

# Deep Water Liquid and Gas Properties

## 1. Introduction

This Jupyter notebook performs the calculations of the liquid and gas properties at pressures and temperatures that vary from the water surface to the deep ocean (3500 m depth and 1.5 °C temperature) for use in modeling bubble oscillations and sound production by fish swim bladders for the paper Mark W. Sprague, Michael L. Fine, and Timothy M. Cameron (2022), “An investigation of bubble resonance and its implications for sound production by deep-water fishes.” Julia version 1.7.2 was used for the calculations. Symbolic calculations use the SymPy package (which calls the Python SymPy package). Symbolic expressions are converted to Julia functions to calculate numerical values. For each parameter we calculate values for the warm surface (temperature 20 °C, salinity 35 g/kg), cold surface (temperature 1.5 °C, salinity 35 g/kg), and 3500 m deep (temperature 1.5 °C, salinity 35 g/kg) environments. We also calculate values a 1 m depth intervals for an ocean with constant temperature 1.5 °C and salinity 35 g/kg. The depth profile values required for our acoustic calculations are stored in dataframes in tabular form exported to CSV files. See the main paper for all references cited here.

This notebook uses the following Julia packages.

- SymPy - symbolic calculations.
- Roots - numerical root finding.
- DataFrames - store tabulated values in a dataframe for export.
- CSV - export dataframes with tabulated values into a CSV file.

Many of the symbolic calculations in this notebook produce long symbolic expressions as output. These expressions are many lines long (sometimes over a page long) and often do not fit within the page margins or screen size. Output from these expressions has been suppressed using a trailing semicolon (;). To view the output, delete the trailing semicolon before entering the input cell.

## 2. Initializations

Load the necessary packages and import the symbols defined by SymPy.

```
[1]: using SymPy, Roots, CSV, DataFrames
import_from(sympy)
```

## 3. Parameters

Define some parameters.

```
[2]: tcold = 1.5; # °C, cold water temperature
```

```
[3]: Tcold = tcold + 273.15; # K, cold water absolute temperature
```

```
[4]: sal = 35.0; # g/kg, salinity
```

```
[5]: ts = 20.0; # °C, warm surface temperature
```

```
[6]: Ts = 293.15; # K, warm surface absolute temperature
```

```
[7]: ps = 1.01325e5; # Pa, surface pressure
```

```
[8]: phi0 = 30.0 * pi/180; # degrees, latitude for gravitational acceleration  
      # term in pressure-depth calculations
```

```
[9]: dvals = 0:3500; # m, range of depth values for calculation
```

Note that the array `dvals` contains depths at 1 m intervals from 0 m to 3500 m. A depth `d` that is a whole number value in meters is at index `d + 1` in `dvals`. This is useful because we do not have to repeat indexed calculations based on `dvals` when we need values at specific depths.

For calculations a depths 1000 m and 2000 m, locate the `dvals` elements that represent these depths.

```
[10]: dvals[1001]
```

```
[10]: 1000
```

```
[11]: dvals[2001]
```

```
[11]: 2000
```

Initialize dataframes for storing tabulated parameter values. The dataframe `valso2` will hold the water and oxygen gas properties required for the acoustic calculations, and the dataframe `valsn2` will hold the water and nitrogen gas properties required for the acoustic calculations.

```
[12]: valso2 = DataFrame(depth=dvals);  
      valsn2 = DataFrame(depth=dvals);
```

## 4. Liquid Properties

These are the relations for the properties of the liquid (seawater).

Define some symbols.

```
[13]: @vars phi p P z S Sfrac t pPa
```

```
[13]: ( $\phi$ ,  $p$ ,  $P$ ,  $z$ ,  $S$ ,  $Sfrac$ ,  $t$ ,  $pPa$ )
```

### 4.1. Pressure vs. Depth

Pressure vs. depth relationship from Saunders and Fofonoff [52].

Define parameters used in calculation.

```
[14]: cd = [0.712953, 1.113e-7, -3.434e-12, 14190.7];
```

The expression below is for the effective gravitational acceleration in terms of the latitude angle  $\phi$ .

```
[15]: g0 = 9.780318 * (1 + 5.3024e-3 * sin(phi)^2 - 5.9e-6 * sin(2 * phi)^2) # m/s^2,  $\rho$   
      ↪gravitational acceleration
```

```
[15]: 0.0518591581632 sin^2(phi) - 5.77038762 * 10^-5 sin^2(2phi) + 9.780318
```

This is the gravitational acceleration at latitude  $\phi_0 = 30^\circ$  N.

```
[16]: g0(phi=>phi0)
```

```
[16]: 9.79323951163365
```

```
[17]: pg = p - ps # Pa, pressure gradient with surface
```

```
[17]: p - 101325.0
```

```
[18]: pdb = pg/10^4 # dbar, pressure in decibars; used to compare values in the reference
```

```
[18]:  $\frac{p}{10000}$  - 10.1325
```

```
[19]: yprime = 2.226e-6; # m s^-2 dbar^-1
```

We ignore the  $\Delta D$  term Eq. (4) in Saunders and Fofonoff [52] to use a standard ocean.

```
[20]:  $\Delta D = 0$ ; # Ignore this term.
```

This is Eq. (4) in Saunders and Fofonoff [52] with the pressure  $p$  in Pa.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[21]: zpeq = Eq(z, simplify(sum(((cd .* (pdb, pdb^2, pdb^3, log(1 + 1.83e-5 * pdb))) ./  
    ((100 * g0 + 1/2 * yprime * pdb) * 10^-3) .+  $\Delta D$  /  
    0.98)))));
```

Calculate depth for various pressure gradients to compare with the value in Table 1 in Saunders and Fofonoff [52].

```
[22]: zpeq(phi => phi0, p => 1.01325e5 + 500e4)
```

```
[22]: z = 496.013686442597
```

```
[23]: zpeq(phi => phi0, p => 1.01325e5 + 1000e4)
```

```
[23]: z = 990.88969207793
```

```
[24]: zpeq(phi => phi0, p => 1.01325e5 + 3000e4)
```

```
[24]: z = 2959.38223978458
```

```
[25]: zpeq(phi => phi0, p => 1.01325e5 + 4000e4)
```

```
[25]: z = 3937.26224667999
```

```
[26]: (3937.26224667999 - 3935.49)/3935.49 * 100
```

```
[26]: 0.045032427473836185
```

These values are consistent with the table to better than 0.05%, which is OK for our calculations.

Now create a Julia function we can solve numerically.

```
[27]: zpj1 = lambdify(lhs(zpeq) - rhs(zpeq),(phi, z, p))
```

```
[27]: #118 (generic function with 1 method)
```

The function psub gives the pressure at a given depth.

```
[28]: psub(phi, z, p0=100.e5) = find_zero(p1 -> zpj1(phi, z, p1), p0)
```

```
[28]: psub (generic function with 2 methods)
```

Create a Julia function that converts the calculated pressure to dbar so we can compare calculations to Table 1 in Saunders and Fofonoff [52].

```
[29]: pdbj1 = lambdify(pdb, (p,))
```

```
[29]: #118 (generic function with 1 method)
```

Now test this for some values in Table 1 in in Saunders and Fofonoff [52].

```
[30]: pdbj1(psub(phi0, 495.99))
```

```
[30]: 499.97609563134597
```

```
[31]: pdbj1(psub(phi0, 990.77))
```

```
[31]: 999.8789310233103
```

```
[32]: pdbj1(psub(30*pi/180, 2958.38))
```

```
[32]: 2998.9772647391114
```

```
[33]: pdbj1(psub(30*pi/180, 3935.49))
```

```
[33]: 3998.183851177998
```

```
[34]: (4000 - pdbj1(psub(30*pi/180, 3935.49))) / 4000 * 100
```

```
[34]: 0.04540372055005264
```

These values are also consistent with those in Table 1 in Saunders and Fofonoff [52] to better than 0.05%.

Create a table of pressures at the depths in dvals.

Warm surface pressure.

```
[35]: psub( $\phi_0$ , 0)
```

```
[35]: 101325.0
```

Cold surface pressure.

```
[36]: psub( $\phi_0$ , 0)
```

```
[36]: 101325.0
```

Pressure at depth 1000 m.

```
[37]: psub( $\phi_0$ , 1000)
```

```
[37]: 1.0193478046816997e7
```

Pressure at depth 2000 m.

```
[38]: psub( $\phi_0$ , 2000)
```

```
[38]: 2.0331946613939572e7
```

Deep water pressure.

```
[39]: psub( $\phi_0$ , 3500)
```

```
[39]: 3.562456759610306e7
```

```
[40]: ptab = map(d1 -> psub(30*pi/180, d1), dvals);
```

```
[41]: ptab[1], ptab[end]
```

```
[41]: (101325.0, 3.562456759610306e7)
```

Store these pressures in the two dataframes.

```
[42]: valso2.pressure = ptab;  
      valsn2.pressure = ptab;
```

## 4.2. Density

We calculate seawater density using Eqs. (7) from Sharqaway *et al.* [53].

Define the parameters in the equation.

```
[43]: arho = (9.992e2, 9.539e-2, -2.581e-5, 3.131e-5, -6.174e-8,  
            4.337e-1, 2.549e-5, -2.899e-7, 9.578e-10, 1.763e-3, -1.231e-4,  
            1.366e-6, 4.045e-9, -1.467e-5, 8.839e-7, -1.102e-9,  
            4.247e-11, -3.959e-14)
```

```
[43]: (999.2, 0.09539, -2.581e-5, 3.131e-5, -6.174e-8, 0.4337, 2.549e-5, -2.899e-7,
9.578e-10, 0.001763, -0.0001231, 1.366e-6, 4.045e-9, -1.467e-5, 8.839e-7,
-1.102e-9, 4.247e-11, -3.959e-14)
```

```
[44]: brho = (-7.999e-1, 2.409e-3, -2.581e-5, 6.856e-8,
6.298e-4, -9.363e-7)
```

```
[44]: (-0.7999, 0.002409, -2.581e-5, 6.856e-8, 0.0006298, -9.363e-7)
```

This is Eq. (7) from Sharqaway *et al.* [53]. Note that the pressure  $p$  is in MPa, and the temperature  $t$  is in °C. Note that the stated accuracy of this equation is  $\pm 2.5\%$ .

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[45]: psw = simplify(sum(arho .* (1, t, t^2, t^3, t^4, p, p*t^2, p*t^3,
p*t^4, p^2, p^2*t, p^2*t^2, p^2*t^3, p^3, p^3*t, p^3*t^2,
p^3*t^3, p^3*t^4)) - sum(brho .* (S, S*t, S*t^2, S*t^3, S*p,
S*p^2)));
```

```
[46]: psw(t=>15, p=>1.01325e5/1e6, S=>0)
```

```
[46]: 1000.77202240146
```

```
[47]: psw(t=>20, p=>1.01325e5/1e6, S=>35)
```

```
[47]: 1028.03294469513
```

```
[48]: psw(t=>tcold, p=>ptab[end]/1e6, S=>sal)
```

```
[48]: 1043.32748758591
```

These values are reasonable given the accuracy of the equation.

Create a Julia function to calculate seawater density.

```
[49]: pswjl = lambdaify(psw(p=>pPa/1e6), (t, pPa, S))
```

```
[49]: #118 (generic function with 1 method)
```

Warm surface density.

```
[50]: pswjl(ts, ptab[1], sal)
```

```
[50]: 1028.032944695128
```

Cold surface density.

```
[51]: pswjl(tcold, ptab[1], sal)
```

```
[51]: 1027.2569176419536
```

Density at depth 1000 m (dvals index 1001)

```
[52]: pswjl(tcold, ptab[1001], sal)
```

```
[52]: 1031.5655667337887
```

Density at depth 2000 m (dvals index 2001)

```
[53]: pswjl(tcold, ptab[2001], sal)
```

```
[53]: 1036.1412358223129
```

Deep water density

```
[54]: pswjl(tcold, ptab[end], sal)
```

```
[54]: 1043.3274875859083
```

Tabulate density values for the depths in dvals.

```
[55]: pswtab = map(p1 -> pswjl(tcold, p1, sal), ptab);
```

```
[56]: pswtab[1], pswtab[end]
```

```
[56]: (1027.2569176419536, 1043.3274875859083)
```

Add these values to the two dataframes.

```
[57]: valso2.water_density = pswtab  
      valsn2.water_density = pswtab;
```

### 4.3. Dynamic Viscosity

We calculate the dynamic viscosity of seawater using Eqs. (22) and (23) from Sharqaway *et al.* [53].

This is Eq. (23).

```
[58]: μw = 4.2844e-5 + (0.157*(t + 64.993)^2 - 91.296)^-1
```

```
[58]: 4.2844 · 10-5 +  $\frac{1}{663.182137693(0.0153862723677935t+1)^2 - 91.296}$ 
```

```
[59]: Aμ = 1.541 + 1.998e-2*t - 9.52e-5*t^2
```

```
[59]: -9.52 · 10-5t2 + 0.01998t + 1.541
```

```
[60]: Bμ = 7.974 - 7.561e-2*t + 4.724e-4*t^2
```

```
[60]: 0.0004724t2 - 0.07561t + 7.974
```

This is Eq. (22). The salinity value  $S_{\text{frac}}$  in the following equation is in kg/kg. We need to divide the traditional salinity in g/kg by 1000 to convert it.

Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.

```
[61]: μsw = μw*(1 + Amu*Sfrac + Bmu*Sfrac^2);
```

Create a Julia function for dynamic viscosity.

```
[62]: μswjl = lambdify(μsw(Sfrac=>S/1000), (t, S))
```

```
[62]: #118 (generic function with 1 method)
```

Warm surface value

```
[63]: μswjl(ts, sal)
```

```
[63]: 0.0010766289252529318
```

Cold surface value

```
[64]: μswjl(tcold, sal)
```

```
[64]: 0.0018115654847495556
```

Value at depth 1000 m

```
[65]: μswjl(tcold, sal)
```

```
[65]: 0.0018115654847495556
```

Value at depth 2000 m

```
[66]: μswjl(tcold, sal)
```

```
[66]: 0.0018115654847495556
```

Deep water value

```
[67]: μswjl(tcold, sal)
```

```
[67]: 0.0018115654847495556
```

This parameter only depends on temperature and salinity, which we are holding constant for this depth profile. Calculate the constant value and multiply it by the ones vector.

```
[68]: μswtab = μswjl(tcold, sal) .* ones(length(dvals));
```

Store these values in the dataframes.

```
[69]: valso2.water_dyn_viscosity = μswtab  
      valsn2.water_dyn_viscosity = μswtab;
```



#### 4.4. Surface Tension

We use Eqs. (27) and (28) from Sharqaway *et al.* [53] for the water surface tension.

This is Eq. (27).

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[70]:  $\sigma_w = 0.2358 * (1 - (t + 273.15)/647.096)^{1.256} * (1 - 0.625*(1 - (t + 273.15)/647.096));$ 
```

This is Eq. (38) solved for the seawater surface tension.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[71]:  $\sigma_{sw} = (1 + (0.000226*t + 0.00946) * \log(1 + 0.0331 * S)) * \sigma_w;$ 
```

Create a Julia function.

```
[72]:  $\sigma_{swjl} = \text{lambdify}(\sigma_{sw}, (t, S))$ 
```

```
[72]: #118 (generic function with 1 method)
```

Warm surface value

```
[73]:  $\sigma_{swjl}(ts, sal)$ 
```

```
[73]: 0.0735185195321562
```

Cold surface value

```
[74]:  $\sigma_{swjl}(tcold, sal)$ 
```

```
[74]: 0.07600619501340314
```

Value at depth 1000 m

```
[75]:  $\sigma_{swjl}(tcold, sal)$ 
```

```
[75]: 0.07600619501340314
```

Value at depth 2000 m

```
[76]:  $\sigma_{swjl}(tcold, sal)$ 
```

```
[76]: 0.07600619501340314
```

Deep water value

```
[77]:  $\sigma_{swjl}(tcold, sal)$ 
```

[77]: 0.07600619501340314

This parameter only depends on temperature and salinity, which we are holding constant for this depth profile. Calculate the constant value and multiply it by the ones vector.

```
[78]: oswtab = oswjl(tcold, sal) .* ones(length(dvals));
```

Add these values to the dataframes.

```
[79]: valso2.water_surface_tension = oswtab  
      valsn2.water_surface_tension = oswtab;
```

## 4.5. Sound Speed

We calculate sound speed from the UN equation in Wong and Zhu [54].

The parameter P is the pressure in bar. (1 bar = 105 Pa.)

Define the other parameters in the equation.

```
[80]: Asw = (  
      (1.389, -1.262e-2, 7.166e-5, 2.008e-6, -3.21e-8),  
      (9.4742e-5, -1.2583e-5, -6.4928e-8, 1.0515e-8, -2.0142e-10),  
      (-3.9064e-7, 9.1061e-9, -1.6009e-10, 7.994e-12),  
      (1.100e-10, 6.651e-12, -3.391e-13)  
      )
```

```
[80]: ((1.389, -0.01262, 7.166e-5, 2.008e-6, -3.21e-8), (9.4742e-5, -1.2583e-5,  
-6.4928e-8, 1.0515e-8, -2.0142e-10), (-3.9064e-7, 9.1061e-9, -1.6009e-10,  
7.994e-12), (1.1e-10, 6.651e-12, -3.391e-13))
```

```
[81]: Bsw = ((-1.922e-2, -4.42e-5), (7.3637e-5, 1.7950e-7))
```

```
[81]: ((-0.01922, -4.42e-5), (7.3637e-5, 1.795e-7))
```

```
[82]: Dsw = (1.727e-3, -7.9836e-6)
```

```
[82]: (0.001727, -7.9836e-6)
```

```
[83]: Cww = ((1402.388, 5.03830, -5.81090e-2, 3.3432e-4, -1.47797e-6,  
3.1419e-9), (0.153563, 6.8999e-4, -8.1829e-6, 1.3632e-7,  
-6.1260e-10), (3.1260e-5, -1.7111e-6, 2.5986e-8, -2.5353e-10,  
1.0415e-12), (-9.7729e-9, 3.8513e-10, -2.3654e-12))
```

```
[83]: ((1402.388, 5.0383, -0.058109, 0.00033432, -1.47797e-6, 3.1419e-9), (0.153563,  
0.00068999, -8.1829e-6, 1.3632e-7, -6.126e-10), (3.126e-5, -1.7111e-6,  
2.5986e-8, -2.5353e-10, 1.0415e-12), (-9.7729e-9, 3.8513e-10, -2.3654e-12))
```

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[84]: AtP = (sum(Asw[1] .* (1, t, t^2, t^3, t^4)) +
        sum(Asw[2] .* (1, t, t^2, t^3, t^4)) * P +
        sum(Asw[3] .* (1, t, t^2, t^3)) * P^2 + sum(Asw[4] .* (1, t, t^2)) * P^3);
```

```
[85]: BtP = sum(Bsw[1] .* (1, t)) + sum(Bsw[2] .* (1, t)) * P
```

```
[85]: P(1.795 · 10-7t + 7.3637 · 10-5) - 4.42 · 10-5t - 0.01922
```

```
[86]: DtP = sum(Dsw .* (1, P))
```

```
[86]: 0.001727 - 7.9836 · 10-6P
```

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[87]: CwtP = sum(Cww[1] .* (1, t, t^2, t^3, t^4, t^5)) + sum(Cww[2] .* (1,
        t, t^2, t^3, t^4)) * P + sum(Cww[3] .* (1, t, t^2, t^3, t^4)) *
        P^2 + sum(Cww[4] .* (1, t, t^2)) * P^3;
```

The following expression is the sound speed as a function of temperature, salinity, and pressure.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[88]: CStP = CwtP + AtP*S + BtP*S^(3/2) + DtP*S^2;
```

Create a Julia function with the pressure value in Pa.

```
[89]: CtSpjl = lambdify(CStP(P=>p/1e5),(t, S, p))
```

```
[89]: #118 (generic function with 1 method)
```

Warm surface value

```
[90]: CtSpjl(ts, sal, ptab[1])
```

```
[90]: 1521.6469588481918
```

Cold surface value

```
[91]: CtSpjl(tcold, sal, ptab[1])
```

```
[91]: 1456.0611774871181
```

Value at depth 1000 m (index 1001 in dvals)

```
[92]: CtSpjl(tcold, sal, ptab[1001])
```

```
[92]: 1472.6428237138698
```

Value at depth 2000 m (index 2001 in dvals)

```
[93]: CtSpjl(tcold, sal, ptab[2001])
```

```
[93]: 1489.5878214658405
```

Deep water value

```
[94]: CtSpjl(tcold, sal, ptab[end])
```

```
[94]: 1515.6224501126085
```

Calculate values for the depth profile.

```
[95]: ctab = map(p1 -> CtSpjl(tcold, sal, p1), ptab);
```

```
[96]: ctab[1], ctab[end]
```

```
[96]: (1456.0611774871181, 1515.6224501126085)
```

Add these values to the dataframes.

```
[97]: valso2.water_sound_speed = ctab  
      valsn2.water_sound_speed = ctab;
```

## 5. Gas Properties

```
[98]: R = 8.314510 # J mol^-1 K^-1, universal gas constant
```

```
[98]: 8.31451
```

### 5.1. Oxygen

We calculate oxygen densities, heat capacities, and sound speeds using the relationships from Schmidt and Wagner [56]. We calculate thermal conductivities using the relationships in Lemmon and Jacobsen [58]. We calculate thermal diffusivities using the relationship in Ainslie and Leighton [1].

Define some gas parameters used by Schmidt and Wagner [56].

```
[99]: M02 = 31.9988/1000; # kg, O2 Molar mass
```

```
[100]: T0 = 298.15; # K
```

```
[101]: p0 = 1.01325e5; # Pa
```

```
[102]: pc = 13.63e3; # mol/m3
```

```
[103]: Tc = 154.581; # K
```

```
[104]: δ0 = p0 / (R * T0 * pc);
```

```
[105]:  $\tau_0 = T_c / T_0;$ 
```

Define variables used in symbolic calculations.

```
[106]: @vars  $\delta \tau T \rho M$ 
```

```
[106]: ( $\delta, \tau, T, \rho, M$ )
```

Define the coefficients in the equations.

```
[107]: no2 = (0.3983768749, -0.1846157454e1, 0.4183473197, 0.2370620711e-1,  
0.9771730573e-1, 0.3017891294e-1, 0.2273353212e-1,  
0.1357254086e-1, -0.4052698943e-1, 0.5454628515e-3,  
0.5113182277e-3, 0.2953466883e-6, -0.8687645072e-4,  
-0.2127082589, 0.8735941958e-1, 0.1275509190, -0.9067701064e-1,  
-0.3540084206e-1, -0.3623278059e-1, 0.1327699290e-1,  
-0.3254111865e-3, -0.8313582932e-2, 0.2124570559e-2,  
-0.8325206232e-3, -0.2626173276e-4, 0.2599581482e-2,  
0.9984649663e-2, 0.2199923153e-2, -0.2591350486e-1,  
-0.1259630848, 0.1478355637, -0.1011251078e-1)
```

```
[107]: (0.3983768749, -1.846157454, 0.4183473197, 0.02370620711, 0.09771730573,  
0.03017891294, 0.02273353212, 0.01357254086, -0.04052698943, 0.0005454628515,  
0.0005113182277, 2.953466883e-7, -8.687645072e-5, -0.2127082589, 0.08735941958,  
0.127550919, -0.09067701064, -0.03540084206, -0.03623278059, 0.0132769929,  
-0.0003254111865, -0.008313582932, 0.002124570559, -0.0008325206232,  
-2.626173276e-5, 0.002599581482, 0.009984649663, 0.002199923153, -0.02591350486,  
-0.1259630848, 0.1478355637, -0.01011251078)
```

```
[108]: kko2 = (-0.740775e-3, -0.664930e-4, 0.250042e1, -0.214487e2,  
0.101258e1, -0.944365, 0.145066e2, 0.749148e2, 0.414817e1)
```

```
[108]: (-0.000740775, -6.6493e-5, 2.50042, -21.4487, 1.01258, -0.944365, 14.5066,  
74.9148, 4.14817)
```

```
[109]: ro2 = (1, 1, 1, 2, 2, 2, 3, 3, 3, 6, 7, 7, 8, 1, 1, 2, 2, 3, 3, 5, 6,  
7, 8, 10, 2, 3, 3, 4, 4, 5, 5, 5)
```

```
[109]: (1, 1, 1, 2, 2, 2, 3, 3, 3, 6, 7, 7, 8, 1, 1, 2, 2, 3, 3, 5, 6, 7, 8, 10, 2, 3,  
3, 4, 4, 5, 5, 5)
```

```
[110]: so2 = (0, 1.5, 2.5, -0.5, 1.5, 2, 0, 1, 2.5, 0, 2, 5, 2, 5, 6, 3.5,  
5.5, 3, 7, 6, 8.5, 4, 6.5, 5.5, 22, 11, 18, 11, 23, 17, 18, 23)
```

```
[110]: (0, 1.5, 2.5, -0.5, 1.5, 2, 0, 1, 2.5, 0, 2, 5, 2, 5, 6, 3.5, 5.5, 3, 7, 6, 8.5,  
4, 6.5, 5.5, 22, 11, 18, 11, 23, 17, 18, 23)
```

The following is Eq. (15) in Schmidt and Wagner [56] with  $\Phi^{id}$  changed to  $\alpha_0$ .

Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.

```
[111]: α0 = (kko2[1]*τ^1.5 + kko2[2]*τ^-2 + kko2[3]*log(τ) + kko2[4]*τ +
          kko2[5]*log(exp(kko2[7]*τ) - 1) + kko2[6]*log(1 +
          2/3*exp(-kko2[8]*τ)) + kko2[9] + log(6/60));
```

The following is Eq (11) in Lemmon and Jacobsen [58] with  $\Phi^r$  changed to  $\alpha r$ .

Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.

