transport properties of partially ionized air is difficult to evaluate without reliable experimental data for the temperature and pressure ranges considered in this report. Detailed comparisons, however, are provided with the existing calculations of Hansen (ref. 7) and of Peng and Pindroh (ref. 9). Devoto and Bauder (ref. 22) have obtained data for the thermal conductivity of equilibrium air from electric arc measurements at a pressure of 1 atm and temperatures of 8000 to 13 000 K. Their data suggest somewhat higher values for the thermal conductivity when appreciable ionization is present. The electric arc data, however, are not considered to be very accurate because the thermodynamic state of the gas may not be well defined, with some of the internal degrees of freedom partially frozen. This lack of accuracy is reflected in the large scatter of Devoto's data.

Finally, the effects of Coulomb collisions are not obtained very accurately with the first Chapman-Enskog approximation. In the limiting case of a fully ionized gas, the transport properties calculated with this approximation differ from those obtained with an accurate solution of the Boltzmann equation (refs. 23 and 24) by about a factor of 2. References 23 and 24 have also suggested approximations that account for effects of Coulomb collisions more accurately. But a complete solution of the problem is not given for a gas with an arbitrary degree of ionization. In the present calculations, an interpolation procedure is used for the region of partial ionization and involves the approximate formulas (used in the transport properties calculations and given later) using effective Coulomb collision cross sections. These cross sections are chosen (similar to ref. 17) to make the calculated transport properties agree as closely as possible with the results of Spitzer and Härm (ref. 23) for the fully ionized case.

Symbols and Abbreviations

$A_{C_p}, B_{C_p}, C_{C_p}, D_{C_p}, E_{C_p}$	curve-fit coefficients for specific heat at constant pressure C_p (eqs. (14a) and (14b))
A_h, B_h, C_h, D_h, E_h	curve-fit coefficients for enthalpy h (eqs. (13a) and (13b))
A_K, B_K, C_K, D_K, E_K	curve-fit coefficients for total thermal conductivity K (eqs. (30a) and (30b))
$A_{\mathrm{Pr}}, B_{\mathrm{Pr}}, C_{\mathrm{Pr}}, D_{\mathrm{Pr}}, E_{\mathrm{Pr}}, F_{\mathrm{Pr}}$	curve-fit coefficients for Prandtl number N_{Pr} (eq. (31a))
A_Z, B_Z, C_Z, D_Z, E_Z	curve-fit coefficients for compressibility Z (eq. (19a))
$A_\mu, B_\mu, C_\mu, D_\mu, E_\mu, F_\mu$	curve-fit coefficients for viscosity μ (eq. (22a))
C_i	mass fraction of species i, ρ_i/ρ
C_p	specific heat at constant pressure, $C_p = C_{p_f} + C_{p_r} = \left(\frac{\partial h}{\partial T}\right)_p$, cal/g-K
C_{p_f}	frozen specific heat at constant pressure, $\sum_{i=1}^{\mathrm{NS}} C_i C_{p,i}$, cal/g-K

C_{p_r}	reactive specific heat at constant pressure, $\sum_{i=1}^{\mathrm{NS}} h_i \left(\frac{\partial C_i}{\partial T}\right)_p$, cal/g-K
$C_{p,i}$	specific heat at constant pressure of species i, $\left(\frac{\partial h_i}{\partial T}\right)_p$, cal/g-K
D_{ij}	binary diffusion coefficient, cm^2/sec
$\widetilde{D}_{ij}$	multicomponent diffusion coefficient, cm^2/sec
D_{im}	effective binary diffusion coefficient (eq. (4b)), cm^2/sec
$\overline{D}_{im}$	effective binary diffusion coefficient (eq. (5b)), cm^2/sec
H	total enthalpy of mixture, $h + \frac{u^2}{2}$, kcal/g
h	enthalpy of mixture, $\sum_{i=1}^{\mathrm{NS}} C_i h_i$, kcal/g
h_i	enthalpy of species i, kcal/g
J_i	diffusion mass flux of species i, g/cm^2-sec
j	zero for plane flow and one for axisymmetric flow
K	total thermal conductivity, $K_f + K_r$, cal/cm-sec-K
K_f	frozen thermal conductivity, cal/cm-sec-K
K_{int}	internal component of frozen thermal conductivity, cal/cm-sec-K
K_r	reaction component of total thermal conductivity, cal/cm-sec-K
K_s	thermal conductivity from Sutherland's law (eq. (33)), cal/cm-sec-K
K_{tr}	translational component of frozen thermal conductivity, cal/cm-sec-K
k	Boltzmann's constant, 1.38066×10^{-16} erg/K
$\overline{M}$	molecular weight of mixture, g/g-mole
M_i	molecular weight of species i, g/g-mole
M_o	molecular weight of undissociated air, 28.96 g/g-mole
N_A	Avogadro's number, 6.0221×10^{23} molecules/g-mole
N_{Pr}	total Prandtl number, $C_p\mu/K$
$N_{\mathrm{Pr},f}$	frozen Prandtl number, $C_{p_f}\mu/K_f$
n	coordinate measured normal to body, cm
p	pressure, atm
q	wall heat transfer rate, cal/cm^2-sec

R_{univ}	universal gas constant, 1.987 cal/g-mole-K
r	radius measured from axis of symmetry to a point on body surface, cm
s	coordinate measured along body, cm
T	temperature, K
u	velocity component tangent to body surface, cm/sec
v	velocity component normal to body surface, cm/sec
$\dot{w}_i$	mass rate of formation of species i, g/cm^3-sec
x_i	mole fraction of species i
Z	compressibility factor
$\Delta_{ij}^{(1)}$	defined by equation (26), cm-sec
$\Delta_{ij}^{(2)}$	defined by equation (21), cm-sec
θ	local body angle measured from body axis
κ	body curvature, cm^{-1}
μ	viscosity, poise
μ_s	viscosity from Sutherland's law (eq. (32)), poise
ρ	density, g/cm^3
ρ_i	density of species i, g/cm^3
ρ_o	density of undissociated air, g/cm^3
$\overline{\Omega}_{ij}^{(1,1)}$	average collision cross section (used for thermal conductivity) for collisions between species i and j, Å^2 (1Å = 10^{-8} cm)
$\overline{\Omega}_{ij}^{(2,2)}$	average collision cross section (used for viscosity and thermal conductivity) for collisions between species i and j, Å^2

Subscripts:

e	local chemical equilibrium
i	species i
j	species j
l	species l
m	mixture
p	constant pressure

Abbreviations:

NIR	total number of independent reactions
NS	total number of chemical species

Background

This section addresses the usefulness of employing the total properties in place of the frozen values to solve the flow-field equations under chemical-equilibrium conditions. The energy equation for a chemically reacting multicomponent gas mixture can be written in terms of frozen values of thermal conductivity and specific heat at constant pressure. (See ref. 4, for example.) However, if the system remains in equilibrium and the elemental composition is constant throughout the flow (i.e., there is no foreign gas injection or elemental separation[2]), then the equation can be written in terms of total thermal conductivity and total specific heat at constant pressure. (See appendix A.) In such a formulation, the species production term $\dot{w}_i$, the species diffusion mass flux J_i, and species concentration C_i do not appear explicitly in the energy equation but instead are contained in the definitions of total specific heat and total thermal conductivity.

Now the total specific heat at constant pressure C_p is defined as follows (see appendix A and refs. 7, 8, and 25):

$$C_p = \left(\frac{\partial h}{\partial T}\right)_p \tag{1a}$$

$$= \sum_{i=1}^{\mathrm{NS}} C_i C_{p,i} + \sum_{i=1}^{\mathrm{NS}} h_i \left(\frac{\partial C_i}{\partial T}\right)_p \tag{1b}$$

$$= C_{p_f} + C_{p_r} \tag{1c}$$

The first term of equations (1b) and (1c) is the frozen component of the specific heat and the second term represents the contribution from chemical reactions. Similarly, the total thermal conductivity K contains the frozen and reactive components and may be defined as (see refs. 6, 7, 8, 17, and 25)

$$K = K_f + K_r \tag{2a}$$

or

$$K = K_f - \left(\sum_{i=1}^{\mathrm{NS}} h_i J_i\right) \Big/ (\partial T/\partial n) \tag{2b}$$

where K_f consists of the translational K_{tr} and internal K_{int} components, which are defined subsequently (eqs. (24a) and (25)).

The diffusion mass flux of species i, J_i, in equation (2b) is given by (refs. 19, 26, and 27)

$$J_i = -\frac{\rho}{\overline{M}^2} \sum_{j=1}^{\mathrm{NS}} M_i M_j \widetilde{D}_{ij} \frac{\partial x_j}{\partial n} \tag{3}$$

for multicomponent diffusion with pressure and thermal diffusion neglected. For a mixture of more than two species, the multicomponent diffusion coefficients $\widetilde{D}_{ij}$ depend not only on the properties of the individual species i and j but also on the mixture composition and on the properties of all species in the mixture (ref. 28). These multicomponent coefficients can be calculated with the expressions given in reference 19 from the mixture composition and the ordinary binary diffusion coefficients D_{ij} given in reference 8. A simpler form of equation (3)

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[2] Elemental separation under thermochemical equilibrium conditions is generally negligible unless there is a foreign gas injection or ablation at the surface of a body.

can be obtained with the assumption that all the species in the mixture move with the same velocity or are stationary. With this assumption, equation (3) in terms of the mass-fraction gradients becomes (refs. 9, 25, and 26)

$$J_i = -\rho D_{im} \frac{\partial C_i}{\partial n} \tag{4a}$$

with

$$D_{im} = \frac{1 - x_i}{\sum_{\substack{j=1 \\ j \neq i}}^{\mathrm{NS}} x_j / D_{ij}} \tag{4b}$$

or, in terms of the mole-fraction gradients (refs. 29 and 30),

$$J_i = -\rho \overline{D}_{im} \frac{\partial x_i}{\partial n} \tag{5a}$$

with

$$\overline{D}_{im} = \frac{\left(M_i/\overline{M}\right)\left[1 - \left(M_i/\overline{M}\right) x_i\right]}{\sum_{\substack{j=1 \\ j \neq i}}^{\mathrm{NS}} x_j / D_{ij}} \tag{5b}$$

Use of any of the above formulations to obtain total thermal conductivity K requires the solution of equation (2b) simultaneously with the flow-field governing equations for a particular flow problem. Under the chemical equilibrium condition, however, the chemical composition almost comes into equilibrium with the local temperature (ref. 6). For such a case, therefore, one can write

$$\left(\frac{\partial C_i}{\partial T}\right)_e = \frac{\partial C_i/\partial n}{\partial T/\partial n} \tag{6}$$

or

$$\left(\frac{\partial x_i}{\partial T}\right)_e = \frac{\partial x_i/\partial n}{\partial T/\partial n} \tag{7}$$

where the subscript e implies local chemical equilibrium. Using equations (6) and (7) along with equations (3), (4a), and (5a) in equation (2b), one obtains

$$K = K_f + \frac{\rho}{\overline{M}^2} \sum_{i=1}^{\mathrm{NS}} \sum_{j=1}^{\mathrm{NS}} h_i M_i M_j \tilde{D}_{ij} \left(\frac{\partial x_j}{\partial T}\right)_e \tag{8a}$$

$$K = K_f + \rho \sum_{i=1}^{\mathrm{NS}} D_{im} h_i \left(\frac{\partial C_i}{\partial T}\right)_e \tag{8b}$$

or

$$K = K_f + \rho \sum_{i=1}^{\mathrm{NS}} \overline{D}_{im} h_i \left(\frac{\partial x_i}{\partial T}\right)_e \tag{8c}$$

Evaluation of K from either the exact equation (8a) or the approximate equation (8b) or (8c) does not require any details of the flow-field geometry. Obviously, equation (8b) or (8c) is considerably simpler to use than equation 8(a) for the evaluation of K. These equations imply that the total thermal conductivity is being computed at a constant pressure.

If the energy equation is formulated in terms of total enthalpy instead of temperature, then it can be shown that the equation can be written in a simplified form (see appendix A) with the use of one additional total quantity, the total Prandtl number N_{Pr}, defined as

$$N_{\mathrm{Pr}} = C_p \mu / K \tag{9}$$

where the total values of C_p and K are obtained from equations (1) and (2), respectively.

Thus, with the introduction of total properties, it is possible to write the energy equation in terms of either temperature or total enthalpy and the resulting equations have the same form as the corresponding perfect-gas equations. Consequently, the equations for an equilibrium reacting gas mixture can be solved in a manner similar to that for a perfect gas, provided the curve fits to the total values of C_p, K, and N_{Pr} are available for the ranges of temperatures and pressures of interest. Such curve fits have been obtained in this study. As also mentioned previously, these curve fits can be used only for equilibrium air calculations where the elemental composition is constant throughout the flow field.

No curve fits are given here for the frozen values of C_p, K, and N_{Pr}. This is because the energy equation formulated in terms of these quantitites (see eqs. (A2) or (A4)) involves gradients of the species concentrations. This formulation, therefore, requires an explicit solution for the species concentrations in the flow field. Once the concentration (and temperature) distributions are available, the frozen values of C_p, K, and N_{Pr} can easily be obtained from the individual species properties. Therefore, there is no need to obtain curve fits for the frozen values.

Analysis

Curve-Fit Temperature Intervals, Averaging, and Interpolation Procedures

The order of the curve-fit polynomials and the number of temperature intervals for the curve fits have been selected to achieve a 5-percent overall accuracy of the curve-fit values compared with the computed values. Also, less computational effort is needed in computing the properties in flow-field calculations if fewer temperature intervals (or ranges) are used with a lower order polynomial. The entire temperature range of 500 to 30 000 K is broken down to two or more intervals with these criteria. Further, to ensure a smooth variation of the curve-fit properties over the complete temperature range, values of the curve-fit coefficients are linearly averaged at the temperature interval boundaries over a specified overlap region. The overlap region is equally spread on the two sides at the temperature boundaries and is 500 K for temperatures less than 20 000 K and 1000 K for higher temperatures. The averaging procedure for a coefficient in the overlap region can be written as

$$\overline{A}_\phi = (1 - a) A_\phi^L + a A_\phi^U \tag{10a}$$

where

$$a = \left(\frac{T - T_B^L}{T_B^U - T_B^L} \right) \tag{10b}$$

Here, T_B^L and T_B^U are the lower and upper temperature limits, respectively, of the overlap region. Coefficient A_ϕ is one of the curve-fit coefficients for flow-field property ϕ. The superscripts U and L on A_ϕ denote coefficients of the curve fits from the upper and lower sides of the temperature boundaries, respectively. With these definitions, the curve-fit coefficient A_ϕ is replaced by $\overline{A}_\phi$ from equation (10a) when the temperature at which the property is to be evaluated is within an overlap region. An example subroutine, which evaluates the curve fits and performs the linear averaging, is presented in appendix B. This subroutine can be easily modified to suit the user's requirements.

Since the curve fits are obtained for a range of constant pressures (10^{-4} to 10^2 atm) in steps of a factor of 10, an interpolation procedure is required to obtain values of the flow-field properties at intermediate pressures. A simple logarithmic interpolation procedure is suggested here for this purpose. With this procedure, a property $\phi^\star$ may be interpolated at pressure $p^\star$ (for a specified temperature) from the following relation:

$$\log \phi^\star = \left(\frac{\log \phi_2 - \log \phi_1}{\log p_2 - \log p_1} \right) \left(\log p^\star - \log p_1 \right) + \log \phi_1 \tag{11}$$

where ϕ_2 and ϕ_1 are the values of property ϕ evaluated for a specified temperature T at pressures p_2 and p_1, respectively, such that $p_1 \leq p^\star \leq p_2$. Other details of the interpolation procedure are given in reference 15. This reference also provides an alternate interpolation procedure, which gives smaller interpolation error as compared to equation (11).

The curve fits provided herein are in terms of temperature. These may be easily converted to be in terms of enthalpy by using the relation between temperature and enthalpy provided by the curve fits in the next section.

Details of Property Computations and Curve Fits

Enthalpy. The specific enthalpy for equilibrium air can be computed from

$$h = \sum_{i=1}^{\mathrm{NS}} C_i h_i \tag{12}$$

where h_i is the specific enthalpy of individual species obtained from the curve fits of reference 8 and C_i is the concentration of individual species obtained from a free-energy-minimization calculation procedure (ref. 1). These computed values have been curve fit by employing the following curve-fit expression to obtain enthalpy as a function of temperature at constant pressure:

$$h = \exp\left(A_h \chi^4 + B_h \chi^3 + C_h \chi^2 + D_h \chi + E_h \right) \tag{13a}$$

or

$$\ln h = A_h \chi^4 + B_h \chi^3 + C_h \chi^2 + D_h \chi + E_h \tag{13b}$$

where

$$\chi = \ln(T/10\,000) \tag{13c}$$

The coefficients A_h, B_h, C_h, D_h, and E_h have been evaluated from the computed values with a least-squares curve-fit technique and are given in table I. These coefficients are given for several temperature ranges at a specified pressure. As mentioned previously, the number of temperature ranges is established to obtain a smooth and accurate curve fit to the computed values, and generally a larger number of ranges are needed at lower pressures.

Figure 2 shows the curve-fit and computed values for enthalpy at selected pressure values. All the computed values are not shown in this and other figures, especially at temperatures of less than 2000 K. Values from the curve-fit equation (13a) are within 4 percent of the values computed from equation (12) for the seven specified pressures in the range 10^{-4} to 10^2 atm and the entire temperature range (500 to 30 000 K) considered herein.

Total specific heat at constant pressure. The total specific heat at constant pressure can be computed from equation (1b). The species concentration C_i appearing in this equation is obtained from the free-energy-minimization calculation method of reference 1, and $(\partial C_i/\partial T)_p$ is evaluated numerically by differentiating the data from this calculation. The contribution of the chemical reactions to the specific heat (involving $(\partial C_i/\partial T)_p$) becomes neligible for temperatures less than 2000 K at pressures around 10^0 atm.

The following expression is employed to curve fit the values of C_p computed from equation (1b):

$$C_p = \exp\left(A_{C_p}\chi^4 + B_{C_p}\chi^3 + C_{C_p}\chi^2 + D_{C_p}\chi + E_{C_p}\right) \tag{14a}$$

or

$$\ln C_p = A_{C_p}\chi^4 + B_{C_p}\chi^3 + C_{C_p}\chi^2 + D_{C_p}\chi + E_{C_p} \tag{14b}$$

with

$$\chi = \ln(T/10\,000) \tag{14c}$$

The tabulated values of coefficients A_{C_p}, B_{C_p}, C_{C_p}, D_{C_p}, and E_{C_p} are provided in table II. Figure 3 shows the computed and curve-fit values. The curve-fit values are within 4 percent of the computed values for the entire temperature range and pressure values considered herein.

Compressibility factor. The density of equilibrium air can be obtained from the equation of state:

$$\rho = \left(p\overline{M}/R_{\text{univ}}T\right) \times 2.4218 \times 10^{-2} \tag{15}$$

where the factor 2.4218×10^{-2} appears because of the units of thermodynamic variables and the universal gas constant employed here (see list of symbols for the units) and the mixture molecular weight $\overline{M}$ is given by

$$\overline{M} = \frac{1}{\sum_{i=1}^{\text{NS}} \left(C_i/M_i\right)} \tag{16}$$

The density of undissociated air ρ_o can be computed from

$$\rho_o = (pM_o/R_{\text{univ}}T)\, 2.4218 \times 10^{-2} \tag{17}$$

The compressibility factor Z, which is equal to the ratio of the molecular weight of undissociated air to the mean molecular weight, can be obtained from equations (15) and (17) through the relation

$$Z = \frac{M_o}{\overline{M}} = \frac{\rho_o}{\rho} \tag{18}$$

The computed values of the compressibility factor Z have been curve fit by employing the following expression at constant pressure:

$$Z = A_Z + B_Z\chi + C_Z\chi^2 + D_Z\chi^3 + E_Z\chi^4 \tag{19a}$$

where

$$\chi = T/1000 \tag{19b}$$

The coefficients appearing in equation (19a) are given in table III. Accuracy of the curve fit of equation (19a) compared with the computed values from equations (15), (17), and (18) is shown in figure 4. The curve-fit values are within 3 percent of the computed values for the pressure range of 10^{-4} to 10^2 atm.

Viscosity. Viscosity has been computed from the following expression (see refs. 8 and 17):

$$\mu = \sum_{i=1}^{NS} \frac{(M_i/N_A)\,x_i}{\sum_{j=1}^{NS} x_j \Delta_{ij}^{(2)}} \tag{20}$$

where $\Delta_{ij}^{(2)}$ is defined as

$$\Delta_{ij}^{(2)} = \frac{16}{5}(1.5460 \times 10^{-20}) \left[\frac{2M_i M_j}{\pi R_{\rm univ} T \left(M_i + M_j\right)} \right]^{1/2} \pi\overline{\Omega}_{ij}^{(2,2)} \tag{21}$$

In the above equation, $\pi\overline{\Omega}_{ij}^{(2,2)}$ is the average collision cross section for viscosity and is provided in curve-fit form as a function of temperature in reference 8 for the various species interaction pairs.

The following expression has been used to curve fit the viscosity values computed from equation (20):

$$\mu = A_\mu + B_\mu \chi + C_\mu \chi^2 + D_\mu \chi^3 + E_\mu \chi^4 + F_\mu \chi^5 \tag{22a}$$

where

$$\chi = T/1000 \tag{22b}$$

The polynomial coefficients of equation (22a) are given in table IV. The computed and curve-fit values of the viscosity are shown in figure 5 for different pressures. In general, the curve-fit values are within 4 percent of the values computed from equation (20). The accuracy improves with increasing pressure, similar to the other thermodynamic and transport properties.

Total thermal conductivity. The total thermal conductivity K for equilibrium air is obtained from equations (2). The frozen part in these equations is obtained from the translational and internal components:

$$K_f = K_{\rm tr} + K_{\rm int} \tag{23}$$

The translational contribution in the above equation is computed from the relation (see refs. 8 and 17)

$$K_{\rm tr} = (2.3901 \times 10^{-8}) \frac{15}{4} k \sum_{i=1}^{NS} \frac{x_i}{\sum_{j=1}^{NS} \alpha_{ij} x_j \Delta_{ij}^{(2)}} \tag{24a}$$

where $\Delta_{ij}^{(2)}$ is given by equation (21) and α_{ij} is defined as

$$\alpha_{ij} = 1 + \frac{\left[1 - \left(M_i/M_j\right)\right]\left[0.45 - 2.54\left(M_i/M_j\right)\right]}{\left[1 + \left(M_i/M_j\right)\right]^2} \tag{24b}$$

The component of thermal conductivity resulting from the internal excitation energy of the molecules $K_{\rm int}$ is calculated from (refs. 8 and 17)

$$K_{\rm int} = (2.3901 \times 10^{-8}) k \sum_{i=1}^{NS} \frac{\left[\left(C_{p,i}/R_{\rm univ}\right) - (5/2)\right] x_i}{\sum_{j=1}^{NS} x_j \Delta_{ij}^{(1)}} \tag{25}$$

where $\Delta_{ij}^{(1)}$ is defined as

$$\Delta_{ij}^{(1)} = \frac{8}{3}(1.546 \times 10^{-20}) \left[\frac{2M_i M_j}{\pi R_{\text{univ}} T \left(M_i + M_j \right)} \right]^{1/2} \pi \overline{\Omega}_{ij}^{(1,1)} \tag{26}$$

and $\pi \overline{\Omega}_{ij}^{(1,1)}$ is the collision cross section for diffusion, which is provided in curve-fit form in reference 8.

The reaction part of the thermal conductivity K_r is defined in equation (8a) or, through some approximations, in equations (8b) and (8c). As shown for a single reaction in references 31 and 32, the reaction part of equation (8a) is equivalent to

$$K_r = k \times 10^{-4} \sum_{l=1}^{\text{NIR}} \frac{(\Delta h_l / R_{\text{univ}} T)^2}{\sum_{i=1}^{\text{NS}} \left(a_{l,i}/x_i \right) \sum_{j=1}^{\text{NS}} \left(a_{l,i} x_j - a_{l,j} x_i \right) \Delta_{ij}^{(1)}} \tag{27}$$

given in references 7, 8, 9, and 17. Compared with the definition of K_r in equation (8a), equation (27) has been simplified with the expressions from reference 19 to eliminate the multicomponent diffusion coefficient $\widetilde{D}_{ij}$ from the problem. Equation (27), therefore, can be evaluated with a greater degree of accuracy and has been used to evaluate K_r. Equation (27) is equivalent to the reaction part of equation (8a) for those temperature and pressure conditions for which only a single chemical reaction is significant; however, there will be some error in this approximation for conditions in which more than one reaction is proceeding simultaneously. This error has been discussed, for example, in reference 20.

In equation (27), NIR is the total number of independent reactions in the system and $a_{l,i}$ represents the stoichiometric coefficients of components A_i in the lth chemical reaction written in the balanced form:

$$\sum_{i=1}^{\text{NS}} a_{l,i} A_i = 0 \tag{28}$$

and Δh_l is the heat of reaction per gram-mole for the lth reaction given by

$$\Delta h_l = \sum_{i=1}^{\text{NS}} \left(h_i \times 10^3 \right) a_{l,i} M_i \tag{29}$$

The total thermal conductivity K, computed from equations (2a), (23), (24a), (25), and (27), is curve fit with the expression

$$K = \exp \left(A_K \chi^4 + B_K \chi^3 + C_K \chi^2 + D_K \chi + E_K \right) \tag{30a}$$

or

$$\ln K = A_K \chi^4 + B_K \chi^3 + C_K \chi^2 + D_K \chi + E_K \tag{30b}$$

where

$$\chi = \ln(T/10\,000) \tag{30c}$$

The coefficients appearing in equations (30) are given in table V. Figure 6 shows the computed and curve-fit values. The curve-fit values are within 4 percent of the computed values for the entire temperature range and pressure values considered herein.

Total Prandtl number. The total Prandtl number for equilibrium air has been computed from equation (9), with C_p and μ obtained from equations (1) and (20), respectively, and K calculated from equations (2a), (23), (24a), (25), and (27). The computed values of the Prandtl number have been curve fit with the relation

$$N_{\mathrm{Pr}} = A_{\mathrm{Pr}} + B_{\mathrm{Pr}}\chi + C_{\mathrm{Pr}}\chi^2 + D_{\mathrm{Pr}}\chi^3 + E_{\mathrm{Pr}}\chi^4 + F_{\mathrm{Pr}}\chi^5 \qquad (31a)$$

with

$$\chi = T/1000 \qquad (31b)$$

The polynomial coefficients of equation (31a) are provided in table VI. Figure 7 shows the curve-fit values of equation (33a) compared with the computed values. The curve-fit values are within 4 percent of the computed values for the pressure and temperature ranges considered herein.

Variation of the Properties With Pressure

The curve-fit values for enthalpy, total specific heat at constant pressure, compressibility factor, viscosity, total thermal conductivity, and total Prandtl number are shown in figure 8. This figure gives the variation of these properties with pressure. For a given pressure, the temperature dependence of the various properties can be divided roughly into four portions corresponding to the reactions taking place. From 500 K to the temperature at which the curves begin to diverge, the mixture stays essentially inert. Divergence can be attributed to the dissociation of oxygen. The large change in properties at the next temperature portion occurs basically because of nitrogen dissociation. At the third temperature portion, single ionization of nitrogen and oxygen atoms causes the change in properties. Finally, double ionization of nitrogen and oxygen is responsible for the change in properties at the last temperature portion. These changes in the values of C_p, μ, K, and N_{Pr} are reflected, generally, through maxima in their values. With the decrease in pressure these maxima (except for μ) increase in sharpness as they shift to lower temperatures.

Comparison With Existing Results

A comparison is provided in this section of the presently computed results with those existing in the literature and commonly employed in various flow-field computations.

Enthalpy. The computed dimensionless enthalpy values are compared with those of Hansen (ref. 7) in figure 9 for two pressures. As mentioned in the "Introduction," Hansen's values are available only through a temperature of 15 000 K for the pressure range of 10^{-4} to 10^2 atm. Agreement is good between the two results through this temperature range. The present results have been obtained with an 11-species air model (N_2, O_2, N, O, NO, N^+, O^+, NO^+, N^{++}, O^{++}, and e^-), whereas the results of reference 7 are based on a 7-species air model (N_2, O_2, N, O, N^+, O^+, and e^-). Obviously the small concentrations of NO^+, N^{++}, and O^{++} ($C_i < 10^{-3}$) do not affect the equilibrium air enthalpy significantly through temperatures less than 15 000 K. For temperatures greater than 15 000 K and pressures less than 10^{-2} atm, however, N^{++} and O^{++} concentrations become quite significant and the equilibrium air calculations need to include these two species, as shown in figures 10(a) and 10(b). A nine-species air model (N_2, O_2, N, O, NO, N^+, O^+, NO^+, and e^-) gives enthalpy values similar to those obtained from a seven-species air model. The enthalpy values obtained from these two models differ considerably from those obtained from an 11-species air model at temperatures greater than 15 000 K.

Total specific heat at constant pressure. The dimensionless values of the total specific heat at constant pressure are compared with those of Hansen (ref. 7) in figure 11. Agreement is quite good except at low pressures and high temperatures, when the production of N^{++} and O^{++} begins to dominate over other species. Clearly the specific heat calculations are affected more than the enthalpy calculations by the production of these two doubly charged ions.

Compressibility factor. The compressibility factors computed presently and those given by Hansen (ref. 7) compare quite well for the entire pressure range (10^{-4} to 10^{2} atm) through a temperature range of 15 000 K, as shown in figure 12. Similar to the enthalpy values, differences in the number of chemical species used in the two calculations do not affect the compressibility factor to any noticeable degree for these pressure and temperature ranges.

Viscosity. The presently computed viscosity values are compared with those of Hansen (ref. 7), Peng and Pindroh (ref. 9), and Svehla (ref. 33) in figure 13(a) for a pressure of 10^{0} atm. Present results obtained with the 11-species air model compare well with the calculations of Peng and Pindroh (based on a 9-species air model) through a temperature of about 7500 K. The discrepancy between the two calculations at higher temperatures may be because of the differences in the mixing law and the cross sections used for charged-neutral and charged-charged particle interactions. Agreement of the present values with those of Hansen is quite poor for almost the entire temperature range shown in figure 13(a), except at temperatures less than about 1500 K. In fact, Hansen's values are similar to those predicted from Sutherland's law of viscosity

$$\mu_s = 1.4584 \times 10^{-5} \frac{T^{3/2}}{T + 110.33} \tag{32}$$

for temperatures less than 5000 K. The agreement of these two values in the temperature range of 2000 to 5000 K is somewhat surprising in view of the fact that oxygen begins to dissociate at 2000 K and is fully dissociated at 5000 K. Sutherland's law of viscosity is applicable only to undissociated air. All the computed values approach Sutherland's values at temperatures less than 2000 K, as shown in figure 13(a). Also included in this figure are the viscosity values computed by Svehla (ref. 33) for unionized air. These values compare well with the present values and with those predicted by Peng and Pindroh through a temperature of about 4000 K.

