CO_2 Dissolution in Water

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0 Introduction

0.A Henry's Law

We will be using Henry's Law to mathematically model the solubility of carbon dioxide in seawater. Henry's Law states that for a gaseous mixture that is in contact with a solution, the amount of gas in the mixture that dissolves in the solution is directly proportional to the partial pressure of the gas [1]. Here, partial pressure refers to the pressure contributed solely by the gas in the liquid-gas mixture [1]. For this law to hold true, we assume that the temperature of the system is constant and doesn't change (although in reality, the temperature changes so slowly that its derivative, with respect to time, is close to zero) [4]. Therefore, if the pressure of the gas above the liquid increases, the amount of gas dissolved in the liquid also increases proportionally. Similarly, as the pressure of the gas decreases, the amount of gas dissolved decreases proportionally. This proportionality depends on the Henry's Law constant [2] and can be simplified as shown below:

$$\frac{C_1}{P_1} = \frac{C_2}{P_2} = const.$$

Where C_1 is the concentration of the gas dissolved in the liquid in the system's first state, P_1 is the partial pressure of the gas in the system's first state, C_2 is the concentration of the gas dissolved in the liquid in the system's second state and P_2 is the partial pressure of the gas in the system's second state [1]. This can therefore be rewritten in the form:

$$\therefore \frac{\mathrm{C}}{P} = \mathrm{k}$$

Where C is the concentration of the gas dissolved in the liquid, P is the partial pressure of the gas and k is the Henry's Law constant [3].

To apply this to our context of ocean acidification, we will primarily use the following simplifications:

1. We will assume that the seawater behaves like pure water. [4]
2. We will ignore all other gases in the atmosphere apart from H_2O and CO_2 and assume that the atmosphere is made up of only H_2O and CO_2. [4]

0.B Relation Equations

Henry's Law can be used to give the following relation equations which are said to be valid when the system is in equilibrium [4]:

$$x_1 P_{v,1} = y_1 \phi_1 P \quad (1.1)$$
$$x_2 H_{21} = y_2 \phi_2 P \quad (1.2)$$

In the above equations, x_1 refers to the molar fraction of water in liquid phase, x_2 refers to the molar fraction of carbon dioxide in liquid phase, y_1 refers to the molar fraction of water in gaseous phase and y_2 refers to the molar fraction of carbon dioxide in gaseous phase.

As for the remaining variables, $P_{v,1}$ is the vapour pressure of water and H_{21} is Henry's Constant which we saw earlier. $P_{v,1}$ can be calculated using the following equation [4]:

$$\ln\frac{P_{v,1}}{P_c} = (\alpha_1 x + \alpha_2 x^{1.5} + \alpha_3 x^3 + \alpha_4 x^{3.5} + \alpha_5 x^4 + \alpha_6 x^{7.5})T_r^{-1} \quad (1.3)$$

In the above equation, $x = 1 - T_r$, $T_r = T \cdot T_c^{-1}$ and coefficients α_1 to α_6 are given in Table 1 below [4]:

α_1	-7.85951783
α_2	1.84408259
α_3	-11.7866497
α_4	22.6807411
α_5	-15.9618719
α_6	1.80122502

Table 1

The variables x_1, x_2, y_1 and y_2 can be modelled in terms of mass fractions which gives us 2 more formulae [4]:

$$\sum_i y_i = y_1 + y_2 = 1 \quad (2.1)$$

$$\sum_i x_i = x_1 + x_2 = 1 \quad (2.2)$$

Φ_2 and Φ_1 refer to the fugacity ratio in liquid and gaseous phases, respectively and can be solved with the equations below [4]:

$$\phi_1 = \frac{\phi_1^v}{\phi_1^l} \quad (2.3)$$

$$\phi_2 = \phi_2^v \quad (2.3)$$

Also, Henry's Constant can be defined with the following equation [4]:

$$\ln(\frac{H_{21}(T)}{1MPa}) = h_1 + \frac{h_2}{T} + \frac{h_3}{T^2} + \frac{h_4}{T^3} \quad (4)$$