```
[112]: αr = (
          sum(map(m -> no2[m] * δ^ro2[m] * τ^so2[m], 1:13)) +
          exp(-δ^2) *
          sum(map(m -> no2[m] * δ^ro2[m] * τ^so2[m], 14:24)) +
          exp(-δ^4) *
          sum(map(m -> no2[m] * δ^ro2[m] * τ^so2[m], 25:32))
        );
```

### 5.1.1. Density

Find the molar density from the root of Eq. (A1) in Schmidt and Wagner [56]. The term  $\rho$  in this equation is molar density with SI unit mol/m<sup>3</sup>.

Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.

```
[113]: peq = Eq(ρ, ρ * R * T * (1 + δ * diff(αr, δ)))(δ => ρ/ρc, τ => Tc/T);
```

Create a Julia function that we can use to find roots numerically.

```
[114]: peqjl = lambdify(lhs(peq) - rhs(peq), (ρ, T, ρ))
```

```
[114]: #118 (generic function with 1 method)
```

Now create a function that numerically finds a root for the density at a given value of pressure and temperature.

```
[115]: ρo2(ρ, T, ρ0=24000.0) = find_zero(ρ1 -> peqjl(ρ, T, ρ1), ρ0)
```

```
[115]: ρo2 (generic function with 2 methods)
```

Now we comparing to densities tabulated by Weber [57] for O<sub>2</sub>.

Find the density at  $p = 700$  bar (or  $700 \times 10^5$  Pa) and  $T = 270$  K.

```
[116]: ρo2(700e5, 270)
```

```
[116]: 22886.84924777297
```

The Weber [57] gives a volume of 1.3657 cm<sup>3</sup>/g at this pressure and temperature (Table VIa). Convert this to density in mol/m<sup>3</sup>.

```
[117]: (1/(1.3657 #= cm^3/g =#) * (1 #= kg =# / 1000 #= g =#) *
        (1 / M02 #= kg/mol =#) * (100 #= cm =# / 1 #= m =#)^3 )
```

```
[117]: 22882.89662367062
```

The calculated value is consistent to 4 significant figures. This is good.

Now find the density at  $p = 700$  bar (or  $700 \times 10^5$  Pa) and  $T = 300$  K.

```
[118]: po2(700e5, 300)
```

```
[118]: 20920.324839551213
```

Weber [57] gives a volume of 1.4941 cm<sup>3</sup>/g (Table VIa). Convert this to density in mol/m<sup>3</sup>.

```
[119]: (1/(1.4941 #= cm^3/g =#) * (1 #= kg =# / 1000 #= g =#) *
        (1 / M02 #= kg/mol =#) * (100 #= cm =# / 1 #= m =#)^3 )
```

```
[119]: 20916.385729835325
```

This also agrees to four significant figures.

Now tabulate mass density values by multiplying each molar density by the molar mass.

```
[120]: po2tab = map(p1 -> po2(p1, Tcold) * M02, ptab);
```

The values below are the mass densities for oxygen at the cold surface, depth 1000 m, depth 2000 m, and depth 3500 m.

```
[121]: po2tab[1], po2tab[1001], po2tab[2001], po2tab[end]
```

```
[121]: (1.4211670046377123, 154.7115917256005, 314.00236160237546, 500.93121320697526)
```

### 5.1.2. Isochoric Heat Capacity $c_v$

The following is Eq. (A6) from Schmidt and Wagner [56].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[122]: cv = -τ^2 * (diff(α0, τ, τ) + diff(αr, τ, τ)) * R;
```

Substitute the values of  $\delta$  and  $\tau$  in terms of molar density and temperature.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[123]: cv(δ => ρ/ρc, τ => Tc/T);
```

Define a Julia function for calculations.

```
[124]: cvjl = lambdify(cv(δ => ρ/ρc, τ => Tc/T), (ρ, T))
```

```
[124]: #118 (generic function with 1 method)
```

Calculate some values.

```
[125]: cvjl(po2(700e5, 270), 270)
```

```
[125]: 23.898882530084624
```

Define another Julia function that uses an input pressure and temperature to calculate the needed density value.

```
[126]: cvpTo2(p, T) = cvjl(po2(p, T), T)
```

```
[126]: cvpTo2 (generic function with 1 method)
```

```
[127]: cvpTo2(1e5, 300)
```

```
[127]: 21.078866720527625
```

```
[128]: cvpTo2(1e5, 270)
```

```
[128]: 20.95584051862463
```

Weber [57] reports specific heat  $C_v$  values in J/(g K). Get these by dividing the `cvpTo2` values by the molar mass in g, which is  $1000 M_{O2}$ .

```
[129]: cvpTo2(10e5, 300) / (1000 * MO2)
```

```
[129]: 0.660918602988702
```

```
[130]: cvpTo2(25e5, 300) / (1000 * MO2)
```

```
[130]: 0.6644992914305471
```

These values are very close to Weber's results. They begin to diverge at higher pressures.

```
[131]: cvpTo2(300e5, 300) / (1000 * MO2)
```

```
[131]: 0.7089086969553833
```

### 5.1.3. Isobaric Heat Capacity $c_p$

Use Eq. (A7) from Schmidt and Wagner [56] to calculate  $c_p$ .

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*



```
[132]: cp = (cv + (1 + δ * diff(αr, δ) - δ * τ *  
diff(αr, δ, τ))^2 / (1 + 2 * δ * diff(αr, δ) +  
δ^2 * diff(αr, δ, δ)) * R);
```

Define a Julia function to calculate values.

```
[133]: cpjl = lambdify(cp(δ => ρ/ρc, τ => Tc/T),(ρ, T))
```

```
[133]: #118 (generic function with 1 method)
```

Define another Julia function that uses an input pressure and temperature to calculate the needed density value.

```
[134]: cppTo2(p, T) = cpjl(ρo2(p, T), T)
```

```
[134]: cppTo2 (generic function with 1 method)
```

Calculate some values.

```
[135]: cppTo2(1e5, 300)
```

```
[135]: 29.435205927984697
```

```
[136]: cppTo2(1e5, 300) / (1000 * M02)
```

```
[136]: 0.9198846809250565
```

Weber [57] reports specific heat  $C_p$  values in J/(g K). Get these by dividing the `cppTo2` values by the molar mass in g, which is `1000 M02`.

```
[137]: cppTo2(10e5, 300) / (1000 * M02)
```

```
[137]: 0.9340227201860647
```

```
[138]: cppTo2(25e5, 300) / (1000 * M02)
```

```
[138]: 0.9582613365905686
```

These values are very close to Weber's results. They begin to diverge at higher pressures.

```
[139]: cppTo2(300e5, 300) / (1000 * M02)
```

```
[139]: 1.3072282411638052
```

#### 5.1.4. Ratio of Specific Heats $\gamma$

Use the values of the two specific heats to calculate  $\gamma = c_p/c_v$ .

```
[140]: γo2(p, T) = cppTo2(p, T) / cvpTo2(p, T)
```

[140]: `yo2` (generic function with 1 method)

Warm surface value

```
[141]: yo2(ptab[1], Ts)
```

[141]: 1.3971781560134038

Cold surface value

```
[142]: yo2(ptab[1], Tcold)
```

[142]: 1.398953943344819

Value at depth 1000 m (index 1001 in `dvals`)

```
[143]: yo2(ptab[1001], Tcold)
```

[143]: 1.6680921647387352

Value at depth 2000 m (index 2001 in `dvals`)

```
[144]: yo2(ptab[2001], Tcold)
```

[144]: 1.8968036632857108

Deep water value

```
[145]: yo2(ptab[end], Tcold)
```

[145]: 1.9497207685437572

Calculate values for the depth profile.

```
[146]: yo2tab = map(p1 -> yo2(p1, Tcold), ptab);
```

```
[147]: yo2tab[1], yo2tab[1001], yo2tab[2001], yo2tab[end]
```

[147]: (1.398953943344819, 1.6680921647387352, 1.8968036632857108, 1.9497207685437572)

Add these values to the dataframe.

```
[148]: valso2.gamma = yo2tab;
```

### 5.1.5. Sound Speed

Use Eq. (A8) from Schmidt and Wagner [56] to calculate the sound speed in oxygen.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[149]: w = sqrt( R * T / M * (1 + 2 * δ * diff(αr, δ) + δ^2 * diff(αr, δ, δ) -  
    (1 + δ * diff(αr, δ) - δ * τ * diff(αr, δ, τ))^2 / (τ^2 *  
    (diff(α0, τ, τ) + diff(αr, τ, τ))));
```

Define a Julia function.

```
[150]: wjl = lambdify(w(δ => ρ/ρc, τ => Tc/T),(ρ, T, M))
```

```
[150]: #118 (generic function with 1 method)
```

Define a function of pressure and temperature as before.

```
[151]: wpT(p, T) = wjl(ρo2(p, T), T, M02)
```

```
[151]: wpT (generic function with 1 method)
```

```
[152]: wpT(300e5, 300)
```

```
[152]: 415.3954022737472
```

This value is similar to that of Weber [57].

Warm surface value

```
[153]: wpT(ptab[1], Ts)
```

```
[153]: 325.9996893882054
```

Cold surface value

```
[154]: wpT(ptab[1], Tcold)
```

```
[154]: 315.66916929963963
```

Value at depth 1000 m (index 1001 in dvals)

```
[155]: wpT(ptab[1001], Tcold)
```

```
[155]: 322.7128276738636
```

Value at depth 2000 m (index 2001 in dvals)

```
[156]: wpT(ptab[2001], Tcold)
```

```
[156]: 358.2715926515373
```

Deep water value

```
[157]: wpT(ptab[end], Tcold)
```

```
[157]: 447.86433243536436
```

Tabulate values for depth profile.

```
[158]: wo2tab = map(p1 -> wpT(p1, Tcold), ptab);
```

```
[159]: wo2tab[1], wo2tab[1001], wo2tab[2001], wo2tab[end]
```

```
[159]: (315.66916929963963, 322.7128276738636, 358.2715926515373, 447.86433243536436)
```

### 5.1.6. Viscosity

Use the relationships from Lemmon and Jacobsen [58].

Define parameters and coefficients.

```
[160]: pc = 5.043e6; # Pa
```

```
[161]: bi = (0.431, -0.4623, 0.08406, 0.005341, -0.00331);
```

The following is the collision integral required for Eq. (2) in Lemmon and Jacobsen [58].

```
[162]: Ω(Tstar) = exp(sum(bi[i+1] * (log(Tstar))^i for i in 0:4))
```

```
[162]: Ω (generic function with 1 method)
```

```
[163]: eoverk = 118.5 # K
```

```
[163]: 118.5
```

```
[164]: Ω(300/eoverk)
```

```
[164]: 1.0788836619239601
```

```
[165]: σvis = 0.3428e-9
```

```
[165]: 3.428e-10
```

The following is Eq. (2) from Lemmon and Jacobsen [58] with the constants adjusted so all values are in SI units. The resulting value is in Pa s.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[166]: η0 = 0.0266958e-24 * sqrt(1000 * M * T) / (σvis^2*Ω(T/eoverk));
```

The following parameters are needed for Eq. (3) in Lemmon and Jacobsen [58].

```
[167]: Nvis = (17.67, 0.4042, 0.0001077, 0.3510, -13.67)
```

```
[167]: (17.67, 0.4042, 0.0001077, 0.351, -13.67)
```

```
[168]: tvis = (0.05, 0, 2.10, 0, 0.5)
```

```
[168]: (0.05, 0, 2.1, 0, 0.5)
```

```
[169]: dvis = (1, 5, 12, 8, 1)
```

```
[169]: (1, 5, 12, 8, 1)
```

```
[170]: lvis = (0, 0, 0, 1, 2)
```

```
[170]: (0, 0, 0, 1, 2)
```

This is Eq. (3) in Lemmon and Jacobsen [58].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[171]: ηr = 10^-6 * sum(Nvis[i] * τ^tvis[i] * δ^dvis[i] *  
    exp(lvis[i] == 0 ? 0 : -δ^lvis[i]) for i in 1:5);
```

This is Eq. (1) in Lemmon and Jacobsen [58]. The viscosity of oxygen is  $\eta$ .

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[172]: η = η0 + ηr;
```

Define a Julia function.

```
[173]: ηjl = lambdify(η(δ => ρ/ρc, τ => Tc/T), (ρ, T, M))
```

```
[173]: #118 (generic function with 1 method)
```

Calculate some values to compare with Lemmon and Jacobsen [58].

```
[174]: ηjl(5e3, 300, M02) * 1e6
```

```
[174]: 23.757700201413066
```

```
[175]: ηjl(35e3, 100, M02) * 1e6
```

```
[175]: 172.13579729510082
```

```
[176]: ηjl(10e3, 200, M02) * 1e6
```

```
[176]: 22.44451567141834
```

These values are consistent with the values in Lemmon and Jacobsen [58].

Define a function of pressure and temperature.

```
[177]: ηpT(p, T) = ηjl(ρo2(p, T), T, M02)
```

```
[177]: ηpT (generic function with 1 method)
```

Warm surface value

```
[178]: ηpT(ptab[1], Ts)
```

```
[178]: 2.027266881737361e-5
```

Cold surface value

```
[179]: ηpT(ptab[1], Tcold)
```

```
[179]: 1.9229098582802137e-5
```

Value at depth 1000 m (dvals index 1001)

```
[180]: ηpT(ptab[1001], Tcold)
```

```
[180]: 2.2091576792708548e-5
```

Value at depth 2000 m (dvals index 2001)

```
[181]: ηpT(ptab[2001], Tcold)
```

```
[181]: 2.726127656589478e-5
```

Deep water value

```
[182]: ηpT(ptab[end], Tcold)
```

```
[182]: 3.692230187855806e-5
```

Calculate values for the depth profile.