Figure 13(b) shows a comparison of the presently computed viscosity values with those of Hansen (ref. 7) and those from Sutherland's law of viscosity (eq. (32)) at a pressure of 10^{-4} atm. The disagreement with Hansen's values is similar to that noted for a pressure of 10^{0} atm (fig. 13(a)). Peng and Pindroh (ref. 9) have not provided viscosity values for $p < 10^{-2}$ atm and, therefore, their calculations are not included for comparison here. Similarly, Svehla (ref. 33) has provided computed values only for 10^{0} atm and his values cannot be compared in figure 13(b).

The differences in the various results shown herein, particularly at higher temperatures, may be attributed to the differences in the viscosities of the constituent air species (resulting from the differences in the species cross sections), mixing laws employed for the mixture calculations, and to a somewhat lesser extent, the number of chemical species considered in the air model.

Total thermal conductivity. The present values of the total thermal conductivity are compared with those given by Hansen (ref. 7) and Peng and Pindroh (ref. 9) in figure 14(a) for a pressure of 10^{0} atm. Figure 14(b) gives a comparison with Hansen's (ref. 7) predictions for a pressure of 10^{-4} atm. As with viscosity, the total conductivity values of reference 9 are not available for pressures less than 10^{-2} atm. Further, the present thermal conductivity values agree better with the results of Peng and Pindroh than with those of Hansen through a temperature of about 9000 K, as shown in figure 14(a). With increasing ionization at higher temperatures the two results begin to differ. Hansen's results underpredict thermal conductivity through a temperature of about 9000 K and overpredict beyond 9500 K compared with the present results (as well as those of Peng and Pindroh). Also included in figures 14(a) and 14(b) are the values obtained from Sutherland's law:

$$K_S = 5.9776 \times 10^{-6} \frac{T^{3/2}}{T + 194.4} \tag{33}$$

All the computed values approach the Sutherland values as the temperature decreases to 500 K, when only the rotational component of the internal energy of the molecular species is fully excited. For temperatures greater than 500 K, the vibrational component becomes excited and the dissociation of oxygen in air is initiated at approximately 2000 K. Therefore, Sutherland's law (eq. (33)) should not be applicable for temperatures greater than about 500 K.

The differences between the values for various computations shown in figures 14(a) and 14(b) exist for reasons similar to those given previously for the differences in viscosity values.

Total Prandtl number. The calculated total Prandtl number values compare qualitatively with those of Hansen (ref. 7) for a temperature up to about 9000 K at a pressure of 10^0 atm, as shown in figure 15(a). However, the values differ quantitatively by as much as 22 percent. For temperatures greater than 9000 K, Hansen's values are much lower than the present results, primarily because of the larger value of the thermal conductivity computed by Hansen. (See fig. 14(a).) Results from the two calculations compare much more favorably at a pressure of 10^{-4} atm (as shown in fig. 15(b)) except for the temperature range of 5500 to 10 500 K. These differences are related directly to the differences in the values of thermal conductivity shown in figure 14(b).

Concluding Remarks

A self-consistent set of values have been computed for enthalpy, total specific heat at constant pressure, compressibility factor, viscosity, total thermal conductivity, and total Prandtl number of equilibrium air from 500 to 30 000 K over a pressure range of 10^{-4} to 10^2 atm. Previous results for most of these properties have been limited to a temperature of 15 000 K. The mixture values are calculated from the transport and thermodynamic properties of the individual species provided in a recent study. The air model considered herein consists of 11 species: O_2, N_2, O, N, NO, O^+, N^+, NO^+, O^{++}, N^{++}, and e^-. For pressures less than 10^{-2} atm and temperatures greater than 14 000 K, the concentrations of N^{++} and O^{++} become dominant. The differences in the computed values given herein and those obtained by other researchers may be attributed to the differences in the properties of the individual species used (including those due to the electron number density correction for the ionized-species transport properties), mixing laws used for the mixture, and to a lesser extent, the number of chemical species considered.

The computed values of the various properties are curve fit as a function of temperature at constant values of pressure through the use of the least-squares curve-fit technique. A logarithmic interpolation relation is provided to obtain values at intermediate pressures. Further, a linear averaging procedure is suggested for the various curve-fit coefficients in order to obtain continuous values of the properties across the curve-fit boundaries. The curve fits are accurate to within 5 percent of the computed results for the pressure values and temperature range considered. These curve fits provide an efficient and fairly accurate means of computing the flow-field properties for equilibrium air calculations.

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Appendix A
Energy Equation in Terms of Frozen and Total Values of Specific Heat, Thermal Conductivity, and Prandtl Number

The viscous-shock-layer form[3] of the energy equation for a chemically reacting multicomponent gas mixture can be written in terms of the frozen values of thermal conductivity and specific heat at constant pressure as follows (ref. 4):

$$\begin{aligned}\rho C_{p_f}&\left(\frac{u}{1+n\kappa}\frac{\partial T}{\partial s}+v\frac{\partial T}{\partial n}\right)-\left(\frac{u}{1+n\kappa}\frac{\partial p}{\partial s}+v\frac{\partial p}{\partial n}\right)\\ &=\frac{\partial}{\partial n}\left(K_f\frac{\partial T}{\partial n}\right)+\left(\frac{\kappa}{1+n\kappa}+\frac{j\cos\theta}{r+n\cos\theta}\right)K_f\frac{\partial T}{\partial n}\\ &\quad-\sum_{i=1}^{\mathrm{NS}}J_iC_{p,i}\frac{\partial T}{\partial n}+\mu\left(\frac{\partial u}{\partial n}-\frac{\kappa u}{1+n\kappa}\right)^2-\sum_{i=1}^{\mathrm{NS}}h_i\dot{w}_i\end{aligned}\tag{A1}$$

If the species continuity equation (5) of reference 4 is multiplied by h_i, summed over all the species, and then subtracted from equation (A1), the following form of the energy equation is obtained:

$$\begin{aligned}\rho C_{p_f}&\left(\frac{u}{1+n\kappa}\frac{\partial T}{\partial s}+v\frac{\partial T}{\partial n}\right)-\left(\frac{u}{1+n\kappa}\frac{\partial p}{\partial s}+v\frac{\partial p}{\partial n}\right)\\ &=\frac{\partial}{\partial n}\left(K_f\frac{\partial T}{\partial n}-\sum_{i=1}^{\mathrm{NS}}h_iJ_i\right)\\ &\quad+\left(\frac{\kappa}{1+n\kappa}+\frac{j\cos\theta}{r+n\cos\theta}\right)\left(K_f\frac{\partial T}{\partial n}-\sum_{i=1}^{\mathrm{NS}}h_iJ_i\right)\\ &\quad+\mu\left(\frac{\partial u}{\partial n}-\frac{\kappa u}{1+n\kappa}\right)^2-\rho\left(\frac{u}{1+n\kappa}\sum_{i=1}^{\mathrm{NS}}h_i\frac{\partial C_i}{\partial s}+v\sum_{i=1}^{\mathrm{NS}}h_i\frac{\partial C_i}{\partial n}\right)\end{aligned}\tag{A2}$$

Equation (A2) may be further rewritten, in terms of the total thermal conductivity and total specific heat at constant pressure, as follows:

$$\begin{aligned}\rho C_p&\left(\frac{u}{1+n\kappa}\frac{\partial T}{\partial s}+v\frac{\partial T}{\partial n}\right)-\left(\frac{u}{1+n\kappa}\frac{\partial p}{\partial s}+v\frac{\partial p}{\partial n}\right)\\ &=\frac{\partial}{\partial n}\left(K\frac{\partial T}{\partial n}\right)+\left(\frac{\kappa}{1+n\kappa}+\frac{j\cos\theta}{r+n\cos\theta}\right)K\frac{\partial T}{\partial n}\\ &\quad+\mu\left(\frac{\partial u}{\partial n}-\frac{\kappa u}{1+n\kappa}\right)^2\end{aligned}\tag{A3}$$

where C_p is the total specific heat at constant pressure and K is the total thermal conductivity defined in equations (1) and (2), respectively. The mass diffusion term J_i in equations (A1) and (A2) is defined by equations (3), (4), or (5).

---

[3] The equations chosen for the purpose of illustration here are of the viscous-shock-layer form for the sake of simplicity. Similar treatment can be extended to the Navier-Stokes equations also.

Equations (A2) and (A3) do not contain the species production rate term $\dot{w}_i$ appearing in equation (A1). This is the term that is responsible for causing stiffness and convergence problems in the solution of equation (A1) when the flow is under (or near) chemical-equilibrium conditions. For such cases, forms of the energy equation given by equations (A2) and (A3) are more desirable. Unlike equation (A2), diffusion terms do not appear explicitly in equation (A3) but instead are contained in the definitions of total specific heat and total thermal conductivity (eqs. (1) and (2)).

Reference 4 provides an alternate form of the energy equation (A1) in terms of total enthalpy for chemical-equilibrium flow calculations:

$$\rho\left(\frac{u}{1+n\kappa}\frac{\partial H}{\partial s}+v\frac{\partial H}{\partial n}\right)-v\frac{\partial p}{\partial n}+\rho\frac{\kappa u^2 v}{1+n\kappa}=\frac{\partial \Phi}{\partial n}+\left(\frac{\kappa}{1+n\kappa}+\frac{j\cos\theta}{r+n\cos\theta}\right)\Phi \tag{A4}$$

where

$$\Phi=\frac{\mu}{N_{\mathrm{Pr},f}}\frac{\partial H}{\partial n}-\frac{\mu}{N_{\mathrm{Pr},f}}\sum_{i=1}^{\mathrm{NS}}h_i\frac{\partial C_i}{\partial n}-\rho\sum_{i=1}^{\mathrm{NS}}h_i J_i+\frac{\mu}{N_{\mathrm{Pr},f}}\left(N_{\mathrm{Pr},f}-1\right)u\frac{\partial u}{\partial n}-\frac{\mu\kappa u^2}{1+n\kappa} \tag{A5}$$

Similar to equations (A2) and (A3), equation (A4) also does not contain the species production rate term $\dot{w}_i$ and is a desired form for equilibrium flow calculations.

If the frozen Prandtl number $N_{\mathrm{Pr},f}$ appearing in equation (A5) is replaced by the total Prandtl number N_{Pr}, equation (A5) becomes

$$\Phi=\frac{\mu}{N_{\mathrm{Pr}}}\frac{\partial h}{\partial n}+\mu u\left(\frac{\partial u}{\partial n}-\frac{\kappa u}{1+n\kappa}\right) \tag{A6}$$

where the total Prandtl number N_{Pr} is defined as (eq. (9))

$$N_{\mathrm{Pr}}=C_p\mu/K$$

and total values for C_p and K are defined in equations (1) and (2), respectively. Equation (A6) is preferred over equation (A5) because the diffusion terms do not appear explicitly.

Equations (A3) and (A4) (with Φ defined in equation (A6)) have the same form as that for a perfect gas and may be solved in a similar manner without the need to solve for the species concentrations, provided the curve fits to the total values of C_p, K, and N_{Pr} are available for the ranges of temperatures and pressures of interest.

There is a specific advantage to using equation (A3) instead of equation (A4) (with Φ given by equation (A6)) for equilibrium flow calculations because the expensive iterative process of obtaining the temperature (needed for computing the thermodynamic and transport properties) from the mixture enthalpy at every point in the flow field is avoided. Another advantage of using the energy equation with temperature as the dependent variable is that this form can also be used for finite-rate chemistry calculations. For such calculations, however, equation (A2), which separates the frozen and reactive components of C_p and K, is more desirable.

Appendix B

Sample Program To Evaluate Transport and Thermodynamic Properties for Equilibrium Air From Polynomial Curve Fit at a Given Pressure

This appendix is a sample FORTRAN subroutine that evaluates the thermodynamic properties for equilibrium air (with 11 constituent species) with polynomial curve fits used as functions of temperature. The same subroutine can also be modified for evaluation of the transport properties. Different temperature ranges are used at different pressures. Properties evaluated near the temperature range boundaries are smoothed by linearly averaging the polynomial coefficients to assure continuous derivatives. The subroutine may be easily modified for different needs.

```
      SUBROUTINE THERMO(T,H)
C  Computes enthalpy of equilibrium air by approximating polynomials.
C  Polynomial coefficients are stored in arrays A1 to A5 and are
C  linearly averaged at the temperature range boundaries.  The
C  temperature ranges are for pressure at 0.0001 atm.
C
C  input:  T    temperature, K
C  output: H    enthalpy, kcal/g
C
      DIMENSION A1(6),A2(6),A3(6),A4(6),A5(6)
      DIMENSION P(5),COEF(6,5)
      EQUIVALENCE (A1,COEF)
C
C Coefficients are input for six temperature ranges
C
      K=5
      L=6
      IF(T.GT.11000.) GO TO 10
      K=4
      L=5
      IF(T.GT.7000.) GO TO 20
      K=3
      L=4
      IF(T.GT.4500.) GO TO 30
      K=2
      L=3
      IF(T.GT.2500.) GO TO 40
      K=1
```

```
      L=2
      PA=1.0
      PB=0.0
      IF(T.LE.2000.) GO TO 50
      PB=0.002*(T-2000.)
      PA=1.0-PB
      GO TO 50
   10 CONTINUE
      PA=0.0
      PB=1.0
      IF(T.GE.18000.) GO TO 50
      PA=1.0
      PB=0.0
      IF(T.LE.17500.) GO TO 50
      PB=0.002*(T-17500.)
      PA=1.0-PB
      GO TO 50
   20 CONTINUE
      PA=1.0
      PB=0.0
      IF(T.LE.10500.) GO TO 50
      PB=0.002*(T-10500.)
      PA=1.0-PB
      GO TO 50
   30 CONTINUE
      PA=1.0
      PB=0.0
      IF(T.LE.6500.) GO TO 50
      PB=0.002*(T-6500.)
      PA=1.0-PB
      GO TO 50
   40 CONTINUE
      PA=1.0
      PB=0.0
      IF(T.LE.4000.) GO TO 50
```

```
      PB=0.002*(T-4000.)
      PA=1.0-PB
   50 CONTINUE
C
      DO 100 I=1,5
  100 P(I)=PA*COEF(K,I)+PB*COEF(L,I)
C
      TLN=ALOG(T/10000.)
      TLN2=TLN*TLN
      TLN3=TLN2*TLN
      TLN4=TLN3*TLN
C
      H=P(1)*TLN4+P(2)*TLN3+P(3)*TLN2+P(4)*TLN+P(5)
      H=EXP(H)
C
      RETURN
      END
```

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Table I. Curve-Fit Coefficients for Enthalpy of Equilibrium Air

[Enthalpy obtained in kcal/g; curve fits obtained from enthalpies of individual species referenced to $T = 0$ K]

Pressure, atm	A_h	B_h	C_h	D_h	E_h	Temperature range[a], K
10^{-4}	0.128180E + 01	0.121182E + 02	0.424907E + 02	0.665524E + 02	0.385195E + 02	500– 2250
	0.125380E + 02	0.720107E + 02	0.148949E + 03	0.133853E + 03	0.451550E + 02	2250– 4250
	0.426138E + 02	0.123001E + 03	0.121801E + 03	0.509305E + 02	0.995964E + 01	4250– 6750
	0.885088E + 01	−0.207380E + 02	−0.134604E + 02	0.166408E + 01	0.356570E + 01	6750–10750
	0.151569E + 02	−0.713138E + 01	−0.172524E + 00	0.643645E + 00	0.356353E + 01	10750–17750
	0.101759E + 02	−0.161956E + 02	−0.336892E + 01	0.161274E + 02	−0.201068E + 01	17750–25000
10^{-3}	0.902850E + 00	0.839944E + 01	0.289458E + 02	0.448640E + 02	0.256452E + 02	500– 2250
	0.237222E + 02	0.118014E + 03	0.214780E + 03	0.171168E + 03	0.513939E + 02	2250– 4250
	0.880011E + 02	0.213329E + 03	0.181623E + 03	0.661367E + 02	0.110476E + 02	4250– 6750
	−0.333238E + 02	−0.316397E + 02	−0.401000E + 01	0.379639E + 01	0.325469E + 01	6750–11750
	0.196866E + 02	−0.201771E + 02	0.635249E + 01	−0.174347E + 00	0.354258E + 01	11750–18750
	0.446869E + 02	−0.141086E + 03	0.159412E + 03	−0.738595E + 02	0.155141E + 02	18750–28000
10^{-2}	0.653358E + 00	0.596886E + 01	0.201689E + 02	0.309518E + 02	0.174843E + 02	500– 2750
	0.431122E + 01	0.267604E + 02	0.541203E + 02	0.462077E + 02	0.152182E + 02	2750– 5250
	−0.126229E + 01	0.113432E + 02	0.109117E + 02	0.400303E + 01	0.284253E + 01	5250– 9750
	0.209845E + 02	−0.181381E + 02	−0.399635E + 00	0.387388E + 01	0.283981E + 01	9750–17750
	0.268647E + 02	−0.104256E + 03	0.145439E + 03	−0.846045E + 02	0.212051E + 02	17750–30000
10^{-1}	0.363885E + 00	0.329839E + 01	0.110641E + 02	0.173605E + 02	0.999025E + 01	500– 3250
	−0.865884E + 01	−0.208034E + 02	−0.132700E + 02	0.242899E + 01	0.417259E + 01	3250– 6250
	−0.164319E + 02	−0.285858E + 00	0.447878E + 01	0.196275E + 01	0.256061E + 01	6250–15250
	−0.207249E + 02	0.633182E + 02	−0.678713E + 02	0.312942E + 02	−0.158288E + 01	15250–30000
10^{0}	0.209284E + 00	0.187458E + 01	0.622153E + 01	0.101561E + 02	0.603650E + 01	500– 3750
	−0.171560E + 02	−0.416138E + 02	−0.332532E + 02	−0.747816E + 01	0.178858E + 01	3750– 8250
	−0.134978E + 02	0.801118E + 01	0.192371E + 01	0.930272E + 00	0.244209E + 01	8250–17750
	−0.564265E + 01	0.262889E + 02	−0.396119E + 02	0.251297E + 02	−0.207198E + 01	17750–30000
10^{1}	0.124937E + 00	0.109286E + 01	0.355163E + 01	0.617946E + 01	0.386028E + 01	500– 4250
	−0.120314E + 02	−0.229170E + 02	−0.129249E + 02	0.262066E + 00	0.235363E + 01	4250– 9250
	−0.913636E + 01	0.113996E + 02	−0.259796E + 01	0.114665E + 01	0.236890E + 01	9250–18750
	0.639208E + 01	−0.149544E + 02	0.882252E + 01	0.258596E + 01	0.107086E + 01	18750–30000
10^{2}	−0.755123E − 02	0.164258E − 01	0.366590E + 00	0.210603E + 01	0.195195E + 01	500– 6250
	−0.117469E + 01	−0.592622E + 01	−0.214181E + 01	0.251111E + 01	0.212013E + 01	6250–12750
	−0.245329E + 01	0.371340E + 01	−0.288683E + 00	0.421200E + 00	0.239842E + 01	12750–30000

[a] For temperatures less than 500 K, enthalpy for air may be obtained from the relation $h = 0.24 \times 10^{-3} T$.

Table II. Curve-Fit Coefficients for Specific Heat of Equilibrium Air

[Specific heat obtained in cal/g-K]

Pressure, atm	A_{C_p}	B_{C_p}	C_{C_p}	D_{C_p}	E_{C_p}	Temperature range[a], K
10^{-4}	0.349023E + 00	0.344158E + 01	0.126715E + 02	0.208154E + 02	0.116592E + 02	500– 1250
	0.152264E + 02	0.129277E + 03	0.411057E + 03	0.580300E + 03	0.305728E + 03	1250– 1750
	−0.159675E + 02	−0.136508E + 03	−0.411657E + 03	−0.525250E + 03	−0.241298E + 03	1750– 2750
	−0.108293E + 03	−0.515276E + 03	−0.882748E + 03	−0.642505E + 03	−0.166628E + 03	2750– 4750
	−0.116246E + 04	−0.266973E + 04	−0.221802E + 04	−0.791376E + 03	−0.102433E + 03	4750– 6250
	−0.238707E + 02	−0.104336E + 03	−0.890658E + 02	−0.182697E + 02	0.138792E + 01	6250– 9750
	−0.209557E + 02	0.253228E + 02	0.212355E + 02	−0.128857E + 02	0.135712E + 01	9750–14250
	0.762671E + 03	−0.167407E + 04	0.130713E + 04	−0.422349E + 03	0.482128E + 02	14250–19750
	−0.789820E + 03	0.263864E + 04	−0.326378E + 04	0.176381E + 04	−0.348874E + 03	19750–25000
10^{-3}	0.199532E + 00	0.192597E + 01	0.694347E + 01	0.112521E + 02	0.570825E + 01	500– 1250
	0.345376E + 01	0.315624E + 02	0.107177E + 03	0.160585E + 03	0.884544E + 02	1250– 2250
	−0.369572E + 02	−0.128366E + 03	−0.129698E + 03	−0.169299E + 02	0.207647E + 02	2250– 3750
	−0.146237E + 03	−0.581296E + 03	−0.848597E + 03	−0.532403E + 03	−0.119389E + 03	3750– 5250
	−0.758521E + 03	−0.139794E + 04	−0.900003E + 03	−0.238528E + 03	−0.216169E + 02	5250– 7250
	−0.330240E + 02	−0.866157E + 02	−0.489572E + 02	−0.182071E + 01	0.229104E + 01	7250–10750
	−0.618098E + 02	0.103127E + 03	−0.262275E + 02	−0.850086E + 01	0.253250E + 01	10750–17250
	0.125063E + 03	−0.298121E + 03	0.210795E + 03	−0.295269E + 02	−0.792067E + 01	17250–28000
10^{-2}	0.669436E + 00	0.644478E + 01	0.230631E + 02	0.365225E + 02	0.203928E + 02	500– 1750
	−0.453138E + 02	−0.292666E + 03	−0.699603E + 03	−0.730849E + 03	−0.281133E + 03	1750– 2750
	−0.151035E + 03	−0.591051E + 03	−0.835692E + 03	−0.502696E + 03	−0.107793E + 03	2750– 4750
	0.539167E + 03	0.126894E + 04	0.106221E + 04	0.370582E + 03	0.457650E + 02	4750– 6750
	0.217707E + 02	−0.450370E + 02	−0.192634E + 02	0.517928E + 01	0.180195E + 01	6750–12750
	−0.122810E + 03	0.240030E + 03	−0.138486E + 03	0.225676E + 02	0.100733E + 01	12750–19750
	0.162348E + 03	−0.497482E + 03	0.525270E + 03	−0.216688E + 03	0.277132E + 02	19750–30000
10^{-1}	0.291577E + 00	0.278787E + 01	0.992221E + 01	0.157475E + 02	0.820277E + 01	500– 1750
	−0.662937E + 01	−0.382984E + 02	−0.779456E + 02	−0.627915E + 02	−0.154364E + 02	1750– 2750
	0.128388E + 03	0.596922E + 03	0.101945E + 04	0.757047E + 03	0.205793E + 03	2750– 4250
	−0.296048E + 02	−0.133243E + 03	−0.187832E + 03	−0.100614E + 03	−0.168003E + 02	4250– 6750
	−0.308894E + 03	−0.267701E + 03	−0.478605E + 02	0.326629E + 01	0.838365E + 00	6750– 9750
	0.104767E + 03	−0.105447E + 03	0.127166E + 02	0.595868E + 01	0.821623E + 00	9750–15750
	−0.188079E + 03	0.472158E + 03	−0.407311E + 03	0.141182E + 03	−0.156018E + 02	15750–21500
	0.232697E + 03	−0.869061E + 03	0.117775E + 04	−0.682883E + 03	0.143551E + 03	21500–30000

[a] For temperatures less than 500 K, a value of 0.24 cal/g-K for the specific heat of air may be used.

Table II. Concluded

[Specific heat obtained in cal/g-K]

Pressure, atm	A_{C_p}	B_{C_p}	C_{C_p}	D_{C_p}	E_{C_p}	Temperature range[a], K
10^0	$0.164992E+00$	$0.156336E+01$	$0.552429E+01$	$0.879873E+01$	$0.412806E+01$	500– 1750
	$-0.830572E+01$	$-0.483112E+02$	$-0.101598E+03$	$-0.897230E+02$	$-0.280651E+02$	1750– 3250
	$0.848335E+02$	$0.361629E+03$	$0.561712E+03$	$0.376565E+03$	$0.915792E+02$	3250– 4750
	$-0.945467E+01$	$-0.640807E+02$	$-0.893740E+02$	$-0.403342E+02$	$-0.458728E+01$	4750– 7750
	$-0.153176E+03$	$-0.476111E+02$	$0.217674E+02$	$0.314736E+01$	$0.922570E-01$	7750–11750
	$0.975058E+02$	$-0.158721E+03$	$0.753693E+02$	$-0.936668E+01$	$0.987515E+00$	11750–20500
	$-0.473648E+02$	$0.818135E+02$	$0.169726E+02$	$-0.836769E+02$	$0.339060E+02$	20500–30000
10^1	$0.111751E+00$	$0.105018E+01$	$0.368846E+01$	$0.591074E+01$	$0.244269E+01$	500– 1750
	$0.252675E+00$	$0.341131E+01$	$0.131529E+02$	$0.203259E+02$	$0.100197E+02$	1750– 3250
	$0.450386E+02$	$0.167261E+03$	$0.224425E+03$	$0.128924E+03$	$0.263694E+02$	3250– 5750
	$0.231376E+02$	$-0.104484E+01$	$-0.271807E+02$	$-0.102436E+02$	$-0.333185E-01$	5750– 9250
	$-0.799940E+02$	$0.170114E+02$	$0.187072E+02$	$-0.350311E+01$	$0.184168E+00$	9250–13750
	$0.491689E+02$	$-0.116351E+03$	$0.889977E+02$	$-0.242638E+02$	$0.263659E+01$	13750–22500
	$-0.253231E+03$	$0.955890E+03$	$-0.132457E+04$	$0.798459E+03$	$-0.175990E+03$	22500–30000
10^2	$0.986591E-01$	$0.923581E+00$	$0.323392E+01$	$0.519284E+01$	$0.202191E+01$	500– 1750
	$0.974261E-01$	$0.146776E+01$	$0.575473E+01$	$0.896935E+01$	$0.384233E+01$	1750– 3750
	$0.210207E+02$	$0.677318E+02$	$0.778089E+02$	$0.381171E+02$	$0.628850E+01$	3750– 6750
	$0.143729E+02$	$-0.128820E+02$	$-0.173603E+02$	$-0.137585E+01$	$0.743313E+00$	6750–10750
	$-0.347606E+02$	$0.320177E+02$	$0.148249E+01$	$-0.510951E+01$	$0.877002E+00$	10750–17750
	$0.450529E+02$	$-0.143364E+03$	$0.161302E+03$	$-0.752038E+02$	$0.129598E+02$	17750–30000

[a] For temperatures less than 500 K, a value of 0.24 cal/g-K for the specific heat of air may be used.

Table III. Curve-Fit Coefficients for Compressibility of Equilibrium Air

Pressure, atm	A_Z	B_Z	C_Z	D_Z	E_Z	Temperature range^a,K
10^{-4}	$0.710750E+00$	$0.107229E+01$	$-0.125673E+01$	$0.564944E+00$	$-0.822333E-01$	500– 2750
	$-0.614415E+01$	$0.861656E+01$	$-0.370256E+01$	$0.681208E+00$	$-0.443045E-01$	2750– 5750
	$-0.632086E+02$	$0.370722E+02$	$-0.776456E+01$	$0.706484E+00$	$-0.233636E-01$	5750– 8750
	$-0.467833E+02$	$0.139011E+02$	$-0.138693E+01$	$0.592861E-01$	$-0.903887E-03$	8750–17750
	$0.556705E+02$	$-0.135009E+02$	$0.118386E+01$	$-0.427210E-01$	$0.551468E-03$	17750–25000
10^{-3}	$0.824286E+00$	$0.625098E+00$	$-0.689867E+00$	$0.286982E+00$	$-0.376727E-01$	500– 3250
	$0.746758E+01$	$-0.460729E+01$	$0.109594E+01$	$-0.898428E-01$	$0.162238E-02$	3250– 6750
	$-0.385889E+02$	$0.209649E+02$	$-0.398276E+01$	$0.327436E+00$	$-0.970559E-02$	6750– 9750
	$-0.455262E+02$	$0.121138E+02$	$-0.108251E+01$	$0.415356E-01$	$-0.569596E-03$	9750–19750
	$0.809623E+02$	$-0.162146E+02$	$0.120105E+01$	$-0.375039E-01$	$0.424122E-03$	19750–28000
10^{-2}	$0.873086E+00$	$0.434929E+00$	$-0.454400E+00$	$0.176448E+00$	$-0.212727E-01$	500– 3250
	$-0.195828E+01$	$0.324383E+01$	$-0.123210E+01$	$0.198816E+00$	$-0.110471E-01$	3250– 7250
	$-0.417508E+02$	$0.199010E+02$	$-0.334091E+01$	$0.243749E+00$	$-0.644569E-02$	7250–11750
	$-0.431463E+02$	$0.101757E+02$	$-0.804882E+00$	$0.274096E-01$	$-0.334336E-03$	11750–21500
	$0.208036E+03$	$-0.342626E+02$	$0.210825E+01$	$-0.563525E-01$	$0.555405E-03$	21500–30000
10^{-1}	$0.904213E+00$	$0.311295E+00$	$-0.302086E+00$	$0.107468E+00$	$-0.116924E-01$	500– 3750
	$0.124751E+01$	$0.485004E+00$	$-0.321087E+00$	$0.632573E-01$	$-0.364522E-02$	3750– 8250
	$-0.325326E+02$	$0.137742E+02$	$-0.203163E+01$	$0.130377E+00$	$-0.302863E-02$	8250–13750
	$-0.428667E+02$	$0.888031E+01$	$-0.620696E+00$	$0.188157E-01$	$-0.206237E-03$	13750–23500
	$0.217096E+03$	$-0.309522E+02$	$0.165245E+01$	$-0.384201E-01$	$0.330019E-03$	23500–30000
10^{0}	$0.102671E+01$	$-0.465274E-01$	$0.972123E-02$	$0.417402E-02$	$-0.536830E-03$	500– 5750
	$0.387376E+02$	$-0.204439E+02$	$0.404607E+01$	$-0.344141E+00$	$0.107287E-01$	5750– 9250
	$-0.161621E+02$	$0.637080E+01$	$-0.827695E+00$	$0.466769E-01$	$-0.941988E-03$	9250–15750
	$-0.255245E+02$	$0.419968E+01$	$-0.208573E+00$	$0.395832E-02$	$-0.175392E-04$	15750–23500
	$-0.784807E+02$	$0.129796E+02$	$-0.758996E+00$	$0.194343E-01$	$-0.182292E-03$	23500–30000
10^{1}	$0.970875E+00$	$0.869030E-01$	$-0.737745E-01$	$0.218303E-01$	$-0.179762E-02$	500– 5750
	$-0.100200E+01$	$0.186655E+01$	$-0.540958E+00$	$0.639254E-01$	$-0.255478E-02$	5750– 9750
	$-0.993188E+01$	$0.353080E+01$	$-0.389667E+00$	$0.187431E-01$	$-0.320898E-03$	9750–17250
	$0.398457E-01$	$-0.612253E+00$	$0.997312E-01$	$-0.411847E-02$	$0.542207E-04$	17250–30000
10^{2}	$0.103304E+01$	$-0.585872E-01$	$0.237877E-01$	$-0.281715E-02$	$0.168221E-03$	500– 8750
	$-0.555015E+01$	$0.157079E+01$	$-0.115055E+00$	$0.324023E-02$	$-0.188832E-04$	8750–17750
	$0.202955E+02$	$-0.323532E+01$	$0.203092E+00$	$-0.525620E-02$	$0.489857E-04$	17750–30000

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[a] For temperatures less than 500 K, a compressibility factor of unity may be used for air.