Here, the variables h_1, h_2 h_3 and h_4 are given in Table 2 below [4]:

h_1	-6.8346
h_2	1.2817×10^4
h_3	-3.7668×10^6
h_4	2.997×10^8

Table 2

The Peng-Robinson Equation helps calculate the fugacity ratios and is given in the following equations [4]:

$$\ln\phi^v = Z_v - 1 - \ln(Z_v - B) - \frac{A}{2\sqrt{2}B}\ln(\frac{Z_v + (1+\sqrt{2})B}{Z_v + (1-\sqrt{2})B}) \quad (5.1)$$

$$\ln\phi^l = Z_l - 1 - \ln(Z_l - B) - \frac{A}{2\sqrt{2}B}\ln(\frac{Z_l + (1+\sqrt{2})B}{Z_l + (1-\sqrt{2})B}) \quad (5.2)$$

In the above equations, ϕ^v refers to fugacity ratios in the vapour phase and ϕ^l refers to fugacity ratios in the liquid phase. Also, Z is given by the roots of the following equation [4]:

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \tag{5.3}$$

Furthermore, variables A and B can be solved with the equations below [4]:

$$A = \frac{a^* P}{(RT)^2} \tag{5.4}$$

$$B = \frac{bP}{RT} \tag{5.5}$$

Where a and b are related in the equations [4]:

$$\frac{aP_c}{(RT_c)^2} = 0.45724 \tag{5.6}$$

$$\frac{bP_c}{RT_c} = 0.0778 \tag{5.7}$$

Also, a^* is given below [4]:

$$a^* = a\alpha(T_r, w) \tag{5.8}$$

And α is given as [4]:

$$\alpha(T_r, w) = [1 + (0.37464 + 1.54226w - 0.2699w^2)(1 - {T_r}^{0.5})]^2 \tag{5.9}$$

0.C Reaction Kinetics

Coming to reaction kinetics, we have a system of 6 differential equations [4]:

$$\frac{d}{dt}[CO_2(g)] = -k_1[CO_2(g)] + k_{-1}[CO_2(aq)] \tag{6.1}$$

$$\frac{d}{dt}[CO_2(aq)] = k_1[CO_2(g)] - (k_{-1} + k_2)[CO_2(aq)] + k_{-2}[H_2CO_3] \tag{6.2}$$

$$\frac{d}{dt}[H_2CO_3] = k_2[CO_2(aq)] - (k_{-2} + k_3)[H_2CO_3] + k_{-3}[H^+][{HCO_3}^-] \tag{6.3}$$

$$\frac{d}{dt}[{H_2CO_3}^-] = k_3[H_2CO_3] - k_{-3}[H^+][{HCO_3}^-] - k_4[HCO_3^-] + k_{-4}[H^+][{CO_3}^{2-}] \tag{6.4}$$

$$\frac{d}{dt}[{CO_3}^{2-}] = k_4[{HCO_3}^-] - k_{-4}[H^+][{CO_3}^{2-}] \tag{6.5}$$

$$\frac{d}{dt}[H^+] = k_3[H_2CO_3] - k_{-3}[H^+][{HCO_3}^-] + k_4[HCO_3^-] - k_{-4}[H^+][{CO_3}^{2-}] \tag{6.6}$$

Additionally, the variables k_1 to k_4 and k_{-1} to k_{-4} (s^{-1}) are given in Table 3 below [4]:

k_1	1×10^{10}	k_{-1}	1×10^{10}
k_2	6×10^{-2}	k_{-2}	2×10^{1}
k_3	1×10^{7}	k_{-3}	5×10^{10}
k_4	3×10^{0}	k_{-4}	5×10^{10}

Table 3

And lastly, there are 4 reaction equations as shown below [4]:

$$CO_2(g) \leftrightarrow CO_2(aq) \quad \text{(R1)}$$
$$CO_2(aq) + H_2O \leftrightarrow H_2CO_3 \quad \text{(R2)}$$
$$H_2CO_3 \leftrightarrow H^+ + {HCO_3}^- \quad \text{(R3)}$$
$$HCO_3^- \leftrightarrow H^+ + {CO_3}^{2-} \quad \text{(R4)}$$

1 Task 1

1.A Mathematical Task

Looking at equations 1.1, 1.2, 2.1 and 2.2, we can see that there are 4 key variables: x_1, x_2, y_1 and y_2. To get a matrix in terms of these variables, we must make sure that the equations are all in the correct format so that there are no variables on the right-hand side of the equation. Therefore, the equations can be written as:

$$x_1 P_{v,1} - y_1 \phi_1 P = 0 \quad (1.1)$$
$$x_2 H_{21} - y_2 \phi_2 P = 0 \quad (1.2)$$
$$y_1 + y_2 = 1 \quad (2.1)$$
$$x_1 + x_2 = 1 \quad (2.2)$$