```
[183]: ηo2tab = map(p1 -> ηpT(p1, Tcold), ptab);
```

```
[184]: ηo2tab[1], ηo2tab[1001], ηo2tab[2001], ηo2tab[end]
```

```
[184]: (1.9229098582802137e-5, 2.2091576792708548e-5, 2.726127656589478e-5,  
3.692230187855806e-5)
```

### 5.1.7. Thermal Conductivity

Use the relationships from Lemmon and Jacobsen [58].

Define the coefficients for the calculations (Table IV in Lemmon and Jacobsen [58]).

```
[185]: Ncon = (1.036, 6.283, -4.262, 15.31, 8.898, -0.7336,  
6.728, -4.374, -0.4747)
```

```
[185]: (1.036, 6.283, -4.262, 15.31, 8.898, -0.7336, 6.728, -4.374, -0.4747)
```

The first term in the list below is for  $i = 2$ .

```
[186]: tcon = (-0.9, -0.6, 0, 0, 0.3, 4.3, 0.5, 1.8)
```

```
[186]: (-0.9, -0.6, 0, 0, 0.3, 4.3, 0.5, 1.8)
```

The first term in the list below is for  $i = 4$ .

```
[187]: dcon = (1, 3, 4, 5, 7, 10)
```

```
[187]: (1, 3, 4, 5, 7, 10)
```

The first term in the list below is for  $i = 4$ .

```
[188]: lcon = (0, 0, 0, 2, 2, 2)
```

```
[188]: (0, 0, 0, 2, 2, 2)
```

The equation below is Eq. (5) in Lemmon and Jacobsen [58] adjusted so all parameters are in SI units.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[189]: λ0 = 10^-3 * (Ncon[1] * (η0 / 10^-6) + Ncon[2] * τ^tcon[2 - 1] + Ncon[3]*τ^tcon[3 - 1]);
```

Define a Julia function for calculations.

```
[190]: λ0jl = lambdify(λ0(τ=>Tc/T), (T, M))
```

```
[190]: #118 (generic function with 1 method)
```

Compare symbolic and Julia function calculations.

```
[191]: N(λ0(τ=>Tc/T, M=>M02) (T=>100))
```

```
[191]: 0.008943340238199921795214540684620835839186806243358885993985347078141679335627  
102
```

```
[192]: λ0jl(100, M02)
```

```
[192]: 0.008943340238199926
```

```
[193]: N(λ0(τ=>Tc/T, M=>M02) (T=>300))
```

```
[193]: 0.026440301365016987601270266915169642137333227786556723239898346838396525273494  
83
```

```
[194]: λ0jl(300, M02)
```

```
[194]: 0.026440301365017002
```

These are consistent.

This is Eq. (6) in Lemmon and Jacobsen [58].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[195]: λr = 10^-3 * sum( Ncon[i] * τ^tcon[i - 1] * δ^dcon[i - 3] * exp(lcon[i - 3] == 0 ? 0 : -δ^lcon[i - 3]) for i in 4:9);
```

Define a Julia function for this.

```
[196]: λrjl = lambdify(λr(δ => ρ/ρc, τ => Tc/T), (ρ, T))
```

```
[196]: #118 (generic function with 1 method)
```

Compare symbolic and Julia function values.

```
[197]: N(λr(δ => ρ/ρc, τ => Tc/T)(ρ => ρ2tab[end], T=>Tcold))
```

```
[197]: 0.0005631153755697235
```

```
[198]: λrjl(ρ2tab[end], Tcold)
```

```
[198]: 0.0005631153755697235
```

These are consistent.

In order to calculate  $\lambda^c$  in Eq. (7) in Lemmon and Jacobsen [58], we must calculate the parameters in Eqs. (8-11).

First, we define some of the parameters in these equations.

```
[199]: ξ0 = 0.24e-9 # m
```

```
[199]: 2.4e-10
```

```
[200]: ρc = 5.043e6 # Pa
```

```
[200]: 5.043e6
```

```
[201]: ρc = 13.63e3 # mol/m^3
```

```
[201]: 13630.0
```

We need  $\left(\frac{\partial \rho}{\partial p}\right)_T$ . Use the equation of state from Eq. (A1) in Schmidt and Wagner [56] to get  $\left(\frac{\partial p}{\partial \rho}\right)_T$ , and invert it.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[202]: dpdp = diff(ρ * R * T * (1 + δ * diff(αr, δ))(δ => ρ/ρc, τ => Tc/T), ρ);
```



$\left(\frac{\partial \rho}{\partial p}\right)_T$  is the reciprocal of the previous result.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[203]: dpdp = 1/dpdp;
```

The following is Eq. (11) from Lemmon and Jacobsen [58].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[204]: χn = pc * ρ/ρc^2 * dpdp;
```

Calculate some values to test this.

```
[205]: χn(ρ => 15654, T => 309.162)
```

```
[205]: 0.100290882386026
```

```
[206]: N(χn(ρ => 15654, T => 309.162))
```

```
[206]: 0.10029088238602606
```

Compare the symbolic calculations above to values calculated by a Julia function.

```
[207]: lambdify(χn(T=>309.162), (ρ,))(15654)
```

```
[207]: 0.1016422565742757
```

```
[208]: lambdify(χn, (ρ,T))(BigFloat("15654."), BigFloat("309.162"))
```

```
[208]: 0.100290882386026026561986816030949345798372149081095358519805036184306650964384
```

```
[209]: convert(Float64, lambdify(χn, (ρ,T))(BigFloat("15654."), BigFloat("309.162")))
```

```
[209]: 0.10029088238602603
```

There is a significant loss in precision when we go to a Julia floating point calculation from the symbolic calculation. We are going to have to use BigFloat (extended precision) numbers in Julia for  $\chi_n$  and the parameters that depend on it.

Define a Julia function.

```
[210]: χnjl = lambdify(χn, (ρ,T))
```

```
[210]: #118 (generic function with 1 method)
```

Define some more needed parameters.

```
[211]: Γ = 0.055
```

```
[211]: 0.055
```

```
[212]: v = 0.63
```

```
[212]: 0.63
```

```
[213]:  $\gamma_{tc} = 1.2415$ 
```

```
[213]: 1.2415
```

```
[214]: Tref = 309.162 # K
```

```
[214]: 309.162
```

Compare some symbolic and Julia calculations to make sure everything is consistent.

```
[215]: N( $\chi_n(\rho \Rightarrow \rho_2(\text{ptab}[\text{end}], T_{\text{cold}}), T \Rightarrow T_{\text{cold}})$ )
```

```
[215]: 0.12908846305731383
```

```
[216]:  $\chi_{nj\ell}(\text{BigFloat}(\rho_2(\text{ptab}[\text{end}], T_{\text{cold}})), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[216]: 0.129088463057313870706571123749547161889231947922284239137986742847161896906720  
7
```

```
[217]: N( $\chi_n(\rho \Rightarrow \rho_2(\text{ptab}[\text{end}], T_{\text{ref}}), T \Rightarrow T_{\text{ref}})$ )
```

```
[217]: 0.1042176516484715
```

```
[218]:  $\chi_{nj\ell}(\text{BigFloat}(\rho_2(\text{ptab}[\text{end}], T_{\text{ref}})), \text{BigFloat}(T_{\text{ref}}))$ 
```

```
[218]: 0.104217651648471459600972432808902764535549691366036930550613313060397595730888  
1
```

The values above are consistent.

This is Eq. (10) in Lemmon and Jacobsen [58]. We define it here as a symbolic function (which produces a SymPy expression).

```
[219]:  $\xi(\rho_1, T_1) = \xi_0 * ((\chi_n(\rho \Rightarrow \rho_1, T \Rightarrow T_1)) -$   
       $(\chi_n(\rho \Rightarrow \rho_1, T \Rightarrow T_{\text{ref}})) * (T_{\text{ref}}/T_1)) /$   
       $\Gamma^{(v/\gamma_{tc})}$ 
```

```
[219]:  $\xi$  (generic function with 1 method)
```

Define a Julia function for this.

```
[220]:  $\xi_{j\ell}(\rho_1, T_1) = \xi_0 * ((\chi_{nj\ell}(\rho_1, T_1)) - (\chi_{nj\ell}(\rho_1, T_{\text{ref}})) * (T_{\text{ref}}/T_1)) / \Gamma^{(v/\gamma_{tc})}$ 
```

```
[220]:  $\xi_{j\ell}$  (generic function with 1 method)
```

Compare symbolic and Julia floating point calculations.

```
[221]: N(ξ(po2tab[end], Tcold), Tcold)
```

```
[221]: 1.2906193451956456e-10
```

```
[222]: N(ξ(po2tab[end]/M02, Tcold))
```

```
[222]: 1.2906193451956456e-10
```

```
[223]: ξjl(po2tab[end]/M02, Tcold)
```

```
[223]: 1.2906193451956505e-10
```

These are consistent.

Define some more parameters.

```
[224]: R0 = 1.01
```

```
[224]: 1.01
```

```
[225]: k = 1.380658e-23 # J/K
```

```
[225]: 1.380658e-23
```

```
[226]: qD = 0.51e-9 # m
```

```
[226]: 5.1e-10
```

The following is Eq. (8) in Lemmon and Jacobsen [58].

```
[227]: Ωn(ρ1, T1) = (2/π * ((cp - cv) / cp * atan(ξ(ρ1, T1) /  
    qD) + cv / cp * ξ(ρ1, T1) / qD)(δ => ρ/ρc,  
    τ => Tc/T))(ρ => ρ1, T => T1)
```

```
[227]: Ωn (generic function with 1 method)
```

Define a Julia function for this using the Julia functions for the parameters.

```
[228]: Ωnjl(ρ1, T1) = 2/π * ((cpjl(ρ1, T1) - cvjl(ρ1, T1)) /  
    cpjl(ρ1, T1) * atan(ξjl(ρ1, T1) /  
    qD) + cvjl(ρ1, T1) / cpjl(ρ1, T1) * ξjl(ρ1, T1) / qD)
```

```
[228]: Ωnjl (generic function with 1 method)
```

Compare symbolic and Julia calculations.

```
[229]: N(Ωn(po2tab[end]/M02, Tcold))
```

```
[229]: 0.1594910300518962
```

```
[230]: Ωnjl(po2tab[end]/M02, Tcold)
```

[230]: 0.15949103005189677

These are consistent.

The following is Eq. (9) in Lemmon and Jacobsen [58].

```
[231]: Ω0n(ρ1, T1) = (2 / π * (1 - exp(-1 / ((ξ(ρ1, T1) /
    qD)^-1 + 1/3 * (ξ(ρ1, T1) / qD)^2 * (ρc /
    ρ)^2))) (δ => ρ/ρc, τ => Tc/T) (ρ => ρ1, T => T1)
```

[231]: Ω0n (generic function with 1 method)

Define a Julia function for this using the Julia functions for the parameters.

```
[232]: Ω0nj1(ρ1, T1) = 2 / π * (1 - exp(-1 / ((ξj1(ρ1, T1) /
    qD)^-1 + 1/3 * (ξj1(ρ1, T1) / qD)^2 * (ρc /
    ρ1)^2)))
```

[232]: Ω0nj1 (generic function with 1 method)

Compare symbolic and Julia calculations.

```
[233]: N(Ω0n(po2tab[end]/M02, Tcold))
```

[233]: 0.14182550739186106

```
[234]: Ω0nj1(po2tab[end]/M02, Tcold)
```

[234]: 0.14182550739186153

These are consistent.

The following expression is Eq. (7) in Lemmon and Jacobsen [58].

```
[235]: λc(ρ1, T1) =
    if (((χn(ρ => ρ1, T => T1)) - (χn(ρ => ρ1, T =>
        Tref)) * (Tref / T1)) / Γ) > 0
        ((ρ * cp * k * R0 * T1 / (6 * π * ξ(ρ1, T1) * η)
            * (Ωn(ρ1, T1) - Ω0n(ρ1, T1))) (δ =>
            ρ/ρc, τ => Tc/T) (ρ => ρ1, T => T1)
        else
            0
        end
```

[235]: λc (generic function with 1 method)

Define a Julia function for this using the Julia functions for the parameters.

```
[236]: function λcj1(ρ1, T1)
    if (((χnj1(ρ1, T1) - (χnj1(ρ1, Tref)) * (Tref / T1)) / Γ) > 0
        ρ1 * cpj1(ρ1, T1) * k * R0 * T1 / (6 * π * ξj1(ρ1, T1) * nj1(ρ1, T1, M02)) *
```

```

        (Ωnjl(ρ1, T1) - Ω0njl(ρ1, T1))
    else
        0
    end
end
end

```

[236]: λcjl (generic function with 1 method)

Compare symbolic and Julia calculations.

[237]: N(λc(po2tab[end]/M02, Tcold)(M=>M02))

[237]: 0.000530703253670222412185176359432321554010875723549134702061466374871540787203  
1297

[238]: λcjl(po2tab[end]/M02, Tcold)

[238]: 0.0005307032536702239

These are consistent.