Table IV. Curve-Fit Coefficients for Viscosity of Equilibrium Air

[Viscosity obtained in poise]

Pressure, atm	A_μ	B_μ	C_μ	D_μ	E_μ	F_μ	Temperature range[a],K
10^{-4}	−0.1160076E − 04	0.6656010E − 03	−0.2933969E − 03	0.7427050E − 04	−0.6456605E − 05	0.8752161E − 07	500– 7750
	−0.9105422E + 00	0.4949794E + 00	−0.1060568E + 00	0.1123425E − 01	−0.5896774E − 03	0.1229026E − 04	7750–10750
	0.1463029E − 01	−0.5019958E − 02	0.6886543E − 03	−0.4723839E − 04	0.1623374E − 05	−0.2239581E − 07	10750–16750
	−0.2140374E − 02	0.6529285E − 03	−0.7290226E − 04	0.3865996E − 05	−0.9908122E − 07	0.9916638E − 09	16750–25000
10^{-3}	0.2397194E − 04	0.5564725E − 03	−0.1970968E − 03	0.4272210E − 04	−0.2690853E − 05	−0.3009241E − 07	500– 8250
	−0.5784272E + 00	0.2816531E + 00	−0.5377449E − 01	0.5058384E − 02	−0.2352317E − 03	0.4336410E − 05	8250–12250
	0.1658118E − 01	−0.5027652E − 02	0.6106363E − 03	−0.3715711E − 04	0.1135683E − 05	−0.1397984E − 07	12250–18750
	0.6903134E − 02	−0.1345295E − 02	0.1061916E − 03	−0.4234384E − 05	0.8514686E − 07	−0.6893227E − 09	18750–28000
10^{-2}	0.5085043E − 04	0.4774840E − 03	−0.1322133E − 03	0.2362256E − 04	−0.8014978E − 06	−0.6458338E − 07	500– 8750
	−0.3414870E + 00	0.1473594E + 00	−0.2471167E − 01	0.2030404E − 02	−0.8216415E − 04	0.1314540E − 05	8750–14250
	0.2450600E − 01	−0.6697224E − 02	0.7362709E − 03	−0.4070960E − 04	0.1134307E − 05	−0.1276018E − 07	14250–19750
	−0.3561146E − 01	0.7255623E − 02	−0.5837678E − 03	0.2324839E − 04	−0.4590857E − 06	0.3600777E − 08	19750–30000
10^{-1}	0.6394112E − 04	0.4385020E − 03	−0.1024141E − 03	0.1654305E − 04	−0.5014106E − 06	−0.3710875E − 07	500– 9750
	−0.2376368E + 00	0.9006170E − 01	−0.1315352E − 01	0.9370344E − 03	−0.3279124E − 04	0.4529650E − 06	9750–16750
	0.6309492E − 03	0.6108099E − 03	−0.1286661E − 03	0.9381977E − 05	−0.2960969E − 06	0.3444222E − 08	16750–24500
	−0.1622687E + 01	0.3035173E + 00	−0.2266401E − 01	0.8445985E − 03	−0.1570909E − 04	0.1166667E − 06	24500–30000
10^{0}	0.5781887E − 04	0.4438221E − 03	−0.1020840E − 03	0.1688754E − 04	−0.8622324E − 06	−0.2239193E − 09	500–11250
	−0.1844238E + 00	0.6040101E − 01	−0.7566737E − 02	0.4609058E − 03	−0.1377229E − 04	0.1623637E − 06	11250–19750
	0.2606784E − 01	−0.4562535E − 02	0.3111533E − 03	−0.1018512E − 04	0.1576999E − 06	−0.9011456E − 09	19750–30000
10^{1}	0.7256455E − 04	0.4050530E − 03	−0.7626766E − 04	0.1114437E − 04	−0.5020411E − 06	0.7074486E − 10	500–12750
	−0.9524274E − 01	0.2589951E − 01	−0.2593217E − 02	0.1227975E − 03	−0.2772500E − 05	0.2383398E − 07	12750–21500
	0.5037513E − 01	−0.8081647E − 02	0.5209350E − 03	−0.1682098E − 04	0.2731352E − 06	−0.1794872E − 08	21500–30000
10^{2}	0.7609039E − 04	0.3891948E − 03	−0.6458779E − 04	0.8791566E − 05	−0.4216496E − 06	0.4509800E − 08	500–15250
	−0.7868582E − 01	0.1820922E − 01	−0.1543467E − 02	0.6257766E − 04	−0.1234998E − 05	0.9579999E − 08	15250–30000

[a] For temperatures less than 500 K, Sutherland's viscosity law may be used:

$$\mu_s = 1.4584 \times 10^{-5} \frac{T^{3/2}}{T + 110.33}$$

Table V. Curve-Fit Coefficients for Thermal Conductivity of Equilibrium Air

[Thermal conductivity obtained in cal/cm-sec-K]

Pressure, atm	A_K	B_K	C_K	D_K	E_K	Temperature range[a],K
10^{-4}	0.395299$E+01$	0.386816$E+02$	0.140687$E+03$	0.226110$E+03$	0.127138$E+03$	500– 1750
	0.119879$E+02$	0.412181$E+02$	0.717156$E+01$	−0.911924$E+02$	−0.810415$E+02$	1750– 2750
	−0.832682$E+02$	−0.419438$E+03$	−0.751764$E+03$	−0.566912$E+03$	−0.157470$E+03$	2750– 4750
	−0.103603$E+04$	−0.242470$E+04$	−0.206135$E+04$	−0.757541$E+03$	−0.108281$E+03$	4750– 6250
	0.261125$E+02$	0.411940$E+01$	−0.186054$E+02$	−0.645054$E+01$	−0.621476$E+01$	6250–10250
	0.246095$E+02$	−0.507490$E+02$	0.369131$E+02$	−0.897288$E+01$	−0.623025$E+01$	10250–17750
	−0.571805$E+02$	0.168628$E+03$	−0.181577$E+03$	0.859388$E+02$	−0.213335$E+02$	17750–25000
10^{-3}	0.199665$E+01$	0.194822$E+02$	0.706404$E+02$	0.113538$E+03$	0.599079$E+02$	500– 1750
	−0.831120$E+02$	−0.560438$E+03$	−0.140314$E+04$	−0.154128$E+04$	−0.632398$E+03$	1750– 2750
	−0.110139$E+03$	−0.481050$E+03$	−0.757873$E+03$	−0.505860$E+03$	−0.125800$E+03$	2750– 4750
	0.299875$E+03$	0.923042$E+03$	0.992814$E+03$	0.442621$E+03$	0.634709$E+02$	4750– 6250
	0.434485$E+02$	0.464790$E+01$	−0.155778$E+02$	−0.220224$E+01$	−0.558790$E+01$	6250–11250
	0.895136$E+01$	−0.322183$E+02$	0.350726$E+02$	−0.129798$E+02$	−0.498154$E+01$	11250–18250
	−0.422029$E+02$	0.144838$E+03$	−0.182586$E+03$	0.101698$E+03$	−0.270417$E+02$	18250–28000
10^{-2}	0.198558$E+01$	0.189164$E+02$	0.668384$E+02$	0.104546$E+03$	0.527822$E+02$	500– 2250
	0.595832$E+02$	0.288748$E+03$	0.500756$E+03$	0.363789$E+03$	0.844428$E+02$	2250– 3250
	−0.442143$E+02$	−0.206207$E+03$	−0.324643$E+03$	−0.204871$E+03$	−0.494556$E+02$	3250– 5750
	−0.584437$E+03$	−0.873106$E+03$	−0.445088$E+03$	−0.927269$E+02$	−0.128529$E+02$	5750– 7750
	0.373716$E+02$	−0.115449$E+02$	−0.113653$E+02$	0.135799$E+01$	−0.542822$E+01$	7750–12750
	−0.143675$E+02$	0.801073$E+01$	0.146420$E+02$	−0.117248$E+02$	−0.389761$E+01$	12750–18750
	0.502985$E+01$	−0.960227$E+01$	0.196818$E+01$	0.643952$E+01$	−0.896353$E+01$	18750–30000
10^{-1}	0.105928$E+01$	0.100924$E+02$	0.356709$E+02$	0.561818$E+02$	0.249670$E+02$	500– 2250
	0.101351$E+03$	0.490653$E+03$	0.868620$E+03$	0.666792$E+03$	0.180596$E+03$	2250– 4250
	0.830640$E+01$	−0.324274$E+02$	−0.942568$E+02$	−0.647282$E+02$	−0.180857$E+02$	4250– 6750
	−0.318301$E+03$	−0.306306$E+03$	−0.782124$E+02$	−0.466313$E+01$	−0.585083$E+01$	6750– 9250
	0.469099$E+02$	−0.330961$E+02$	−0.146607$E+01$	0.306898$E+01$	−0.562490$E+01$	9250–16750
	0.154279$E+02$	−0.541310$E+02$	0.693640$E+02$	−0.366810$E+02$	0.115271$E+01$	16750–30000

[a] For temperatures less than 500 K, Sutherland's thermal conductivity law may be used:

$$K_s = 5.9776 \times 10^{-6} \frac{T^{3/2}}{T + 194.4}$$

Table V. Concluded

[Thermal conductivity obtained in cal/cm-sec-K]

Pressure, atm	A_K	B_K	C_K	D_K	E_K	Temperature range[a],K
10^0	0.334316E + 00	0.328202E + 01	0.119939E + 02	0.200944E + 02	0.462882E + 01	500– 2250
	0.109992E + 02	0.387106E + 02	0.387282E + 02	0.548304E + 01	−0.120106E + 02	2250– 4250
	0.124072E + 02	−0.147438E + 02	−0.530293E + 02	−0.299886E + 02	−0.961485E + 01	4250– 7750
	−0.189644E + 03	−0.828711E + 02	0.998789E + 01	0.227739E + 01	−0.581069E + 01	7750–10750
	0.298795E + 02	−0.381078E + 02	0.117041E + 02	0.122011E + 01	−0.578171E + 01	10750–19250
	0.844897E + 01	−0.358117E + 02	0.553921E + 02	−0.353787E + 02	0.274595E + 01	19250–30000
10^1	0.413573E + 00	0.383393E + 01	0.131885E + 02	0.207305E + 02	0.427728E + 01	500– 3250
	0.821184E + 02	0.308927E + 03	0.423174E + 03	0.250668E + 03	0.475889E + 02	3250– 5250
	0.113875E + 02	−0.133907E + 02	−0.337860E + 02	−0.122339E + 02	−0.610064E + 01	5250– 8750
	−0.723261E + 02	0.143656E + 02	0.135247E + 02	−0.233991E + 01	−0.556444E + 01	8750–13750
	−0.382696E + 01	0.146502E + 02	−0.187337E + 02	0.107119E + 02	−0.717162E + 01	13750–30000
10^2	0.208749E + 00	0.192122E + 01	0.658813E + 01	0.107630E + 02	−0.127699E + 01	500– 3750
	0.378677E + 02	0.123284E + 03	0.144224E + 03	0.728083E + 02	0.684807E + 01	3750– 6250
	0.223116E + 02	0.336369E + 00	−0.142705E + 02	−0.134534E + 01	−0.498832E + 01	6250–10750
	0.792550E + 01	−0.216552E + 02	0.204578E + 02	−0.597164E + 01	−0.485454E + 01	10750–30000

[a] For temperatures less than 500 K, Sutherland's thermal conductivity law may be used:

$$K_s = 5.9776 \times 10^{-6} \frac{T^{3/2}}{T + 194.4}$$

Table VI. Curve-Fit Coefficients for Prandtl Number of Equilibrium Air

Pressure, atm	A_{Pr}	B_{Pr}	C_{Pr}	D_{Pr}	E_{Pr}	F_{Pr}	Temperature range[a],K
10^{-4}	0.7695318E + 00	−0.2487156E + 00	−0.3371200E − 02	0.5237761E + 00	−0.4272376E + 00	0.9284843E − 01	500– 2250
	0.4081926E + 02	−0.6945482E + 02	0.4642510E + 02	−0.1500926E + 02	0.2350767E + 01	−0.1430131E + 00	2250– 3750
	−0.5060907E + 03	0.5765441E + 03	−0.2594581E + 03	0.5768434E + 02	−0.6333573E + 01	0.2747920E + 00	3750– 5750
	0.3172744E + 02	−0.1923593E + 02	0.6031312E + 01	−0.1191714E + 01	0.1301576E + 00	−0.5625333E − 02	5750– 8250
	−0.7624622E + 04	0.3908646E + 04	−0.7963915E + 03	0.8069517E + 02	−0.4069244E + 01	0.8174707E − 01	8250–10750
	0.1034825E + 03	−0.3861297E + 02	0.5742599E + 01	−0.4251452E + 00	0.1565525E − 01	−0.2291528E − 03	10750–14750
	−0.3414530E + 03	0.1193445E + 03	−0.1639670E + 02	0.1109347E + 01	−0.3701973E − 01	0.4881128E − 03	14750–18250
	0.1398841E + 02	−0.2209182E + 01	0.1254939E + 00	−0.2782377E − 02	0.6736752E − 05	0.3740205E − 06	18250–25000
10^{-3}	0.7483071E + 00	−0.1659050E + 00	−0.3548542E − 01	0.3843113E + 00	−0.2847560E + 00	0.5734562E − 01	500– 2250
	0.4355608E + 02	−0.6751147E + 02	0.4101816E + 02	−0.1204527E + 02	0.1712608E + 01	−0.9453467E − 01	2250– 4750
	0.6877578E + 03	−0.5984367E + 03	0.2059622E + 03	−0.3502408E + 02	0.2943975E + 01	−0.9787067E − 01	4750– 7250
	−0.7024989E + 03	0.4515788E + 03	−0.1153420E + 03	0.1460894E + 02	−0.9148849E + 00	0.2261774E − 01	7250–10250
	−0.3107328E + 03	0.1863582E + 03	−0.3984823E + 02	0.4000552E + 01	−0.1930037E + 00	0.3624133E − 02	10250–12750
	0.9153227E + 02	−0.3041980E + 02	0.4035104E + 01	−0.2667702E + 00	0.8781471E − 02	−0.1150000E − 03	12750–17250
	0.2304245E + 04	−0.6078459E + 03	0.6397478E + 02	−0.3358410E + 01	0.8795057E − 01	−0.9193691E − 03	17250–20500
	−0.1424413E + 02	0.3715427E + 01	−0.3586053E + 00	0.1651461E − 01	−0.3685522E − 03	0.3216955E − 05	20500–28000
10^{-2}	0.7406012E + 00	−0.1629686E + 00	0.8014385E − 01	0.1480977E + 00	−0.1294933E + 00	0.2544039E − 01	500– 2750
	0.3206825E + 02	−0.4531855E + 02	0.2519178E + 02	−0.6755087E + 01	0.8752933E + 00	−0.4395200E − 01	2750– 5250
	0.4409105E + 03	−0.3447078E + 03	0.1064873E + 03	−0.1623127E + 02	0.1221500E + 01	−0.3631877E − 01	5250– 8250
	0.2474049E + 02	0.2323747E + 01	−0.4089151E + 01	0.8375614E + 00	−0.6543669E − 01	0.1793128E − 02	8250–11750
	−0.9639789E + 03	0.3960004E + 03	−0.6388451E + 02	0.5082427E + 01	−0.2000122E + 00	0.3121600E − 02	11750–14250
	0.9436717E + 02	−0.2761116E + 02	0.3229296E + 01	−0.1885223E + 00	0.5488061E − 02	−0.6365539E − 04	14250–18250
	−0.7123564E + 02	0.2178196E + 02	−0.2554952E + 01	0.1451363E + 00	−0.4016437E − 02	0.4349632E − 04	18250–23500
	−0.7846718E + 02	0.1520447E + 02	−0.1165686E + 01	0.4430242E − 01	−0.8360113E − 03	0.6273942E − 05	23500–30000
10^{-1}	0.7548377E + 00	−0.2611566E + 00	0.3168480E + 00	−0.1019887E + 00	−0.1326718E − 01	0.6541023E − 02	500– 2750
	0.6190687E + 02	−0.8052889E + 02	0.4117452E + 02	−0.1025306E + 02	0.1246034E + 01	−0.5926933E − 01	2750– 5250
	−0.2641868E + 03	0.2214640E + 03	−0.7330522E + 02	0.1198777E + 02	−0.9677752E + 00	0.3085867E − 01	5250– 7750
	0.7451996E + 02	−0.2929220E + 02	0.4227110E + 01	−0.2590555E + 00	0.5423023E − 02	0.1836850E − 04	7750–13750
	0.1034771E + 03	−0.2138868E + 02	0.1519602E + 01	−0.3418909E − 01	−0.5284942E − 03	0.2331795E − 04	13750–18250
	−0.1252168E + 03	0.2959573E + 02	−0.2775372E + 01	0.1290359E + 00	−0.2973274E − 02	0.2716070E − 04	18250–25500
	−0.5022975E + 04	0.9203587E + 03	−0.6737887E + 02	0.2463703E + 01	−0.4499464E − 01	0.3283492E − 03	25500–30000

[a] For temperatures less than 500 K, the following relation (employing the Sutherland values for the viscosity and thermal conductivity) may be used to obtain Prandtl number for air:

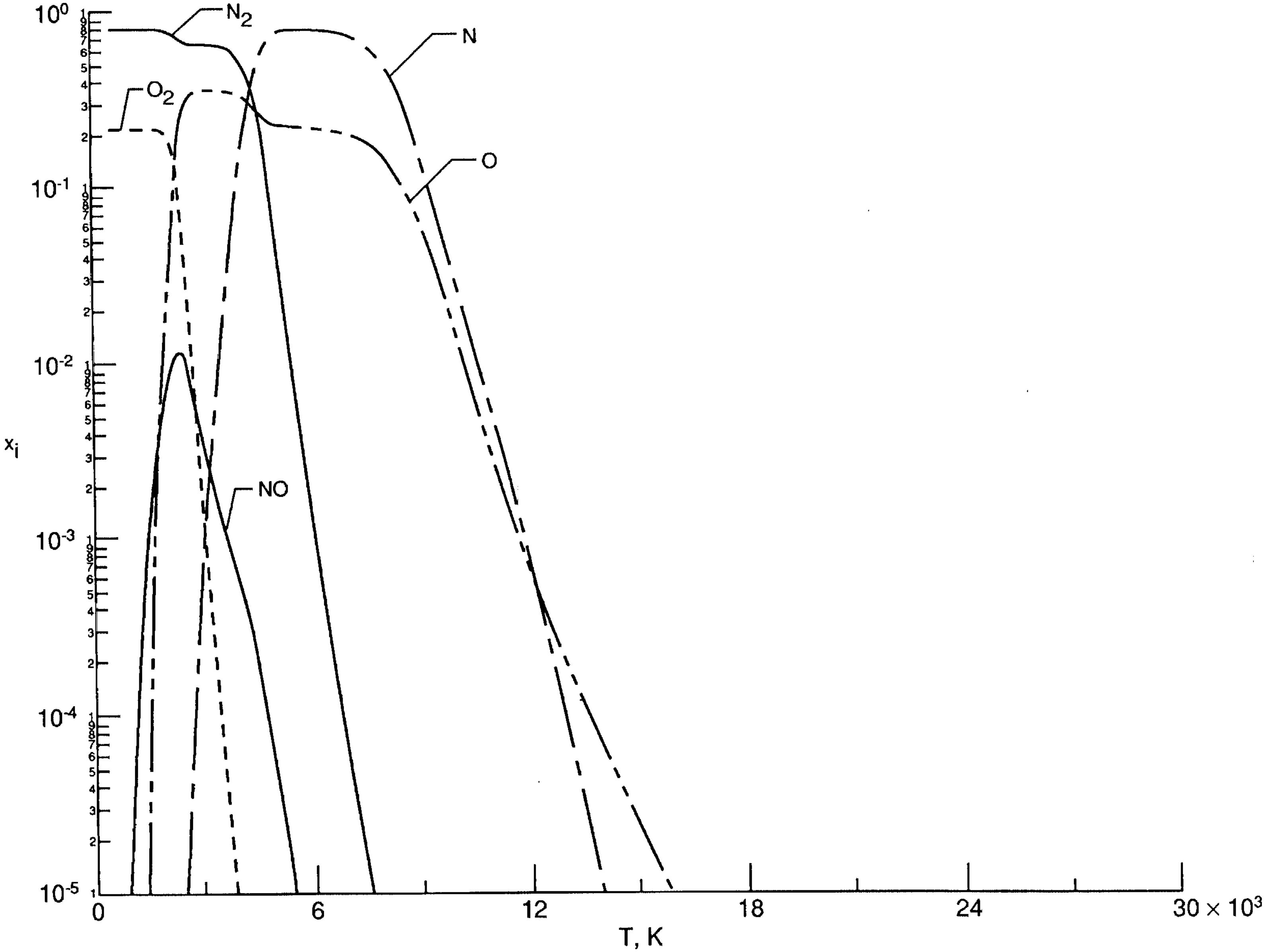
$$N_{\mathrm{Pr}} = 0.24\mu_s/K_s$$

Table VI. Concluded

Pressure, atm	A_{Pr}	B_{Pr}	C_{Pr}	D_{Pr}	E_{Pr}	F_{Pr}	Temperature range[a],K
10^0	$0.8037721E+00$	$-0.5531739E+00$	$0.9090234E+00$	$-0.6243393E+00$	$0.1903222E+00$	$-0.2182155E-01$	500– 2750
	$0.9173178E+02$	$-0.1294114E+03$	$0.7264736E+02$	$-0.2015462E+02$	$0.2763213E+01$	$-0.1497413E+00$	2750– 4750
	$0.1874806E+02$	$-0.1571672E+02$	$0.5656501E+01$	$-0.1040290E+01$	$0.9598832E-01$	$-0.3499282E-02$	4750– 7750
	$-0.1974460E+03$	$0.9815976E+02$	$-0.1915726E+02$	$0.1841274E+01$	$-0.8709938E-01$	$0.1622326E-02$	7750–13250
	$0.5713095E+02$	$-0.2693925E+02$	$0.4625149E+01$	$-0.3686820E+00$	$0.1391085E-01$	$-0.2015436E-03$	13250–17750
	$0.1619271E+03$	$-0.3657252E+02$	$0.3311637E+01$	$-0.1501584E+00$	$0.3407133E-02$	$-0.3092820E-04$	17750–23500
	$-0.1396134E+03$	$0.2786187E+02$	$-0.2213081E+01$	$0.8742029E-01$	$-0.1716422E-02$	$0.1339615E-04$	23500–30000
10^1	$0.8167207E+00$	$-0.6186780E+00$	$0.1015263E+01$	$-0.6989158E+00$	$0.2151091E+00$	$-0.2479595E-01$	500– 2750
	$-0.1857130E+02$	$0.2610712E+02$	$-0.1366805E+02$	$0.3448930E+01$	$-0.4205156E+00$	$0.1987815E-01$	2750–5750
	$-0.4287169E+02$	$0.3082544E+02$	$-0.8483934E+01$	$0.1132069E+01$	$-0.7326105E-01$	$0.1844057E-02$	5750–10750
	$0.6447596E+02$	$-0.2113068E+02$	$0.2725852E+01$	$-0.1705427E+00$	$0.5177594E-02$	$-0.6127611E-04$	10750–20500
	$0.7384318E+02$	$-0.1345184E+02$	$0.9862360E+00$	$-0.3633532E-01$	$0.6720911E-03$	$-0.4987500E-05$	20500–30000
10^2	$0.8147770E+00$	$-0.6129922E+00$	$0.1017670E+01$	$-0.7111724E+00$	$0.2215290E+00$	$-0.2557178E-01$	500– 2750
	$-0.6650000E+01$	$0.9087650E+01$	$-0.4283159E+01$	$0.9588901E+00$	$-0.1026406E+00$	$0.4226421E-02$	2750– 6750
	$-0.2736096E+02$	$0.1729215E+02$	$-0.4132288E+01$	$0.4767165E+00$	$-0.2655841E-01$	$0.5732041E-03$	6750–12750
	$0.4889586E+02$	$-0.1351549E+02$	$0.1493734E+01$	$-0.8122753E-01$	$0.2173037E-02$	$-0.2296542E-04$	12750–20500
	$-0.5525036E+02$	$0.1123889E+02$	$-0.8807574E+00$	$0.3371865E-01$	$-0.6355462E-03$	$0.4740705E-05$	20500–30000

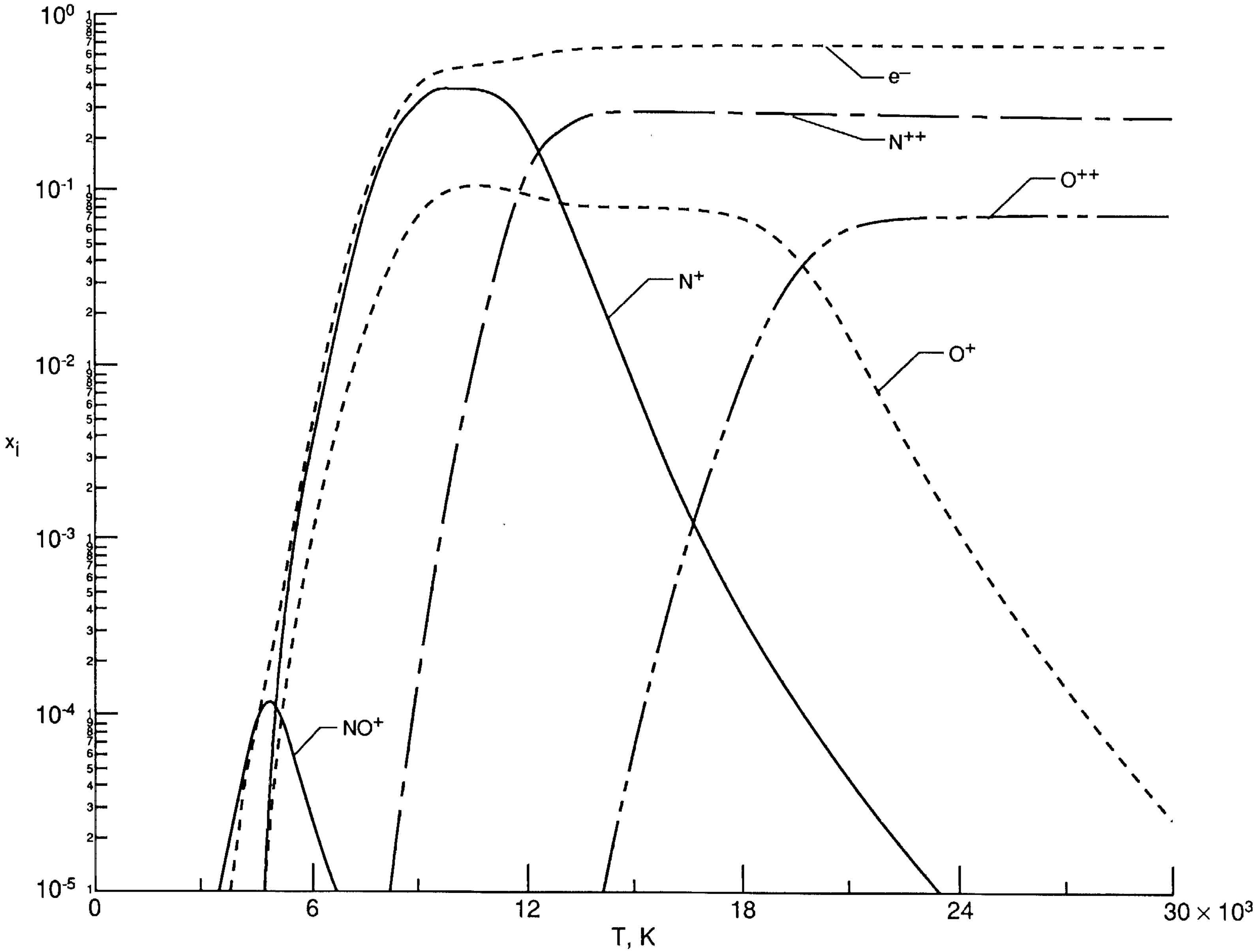
[a] For temperatures less than 500 K, the following relation (employing the Sutherland values for the viscosity and thermal conductivity) may be used to obtain Prandtl number for air:

$$N_{\mathrm{Pr}} = 0.24\mu_s/K_s$$



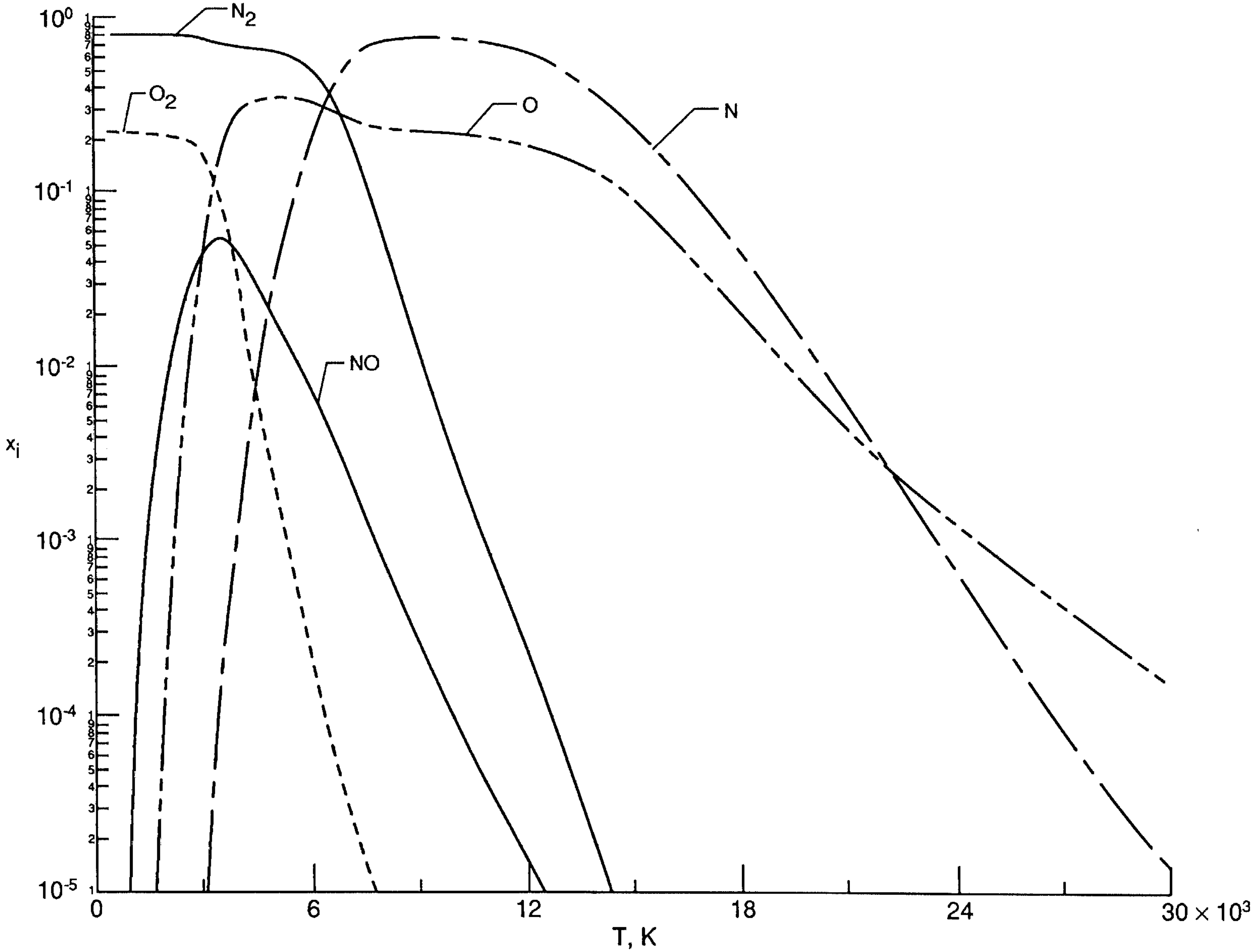
(a) $p = 10^{-4}$ atm; neutral species.