Now let's separate the coefficients and variables for a moment. By doing this, we can now think of the coefficients as being mapped onto the variables to form an equation. We can do exactly this by using matrices:

$$\begin{bmatrix} P_{v,1} & 0 & -\phi_1 P & 0 \\ 0 & H_{21} & 0 & -\phi_2 P \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \quad (2.3)$$

As a result, we can solve for x_1, x_2, y_1 and y_2 by making them the subject to give:

$$\begin{bmatrix} x_1 \\ x_2 \\ y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} P_{v,1} & 0 & -\phi_1 P & 0 \\ 0 & H_{21} & 0 & -\phi_2 P \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \quad (2.4)$$

For the above system of equations to be solvable, the only restriction is the determinant of the 4x4 matrix as it must not be zero. Therefore, if we let the 4x4 matrix be known as A, then $|A| \neq 0$. The determinant of the matrix is given as:

$$|A| = P_{v,1} \begin{vmatrix} H_{21} & 0 & -\phi_2 P \\ 0 & 1 & 1 \\ 1 & 0 & 0 \end{vmatrix} - (0) \begin{vmatrix} 0 & 0 & -\phi_2 P \\ 0 & 1 & 1 \\ 1 & 0 & 0 \end{vmatrix} + (-\phi_1 P) \begin{vmatrix} 0 & H_{21} & -\phi_2 P \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} - (0) \begin{vmatrix} 0 & H_{21} & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}$$

Since the second and fourth terms are zero, this simplifies to:

$$P_{v,1} \begin{vmatrix} H_{21} & 0 & -\phi_2 P \\ 0 & 1 & 1 \\ 1 & 0 & 0 \end{vmatrix} - \phi_1 P \begin{vmatrix} 0 & H_{21} & -\phi_2 P \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}$$

$$= P_{v,1} \left(H_{21} \begin{vmatrix} 1 & 1 \\ 0 & 0 \end{vmatrix} - 0 \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} + (-\phi_2 P) \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \right) - \phi_1 P (0 \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} - H_{21} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} + (-\phi_2 P) \begin{vmatrix} 0 & 0 \\ 1 & 1 \end{vmatrix})$$

$$= P_{v,1} \left(H_{21} \begin{vmatrix} 1 & 1 \\ 0 & 0 \end{vmatrix} - \phi_2 P \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \right) - \phi_1 P \left(-H_{21} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} - \phi_2 P \begin{vmatrix} 0 & 0 \\ 1 & 1 \end{vmatrix} \right)$$

$$= P_{v,1}(H_{21}(0) - \phi_2 P(-1)) - \phi_1 P(-H_{21}(-1) - \phi_2 P(0))$$

$$= P_{v,1}(\phi_2 P) - \phi_1 P(H_{21}) = P_{v,1}\phi_2 P - \phi_1 P H_{21} = P(P_{v,1}\phi_2 - \phi_1 H_{21})$$

To find instances when the model is not true, we have to assume that $|A| = 0$ so $P(P_{v,1}\phi_2 - \phi_1 H_{21}) = 0$. One of the cases that $|A| = 0$ is when P = 0. Therefore, if P=0, pressure is said to be 0 and it implies that no molecules are present – in either phase. However, this is not the case in the real world as it's simply not a vacuum to have a pressure of 0. The other case is when $P_{v,1}\phi_2 = \phi_1 H_{21}$. In this scenario, the gaseous and liquid phases (i.e. atmosphere and ocean) are in equilibrium so the rate at which CO_2 is being dissolved in the water is the same as the rate at which CO_2 is being released from the surface of the water and $P_{v,1}$ is the pressure of the water at which this equilibrium occurs. This 1:1 ratio is essential in oceans as this determines the amount of CO_2 escaping into the atmosphere from the surface of the water. And as CO_2 is a greenhouse gas, excessive release of CO_2 can cause more heat to be trapped in the atmosphere (due to the greenhouse effect), leading to higher global average temperatures, which in turn, accelerates global warming. Any disruptions to this equilibrium could also lead to changes in habitats and the atmosphere – causing more wildlife to rapidly develop adaptations to withstand such sudden changes, disrupting food chains and global ecosystems as a whole.