The following expression is Eq. (4) in Lemmon and Jacobsen [58].

[239]: λ(ρ1, T1) = ((λ0 + λr + λc(ρ1, T1))(δ => ρ/ρc, τ => Tc/T))(ρ => ρ1, T => T1, M => M02)

[239]: λ (generic function with 1 method)

Define a Julia function for this using the Julia functions for the parameters.

[240]: λjl(ρ1, T1) = λ0jl(T1, M02) + λrjl(ρ1, T1) + λcjl(ρ1, T1)

[240]: λjl (generic function with 1 method)

Compare symbolic and Julia calculations.

[241]: N(λ(po2tab[end]/M02, Tcold))

[241]: 0.052752955444510433116782046173814225875561385886768640156582006584237111928273  
48

[242]: λjl(po2tab[end]/M02, Tcold)

[242]: 0.05275295544451044

[243]: λjl(BigFloat(po2tab[end]/M02), BigFloat(Tcold))

[243]: 0.052752955444510435097040430296883057002664877990561645179916718569370718665817  
93

The values calculated above are consistent, but for more extreme parameters, we must use BigFloat (extended precision) number in the Julia calculations to get accurate results.

Compare some more symbolic and Julia values.

```
[244]: N( $\lambda$ (5000, 300))
```

```
[244]: 0.032549088189674745272177722669106169298009244690226531900219840205313025037267  
71
```

```
[245]:  $\lambda$ l(BigFloat(5000), BigFloat(300))
```

```
[245]: 0.032549088189674749235256888276931301378206660675632141193947198318837028272821  
74
```

```
[246]: N( $\lambda$ (10000, 200))
```

```
[246]: 0.034612415901784129551773222073790642974803219930639791353203080869332307171466  
17
```

```
[247]:  $\lambda$ l(BigFloat(10000), BigFloat(200))
```

```
[247]: 0.034612415901784122184802622661381821097952670781125652531965929828868437874540  
69
```

```
[248]: patm = pO2(1.01325e5, 293.15)
```

```
[248]: 41.60020299418699
```

```
[249]: N( $\lambda$ (patm, 293.15))
```

```
[249]: 0.025945926563591421676302437731400475809614162580656869029161562201909570993281  
45
```

Now produce some values to compare to Table V in Lemmon and Jacobsen [58].

```
[250]: N( $\lambda$ (0, 300))
```

```
[250]: 0.026440301365016994529222664434908377718385018837462810152056658015696900130742  
98
```

```
[251]:  $\lambda$ l(BigFloat(0), BigFloat(300))
```

```
[251]: 0.026440301365016998365289370818460662631949267650210060547467109782879850939401  
15
```

```
[252]: N( $\lambda$ (0, 100))
```

```
[252]: 0.008943340238199923166633864347394669058215070422100077280135001759203942532086  
278
```

```
[253]:  $\lambda$ l(BigFloat(0), BigFloat(100))
```

[253]: 0.008943340238199925337625265804124263106635902622932240632661182972401388976083  
374

```
[254]: N( $\lambda$ (35000, 100))
```

[254]: 0.146043656556208452248396112217241429353546548540996561655135001759203942532085  
9

```
[255]:  $\lambda$ jl(BigFloat(35000), BigFloat(100))
```

[255]: 0.146043656556208443823510753481335979183520080951624906434250968639307823456408  
2

```
[256]: N( $\lambda$ (10000, 200))
```

[256]: 0.034612415901784129551773222073790642974803219930639791353203080869332307171466  
17

```
[257]:  $\lambda$ jl(BigFloat(10000), BigFloat(200))
```

[257]: 0.034612415901784122184802622661381821097952670781125652531965929828868437874540  
69

```
[258]: N( $\lambda$ (13600, 154.6))
```

[258]: 0.377493283921180614173728928008880130130253783216826432126167366457387350576113  
2

```
[259]:  $\lambda$ jl(BigFloat(13600), BigFloat(154.6))
```

[259]: 0.377493283920058371625745005351224170932222930290024722551244938730566568268531  
9

These values are consistent.

Produce a Julia function of pressure and temperature.

```
[260]:  $\lambda$ o2pT(p1, T1) =  $\lambda$ jl( $\rho$ o2(p1, T1), T1)
```

[260]:  $\lambda$ o2pT (generic function with 1 method)

Warm surface value

```
[261]:  $\lambda$ o2pT(BigFloat(ptab[1]), BigFloat(Ts))
```

[261]: 0.025945926563591425501461687379475476392469688171268793962554713231377103501947  
19

Cold surface value

```
[262]: λo2pT(BigFloat(ptab[1]), BigFloat(Tcold))
```

```
[262]: 0.024470498314774661002674012752178651275263451258327204003829477523948090263620  
71
```

Value at depth 1000 m (dvals index 1001)

```
[263]: λo2pT(BigFloat(ptab[1001]), BigFloat(Tcold))
```

```
[263]: 0.030377400104053634025203664127849429020382439472413429588153815786206409205391  
84
```

Value at depth 2000 m (dvals index 2001)

```
[264]: λo2pT(BigFloat(ptab[2001]), BigFloat(Tcold))
```

```
[264]: 0.038893942408249203598977578907682186575172363603088298316963006729574767391846  
74
```

Deep water value

```
[265]: λo2pT(BigFloat(ptab[end]), BigFloat(Tcold))
```

```
[265]: 0.052752955444510427850000692062504067249589219155402483190331162606499152333250  
96
```

Calculate values for the depth profile.

```
[266]: λo2tab = map(p -> convert(Float64, λo2pT(BigFloat(p), BigFloat(Tcold))), ptab);
```

```
[267]: λo2tab[1], λo2tab[1001], λo2tab[2001], λo2tab[end]
```

```
[267]: (0.02447049831477466, 0.030377400104053633, 0.038893942408249206,  
0.052752955444510426)
```

### 5.1.8. Thermal Diffusivity

Use the thermal diffusivity definition in Ainslie and Leighton [1].

```
[268]: α(ρ1, T1) = ((λ(ρ1, T1) / (ρ1 * cp))(δ => ρ/ρc, τ => Tc/T))(ρ => ρ1, T => T1, M => M02)
```

```
[268]: α (generic function with 1 method)
```

Calculate a value. Recall that the `po2tab` array is a mass density. We must divide it by molar mass `M02` to get molar density.

```
[269]: N(α(po2tab[end]/M02, Tcold))
```

```
[269]: 7.48721949540435454051145588758847426971599006032218430054735763972069438917396e  
-08
```



Define a Julia function.

```
[270]:  $\alpha_{jl}(\rho_1, T_1) = \lambda_{jl}(\rho_1, T_1) / (\rho_1 * c_{pj}(\rho_1, T_1))$ 
```

```
[270]:  $\alpha_{jl}$  (generic function with 1 method)
```

```
[271]:  $\alpha_{jl}(\text{BigFloat}(\rho_{2\text{tab}}[\text{end}]/M_02), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[271]: 7.487219495404364329811396921172735904625033812475985565163462702756592086379079  
e-08
```

```
[272]:  $\alpha_{2pT}(\rho_1, T_1) = \alpha_{jl}(\rho_2(\rho_1, T_1), T_1)$ 
```

```
[272]:  $\alpha_{2pT}$  (generic function with 1 method)
```

```
[273]:  $\alpha_{2pT}(\text{BigFloat}(p_{\text{tab}}[\text{end}]), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[273]: 7.487219495404364865532554975198480907690881770854359231836399180562323383626429  
e-08
```

Warm surface value

```
[274]:  $\alpha_{2pT}(\text{BigFloat}(p_{\text{tab}}[1]), \text{BigFloat}(T_s))$ 
```

```
[274]: 2.120985841493112653296219166693105071621395430111438146683085448897844454307706  
e-05
```

Cold surface value

```
[275]:  $\alpha_{2pT}(\text{BigFloat}(p_{\text{tab}}[1]), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[275]: 1.877973098323995278124008176810104328920435150793272695302657778424528852338461  
e-05
```

Value at depth 1000 m (dvals index 1001)

```
[276]:  $\alpha_{2pT}(\text{BigFloat}(p_{\text{tab}}[1001]), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[276]: 1.719742443384715854418450771641508186342003600288733110583327019015409320791956  
e-07
```

Value at depth 2000 m (dvals index 2001)

```
[277]:  $\alpha_{2pT}(\text{BigFloat}(p_{\text{tab}}[2001]), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[277]: 9.264192554939795735130225941054086882870839425383077380518022707172419462590197  
e-08
```

Deep water value

```
[278]:  $\alpha_{2pT}(\text{BigFloat}(p_{\text{tab}}[\text{end}]), \text{BigFloat}(T_{\text{cold}}))$ 
```

```
[278]: 7.487219495404364865532554975198480907690881770854359231836399180562323383626429
e-08
```

```
[279]: α2tab = map(p -> convert(Float64, α2pT(BigFloat(p), BigFloat(Tcold))),
ptab);
```

```
[280]: α2tab[1], α2tab[1001], α2tab[2001], α2tab[end]
```

```
[280]: (1.8779730983239953e-5, 1.7197424433847157e-7, 9.264192554939795e-8,
7.487219495404365e-8)
```

```
[281]: valso2.thermal_diffusivity = α2tab;
```

### 5.1.9. Export Oxygen Parameters

We have all the needed oxygen parameters in `valso2`. Export them to a CSV file.

Here are the column names.

```
[282]: names(valso2)
```

```
[282]: 8-element Vector{String}:
 "depth"
 "pressure"
 "water_density"
 "water_dyn_viscosity"
 "water_surface_tension"
 "water_sound_speed"
 "gamma"
 "thermal_diffusivity"
```

Reorder the dataframe columns to match the order that the acoustic calculations require.

```
[283]: select!(valso2, ["depth", "water_density", "pressure", "water_dyn_viscosity",
"water_surface_tension", "water_sound_speed",
"thermal_diffusivity", "gamma"]);
```

```
[284]: CSV.write("DeepWaterProperties02.csv", valso2)
```

```
[284]: "DeepWaterProperties02.csv"
```

## 5.2. Nitrogen

We calculate nitrogen densities, heat capacities, and sound speeds using the relationships from Span *et al.* [55]. We calculate thermal conductivities using the relationships in Lemmon and Jacobsen [58]. We calculate thermal diffusivities using the relationship in Ainslie and Leighton [1].

Define some gas parameters from Span *et al.* [55].

Make sure `R` is defined.

```
[285]: R = 8.314510; # J mol^-1 K^-1, universal gas constant
```

```
[286]: MN2 = 28.01348/1000; # kg, nitrogen molar mass
```

Define variables used in symbolic calculations.

```
[287]: @vars δ τ ρ T M
```

```
[287]: (δ, τ, ρ, T, M)
```

Define the coefficients for Eq. (53) in Span *et al.* [55].

```
[288]: a = (2.5, -12.76952708, -0.00784163, -1.934819e-4, -1.247742e-5,  
6.678326e-8, 1.012941, 26.65788)
```

```
[288]: (2.5, -12.76952708, -0.00784163, -0.0001934819, -1.247742e-5, 6.678326e-8,  
1.012941, 26.65788)
```

This is Eq. (53) in Span *et al.* [55].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[289]: α0 = log(δ) + a[1] * log(τ) + a[2] + a[3] * τ +  
a[4] * τ^-1 + a[5] * τ^-2 + a[6] * τ^-3 +  
a[7] * log(1 - exp(-a[8] * τ));
```

The following parameters are from Table 17 in Span *et al.* [55].