Figure 1. Composition of equilibrium air versus temperature.



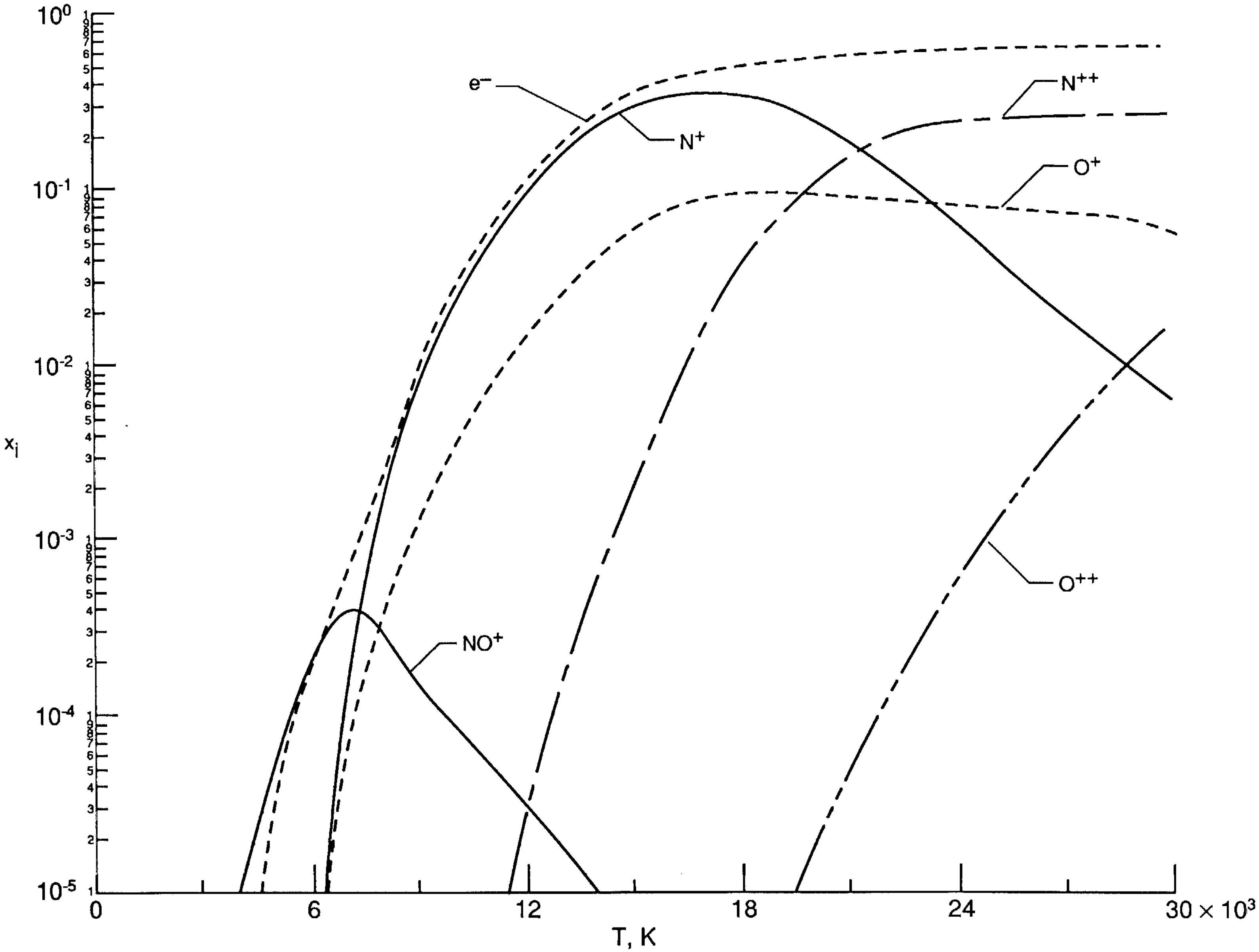
(b) $p = 10^{-4}$ atm; charged species.

Figure 1. Continued.



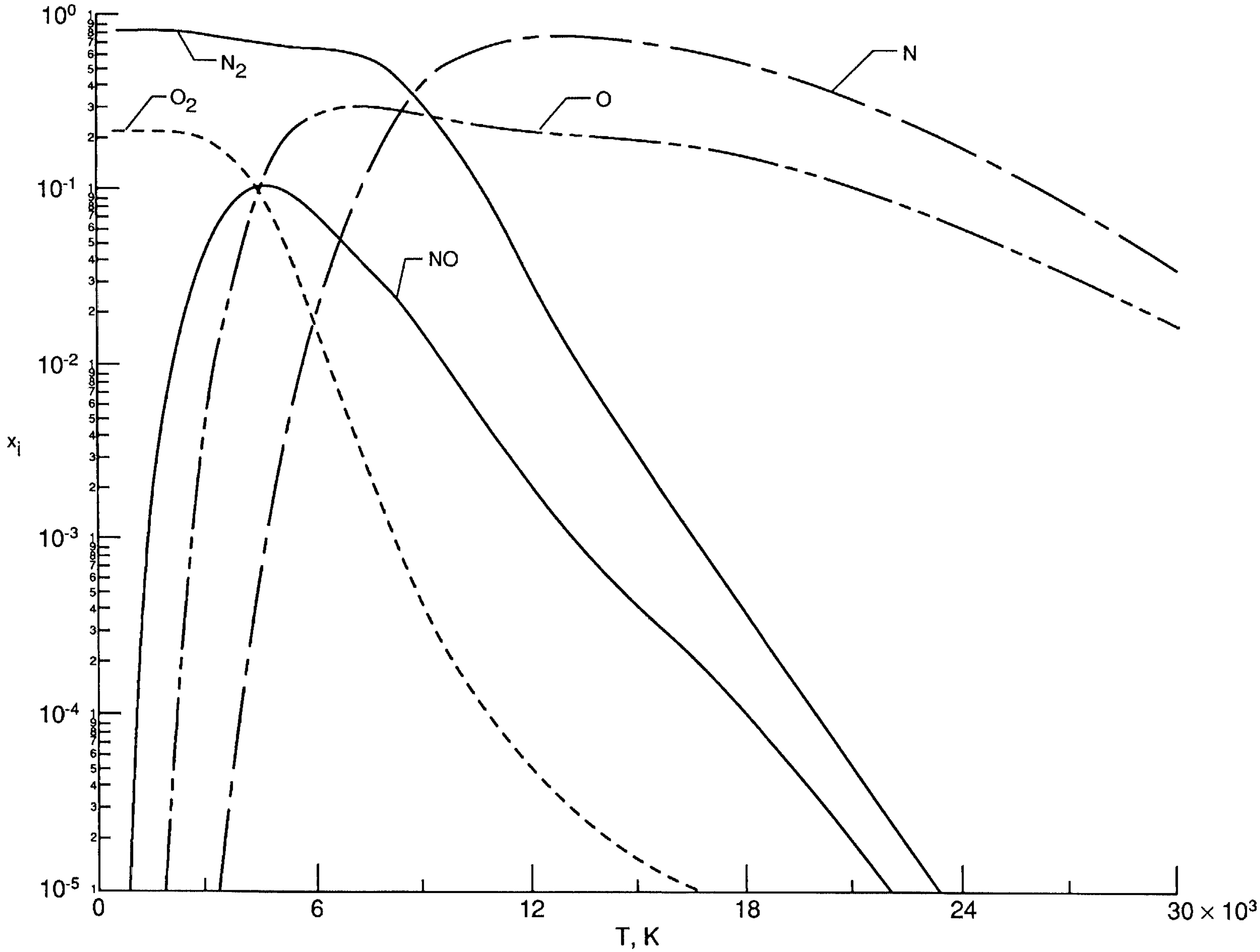
(c) $p = 10^0$ atm; neutral species.

Figure 1. Continued.



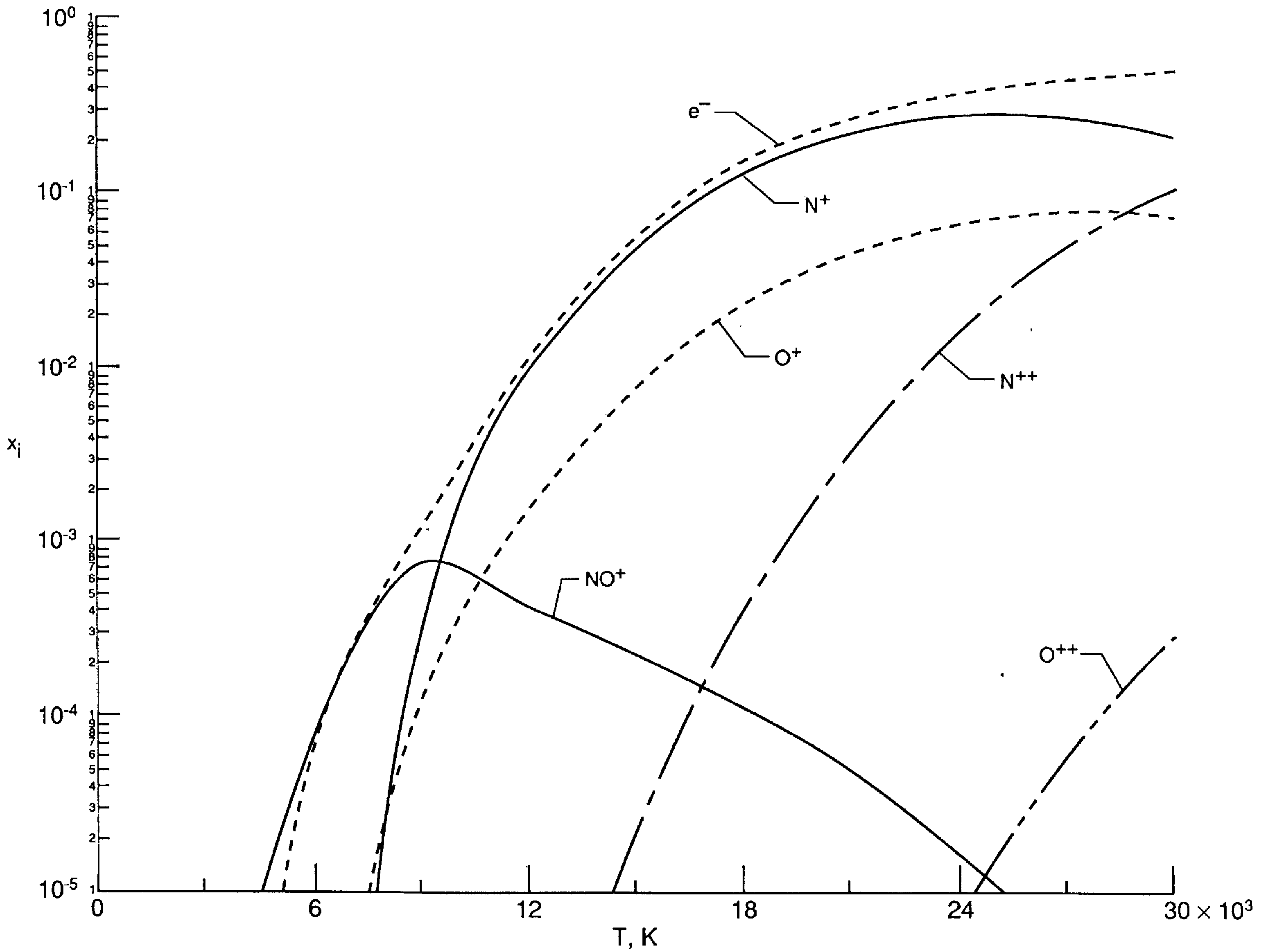
(d) $p = 10^0$ atm; charged species.

Figure 1. Continued.



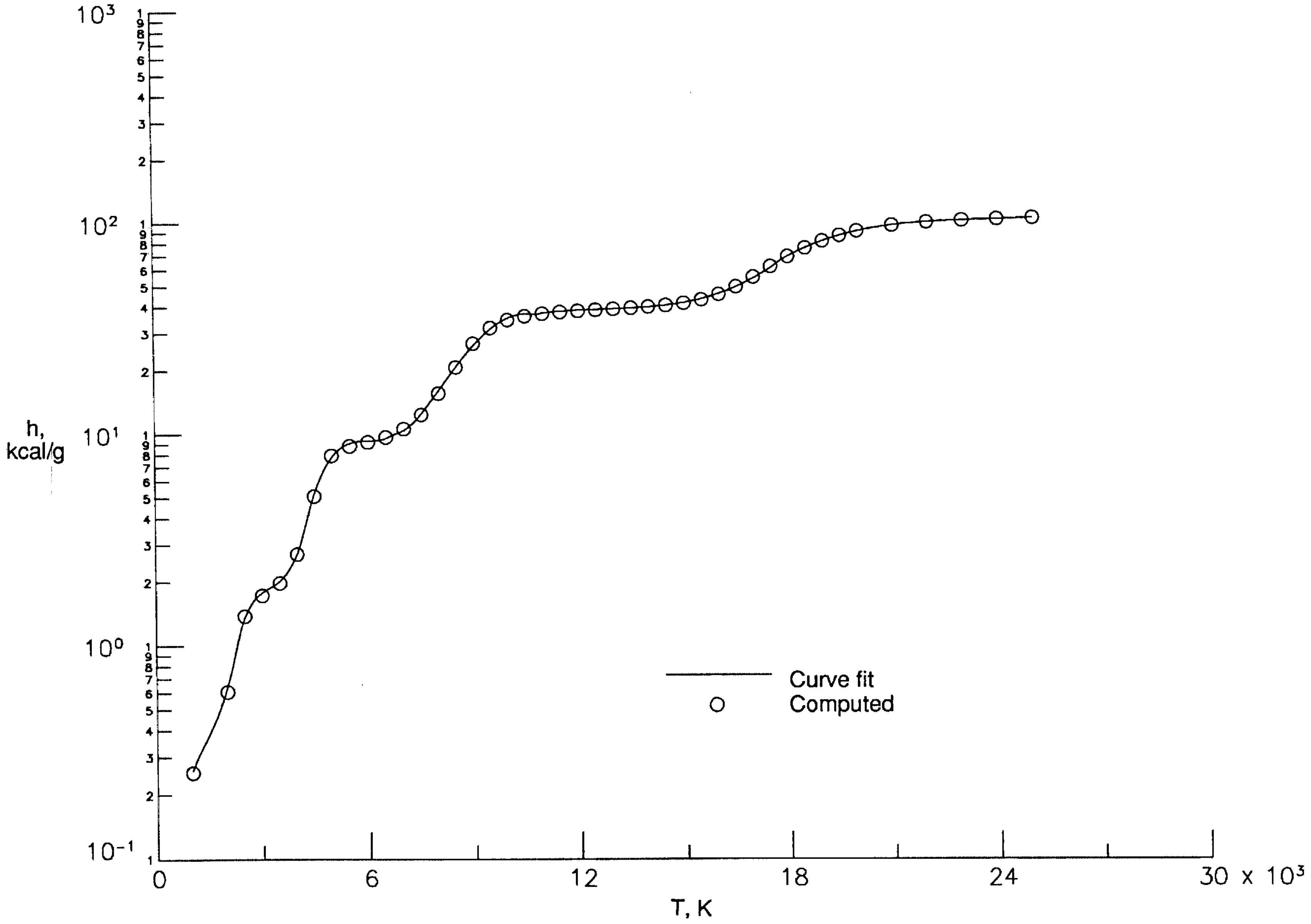
(e) $p = 10^2$ atm; neutral species.

Figure 1. Continued.



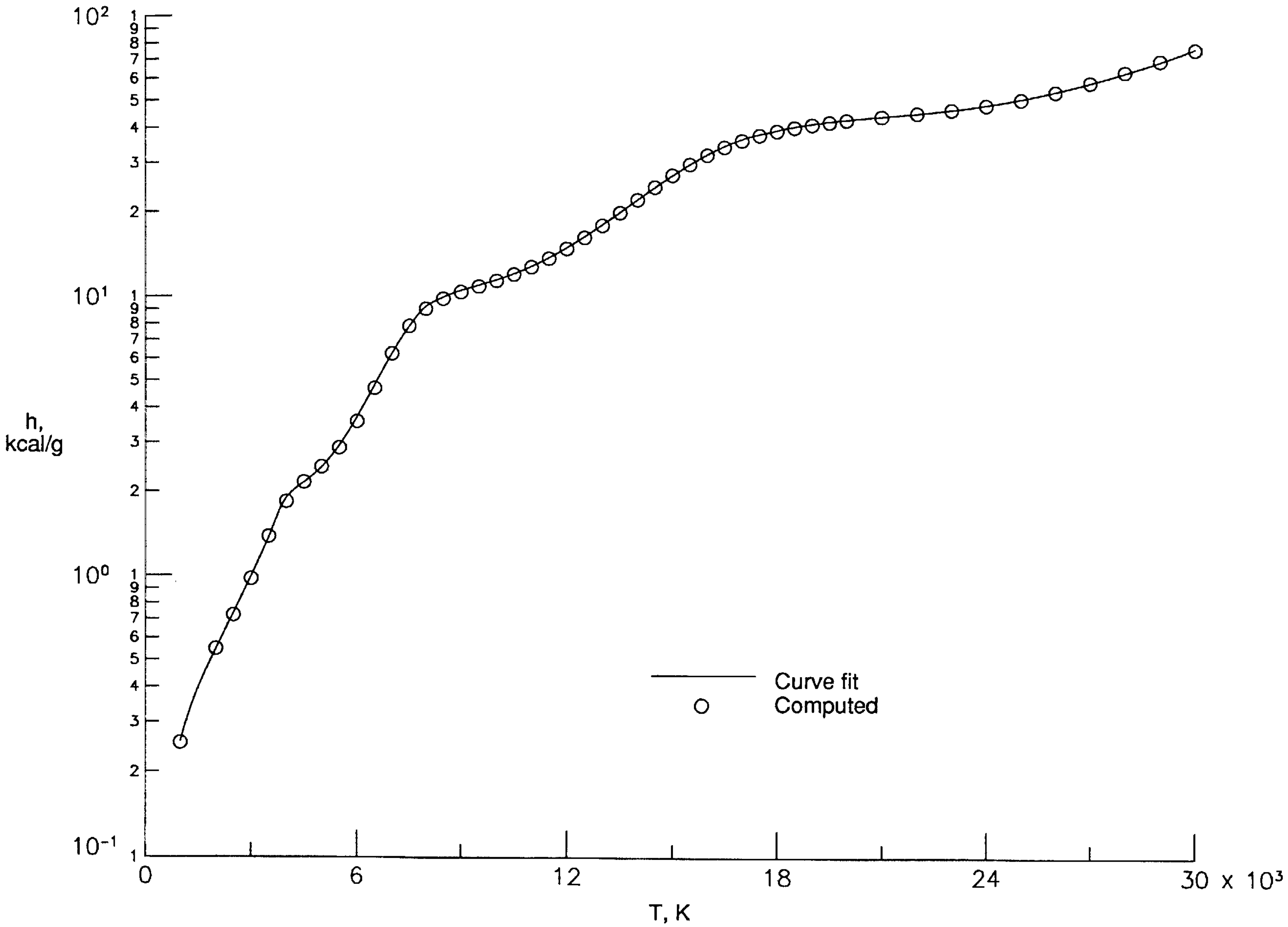
(f) $p = 10^2$ atm; charged species.

Figure 1. Concluded.



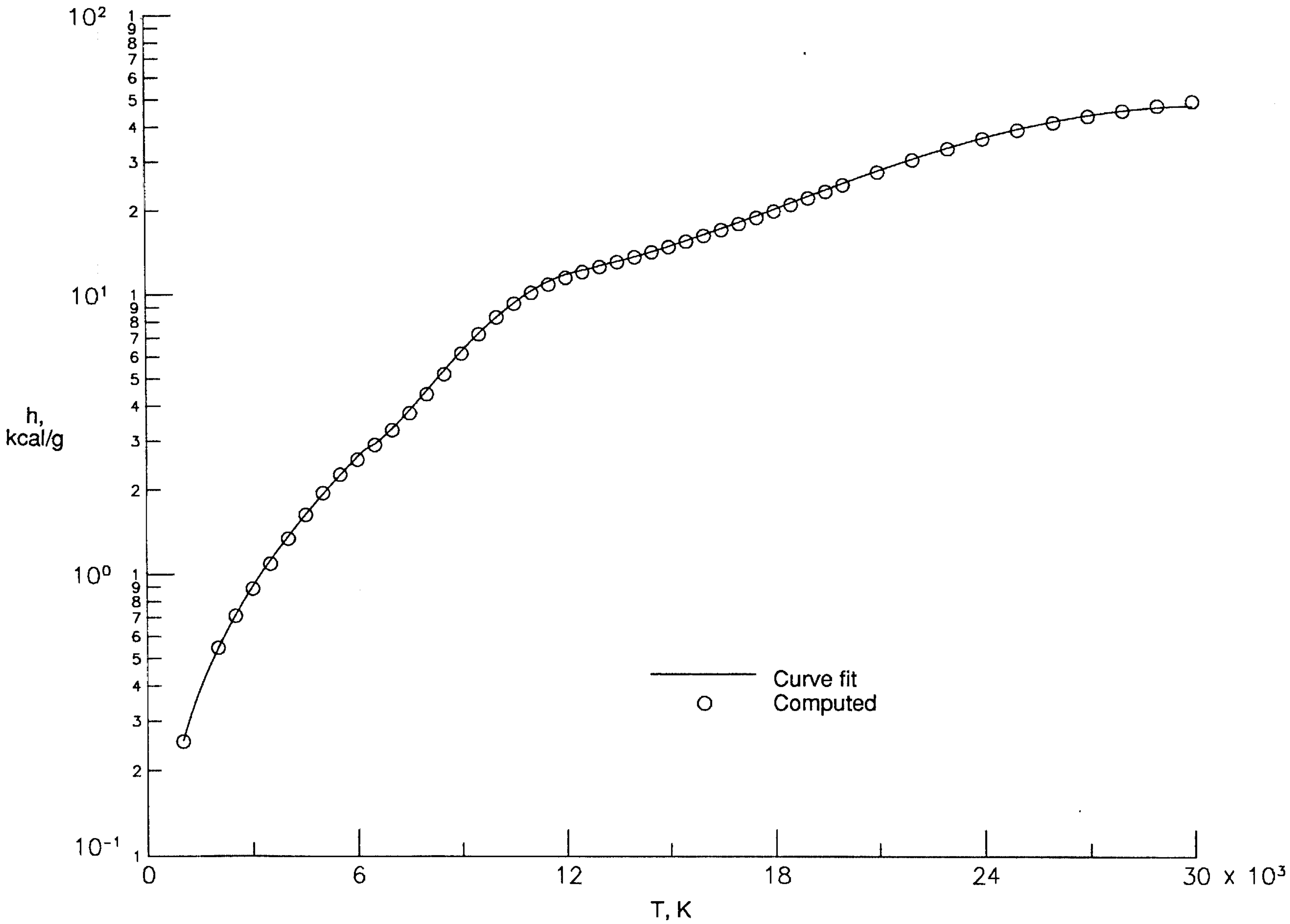
(a) $p = 10^{-4}$ atm.

Figure 2. Enthalpy of equilibrium air.



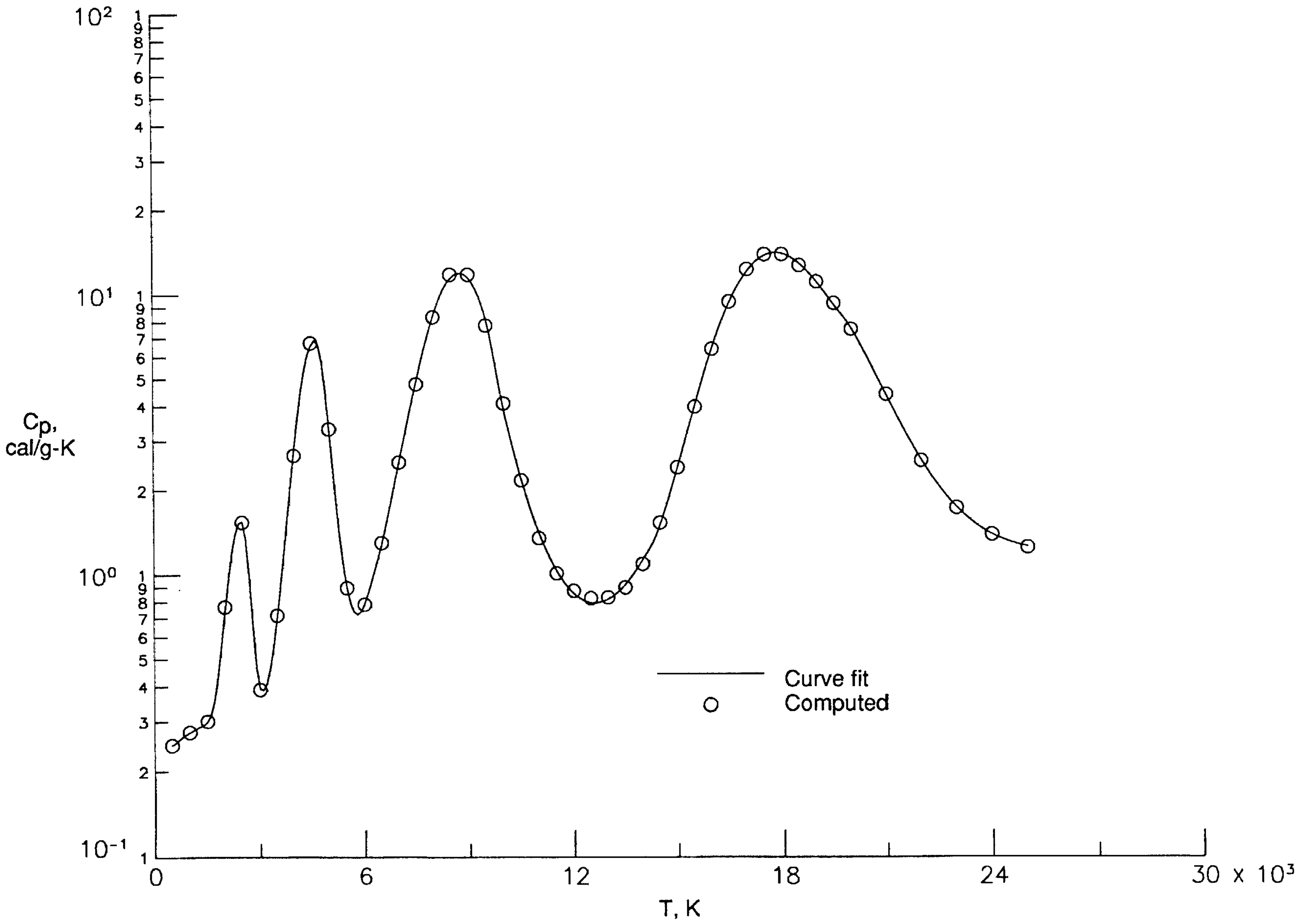
(b) $p = 10^0$ atm.