1.B Communication Task

From the data at hand, we have results for both temperature (°C) and pressure (kPa). With this, we can first work out T_r using the equation, $T_r = \frac{T}{T_c}$. Since our T values are in °C and T_c is in K, we can it to °C by subtracting 273.15. So, T_c = 647.096 - 273.15 = 373.946 °C. Alternatively, the T values in °C can be converted to K by adding 273.15. This value for T_r can then be used to find x using the equation, $x = 1 - T_r$. After that, we can rearrange equation 1.3 for $P_{v,1}$ which gives $P_{v,1} = P_c \cdot e^{(\alpha_1 x + \alpha_2 x^{1.5} + \alpha_3 x^3 + \alpha_4 x^{3.5} + \alpha_5 x^4 + \alpha_6 x^{7.5})T_r^{-1}}$. As for P_c and α_1-α_6, we can use P_c = 22.064MPa (= 22064 kPa) and table 1 to substitute the respective values for α_1 to α_6. This would give us a numerical value for $P_{v,1}$. We can then calculate Henry's Constant using equation 4 and rearranging this for $H_{21}(T)$ gives $H_{21}(T) = 1MPa \cdot e^{h_1 + \frac{h_2}{T} + \frac{h_3}{T^2} + \frac{h_4}{T^3}}$ where H_{21} is a function of temperature. Next, if we come to equation 5.6, we can solve for a to give $a = \frac{0.45724(RT_c)^2}{P_c}$. Since R (8.314 $Jmol^{-1}K^{-1}$), T_c and P_c are all constants, this gives us a numerical value for a. With this value for a, we can now substitute this into equation 5.4, $A = \frac{a^* P}{(RT)^2}$. However, to find A, we have to find a^* using equation 5.8, where $\alpha(T_r, w)$ is given by equation 5.9. As for values of w, these are constants as $w_{H_2O} = 0.348$ and $w_{CO_2} = 0.225$. In a similar way to how we found A, we can do this for equation 5.7 and solve for b to give $b = \frac{0.0778RT_c}{P_c}$. And as we have the same constants, this again gives us a numerical value for b. With this value for b, we can substitute it into equation 5.5, $B = \frac{bP}{RT}$, to find B. Now, we can substitute these values for A and B into the equation 5.3, $Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0$ and find solutions for Z. Since, it's a cubic equation, there will be 3 roots – either all 3 real roots or only 1 real and 2 imaginary roots (which make up a conjugate pair). In the first case, the smallest of the 3 roots will be known as Z_l and the largest will be known as Z_v. The second case will only occur for CO_2 and means that the fluid is supercritical and hence can't exist in liquid form in such thermodynamic conditions. We can now use Z_v to find ϕ^v using equation 5.1 and rearranging it to give $\phi^v = e^{Z_v - 1 - \ln(Z_v - B) - \frac{A}{2\sqrt{2}B}\ln(\frac{Z_v + (1+\sqrt{2})B}{Z_v + (1-\sqrt{2})B})}$. This can then be repeated and can be used to find ϕ_1^v (which is ϕ^v for water) and ϕ_2^v (which is ϕ^v for carbon dioxide). Similarly, we can use Z_l to find ϕ^l using equation 5.2 and rearrange it to give $\phi^l = e^{Z_l - 1 - \ln(Z_l - B) - \frac{A}{2\sqrt{2}B}\ln(\frac{Z_l + (1+\sqrt{2})B}{Z_l + (1-\sqrt{2})B})}$. Again, this can be repeated and used to find ϕ_1^l (which is ϕ^l for water). With these values for ϕ_1^v, ϕ_2^v

and ϕ_1^l, we can then use equations 2.3 and 2.2, $\phi_1 = \frac{\phi_1^v}{\phi_1^l}$ and $\phi_2 = \phi_2^v$ to find ϕ_1 and ϕ_2. After gathering all of these values, we can find x_1, x_2, y_1 and y_2 by inverting the 4x4 matrix and multiplying it by the 4x1 matrix as shown in equation 2.4.