```
[290]: nk = (0.924803575275, -0.492448489428, 0.661883336938,  
-0.192902649201e1, -0.622469309629e-1, 0.349943957581,  
0.564857472498, -0.161720005987e1, -0.481395031883,  
0.421150636384, -0.161962230825e-1, 0.172100994165,  
0.735448924933e-2, 0.168077305479e-1, -0.107626664179e-2,  
-0.137318088513e-1, 0.635466899859e-3, 0.304432279419e-2,  
-0.435762336045e-1, -0.723174889316e-1, 0.389644315272e-1,  
-0.212201363910e-1, 0.408822981509e-2, -0.551990017948e-4,  
-0.462016716479e-1, -0.300311716011e-2, 0.368825891208e-1,  
-0.255856846220e-2, 0.896915264558e-2, -0.441513370350e-2,  
0.133722924858e-2, 0.264832491957e-3, 0.196688194015e2,  
-0.209115600730e2, 0.167788306989e-1, 0.262767566274e4)
```

```
[290]: (0.924803575275, -0.492448489428, 0.661883336938, -1.92902649201,  
-0.0622469309629, 0.349943957581, 0.564857472498, -1.61720005987,  
-0.481395031883, 0.421150636384, -0.0161962230825, 0.172100994165,  
0.00735448924933, 0.0168077305479, -0.00107626664179, -0.0137318088513,  
0.000635466899859, 0.00304432279419, -0.0435762336045, -0.0723174889316,  
0.0389644315272, -0.021220136391, 0.00408822981509, -5.51990017948e-5,  
-0.0462016716479, -0.00300311716011, 0.0368825891208, -0.0025585684622,
```

0.00896915264558, -0.0044151337035, 0.00133722924858, 0.000264832491957,  
19.6688194015, -20.911560073, 0.0167788306989, 2627.67566274)

[291]: `ik = (1, 1, 2, 2, 3, 3, 1, 1, 1, 3, 3, 4, 6, 6, 7, 7, 8, 8, 1, 2, 3,  
4, 5, 8, 4, 5, 5, 8, 3, 5, 6, 9, 1, 1, 3, 2)`

[291]: (1, 1, 2, 2, 3, 3, 1, 1, 1, 3, 3, 4, 6, 6, 7, 7, 8, 8, 1, 2, 3, 4, 5, 8, 4, 5,  
5, 8, 3, 5, 6, 9, 1, 1, 3, 2)

[292]: `jk = (0.25, 0.875, 0.5, 0.875, 0.375, 0.75, 0.5, 0.75, 2, 1.25, 3.5,  
1, 0.5, 3, 0, 2.75, 0.75, 2.5, 4, 6, 6, 3, 3, 6, 16, 11, 15, 12,  
12, 7, 4, 16, 0, 1, 2, 3)`

[292]: (0.25, 0.875, 0.5, 0.875, 0.375, 0.75, 0.5, 0.75, 2, 1.25, 3.5, 1, 0.5, 3, 0,  
2.75, 0.75, 2.5, 4, 6, 6, 3, 3, 6, 16, 11, 15, 12, 12, 7, 4, 16, 0, 1, 2, 3)

[293]: `lk = (0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2,  
2, 2, 2, 3, 3, 3, 3, 4, 4, 4, 4, 2, 2, 2, 2)`

[293]: (0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2,  
3, 3, 4, 4, 4, 4, 2, 2, 2, 2)

The following parameters are from Table 18 in Span *et al.* [55]. The first  $\phi$ ,  $\beta$ , and  $\gamma$  indices in the equation are each 33. these are the first terms below.

[294]: `phi_k = (20, 20, 15, 25)`

[294]: (20, 20, 15, 25)

[295]: `beta_k = (325, 325, 300, 275)`

[295]: (325, 325, 300, 275)

[296]: `gamma_k = (1.16, 1.16, 1.13, 1.25)`

[296]: (1.16, 1.16, 1.13, 1.25)

This is Eq (55) from Span *et al.* [55].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

[297]: `ar = sum(nk[k] * delta^ik[k] * tau^jk[k] for k in 1:6) +  
sum(nk[k] * delta^ik[k] * tau^jk[k] * exp(-delta^lk[k])  
for k in 7:32) + sum(nk[k] * delta^ik[k] * tau^jk[k] *  
exp(-phi_k[k - 32] * (delta - 1)^2 - beta_k[k - 32] * (tau -  
gamma_k[k - 32])^2) for k in 33:36);`

Define the critical temperature and density.

```
[298]: Tc = 126.192; # K
```

```
[299]: ρc = 11.1839e3; # mol/m^3
```

### 5.2.1. Density

This is Eq. (56) from Span *et al.* [55].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[300]: peq = Eq(p, ρ * R * T * (1 + δ * diff(αr, δ))(δ => p/ρc, τ => Tc/T));
```

Create a Julia function that we can use to find roots numerically.

```
[301]: peqjl = lambdify(lhs(peq) - rhs(peq), (p, T, ρ))
```

```
[301]: #118 (generic function with 1 method)
```

Now create a function that numerically finds a root for the density at a given value of pressure and temperature.

```
[302]: pn2(p, T, ρ0=24000.0) = find_zero(ρ1 -> peqjl(p, T, ρ1), ρ0)
```

```
[302]: pn2 (generic function with 2 methods)
```

Now compare to densities from Span *et al.* [55] N2 data. Find the density at  $p = 75$  Mbar ( $750 \times 10^5$  Pa) and  $T = 270$  K.

```
[303]: pn2(750e5, 270)
```

```
[303]: 19395.841644638156
```

Now find the density at  $p = 75$  Mbar ( $750 \times 10^5$  Pa) and  $T = 300$  K.

```
[304]: pn2(750e5, 300)
```

```
[304]: 18053.5804495223
```

These values are consistent.

Warm surface values

```
[305]: pn2(ptab[1], Ts)
```

```
[305]: 41.58105951222148
```

```
[306]: pn2(ptab[1], Ts) * MN2
```

```
[306]: 1.1648301790244262
```

Cold surface values

```
[307]: pn2(ptab[1], Tcold)
```

```
[307]: 44.39057228867911
```

```
[308]: pn2(ptab[1], Tcold) * MN2
```

```
[308]: 1.2435344089974665
```

Values at depth 1000 m (dvals index 1001)

```
[309]: pn2(ptab[1001], Tcold)
```

```
[309]: 4524.56749585226
```

```
[310]: pn2(ptab[1001], Tcold) * MN2
```

```
[310]: 126.74888105370738
```

Values at depth 2000 m (dvals index 2001)

```
[311]: pn2(ptab[2001], Tcold)
```

```
[311]: 8578.084713569095
```

```
[312]: pn2(ptab[2001], Tcold) * MN2
```

```
[312]: 240.30200456187356
```

Deep water values

```
[313]: pn2(ptab[end], Tcold)
```

```
[313]: 13047.278015394078
```

```
[314]: pn2(ptab[end], Tcold) * MN2
```

```
[314]: 365.4996617386817
```

Now tabulate mass density values for the depth profile by multiplying each molar density by the molar mass.

```
[315]: pn2tab = map(p1 -> pn2(p1, Tcold) * MN2, ptab);
```

```
[316]: pn2tab[1], pn2tab[1001], pn2tab[2001], pn2tab[end]
```

```
[316]: (1.2435344089974665, 126.74888105370738, 240.30200456187356, 365.4996617386817)
```

### 5.2.2. Isochoric Heat Capacity $c_v$

The following is Eq. (62) from Span *et al.* [55].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[317]: cv = -τ^2 * (diff(α0, τ, 2) + diff(αr, τ, 2)) * R;
```

Define a Julia function for calculations.

```
[318]: cvjl = lambdify(cv(δ => ρ/ρc, τ => Tc/T), (ρ, T))
```

```
[318]: #118 (generic function with 1 method)
```

Define a function of pressure and temperature.

```
[319]: cvpTn2(p, T) = cvjl(pn2(p, T), T)
```

```
[319]: cvpTn2 (generic function with 1 method)
```

Calculate some values and compare with Span *et al.* [55].

```
[320]: cvpTn2(0.2e6, 290)
```

```
[320]: 20.82243462328305
```

```
[321]: cvpTn2(75e6, 270)
```

```
[321]: 23.810136385096367
```

These values are consistent.

Warm surface value

```
[322]: cvpTn2(ptab[1], Ts)
```

```
[322]: 20.81602794850762
```

Cold surface value

```
[323]: cvpTn2(ptab[1], Tcold)
```

```
[323]: 20.81106217231203
```

Value at depth 1000 m (dvals index 1001)

```
[324]: cvpTn2(ptab[1001], Tcold)
```

```
[324]: 21.575464252247457
```

Value at depth 2000 m (dvals index 2001)

```
[325]: cvpTn2(ptab[2001], Tcold)
```

```
[325]: 22.104361935551182
```

Deep water value

```
[326]: cvpTn2(ptab[end], Tcold)
```

```
[326]: 22.655294332204793
```

### 5.2.3. Isobaric Heat Capacity $c_p$

The following is Eq. (63) from Span *et al.* [55].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[327]: cp = (cv + (1 + δ * diff(αr, δ) - δ * τ *  
diff(αr, δ, τ))^2 / (1 + 2 * δ * diff(αr, δ) +  
δ^2 * diff(αr, δ, δ)) * R);
```

Define a Julia function to calculate values.

```
[328]: cpjl = lambdify(cp(δ => ρ/ρc, τ => Tc/T), (ρ, T))
```

```
[328]: #118 (generic function with 1 method)
```

Define another Julia function that uses an input pressure and temperature to calculate the needed density value.

```
[329]: cppTn2(p, T) = cpjl(ρn2(p, T), T)
```

```
[329]: cppTn2 (generic function with 1 method)
```

Calculate some values.

```
[330]: cppTn2(0.2e6, 290)
```

```
[330]: 29.21999613937129
```

```
[331]: cppTn2(75e6, 270)
```

```
[331]: 39.36103974887872
```

These values are consistent with Span *et al.* [55].

Warm surface value

```
[332]: cppTn2(ptab[1], Ts)
```

```
[332]: 29.171517219967
```



Cold surface value

```
[333]: cppTn2(ptab[1], Tcold)
```

```
[333]: 29.173417101590708
```

Value at depth 1000 m (dvals index 1001)

```
[334]: cppTn2(ptab[1001], Tcold)
```

```
[334]: 34.778572361839494
```

Value at depth 2000 m (dvals index 2001)

```
[335]: cppTn2(ptab[2001], Tcold)
```

```
[335]: 38.42633485169769
```

Deep water value

```
[336]: cppTn2(ptab[end], Tcold)
```

```
[336]: 39.87145571233225
```

#### 5.2.4. Ratio of Specific Heats $\gamma$

Use the values of the two specific heats to calculate  $\gamma = c_p/c_v$ .

```
[337]: yn2(p, T) = cppTn2(p, T) / cvpTn2(p, T)
```

```
[337]: yn2 (generic function with 1 method)
```

Warm surface value

```
[338]: yn2(ptab[1], Ts)
```

```
[338]: 1.4013969087728102
```

Cold surface value

```
[339]: yn2(ptab[1], Tcold)
```

```
[339]: 1.4018225912757267
```

Value at depth 1000 m (dvals index 1001)

```
[340]: yn2(ptab[1001], Tcold)
```

```
[340]: 1.6119501279429806
```

Value at depth 2000 m (dvals index 2001)

```
[341]: yn2(ptab[2001], Tcold)
```

```
[341]: 1.7384050697204398
```

Deep water value

```
[342]: yn2(ptab[end], Tcold)
```

```
[342]: 1.7599177979186287
```

Calculate values for the depth profile.

```
[343]: yn2tab = map(p1 -> yn2(p1, Tcold), ptab);
```

```
[344]: yn2tab[1], yn2tab[1001], yn2tab[2001], yn2tab[end]
```

```
[344]: (1.4018225912757267, 1.6119501279429806, 1.7384050697204398, 1.7599177979186287)
```

Add these values to the dataframe.

```
[345]: valsn2.gamma = yn2tab;
```

### 5.2.5. Sound Speed

The following expression is Eq. (64) from Span *et al.* [55].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[346]: w = sqrt( R * T / M * (1 + 2 * δ * diff(αr, δ) + δ^2 * diff(αr, δ, δ) -  
    (1 + δ * diff(αr, δ) - δ * τ * diff(αr, δ, τ))^2 / (τ^2 *  
    (diff(α0, τ, τ) + diff(αr, τ, τ))));
```

Define a Julia function.

```
[347]: wjl = lambdify(w(δ => ρ/ρc, τ => Tc/T),(ρ, T, M))
```

```
[347]: #118 (generic function with 1 method)
```

Define a function of pressure and temperature as before.

```
[348]: wpT(p, T) = wjl(ρn2(p, T), T, MN2)
```

```
[348]: wpT (generic function with 1 method)
```

Check values for 0.2 MPa

```
[349]: wpT(0.2e6, 290)
```

```
[349]: 347.3589765325666
```

Check values for 75 MPa and 270 K.

```
[350]: wpT(75e6, 270)
```

```
[350]: 749.3016933093184
```

These are consistent with Span *et al.* [55].

Warm surface value

```
[351]: wpT(ps, Ts)
```

```
[351]: 349.1044228816854
```

Cold surface value

```
[352]: wpT(ps, Tcold)
```

```
[352]: 337.89465634739565
```

Value at depth 1000 m (dvals index 1001)

```
[353]: wpT(ptab[1001], Tcold)
```

```
[353]: 363.76133310795603
```

Value at depth 2000 m (dvals index 2001)

```
[354]: wpT(ptab[2001], Tcold)
```

```
[354]: 416.69020841364494
```

Deep water value

```
[355]: wpT(ptab[end], Tcold)
```

```
[355]: 517.0273889822301
```

Tabulate values for depth profile.

```
[356]: wn2tab = map(p1 -> wpT(p1, Tcold), ptab);
```

```
[357]: wn2tab[1], wn2tab[1001], wn2tab[2001], wn2tab[end]
```

```
[357]: (337.89465634739565, 363.76133310795603, 416.69020841364494, 517.0273889822301)
```

### 5.2.6. Viscosity

Use the relationships from Lemmon and Jacobsen [58].