Figure 2. Continued.



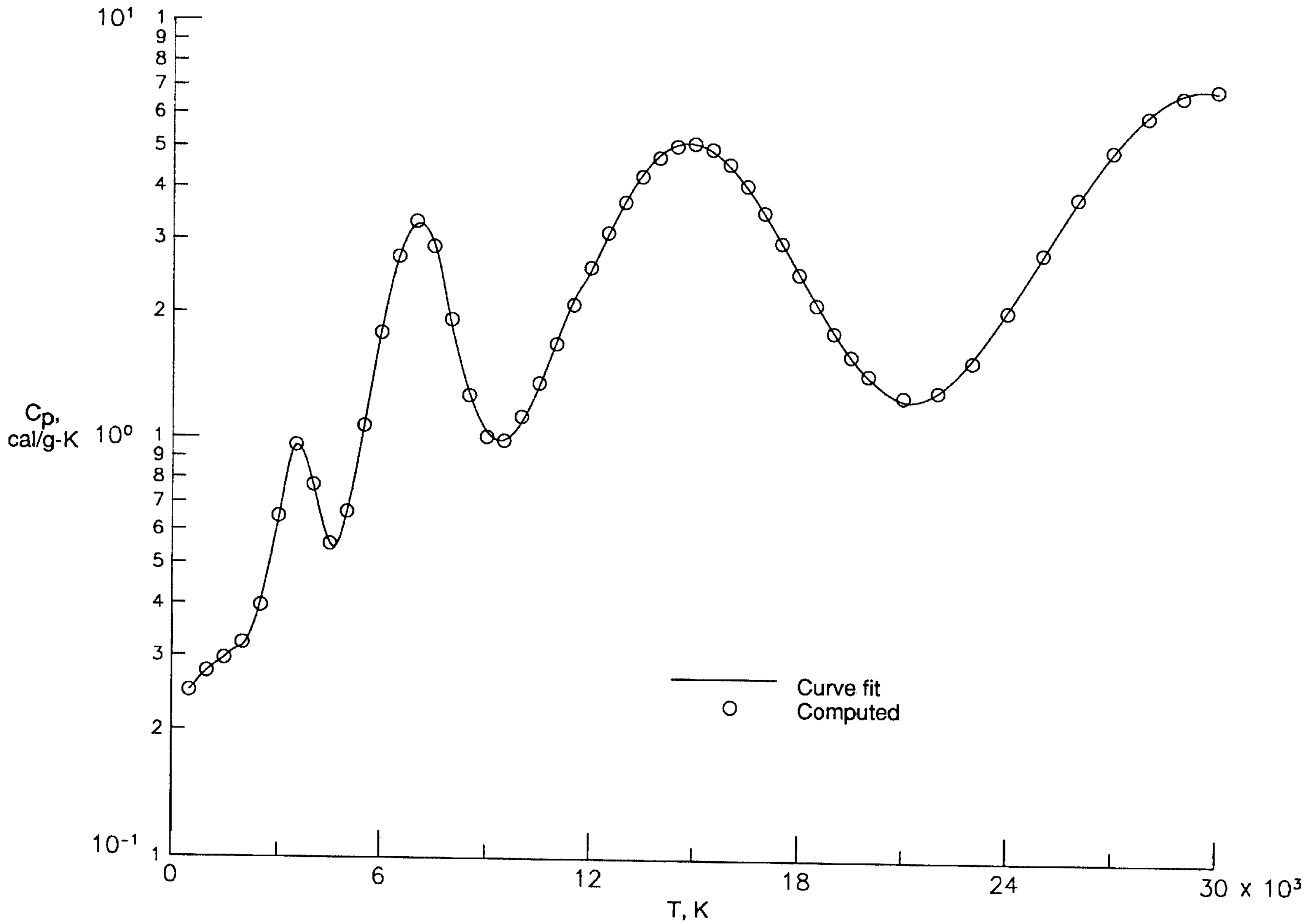
(c) $p = 10^2$ atm.

Figure 2. Concluded.



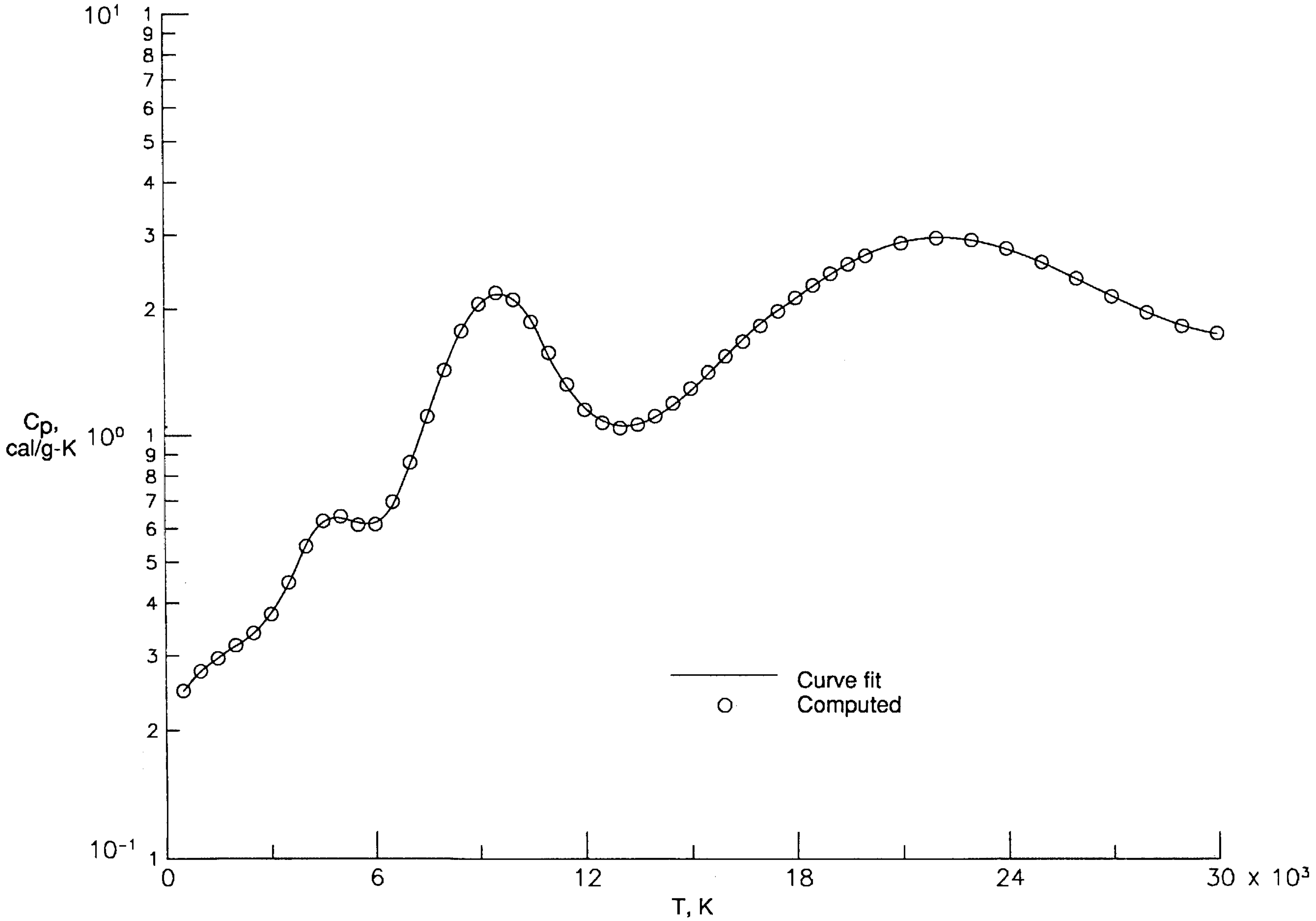
(a) $p = 10^{-4}$ atm.

Figure 3. Specific heat at constant pressure of equilibrium air.



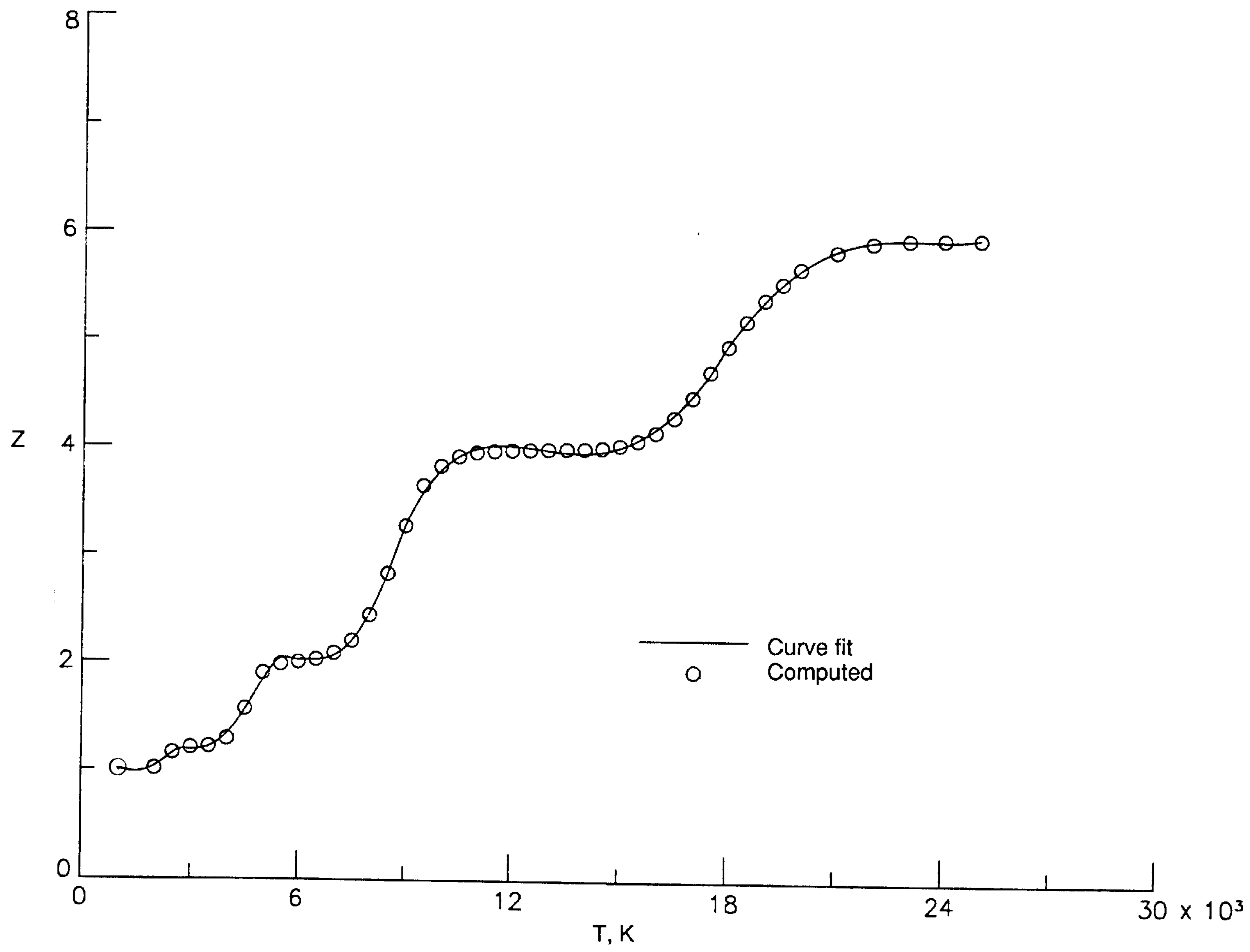
(b) $p = 10^0$ atm.

Figure 3. Continued.



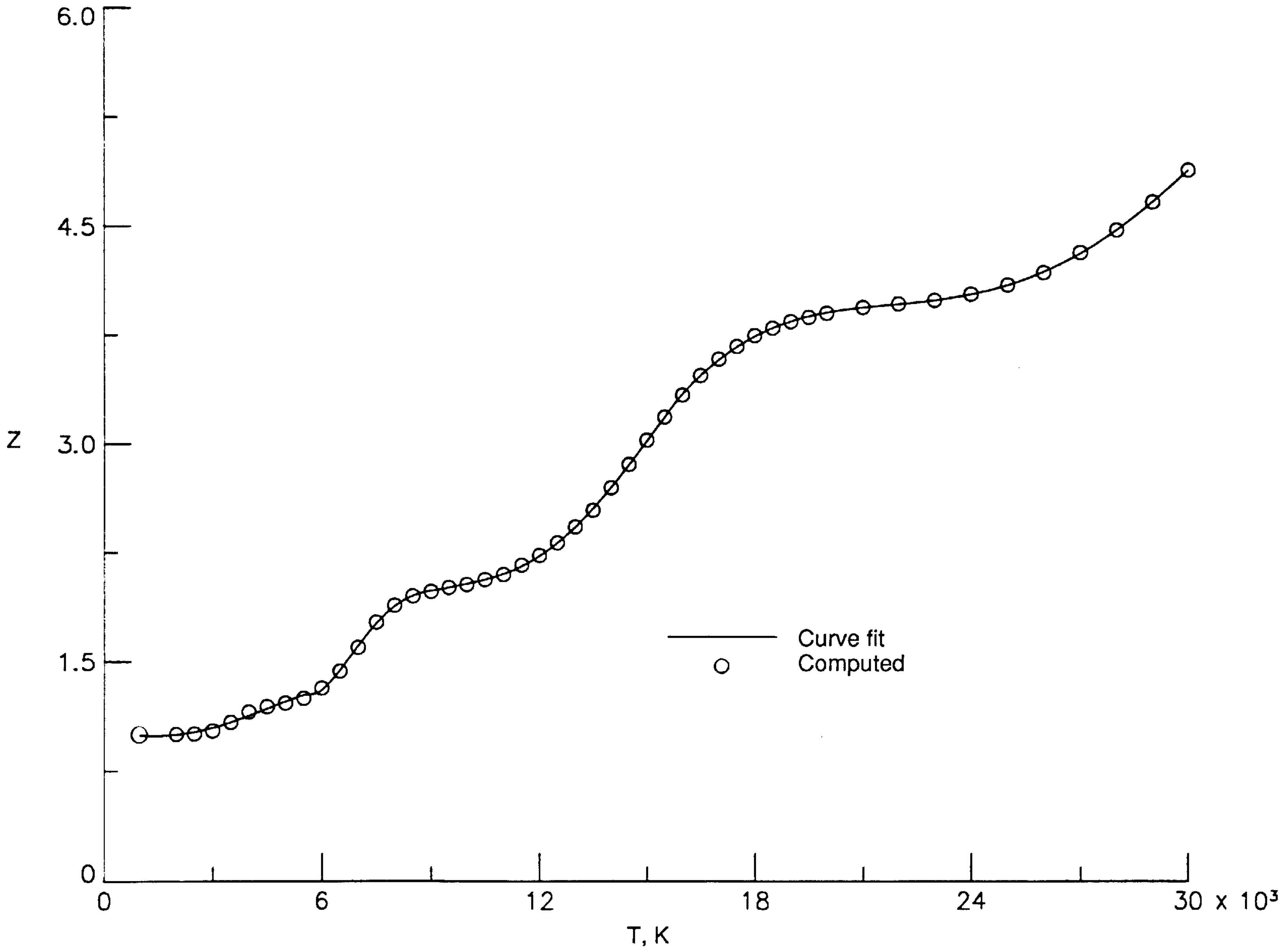
(c) $p = 10^2$ atm.

Figure 3. Concluded.



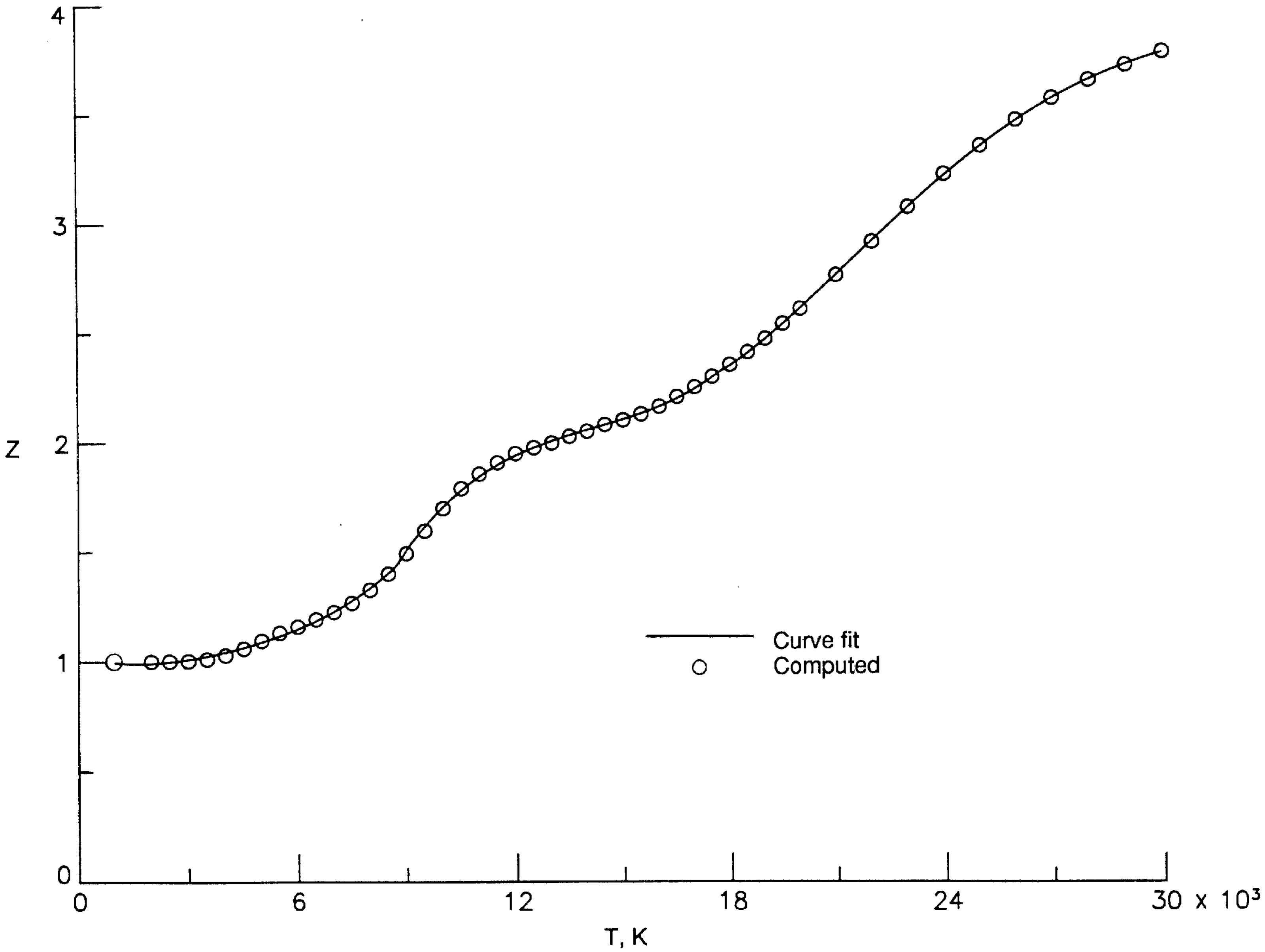
(a) $p = 10^{-4}$ atm.

Figure 4. Compressibility factor for equilibrium air.



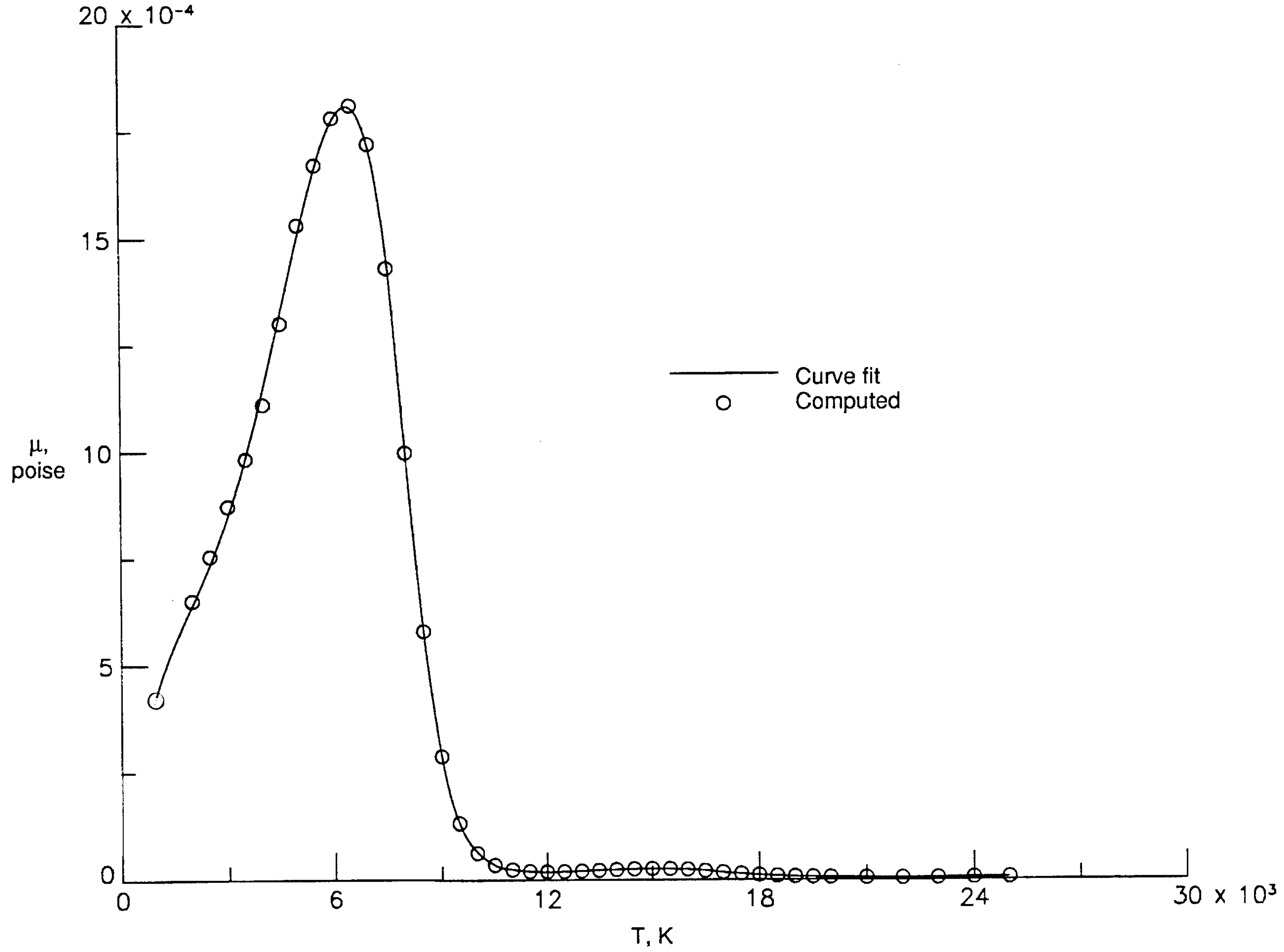
(b) $p = 10^0$ atm.

Figure 4. Continued.



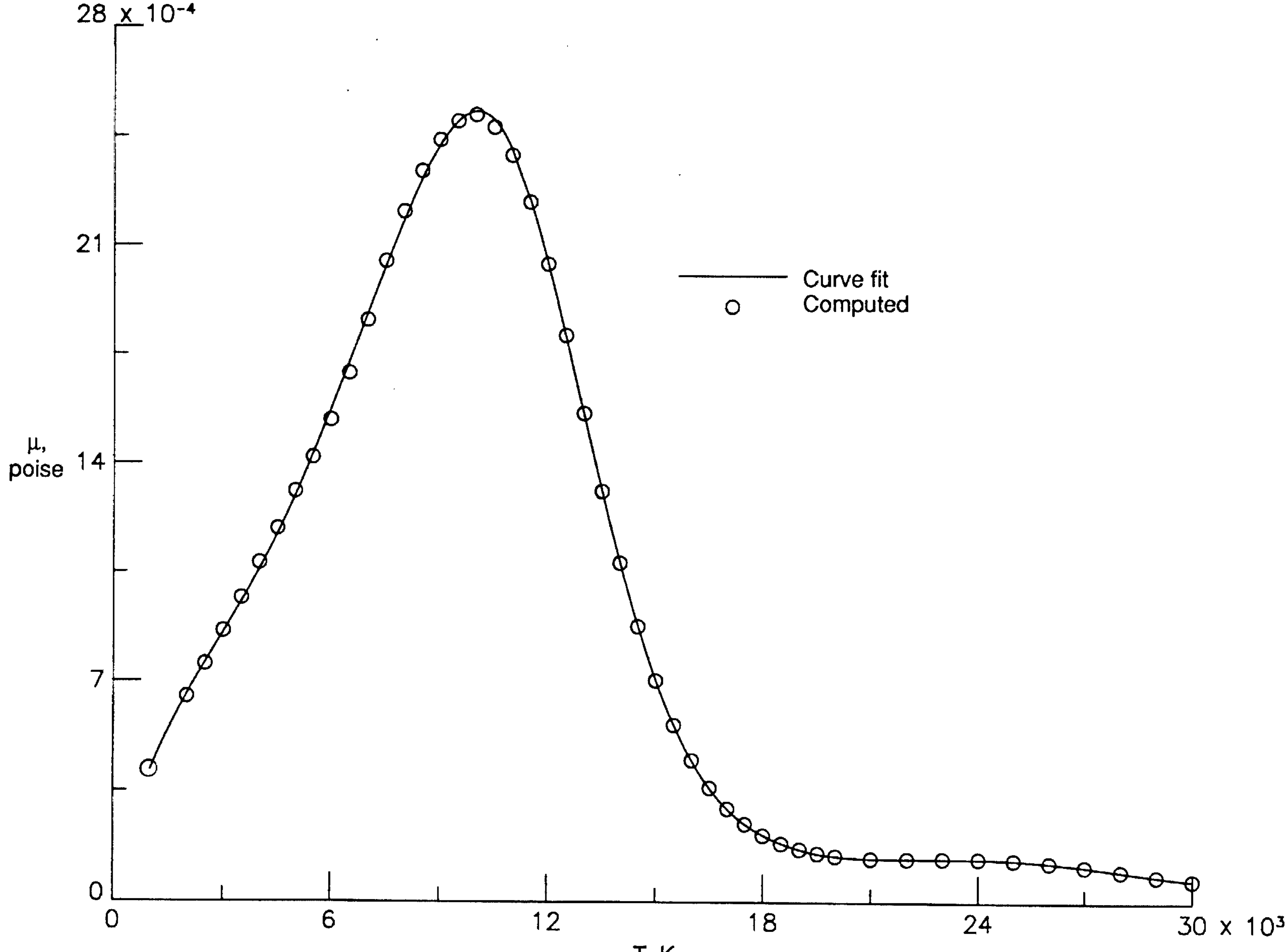
(c) $p = 10^2$ atm.

Figure 4. Concluded.



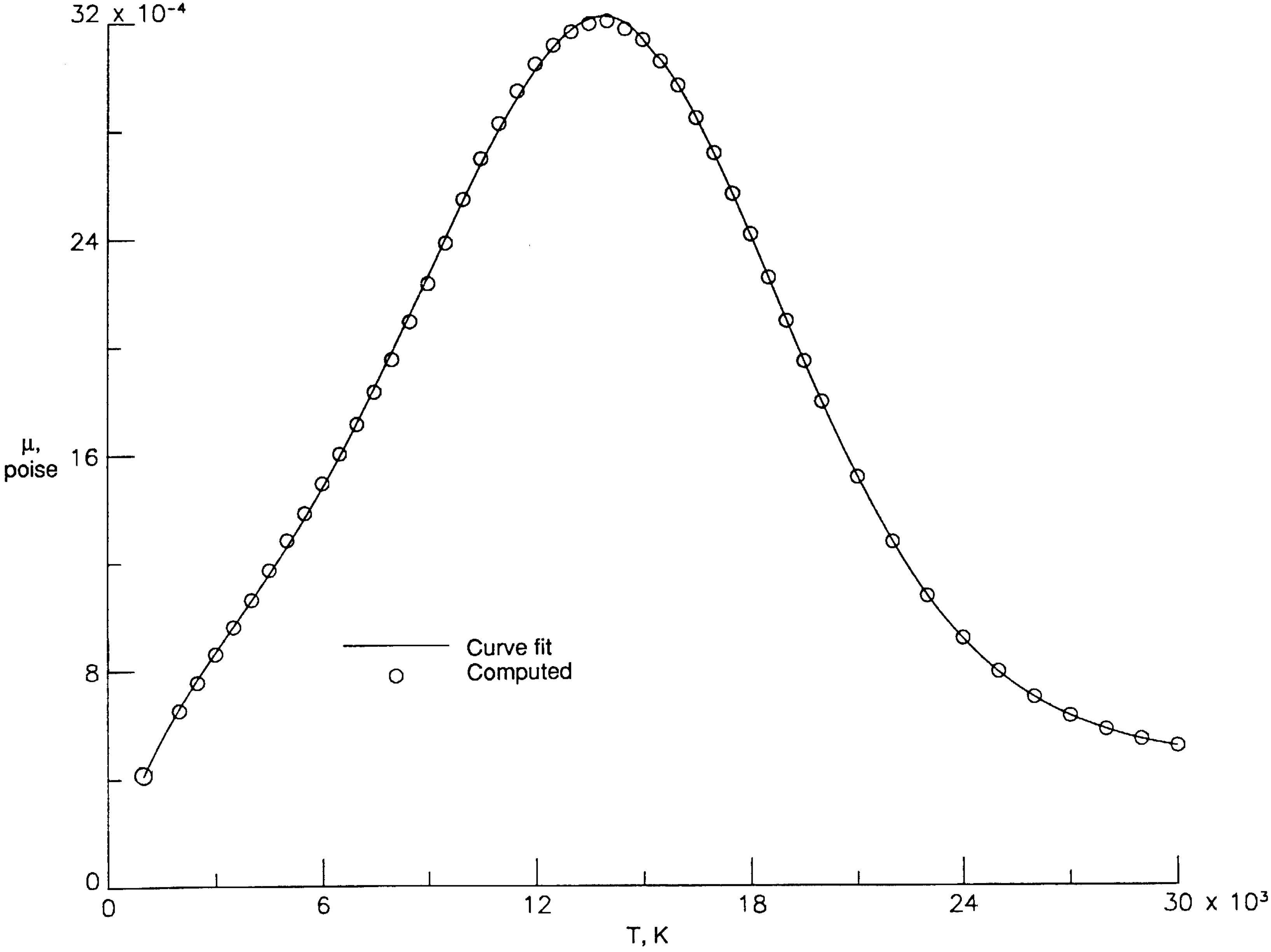
(a) $p = 10^{-4}$ atm.

Figure 5. Viscosity of equilibrium air.



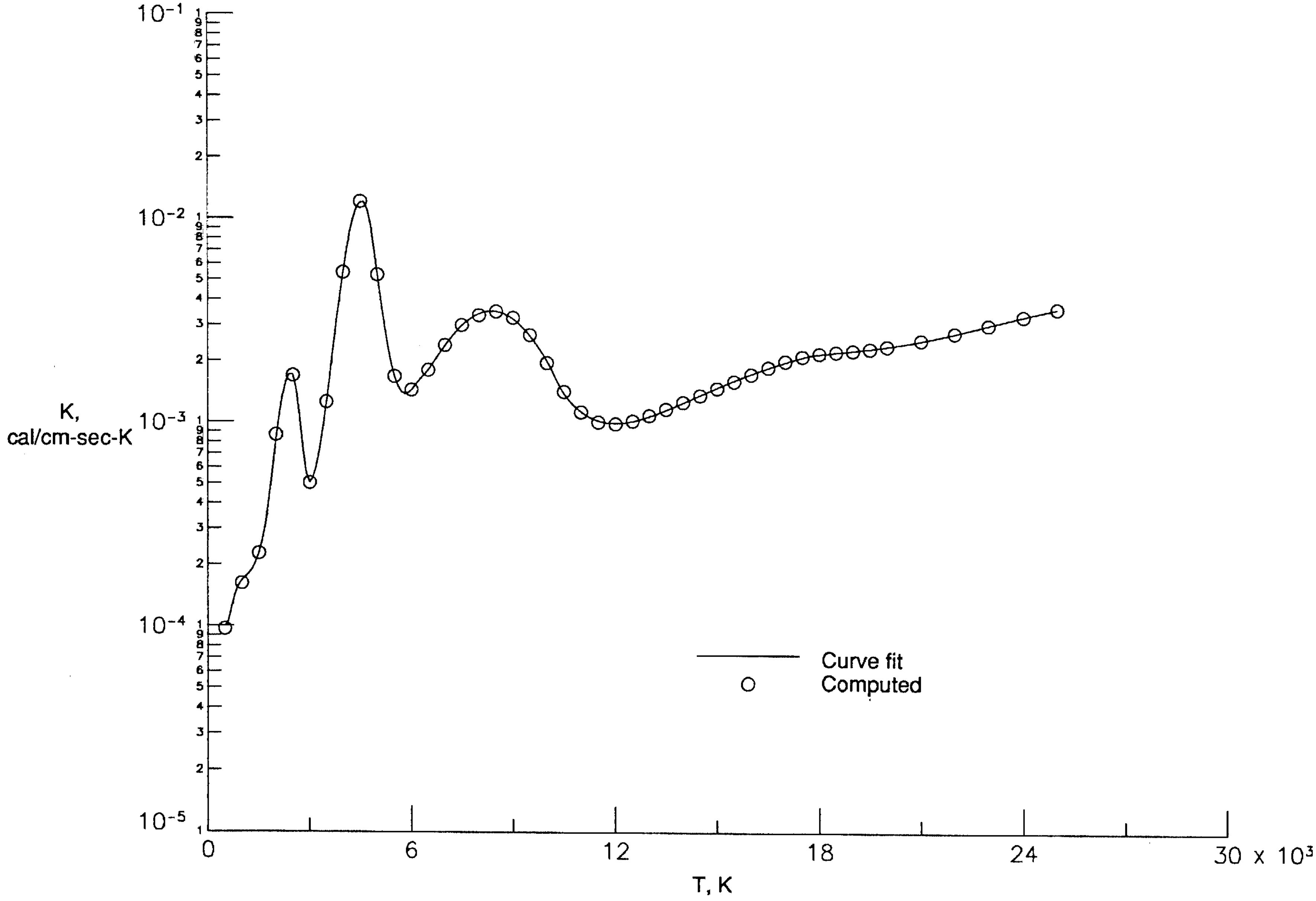
(b) $p = 10^0$ atm.

Figure 5. Continued.



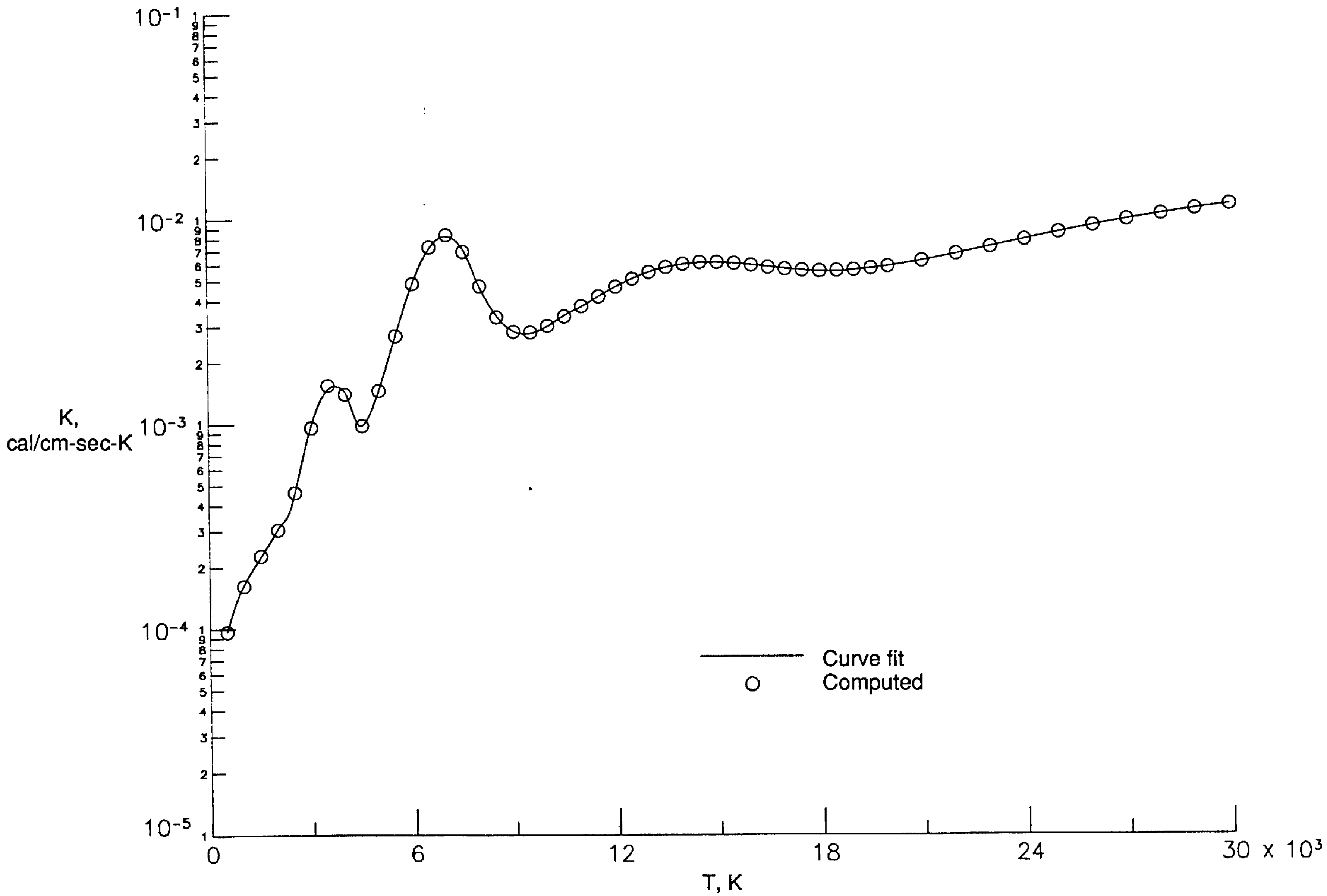
(c) $p = 10^2$ atm.

Figure 5. Concluded.



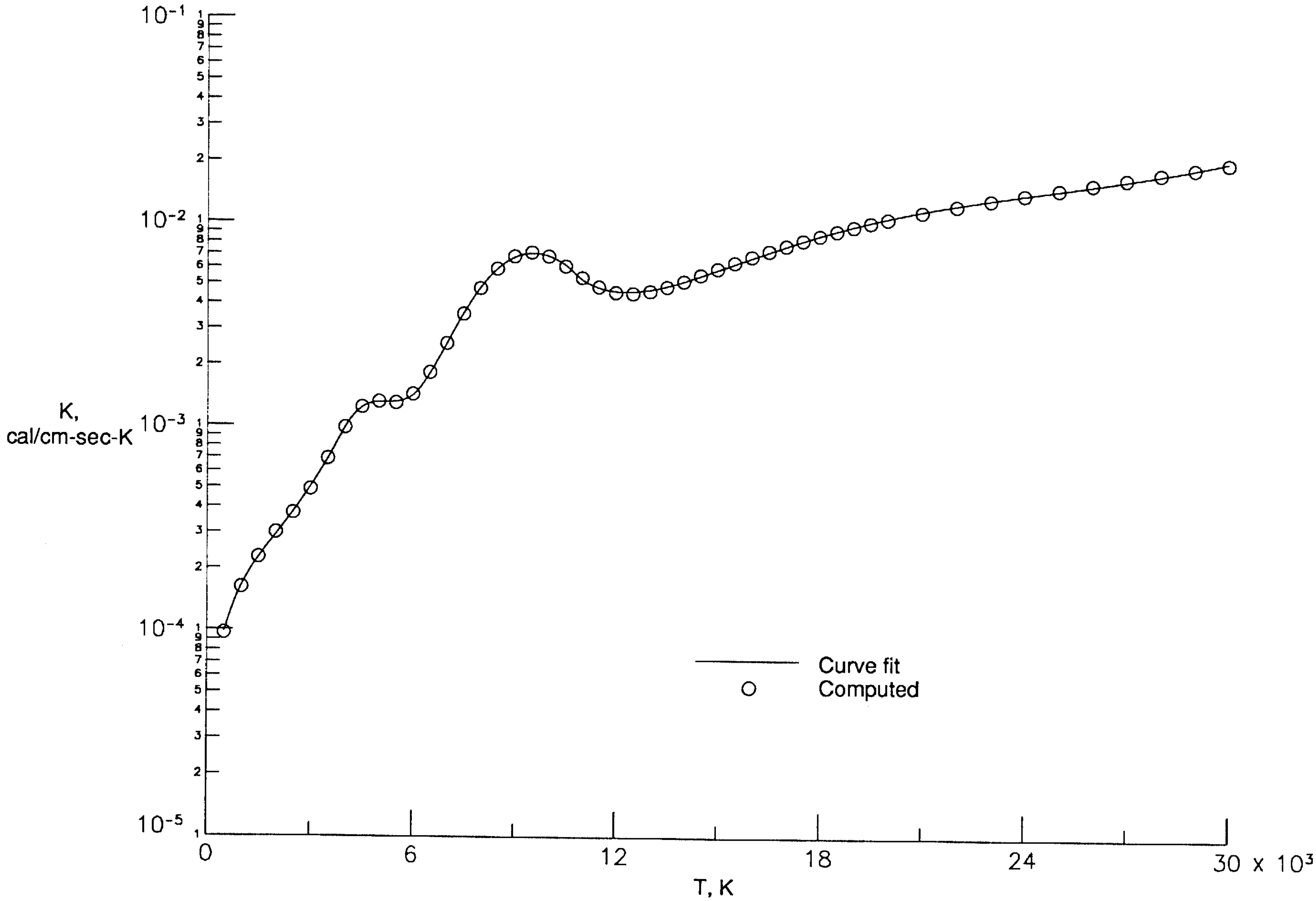
(a) $p = 10^{-4}$ atm.

Figure 6. Thermal conductivity for equilibrium air.



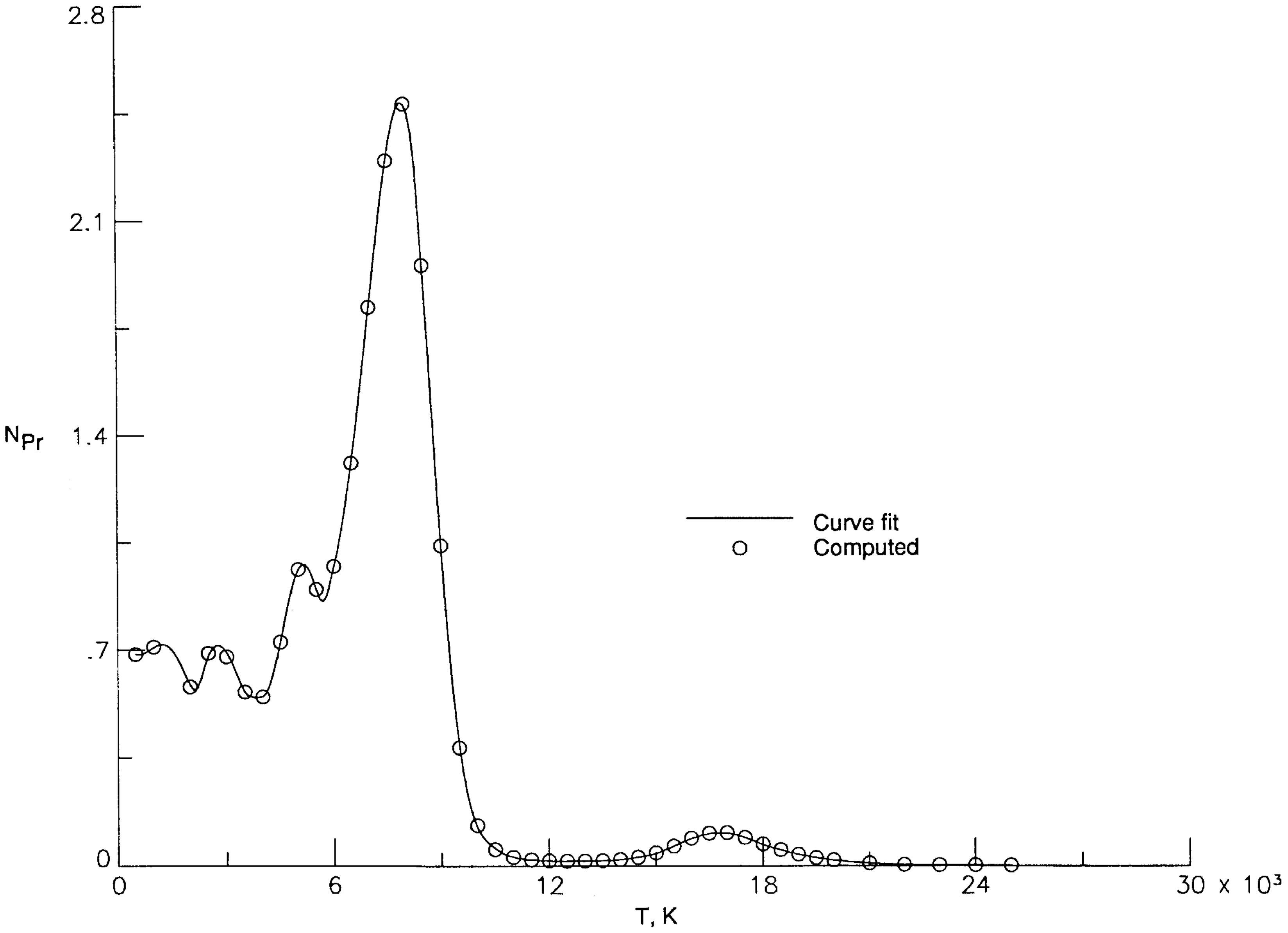
(b) $p = 10^0$ atm.

Figure 6. Continued.



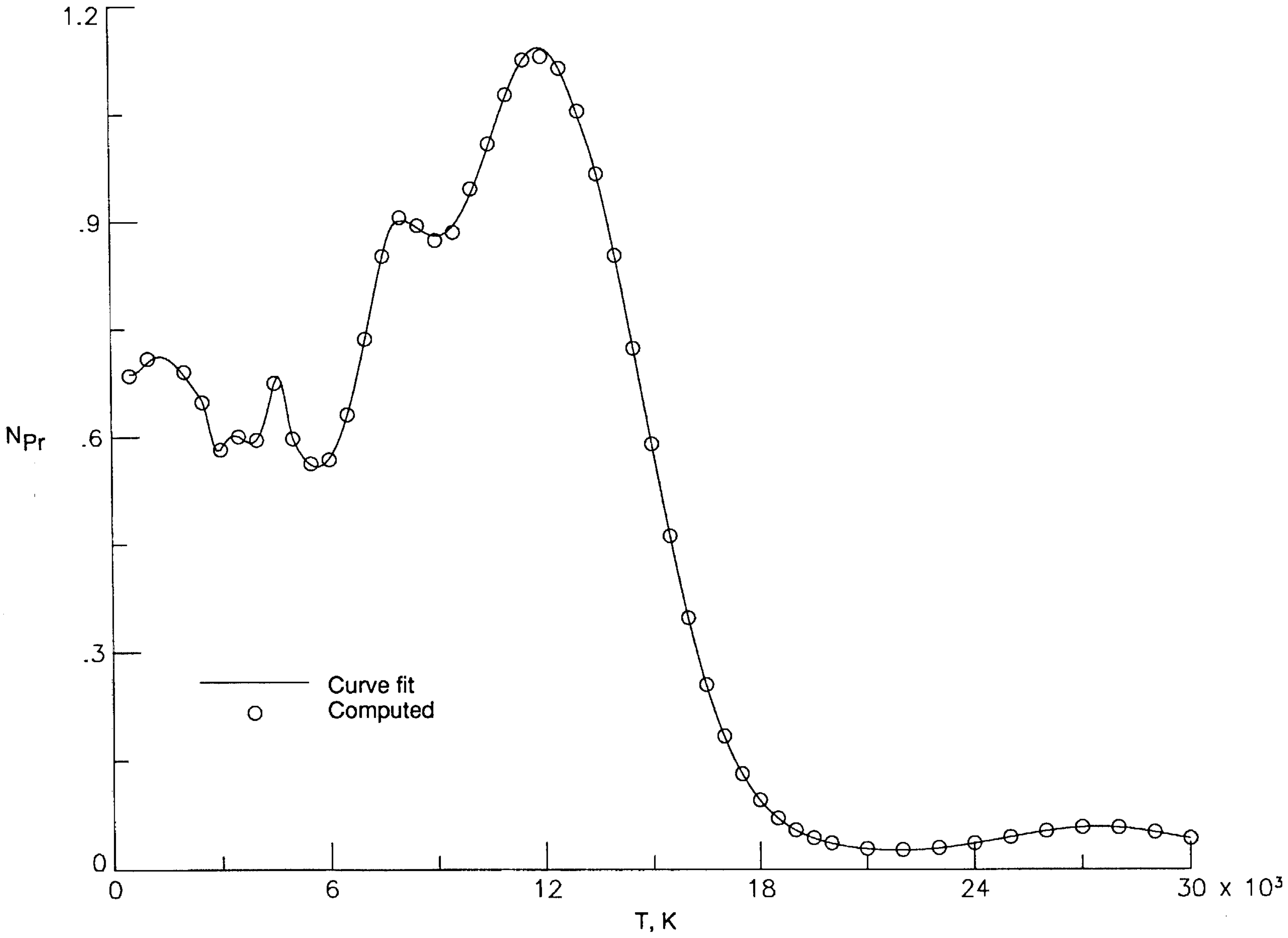
(c) $p = 10^2$ atm.

Figure 6. Concluded.



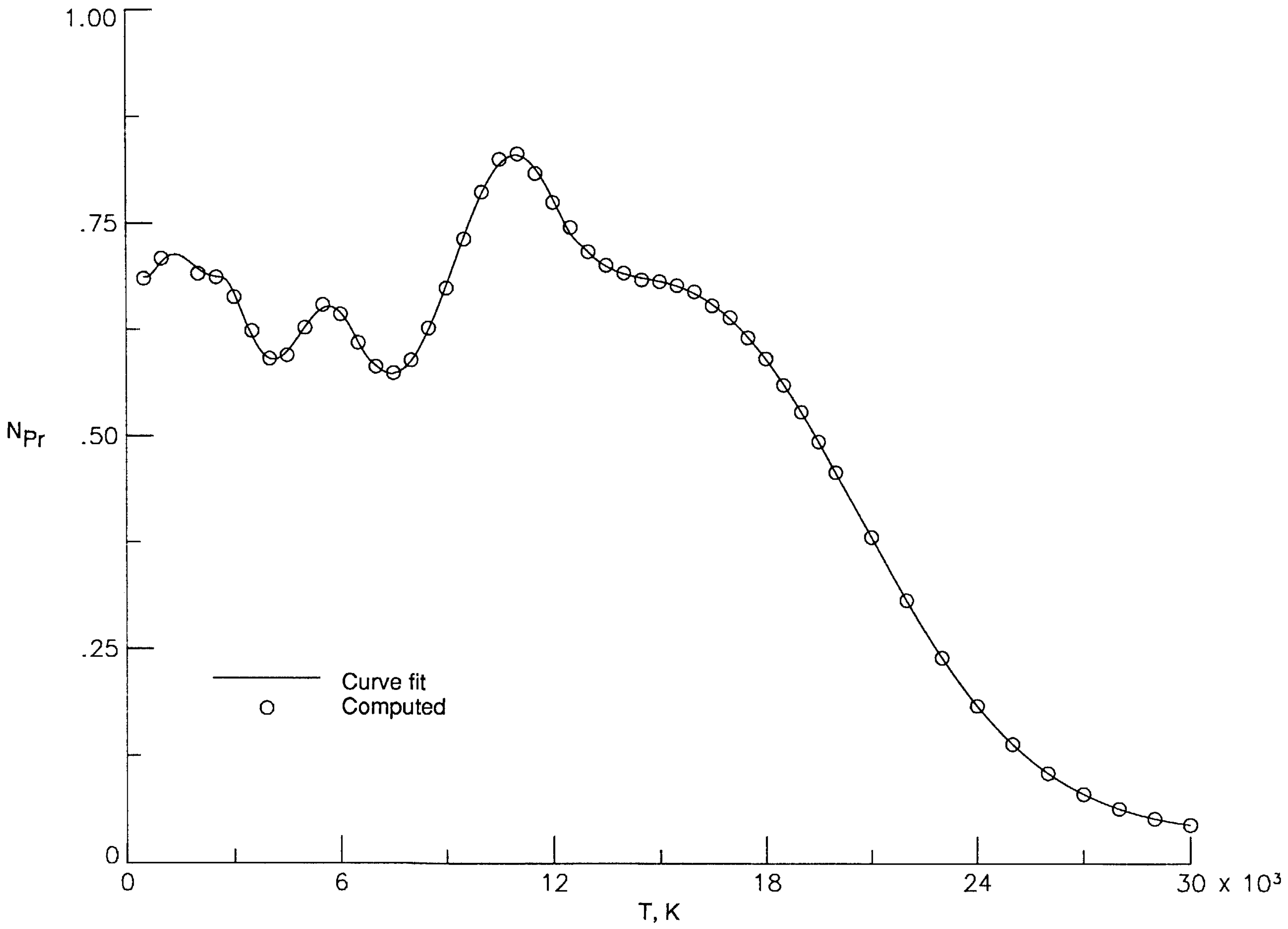
(a) $p = 10^{-4}$ atm.

Figure 7. Prandtl number for equilibrium air.



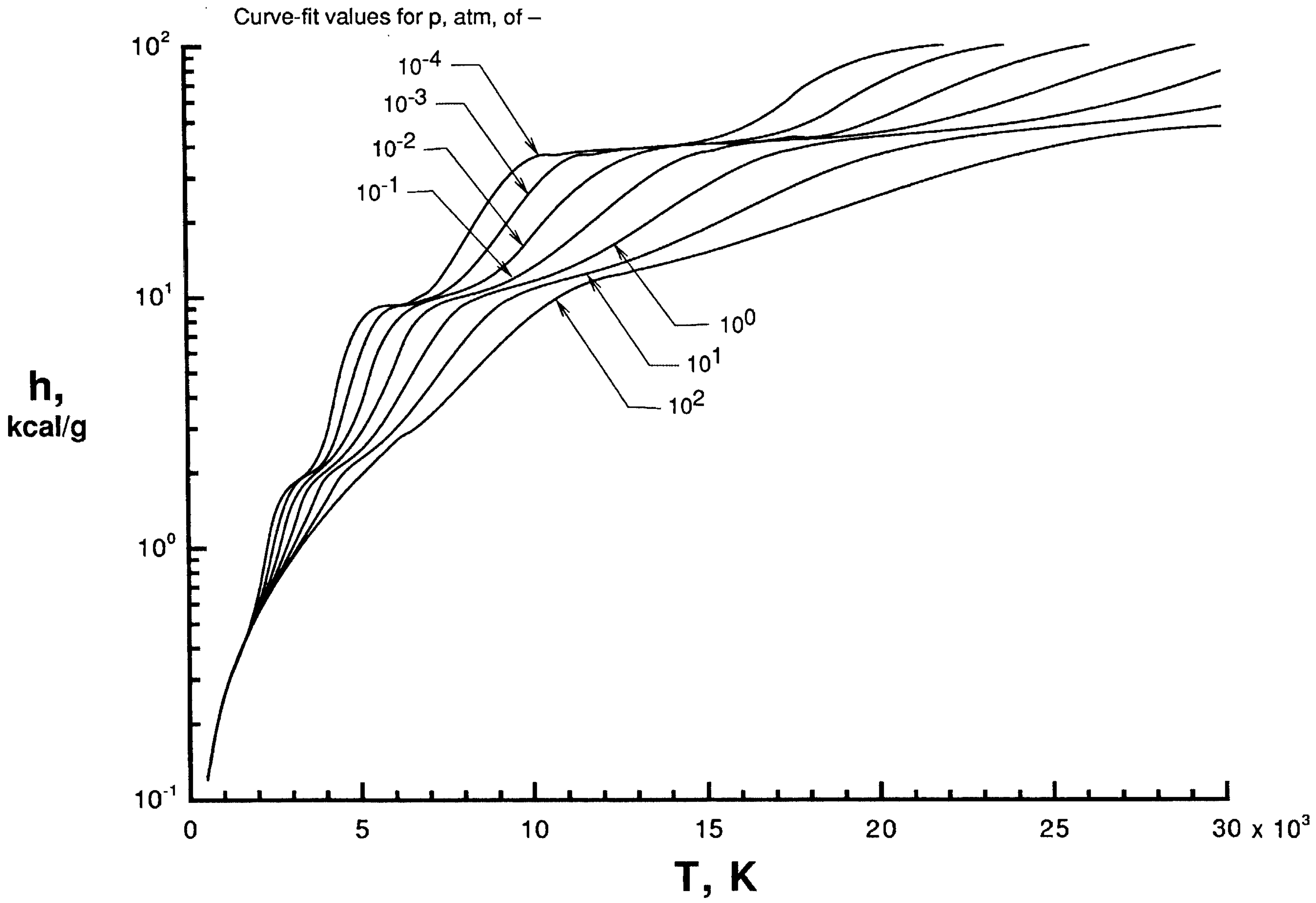
(b) $p = 10^0$ atm.

Figure 7. Continued.



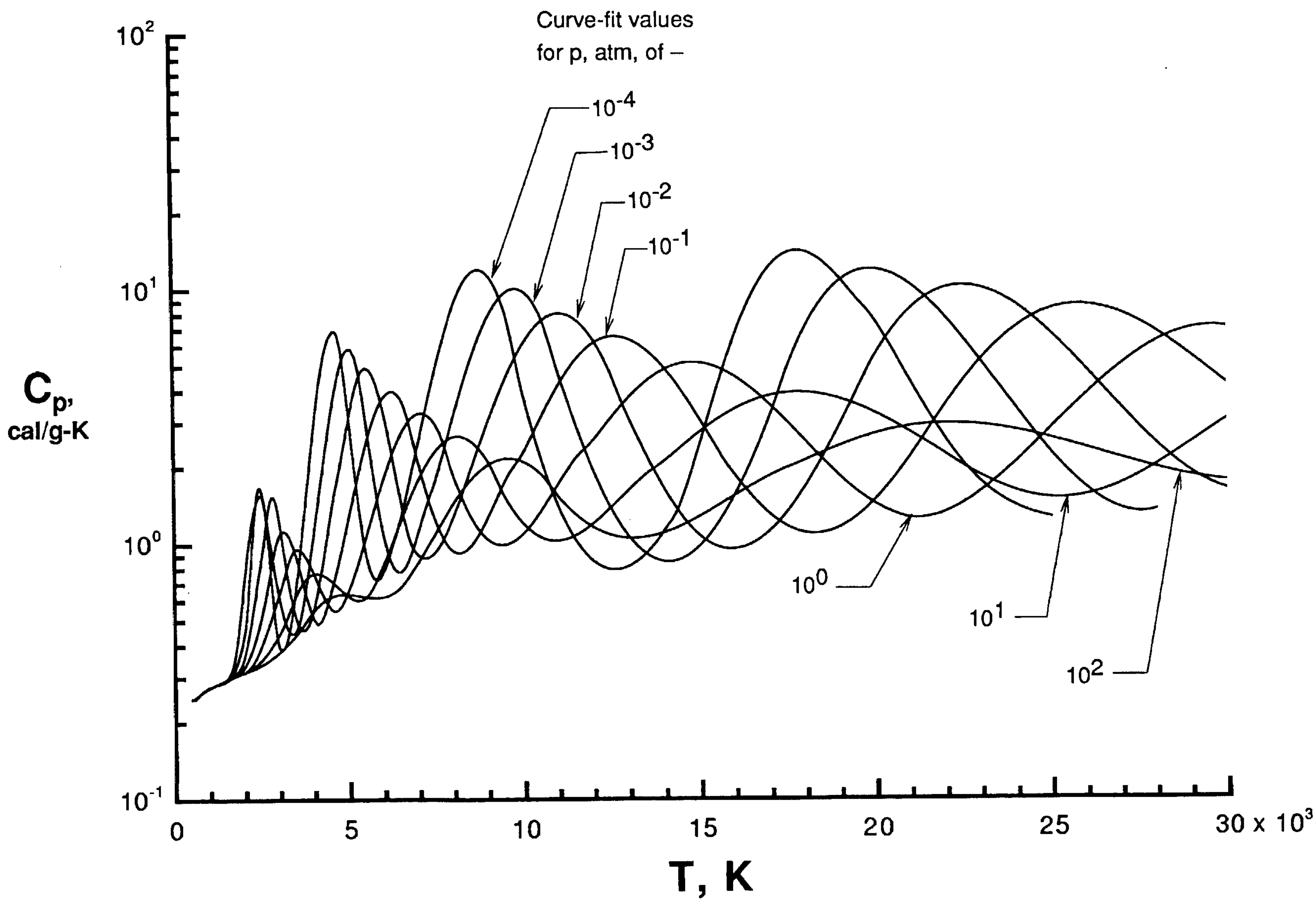
(c) $p = 10^2$ atm.