```
[358]: pc = 3.3958e6; # Pa
```

The following parameters were defined in the oxygen section above. We reuse them here.

[359]: `bi`

[359]: (0.431, -0.4623, 0.08406, 0.005341, -0.00331)

[360]: `Ω(T)`

[360]: 
$$\frac{1.53879554995687e^{-0.00331 \log(T)^4 + 0.005341 \log(T)^3 + 0.08406 \log(T)^2}}{T^{0.4623}}$$

Define some other needed parameters.

[361]: `eoverk = 98.94 # K`

[361]: 98.94

[362]: `Ω(300/eoverk)`

[362]: 1.0241852717016806

[363]: `σvis = 0.3656e-9`

[363]: 3.656e-10

The following is Eq. (2) from Lemmon and Jacobsen [58] with the constants adjusted so all values are in SI units. The resulting value is in Pa s.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

[364]: `η0 = 0.0266958e-24 * sqrt(1000 * M * T) / (σvis^2 * Ω(T/eoverk));`

Calculate a value for  $T = 300$  K.

[365]: `N(η0(T=>300, M=>MN2))`

[365]: 1.787706414600966559101560198695408335590729400220960251909887121698465030839747  
e-05

These are the parameters in Table III in Lemmon and Jacobsen [58].

[366]: `Nvis = (10.72, 0.03989, 0.001208, -7.402, 4.620)`

[366]: (10.72, 0.03989, 0.001208, -7.402, 4.62)

[367]: `tvis = (0.1, 0.25, 3.2, 0.9, 0.3)`

[367]: (0.1, 0.25, 3.2, 0.9, 0.3)

[368]: `dvis = (2, 10, 12, 2, 1)`

[368]: (2, 10, 12, 2, 1)

```
[369]: lvis = (0, 1, 1, 2, 3)
```

```
[369]: (0, 1, 1, 2, 3)
```

This is Eq. (3) in Lemmon and Jacobsen [58].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[370]: ηr = 10^-6 * sum(Nvis[i] * τ^tvis[i] * δ^dvis[i] *  
    exp(lvis[i] == 0 ? 0 : -δ^lvis[i]) for i in 1:5);
```

This is Eq. (1) in Lemmon and Jacobsen [58]. The viscosity of oxygen is  $\eta$ .

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[371]: η = η0 + ηr;
```

Define a Julia function.

```
[372]: ηjl = lambdify(η(δ => ρ/ρc, τ => Tc/T), (ρ, T, M))
```

```
[372]: #118 (generic function with 1 method)
```

Calculate some values to compare with Lemmon and Jacobsen [58].

```
[373]: 1e6 * ηjl(5e3, 300, MN2)
```

```
[373]: 20.743041742625184
```

```
[374]: 1e6 * ηjl(25e3, 100, MN2)
```

```
[374]: 79.7417506134048
```

```
[375]: 1e6 * ηjl(10e3, 200, MN2)
```

```
[375]: 21.081044490030866
```

These values are consistent with the values in Lemmon and Jacobsen [58].

Define a function of pressure and temperature.

```
[376]: ηpT(ρ, T) = ηjl(ρn2(ρ, T), T, MN2)
```

```
[376]: ηpT (generic function with 1 method)
```

Warm surface value

```
[377]: ηpT(ps, Ts)
```

```
[377]: 1.7572933092983353e-5
```

Cold surface value

```
[378]: ηpT(ps, Tcold)
```

```
[378]: 1.6700484916609287e-5
```

Value at depth 1000 m (dvals index 1001)

```
[379]: ηpT(ptab[1001], Tcold)
```

```
[379]: 1.9183615129628023e-5
```

Value at depth 2000 m (dvals index 2001)

```
[380]: ηpT(ptab[2001], Tcold)
```

```
[380]: 2.31078724711162e-5
```

Deep water value

```
[381]: ηpT(ptab[end], Tcold)
```

```
[381]: 2.982149636014933e-5
```

Calculate values for the depth profile.

```
[382]: ηn2tab = map(p1 -> ηpT(p1, Tcold), ptab);
```

```
[383]: ηn2tab[1], ηn2tab[1001], ηn2tab[2001], ηn2tab[end]
```

```
[383]: (1.6700484916609287e-5, 1.9183615129628023e-5, 2.31078724711162e-5,  
2.982149636014933e-5)
```

### 5.2.7. Thermal Conductivity

Use the relationships from Lemmon and Jacobsen [58].

Define the coefficients in Table IV in Lemmon and Jacobsen [58].

```
[384]: Ncon = (1.511, 2.117, -3.332, 8.862, 31.11, -73.13, 20.03, -0.7096, 0.2672)
```

```
[384]: (1.511, 2.117, -3.332, 8.862, 31.11, -73.13, 20.03, -0.7096, 0.2672)
```

The first term in the list below is for  $i = 2$ .

```
[385]: tcon = (-1.0, -0.7, 0, 0.03, 0.2, 0.8, 0.6, 1.9)
```

```
[385]: (-1.0, -0.7, 0, 0.03, 0.2, 0.8, 0.6, 1.9)
```

The first term in the list below is for  $i = 4$ .

```
[386]: dcon = (1, 2, 3, 4, 8, 10)
```

[386]: (1, 2, 3, 4, 8, 10)

The first term in the list below is for  $i = 4$ .

```
[387]: lcon = (0, 0, 1, 2, 2, 2)
```

[387]: (0, 0, 1, 2, 2, 2)

The equation below is Eq (5) in Lemmon and Jacobsen [58] adjusted so all parameters are in SI units.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[388]: λ0 = 10^-3 * (Ncon[1] * (η0 / 10^-6) + Ncon[2] * τ^tcon[2 - 1] + Ncon[3] *  
τ^tcon[3 - 1]);
```

Define a Julia function for calculations.

```
[389]: λ0jl = lambdify(λ0(τ=>Tc/T), (T, M))
```

[389]: #118 (generic function with 1 method)

Compare symbolic and Julia function calculations.

```
[390]: N(λ0(τ=>Tc/T, M=>MN2)(T=>100))
```

[390]: 0.009277493928717767139105141041834353050057249458553867177925127283759715530620  
74

```
[391]: λ0jl(100, MN2)
```

[391]: 0.00927749392871777

```
[392]: N(λ0(τ=>Tc/T, M=>MN2)(T=>300))
```

[392]: 0.025936086671217834185578500179661150105249229268726034868628667377959296136471  
87

```
[393]: λ0jl(300, MN2)
```

[393]: 0.025936086671217842

These values are consistent.

This is Eq. (6) in Lemmon and Jacobsen [58].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[394]: λr = 10^-3 * sum( Ncon[i] * τ^tcon[i - 1] * 6^dcon[i -  
3] * exp(lcon[i - 3] == 0 ? 0 : -6^lcon[i - 3]) for i in
```

```
4:9);
```

Define a Julia function for this.

```
[395]: λrjl = lambdify(λr(δ => ρ/ρc, τ => Tc/T), (ρ, T))
```

```
[395]: #118 (generic function with 1 method)
```

Compare symbolic and Julia function values.

```
[396]: N(λr(δ => ρ/ρc, τ => Tc/T)(ρ => pn2tab[end]/MN2, T=>Tcold))
```

```
[396]: 0.025539505273607738
```

```
[397]: λrjl(pn2tab[end]/MN2, Tcold)
```

```
[397]: 0.025539505273607738
```

In order to calculate  $\lambda^c$  in Eq. (7) in Lemmon and Jacobsen [58], we must calculate the parameters in Eqs. (8-11).

First, we define some of the parameters in these equations.

```
[398]: ξ0 = 0.17e-9; # m
```

```
[399]: ρc = 3.3958e6; # Pa
```

```
[400]: ρc = 11.1839e3; # mol/m^3
```

We need  $\left(\frac{\partial \rho}{\partial p}\right)_T$ . Use the equation of state from Eq. (56) from Lemmon and Jacobsen [58] to get  $\left(\frac{\partial p}{\partial \rho}\right)_T$ , and invert it.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[401]: dpdp = diff(ρ * R * T * (1 + δ * diff(αr, δ))(δ => ρ/ρc, τ => Tc/T), ρ);
```

$\left(\frac{\partial \rho}{\partial p}\right)_T$  is the reciprocal of the previous result.

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[402]: dpdp = 1/dpdp;
```

The following is Eq. (11) from Lemmon and Jacobsen [58].

*Output from the following symbolic calculation has been suppressed. Remove the trailing semicolon before entering the cell to display it.*

```
[403]: χn = ρc * ρ/ρc^2 * dpdp;
```

Calculate some values to test this.



```
[404]:  $\chi_n(\rho \Rightarrow 15654, T \Rightarrow 309.162)$ 
```

```
[404]: 0.0602175741298228
```

```
[405]:  $N(\chi_n(\rho \Rightarrow 15654, T \Rightarrow 309.162))$ 
```

```
[405]: 0.06021757412982283
```

```
[406]:  $\text{lambdify}(\chi_n(T \Rightarrow 309.162), (\rho, ))(15654)$ 
```

```
[406]: 0.05678388205384859
```

```
[407]:  $\text{lambdify}(\chi_n, (\rho, T))(\text{BigFloat}("15654."), \text{BigFloat}("309.162"))$ 
```

```
[407]: 0.06021757412982288700779976306189003702673070912411065870748388041709201066309367
```

```
[408]:  $\text{convert}(\text{Float64}, \text{lambdify}(\chi_n, (\rho, T))(\text{BigFloat}("15654."), \text{BigFloat}("309.162")))$ 
```

```
[408]: 0.060217574129822884
```

There is a significant loss in precision when we go to a floating point calculation from the symbolic calculation. We are going to have to use BigFloat numbers for  $\chi_n$  and the parameters that depend on it.

Define a Julia function.

```
[409]:  $\chi_{njl} = \text{lambdify}(\chi_n, (\rho, T))$ 
```

```
[409]: #118 (generic function with 1 method)
```

Define some more needed parameters.

```
[410]:  $\Gamma = 0.055$ 
```

```
[410]: 0.055
```

```
[411]:  $v = 0.63$ 
```

```
[411]: 0.63
```

```
[412]:  $\gamma_{tc} = 1.2415$ 
```

```
[412]: 1.2415
```

```
[413]:  $T_{ref} = 252.384 \text{ # } K$ 
```

```
[413]: 252.384
```

Compare some symbolic and Julia calculations to make sure everything is consistent.

```
[414]: N(χn(ρ => pn2(ptab[end], Tcold), T => Tcold))
```

```
[414]: 0.08324797739948357
```

```
[415]: χnjℓ(BigFloat(pn2(ptab[end], Ts)), BigFloat(Ts))
```

```
[415]: 0.07614500019331444898864891880754414665567656911879417994408818834904409021383484
```

```
[416]: χnjℓ(BigFloat(pn2(ptab[end], Tref)), BigFloat(Tref))
```

```
[416]: 0.09198684158279236104835953851523045730569138321788117580508021741916668028376403
```

```
[417]: N(χn(ρ => pn2(ptab[end], Tref), T => Tref))
```

```
[417]: 0.09198684158279254
```

```
[418]: χnjℓ(BigFloat(pn2(ptab[end], Tref)), BigFloat(Tref))
```

```
[418]: 0.09198684158279236104835953851523045730569138321788117580508021741916668028376403
```

The values above are consistent.

This is Eq. (10) in Lemmon and Jacobsen [58]. We define it here as a symbolic function (which produces a SymPy expression).

```
[419]: ξ(ρ1, T1) = ξ0 * (((χn(ρ => ρ1, T => T1)) -  
    (χn(ρ => ρ1, T => Tref)) * (Tref/T1)) /  
    Γ)^(ν/γtc)
```

```
[419]: ξ (generic function with 1 method)
```

Define a Julia function for this.

```
[420]: ξjℓ(ρ1, T1) = ξ0 * (((χnjℓ(ρ1, T1)) - (χnjℓ(ρ1, Tref)) * (Tref/T1)) / Γ)^(ν/γtc)
```

```
[420]: ξjℓ (generic function with 1 method)
```

Compare symbolic and Julia floating point calculations.

```
[421]: N(ξ(pn2tab[end]/MN2, Tcold))
```

```
[421]: -1.3442826598788053e-12 + 5.7420423384909375e-11im
```

```
[422]: ξjℓ(BigFloat(pn2tab[end]+ 0im), BigFloat(Tcold+0im))
```

```
[422]: NaN
```

The results above are correct. The temperatures given (and the temperatures in all the underwater environments in the paper) are greater than the critical temperature; therefore  $\xi$  does not contribute to the thermal conductivity through the  $\lambda_c$  term defined in Eq. (7) in Lemmon and Jacobsen [58].

Define some more parameters.

```
[423]: R0 = 1.01;
```

```
[424]: k = 1.380658e-23; # J/K
```

```
[425]: qD = 0.40e-9; # m
```

The following is Eq. (8) in Lemmon and Jacobsen [58].

```
[426]: Ωn(ρ1, T1) = (2/π * ((cp - cv) / cp * atan(ξ(ρ1, T1) /
    qD) + cv / cp * ξ(ρ1, T1) / qD)(δ => ρ/ρc,
    τ => Tc/T))(ρ => ρ1, T => T1)
```

```
[426]: Ωn (generic function with 1 method)
```

Define a Julia function for this using the Julia functions for the parameters.

```
[427]: Ωnjl(ρ1, T1) = 2/π * ((cpjl(ρ1, T1) - cvjl(ρ1, T1)) /
    cpjl(ρ1, T1) * atan(ξjl(ρ1, T1) /
    qD) + cvjl(ρ1, T1) / cpjl(ρ1, T1) * ξjl(ρ1, T1) / qD)
```

```
[427]: Ωnjl (generic function with 1 method)
```

Compare symbolic and Julia calculations.