Figure 7. Concluded.



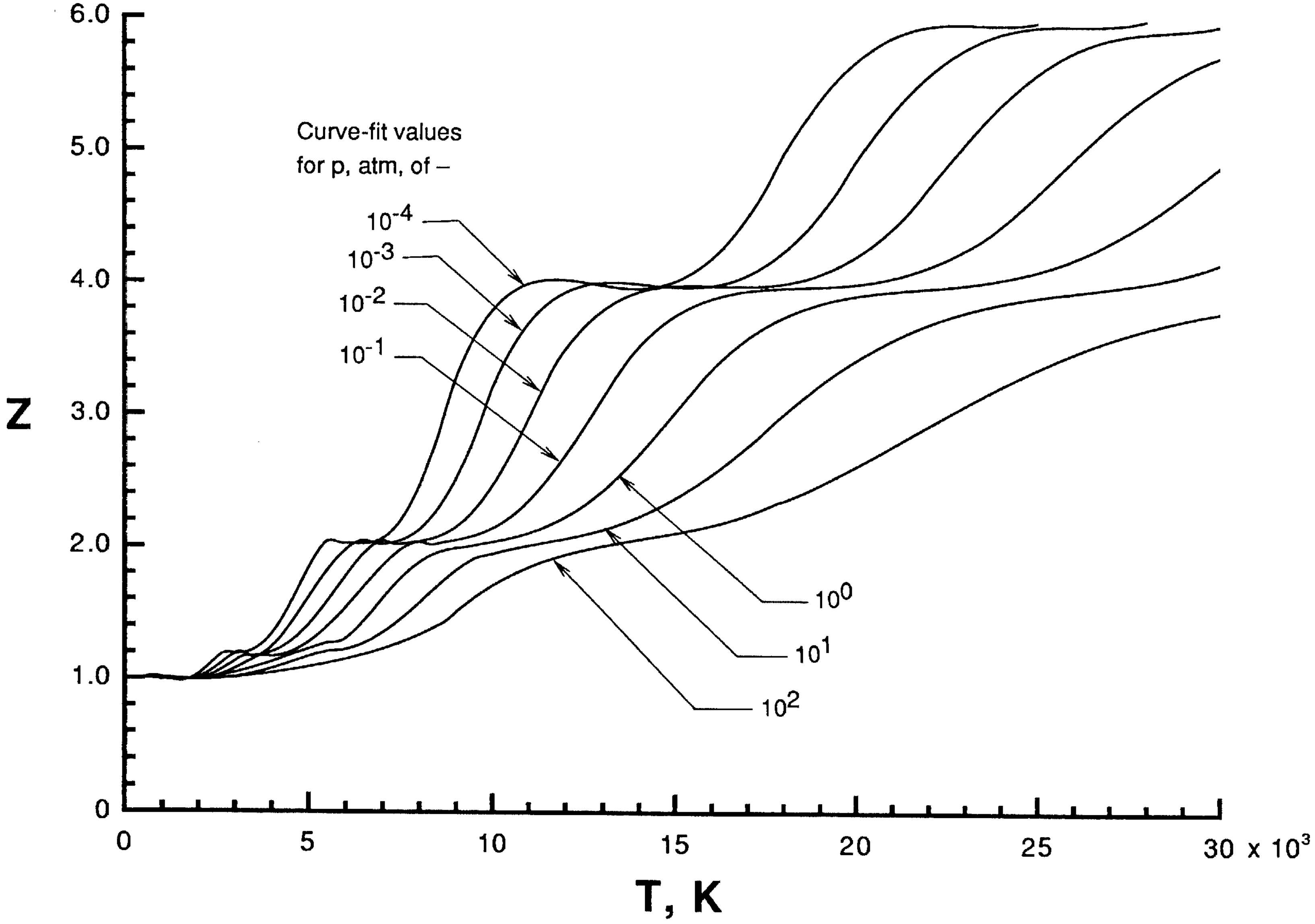
(a) Enthalpy.

Figure 8. Pressure dependence of equilibrium air properties.



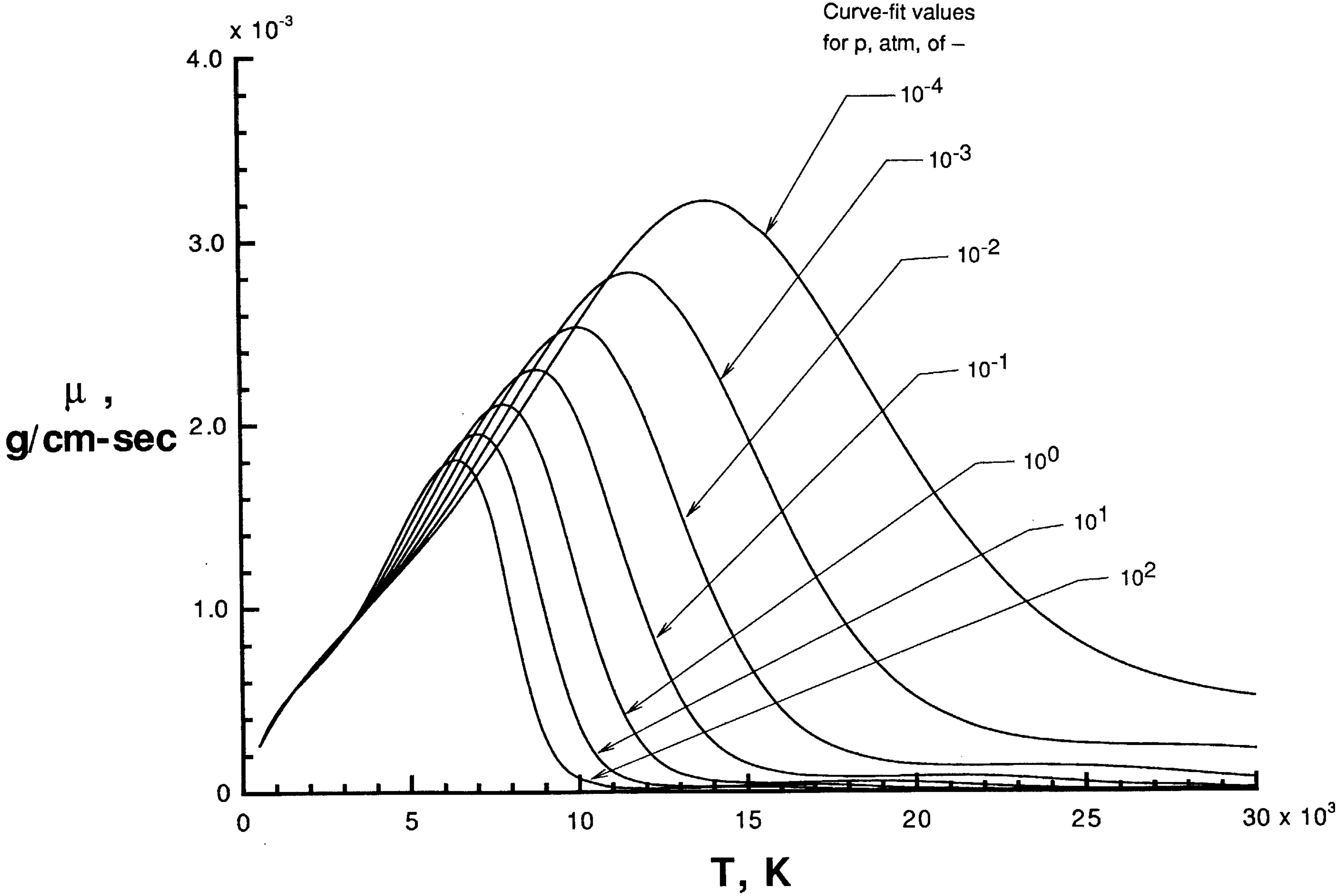
(b) Total specific heat at constant pressure.

Figure 8. Continued.



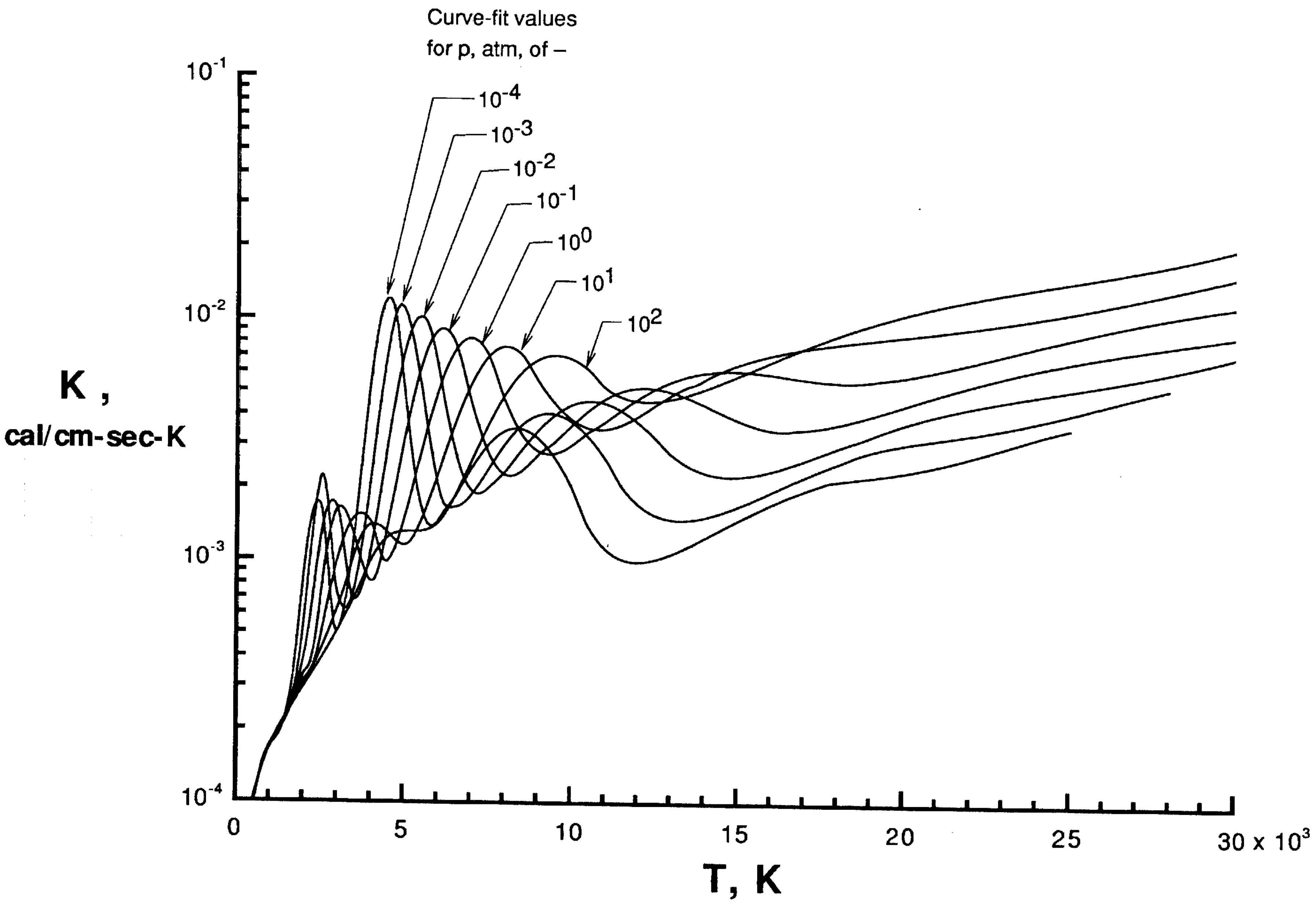
(c) Compressibility factor.

Figure 8. Continued.



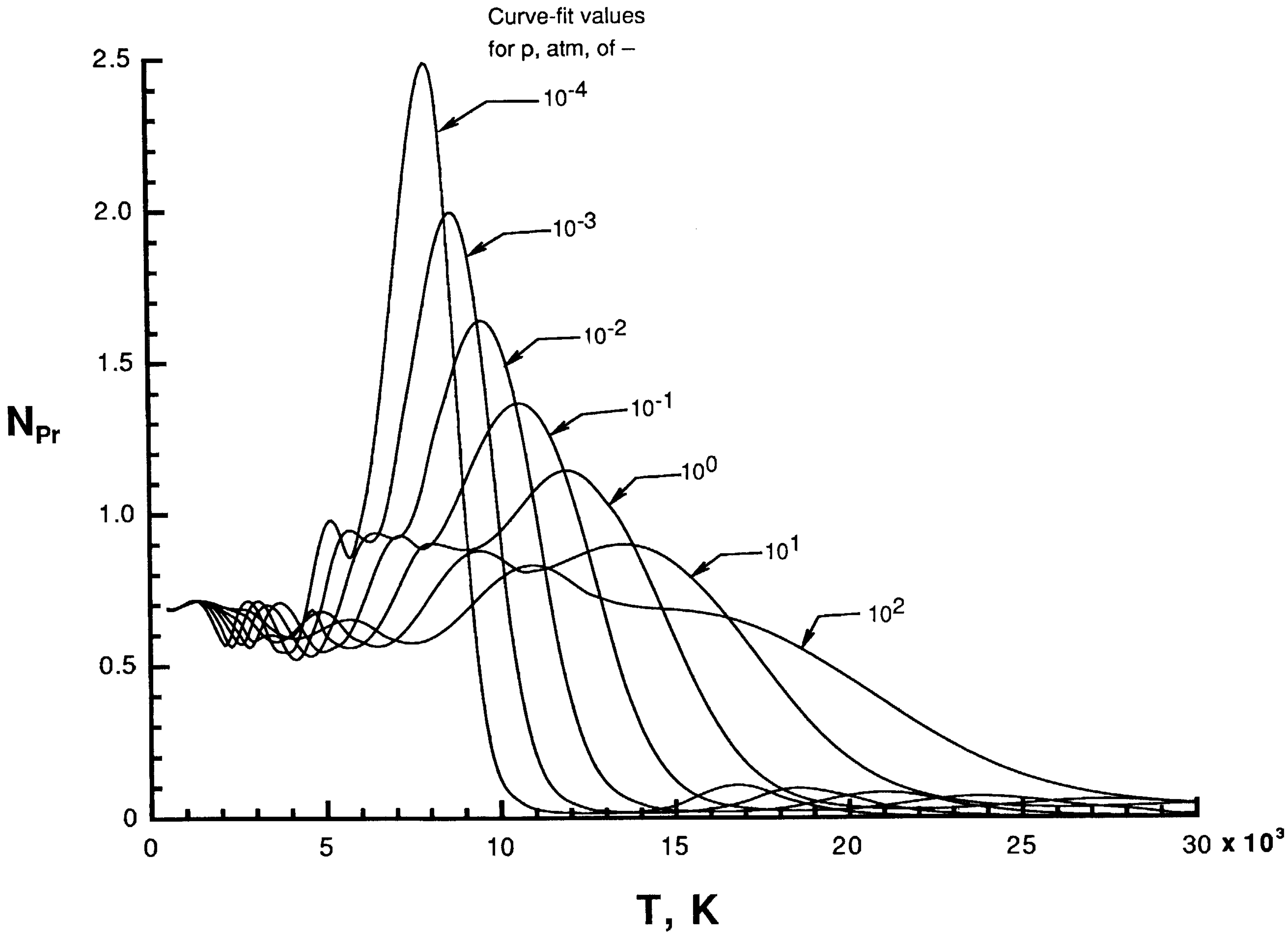
(d) Viscosity.

Figure 8. Continued.



(e) Total thermal conductivity.

Figure 8. Continued.



(f) Total Prandtl number.

Figure 8. Concluded.

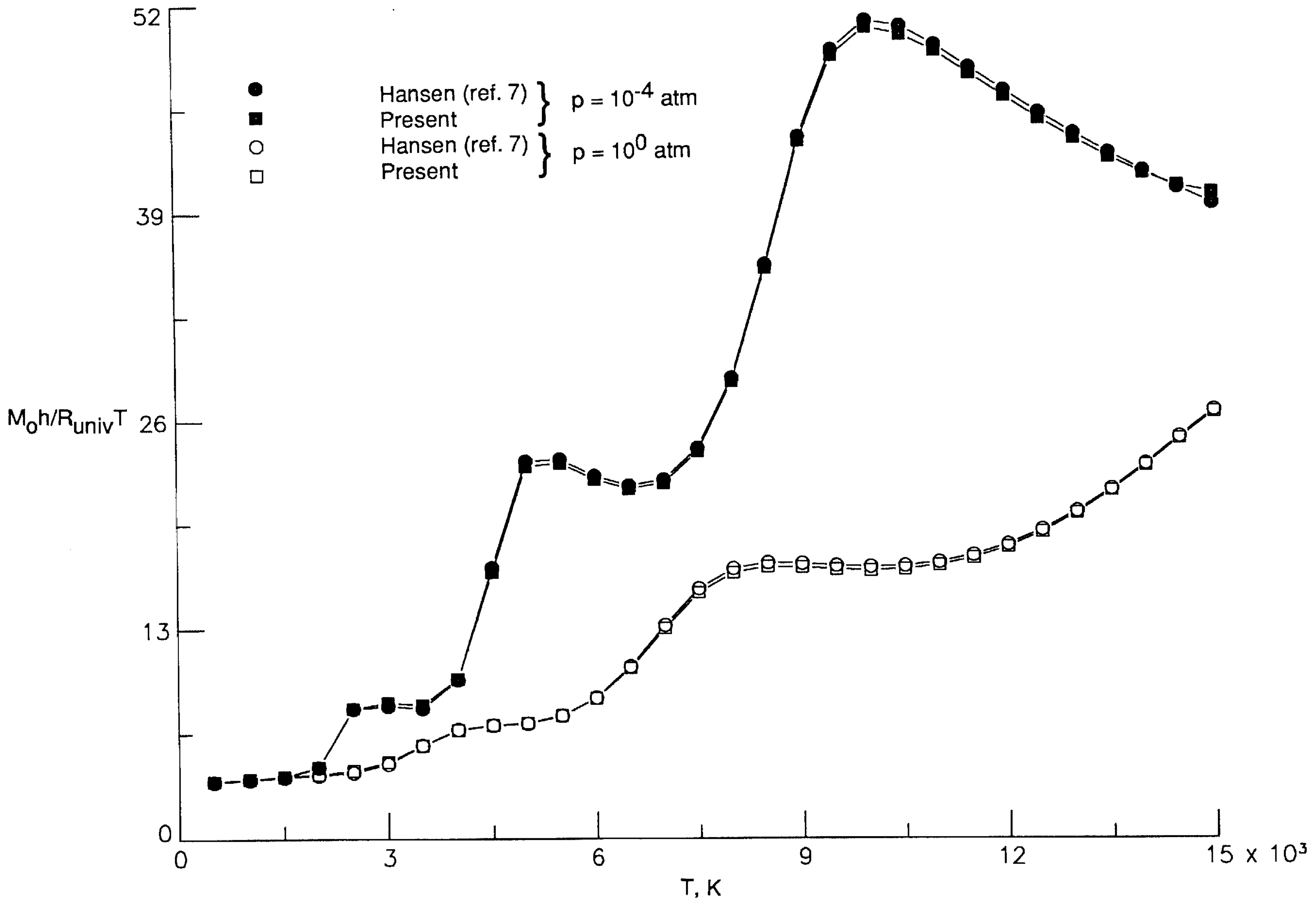
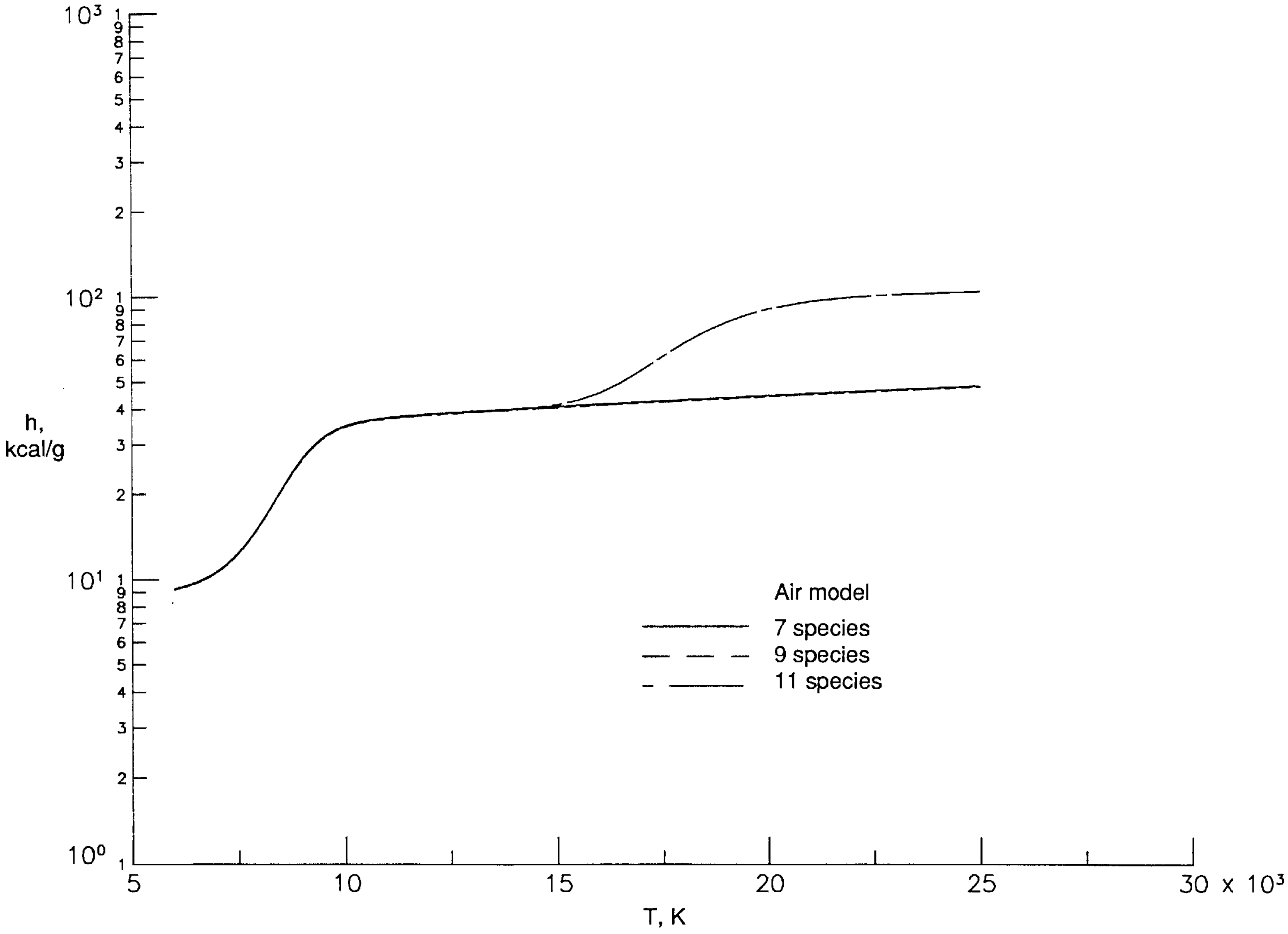
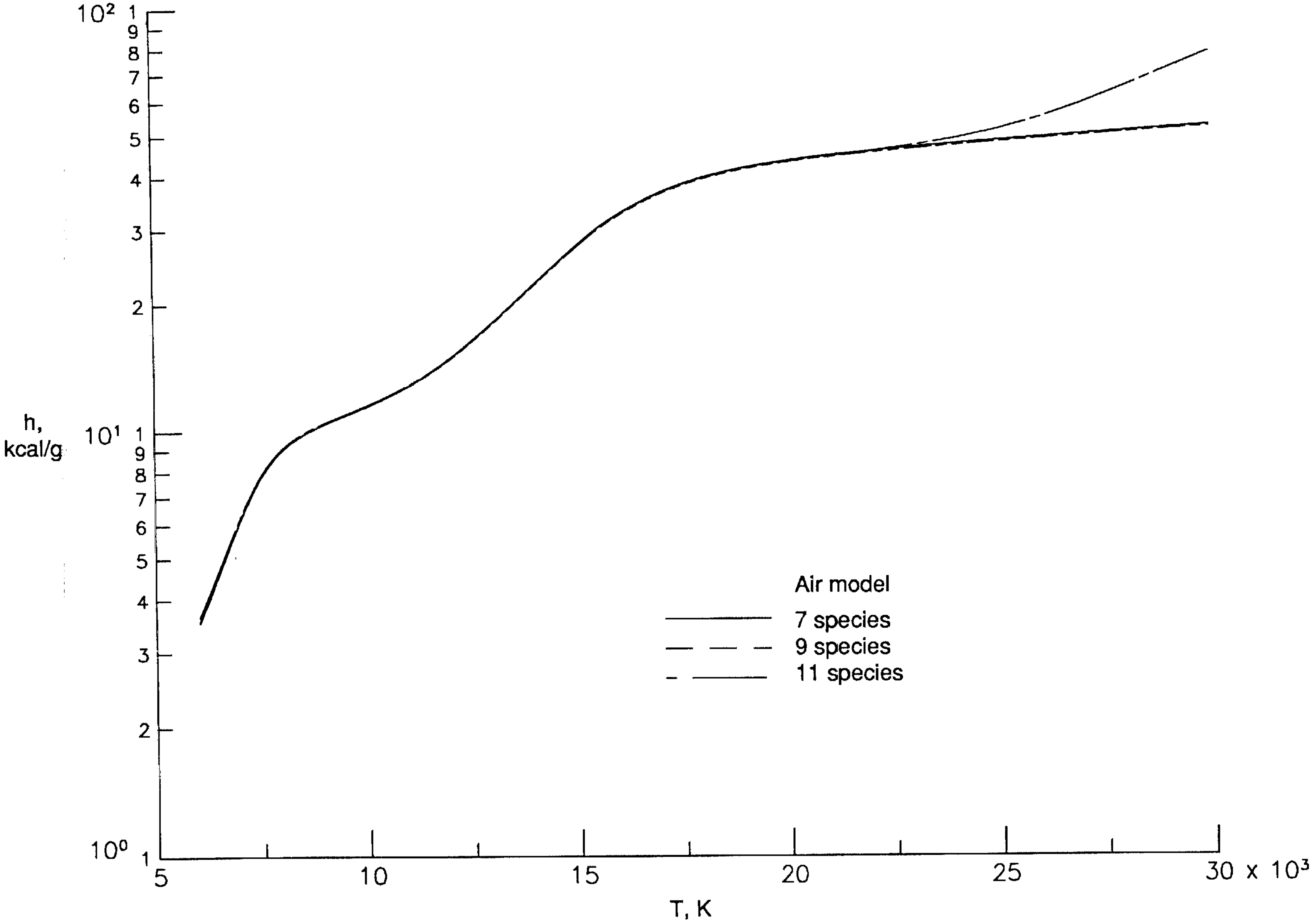


Figure 9. Comparison of dimensionless enthalpy values for equilibrium air.



(a) $p = 10^{-4}$ atm.

Figure 10. Comparison of equilibrium air enthalpy with different species used in air model.



(b) $p = 10^0$ atm.

Figure 10. Concluded.

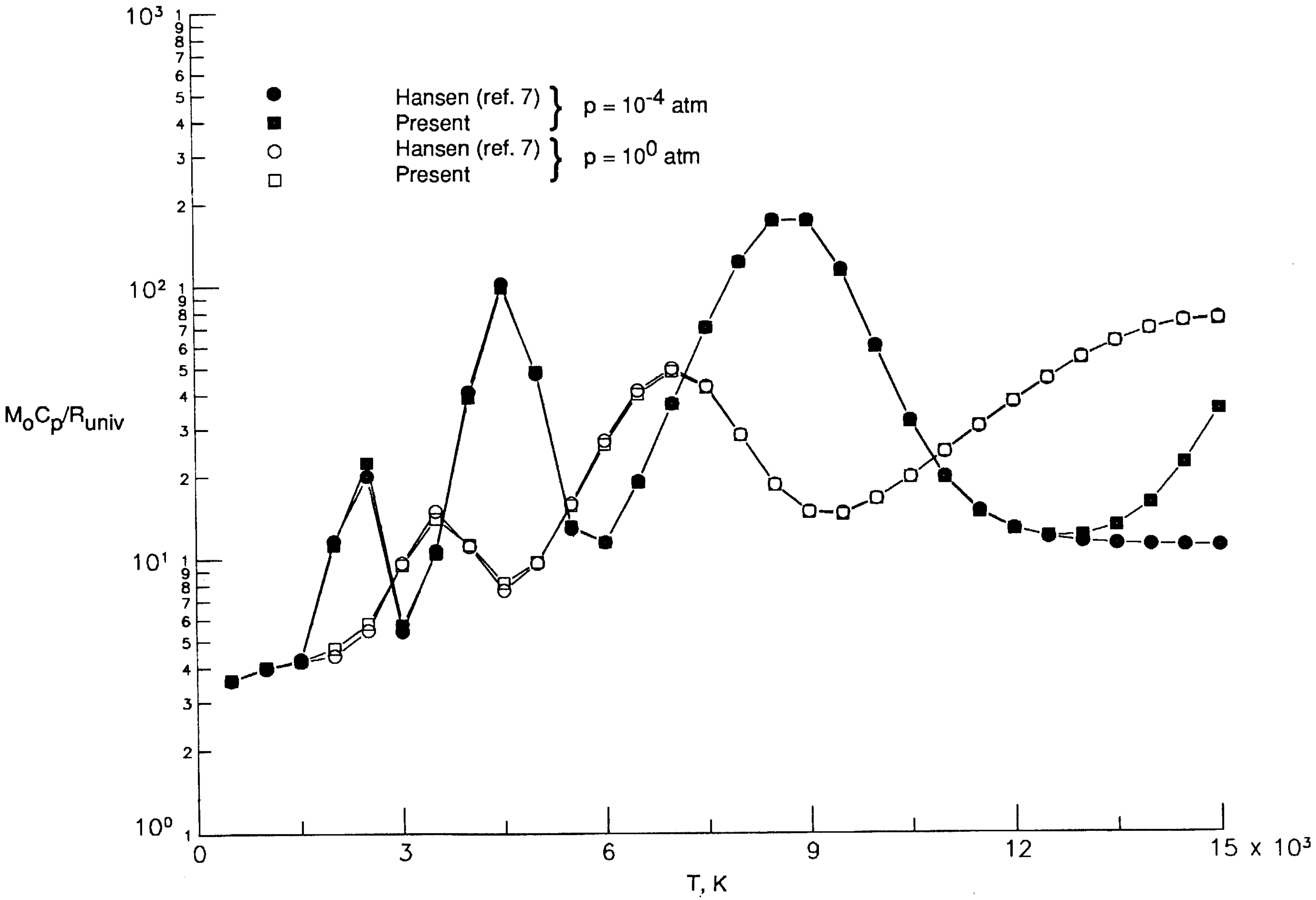


Figure 11. Comparison of dimensionless values of total specific heat ($C_p = C_{p_f} + C_{p_r}$) at constant pressure for equilibrium air.

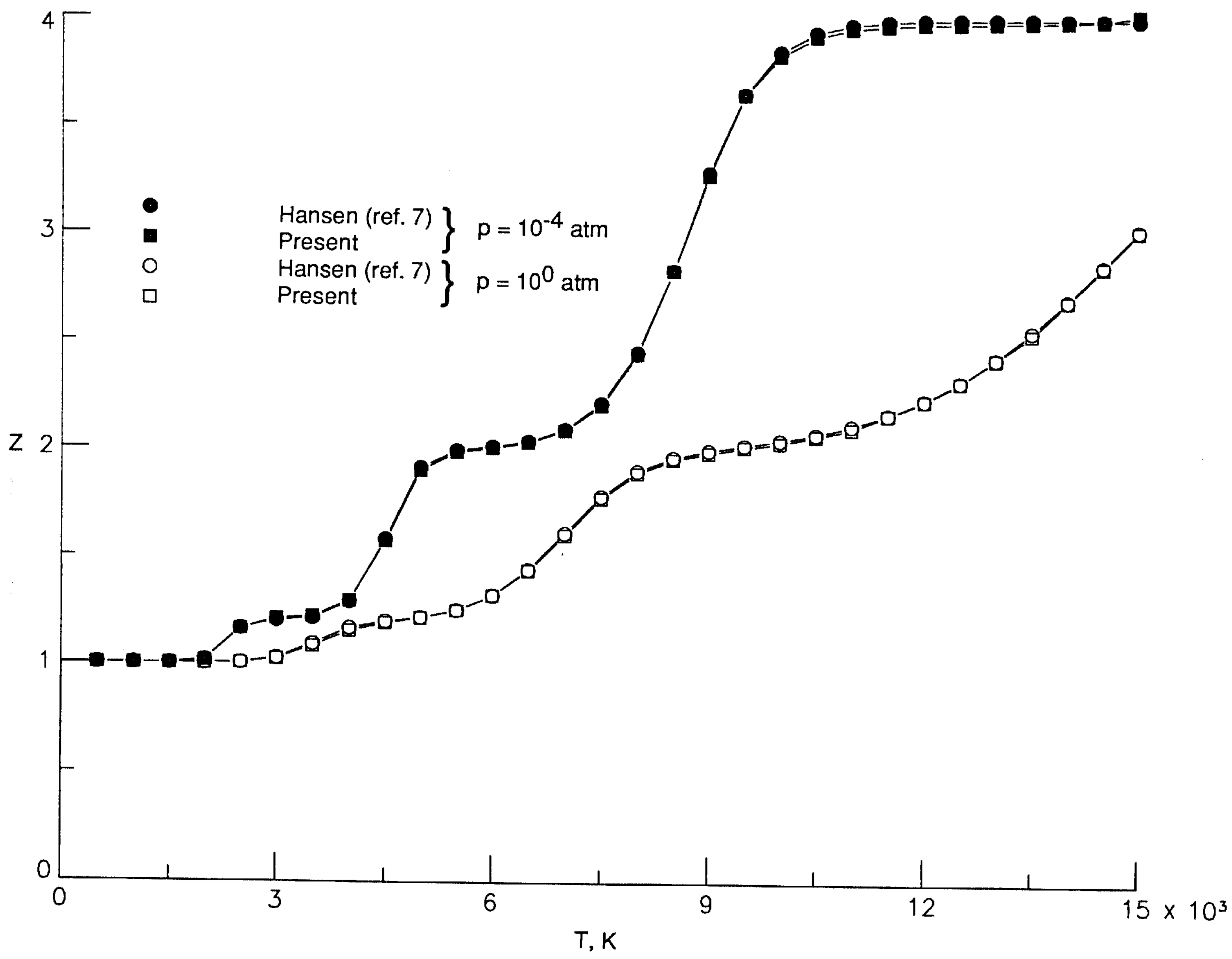
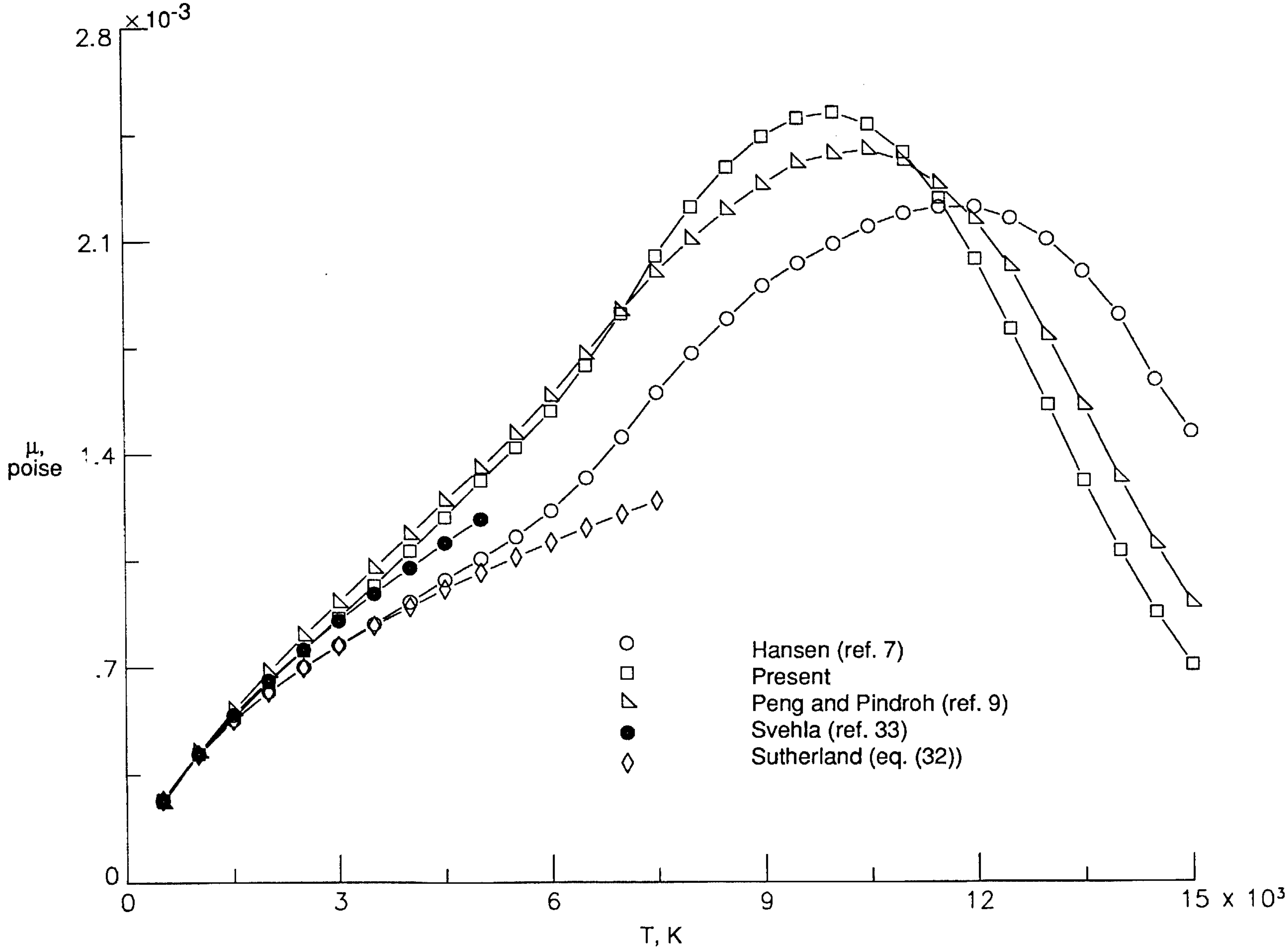
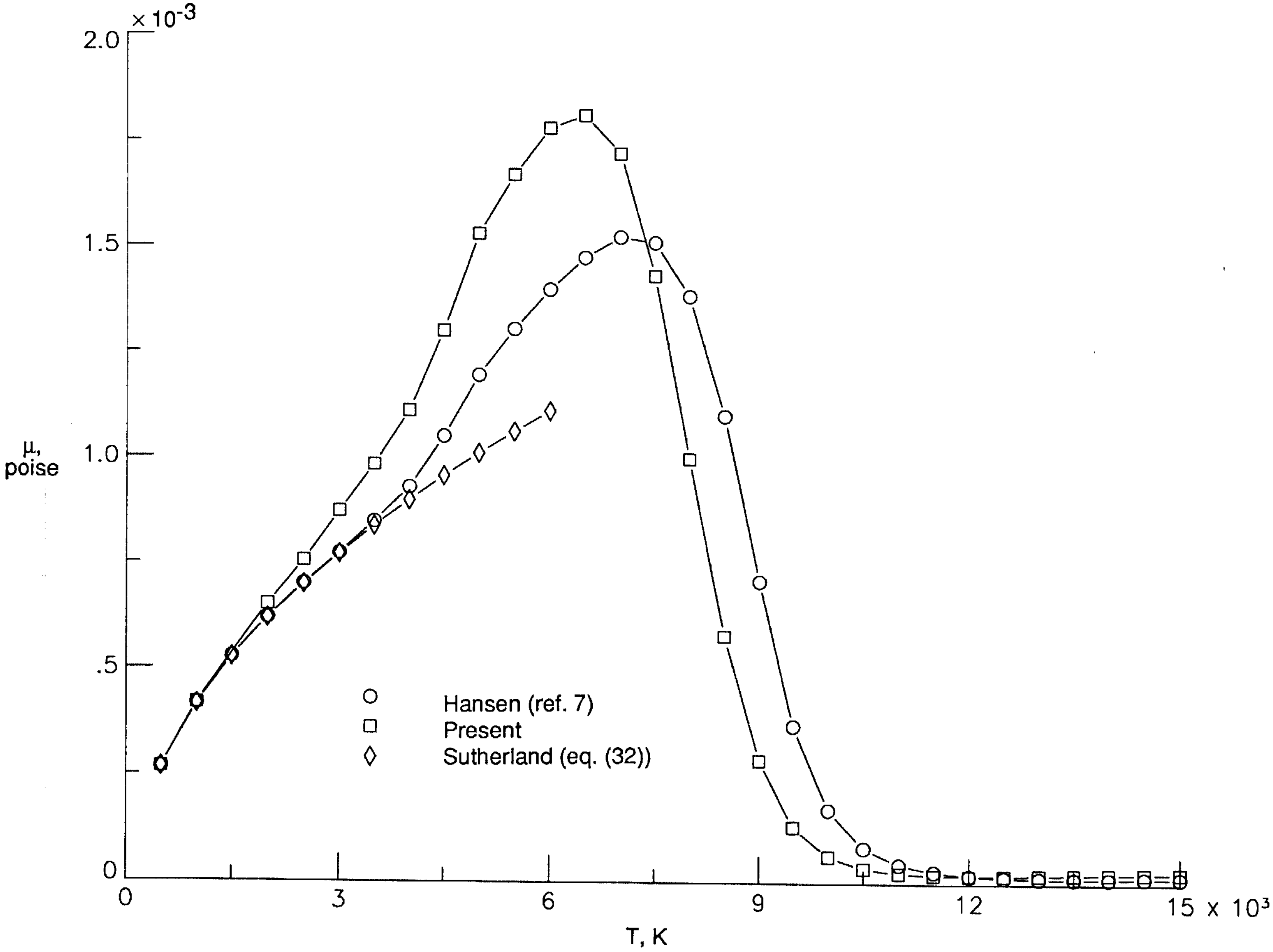


Figure 12. Comparison of compressibility factor values from reference 7 and present computation for equilibrium air.



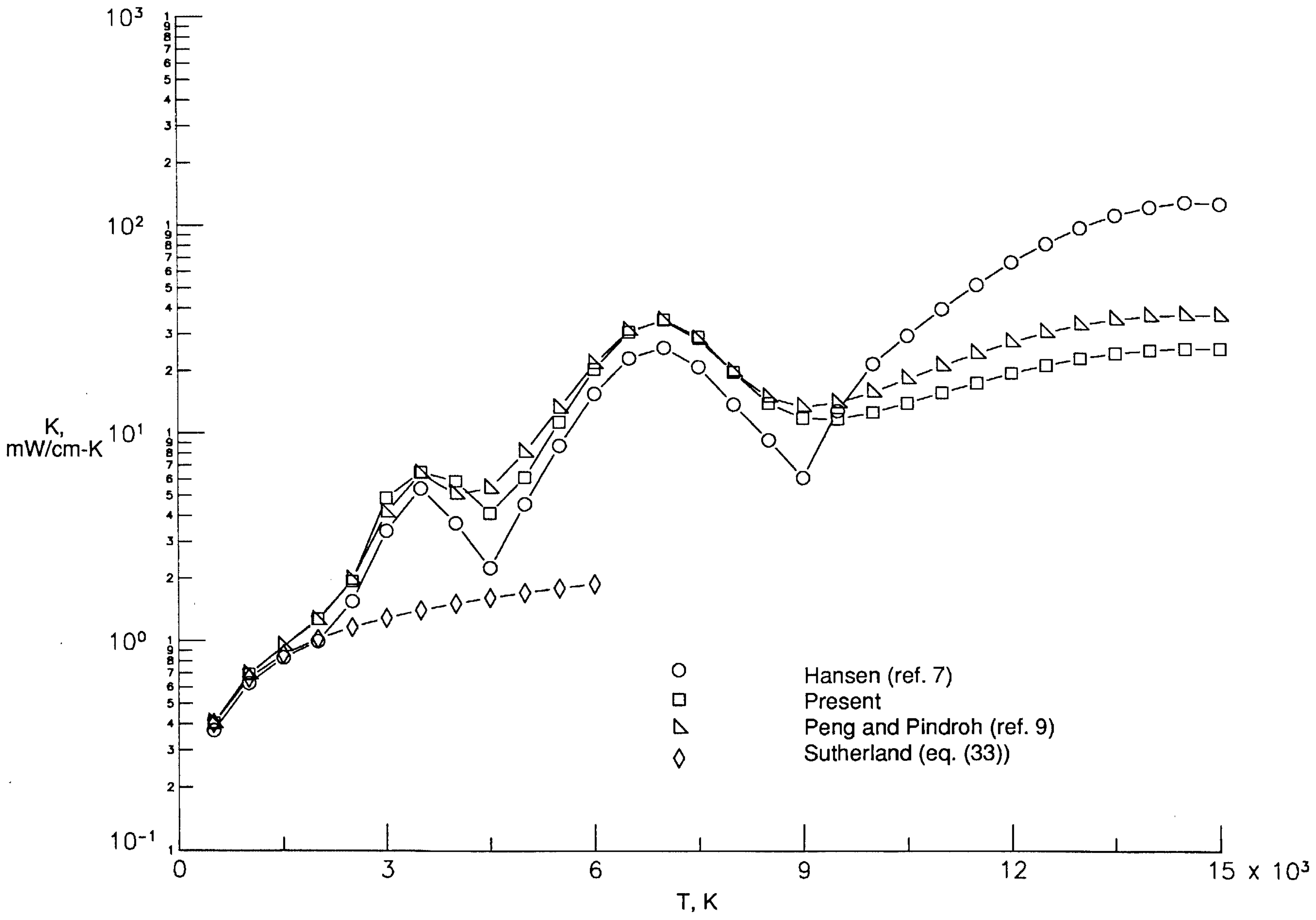
(a) $p = 10^0$ atm.

Figure 13. Comparison of viscosity values from several sources for equilibrium air.



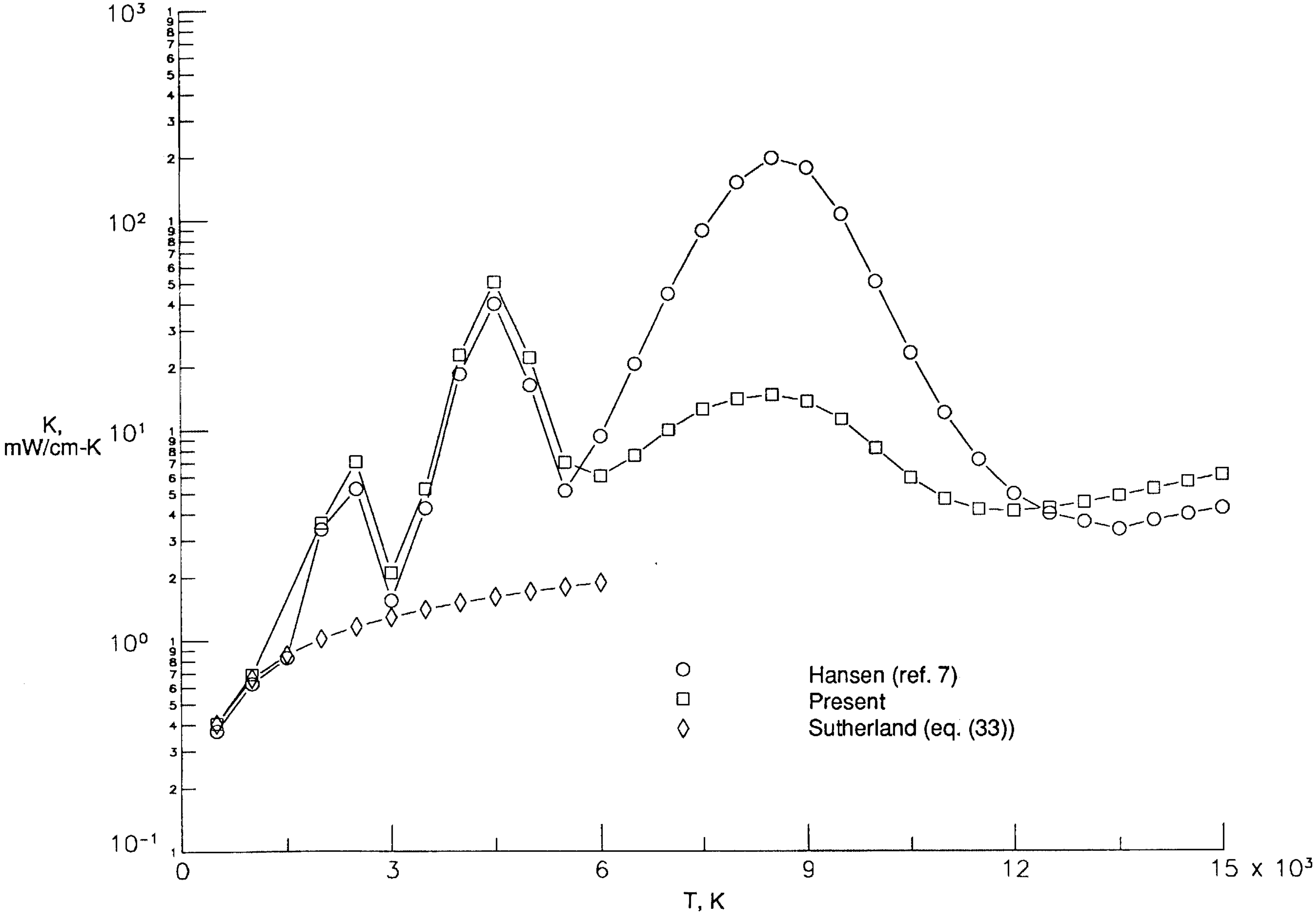
(b) $p = 10^{-4}$ atm.

Figure 13. Concluded.



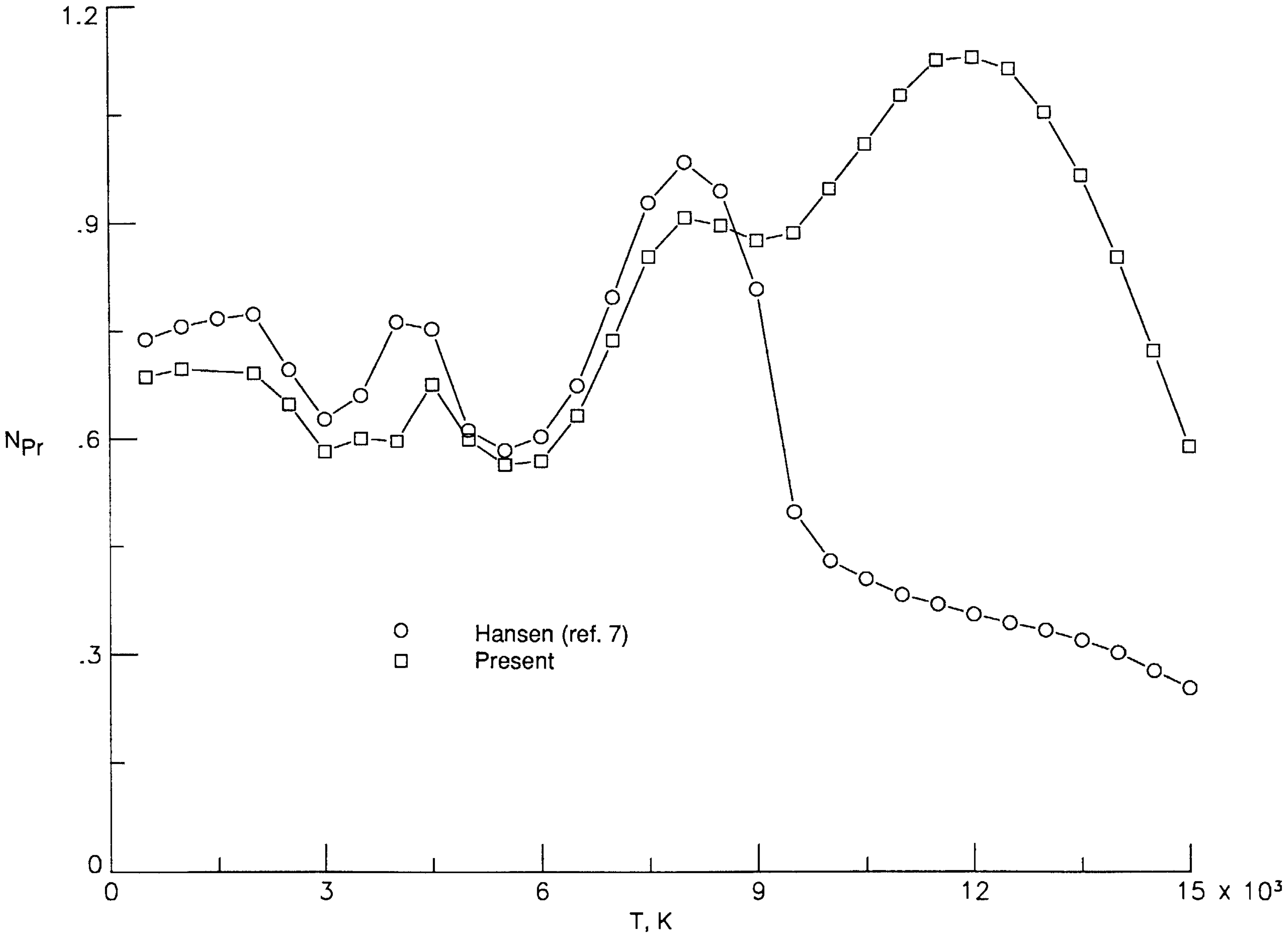
(a) $p = 10^0$ atm.

Figure 14. Comparison of total thermal conductivity values ($K = K_f + K_r$) from several sources for equilibrium air.



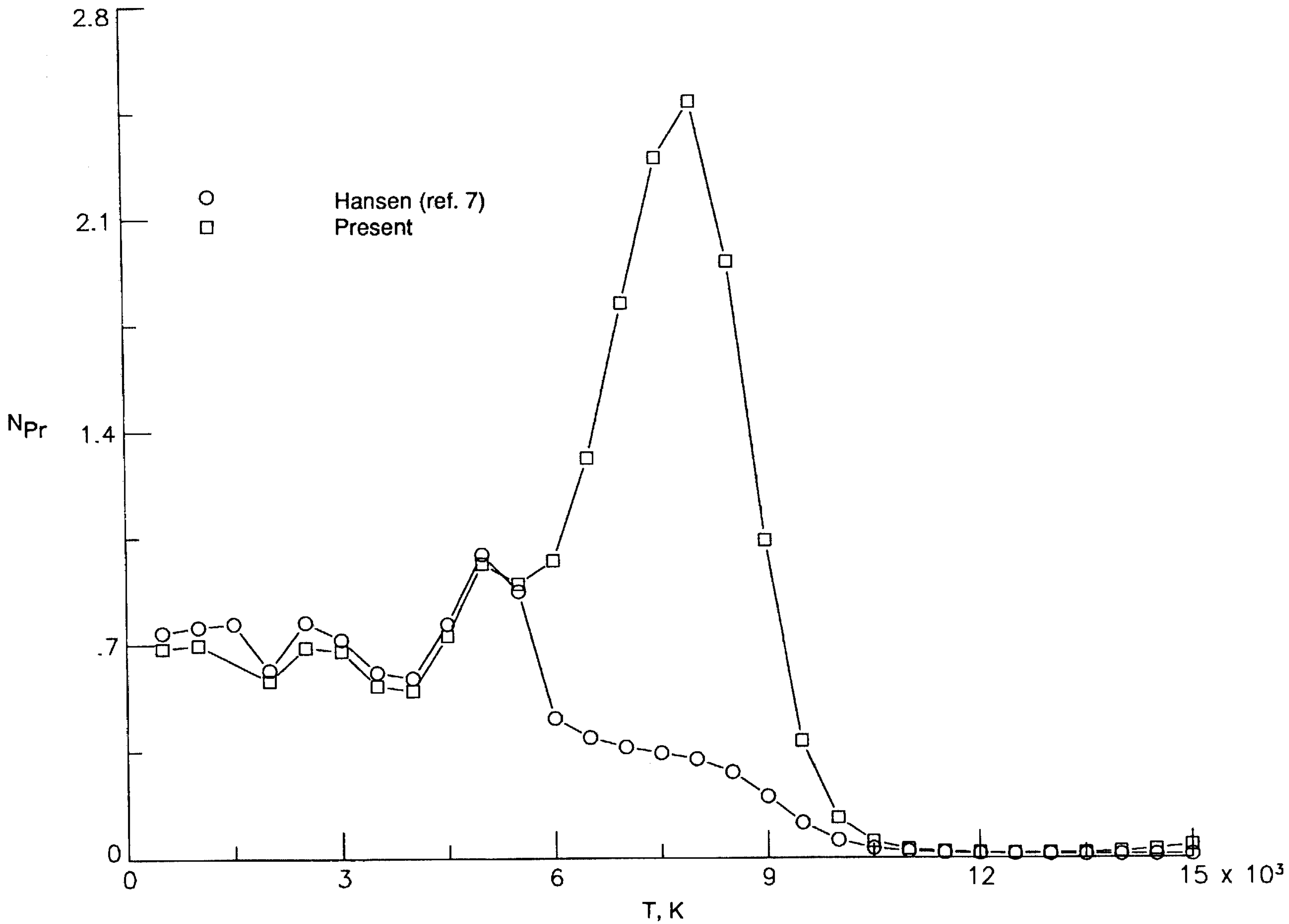
(b) $p = 10^{-4}$ atm.

Figure 14. Concluded.



(a) $p = 10^0$ atm.

Figure 15. Comparison of total Prandtl number values ($C_p\mu/K$) from reference 7 and present computations for equilibrium air.



(b) $p = 10^{-4}$ atm.

Figure 15. Concluded.

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16. Abstract
A self-consistent set of values have been computed for enthalpy, total specific heat at constant pressure, compressibility factor, viscosity, total thermal conductivity, and total Prandtl number of equilibrium air from 500 to 30 000 K over a pressure range of 10^{-4} to 10^{2} atm. Previous results for most of these properties are limited to a temperature of 15 000 K. The mixture values are calculated from the transport and thermodynamic properties of the individual species provided in a recent study by the present authors. The concentrations of the individual species, required in the mixture relations, are obtained from a free-energy-minimization calculation procedure. Present calculations are based on an 11-species air model ($O_2, N_2, O, N, NO, O^+, N^+, NO^+, O^{++}, N^{++}$, and e^-). For pressures less than 10^{-2} atm and temperatures of about 15 000 K and greater, the concentrations of N^{++} and O^{++} become important, and consequently they are included in the calculations for determining the various properties. The differences in the computed values given herein and those obtained by Hansen and Peng and Pindroh (both of which are based on temperatures to 15 000 K) may be attributed to the differences in the properties employed for the individual species, mixing laws used for the mixture, and (to a lesser degree) the number of chemical species considered in the mixture. Finally, all the computed properties are curve fit as a function of temperature at a constant value of pressure. These curve fits reproduce the computed values to within 5 percent for the entire temperature range considered at specific pressures and provide an efficient means for computing the flow-field properties of equilibrium air, provided the elemental composition remains constant at 0.24 for oxygen and 0.76 for nitrogen by mass.

17. Key Words (Suggested by Author(s))
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