```
[428]: N(Ωn(pn2tab[end], Tcold))
```

```
[428]: -0.00010979933356491272 + 0.004689978682126876im
```

```
[429]: Ωnjl(pn2tab[end], Tcold + 0im)
```

```
[429]: -0.00010979933356491013 + 0.004689978682126766im
```

The following is Eq. (9) in Lemmon and Jacobsen [58].

```
[430]: Ω0n(ρ1, T1) = (2 / π * (1 - exp(-1 / ((ξ(ρ1, T1) /
    qD)^-1 + 1/3 * (ξ(ρ1, T1) / qD)^2 * (ρc /
    ρ)^2)))(δ => ρ/ρc, τ => Tc/T))(ρ => ρ1, T => T1)
```

```
[430]: Ω0n (generic function with 1 method)
```

Define a Julia function for this using the Julia functions for the parameters.

```
[431]: Ω0njl(ρ1, T1) = 2 / π * (1 - exp(-1 / ((ξjl(ρ1, T1) /
    qD)^-1 + 1/3 * (ξjl(ρ1, T1) / qD)^2 * (ρc /
    ρ1)^2))
```

[431]:  $\Omega_{njl}$  (generic function with 1 method)

Compare symbolic and Julia calculations.

```
[432]: N( $\Omega_{n}$ (pn2tab[end], Tcold))
```

[432]: -9.311257188915345e-5 + 0.004690669700665422im

```
[433]:  $\Omega_{njl}$ (pn2tab[end], Tcold + 0im)
```

[433]: -9.311257188919424e-5 + 0.004690669700665313im

These are consistent.

The following expression is Eq. (7) in Lemmon and Jacobsen [58].

```
[434]:  $\lambda_c$ ( $\rho_1$ , T1) =  
    if ((( $\chi_n$ ( $\rho \Rightarrow \rho_1$ , T  $\Rightarrow$  T1)) - ( $\chi_n$ ( $\rho \Rightarrow \rho_1$ , T  $\Rightarrow$   
        Tref)) * (Tref / T1)) /  $\Gamma$ ) > 0  
        (( $\rho$  *  $c_p$  *  $k$  *  $R_0$  * T1 / (6 *  $\pi$  *  $\xi$ ( $\rho_1$ , T1) *  $\eta$ )  
         * ( $\Omega_n$ ( $\rho_1$ , T1) -  $\Omega_{0n}$ ( $\rho_1$ , T1)))( $\delta \Rightarrow$   
          $\rho/\rho_c$ ,  $\tau \Rightarrow T_c/T$ ))( $\rho \Rightarrow \rho_1$ , T  $\Rightarrow$  T1)  
    else  
        0  
    end
```

[434]:  $\lambda_c$  (generic function with 1 method)

Define a Julia function for this using the Julia functions for the parameters.

```
[435]: function  $\lambda_{cjl}$ ( $\rho_1$ , T1)  
    if ((( $\chi_{njl}$ ( $\rho_1$ , T1) - ( $\chi_{njl}$ ( $\rho_1$ , Tref)) * (Tref / T1)) /  $\Gamma$ ) > 0  
         $\rho_1$  *  $c_{pjl}$ ( $\rho_1$ , T1) *  $k$  *  $R_0$  * T1 / (6 *  $\pi$  *  $\xi_{jl}$ ( $\rho_1$ , T1) *  $\eta_{jl}$ ( $\rho_1$ , T1, MN2)) *  
        ( $\Omega_{njl}$ ( $\rho_1$ , T1) -  $\Omega_{0njl}$ ( $\rho_1$ , T1))  
    else  
        0  
    end  
end
```

[435]:  $\lambda_{cjl}$  (generic function with 1 method)

Compare symbolic and Julia calculations.

```
[436]:  $\lambda_c$ (pn2tab[end]/MN2, Tcold)
```

[436]: 0

```
[437]:  $\lambda_{cjl}$ (pn2tab[end]/MN2, Tcold)
```

[437]: 0

These are consistent.

The following expression is Eq. (4) in Lemmon and Jacobsen [58].

```
[438]: λ(ρ1, T1) = ((λ0 + λr + λc(ρ1, T1))(δ => ρ/ρc, τ => Tc/T))(ρ => ρ1, T => T1, M => MN2)
```

```
[438]: λ (generic function with 1 method)
```

Define a Julia function for this using the Julia functions for the parameters.

```
[439]: λjl(ρ1, T1) = λ0jl(T1, MN2) + λrjl(ρ1, T1) + λcjl(ρ1, T1)
```

```
[439]: λjl (generic function with 1 method)
```

Compare symbolic and Julia calculations.

```
[440]: N(λ(pn2(ptab[end], Tcold), Tcold))
```

```
[440]: 0.049616519403474207031096168609947088052581303858746925646843920896990484841775  
91
```

```
[441]: λjl(BigFloat(pn2(ptab[end], Tcold)), BigFloat(Tcold))
```

```
[441]: 0.049616519403474200897719979075481186647608518538320295905639954780018200954626  
53
```

Compare some more symbolic and Julia values.

```
[442]: N(λ(5000, 300))
```

```
[442]: 0.032769431881436595764435386959552229104887888057690054045065901402031279198819  
55
```

```
[443]: λjl(BigFloat(5000), BigFloat(300))
```

```
[443]: 0.032769431881436593056666137886092306521561595675800102769380288936416809120920  
59
```

```
[444]: N(λ(10000, 200))
```

```
[444]: 0.036009906646684426440780547760034865817597274455767271744598938205464636453408  
96
```

```
[445]: λjl(BigFloat(10000), BigFloat(200))
```

```
[445]: 0.036009906646684426086009608220607938082101697109938732338886829788792716563352  
82
```

```
[446]: patm = pn2(1.01325e5, 293.15)
```

```
[446]: 41.58105951222148
```

[447]:  $N(\lambda(\text{patm}, 293.15))$

[447]: 0.02547268399436569854852004147471750939605031705263036031149280542692716386774205

[448]:  $N(\lambda(0, 300))$

[448]: 0.02593608667121784255154131527931323480079714976118126498256590140203127919881928

[449]:  $\lambda j l(\text{BigFloat}(0), \text{BigFloat}(300))$

[449]: 0.02593608667121784013963971373148787296652647801054477325138569618925646741186437

[450]:  $N(\lambda(0, 100))$

[450]: 0.00927749392871776713910514104183435305005724945855386717792512728375971553062074

[451]:  $\lambda j l(\text{BigFloat}(0), \text{BigFloat}(100))$

[451]: 0.009277493928717769570614236010251825856602571761573130419573458478105581491863788

[452]:  $N(\lambda(25000, 100))$

[452]: 0.1038342450302420641403411394640530736047340847244110758645760258348835338671782

[453]:  $\lambda j l(\text{BigFloat}(25000), \text{BigFloat}(100))$

[453]: 0.1038342450302421167092440470479961347902925704881382204594676233341878766113536

[454]:  $N(\lambda(10000, 200))$

[454]: 0.03600990664668442644078054776003486581759727445576727174459893820546463645340896

[455]:  $\lambda j l(\text{BigFloat}(10000), \text{BigFloat}(200))$

[455]: 0.03600990664668442608600960822060793808210169710993873233888682978879271656335282

[456]:  $N(\lambda(11.18*1000, 126.195))$

[456]: 0.6758005439333020275702825386057180036631593812691489950818328132721624041932334

```
[457]: λjl(BigFloat(11.18*1000), BigFloat(126.195))
```

```
[457]: 0.675800543906010368981785532559248206105755976052774039976447777713859571563029  
6
```

These values are consistent with Lemmon and Jacobsen [58].

Define a Julia function of pressure and temperature.

```
[458]: λn2pT(p1, T1) = λjl(ρn2(p1, T1), T1)
```

```
[458]: λn2pT (generic function with 1 method)
```

Warm surface value

```
[459]: λn2pT(BigFloat(ptab[1]), BigFloat(Ts))
```

```
[459]: 0.025472683994365702814421504599293940260682950639470834112253777475811761784260  
63
```

Cold surface value

```
[460]: λn2pT(BigFloat(ptab[1]), BigFloat(Tcold))
```

```
[460]: 0.024112663646929646481173735052034339601905749433790170082932129165287497724007  
13
```

Value at depth 1000 m (dvals index 1001)

```
[461]: λn2pT(BigFloat(ptab[1001]), BigFloat(Tcold))
```

```
[461]: 0.030115175702480974874904726458872704060556230069180431206078376955022603534857  
43
```

Value at depth 2000 m (dvals index 2001)

```
[462]: λn2pT(BigFloat(ptab[2001]), BigFloat(Tcold))
```

```
[462]: 0.037676046997134363674845678979295960411033635881113047819727368138175814700286  
05
```

Deep water value

```
[463]: λn2pT(BigFloat(ptab[end]), BigFloat(Tcold))
```

```
[463]: 0.049616519403474198830039019811598479498649519995845358011554803277948977062390  
42
```

Calculate values for the depth profile.

```
[464]: λn2tab = map(p -> convert(Float64, λn2pT(BigFloat(p), BigFloat(Tcold))), ptab);
```

```
[465]: λn2tab[1], λn2tab[1001], λn2tab[2001], λn2tab[end]
```

```
[465]: (0.024112663646929648, 0.030115175702480974, 0.037676046997134366,  
0.049616519403474196)
```

### 5.2.8. Thermal Diffusivity

Use the thermal diffusivity definition in Ainslie and Leighton [1].

```
[466]: α(ρ1, T1) = ((λ(ρ1, T1) / (ρ1 * cp)))(δ => ρ/ρc, τ => Tc/T)(ρ => ρ1,  
T => T1, M => M02)
```

```
[466]: α (generic function with 1 method)
```

Calculate a value. Recall that the `pn2tab` array is a mass density. We must divide it by molar mass `MN2` to get molar density.

```
[467]: N(α(pn2tab[end]/MN2, Tcold))
```

```
[467]: 9.53771380581238216611683959570908533506480226109361649956403874857159298485278e  
-08
```

Define a Julia function.

```
[468]: αjl(ρ1, T1) = λjl(ρ1, T1) / (ρ1 * cpjl(ρ1, T1))
```

```
[468]: αjl (generic function with 1 method)
```

```
[469]: αjl(BigFloat(pn2tab[end]/MN2), BigFloat(Tcold))
```

```
[469]: 9.537713805812383382597846633568194286885392932676980953772982349040826645988277  
e-08
```

```
[470]: αn2pT(ρ1, T1) = αjl(pn2(ρ1, T1), T1)
```

```
[470]: αn2pT (generic function with 1 method)
```

```
[471]: αn2pT(BigFloat(ptab[end]), BigFloat(Tcold))
```

```
[471]: 9.53771380581238389620628978927454593976835927404818426253464594573344068200228e  
-08
```

Warm surface value

```
[472]: αn2pT(BigFloat(ptab[1]), BigFloat(Ts))
```

```
[472]: 2.100004083247022093503946771936644530470311760559136620822034024827056013541225  
e-05
```

Cold surface value



```
[473]: an2pT(BigFloat(ptab[1]), BigFloat(Tcold))
```

```
[473]: 1.861946262897033998571748386675681825481124421867655633040351932072680469144438  
e-05
```

Value at depth 1000 m (dvals index 1001)

```
[474]: an2pT(BigFloat(ptab[1001]), BigFloat(Tcold))
```

```
[474]: 1.913800129237647329608957909779612257816209851330371210293404763124807863569153  
e-07
```

Value at depth 2000 m (dvals index 2001)

```
[475]: an2pT(BigFloat(ptab[2001]), BigFloat(Tcold))
```

```
[475]: 1.14299948890961679506500684513208826851235137428382537456727572856169743355277e  
-07
```

Deep water value

```
[476]: an2pT(BigFloat(ptab[end]), BigFloat(Tcold))
```

```
[476]: 9.53771380581238389620628978927454593976835927404818426253464594573344068200228e  
-08
```

Calculate values for the depth profile.

```
[477]: an2tab = map(p -> convert(Float64, an2pT(BigFloat(p), BigFloat(Tcold))),  
ptab);
```

```
[478]: an2tab[1], an2tab[1001], an2tab[2001], an2tab[end]
```

```
[478]: (1.861946262897034e-5, 1.9138001292376474e-7, 1.1429994889096169e-7,  
9.537713805812384e-8)
```

Add these values to the dataframe.

```
[479]: valsn2.thermal_diffusivity = an2tab;
```

### 5.2.9. Export Nitrogen Parameters

We have all the needed nitrogen parameters in `valsn2`. Export them to a CSV file.

Here are the column names.

```
[480]: names(valsn2)
```

```
[480]: 8-element Vector{String}:  
"depth"  
"pressure"
```

```
"water_density"  
"water_dyn_viscosity"  
"water_surface_tension"  
"water_sound_speed"  
"gamma"  
"thermal_diffusivity"
```

Reorder the dataframe columns to match the order that the acoustic calculations require.

```
[481]: select!(valsn2, ["depth", "water_density", "pressure", "water_dyn_viscosity",  
    "water_surface_tension", "water_sound_speed",  
    "thermal_diffusivity", "gamma"]);
```

```
[482]: CSV.write("DeepWaterPropertiesN2.csv", valsn2)
```

```
[482]: "DeepWaterPropertiesN2.csv"
```