In MATLAB, I would first define the constants T_c, P_c, P, w (acentric factor) and R. I would then make a temperature array in both Celsius for the graph and Kelvin for calculations. Then, after finding T_r and x, I would calculate $P_{v,1}$ and H_{21}. I would then start the cubic equation by calculating a, a*, A, B and α. After substituting in the required values, I'd use the roots and real functions to find Z_v and Z_l for H_2O and CO_2. And substituting those into equation 5.1 and 5.2, this gives me ϕ_1^v, ϕ_2^v and ϕ_1^l. I would then substitute those into equations 2.3 and 2.2 to find ϕ_1 and ϕ_2. And finally, I would plot all 4 variables against temperature in Celsius.

1.C Modelling Task

In order to include other gases also present in the atmosphere, the model has to be altered such that it can be generalised for any gas. Therefore, we can change equation 1.1 to become:

$$x_n H_n = y_n \phi_n P \tag{6.1}$$

Here, x_n is the mass fraction of any gas, n, dissolved in water, y_n is the mass fraction of the gas, H_n is Henry's Law constant for the gas, ϕ_n is the fugacity of the gas and P is the system's pressure. To conserve mass, we would also need to change equations 2.1 and 2.2 to:

$$\sum_n y_n = y_1 + y_2 \ldots + y_n = 1 \tag{6.2}$$

$$\sum_n x_n = x_1 + x_2 \ldots + x_n = 1 \tag{6.3}$$

And keeping in mind that we are designing a model, we need some assumptions:

1. Seawater continues to behave like pure H_2O.
2. The solvent doesn't change (H_2O is constant).
3. Each new gas is modelled individually.

As for examples of gases we could add to the system, these could be nitrogen (N_2), oxygen (O_2), argon (Ar), etc. As a result, we will need to calculate H_n values for each of these gases which can be done with equation 4. However, the coefficients h_1 through to h_4 will be different and these are values that we will have to know/find. A few more of such coefficients would be the gases' T_c, P_c, w_n (acentric factor). After knowing all of these variables' values, we can then calculate the gases' fugacity using the Peng-Robinson equation, 5.1 and 5.2. To solve for variables x_n and y_n, we can still apply the matrix method seen in Task 1. However, since we have more sets of simultaneous equations, the matrix may appear larger than the previous 4x4. More specifically, adding just one extra gas increases the size of the matrix to 6x6, 2 extra gases increasing it to 8x8, etc. However, doing this computationally will hopefully make it easier to calculate. And to add, we will also need a range of T and P values to serve as data points which we can use to complete the model.

2 Task 2

2.A Coding Task

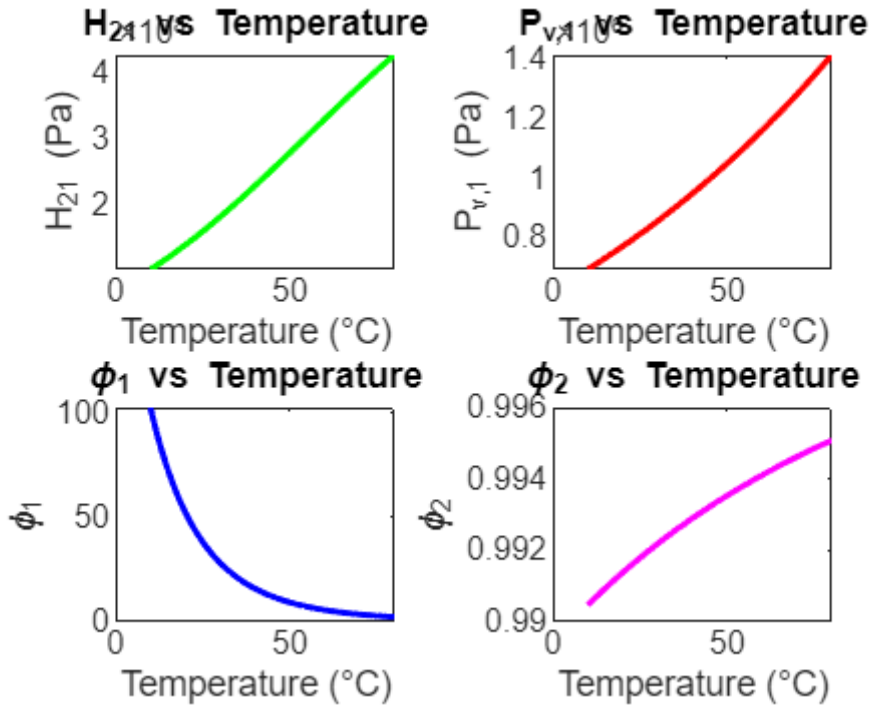

Figure 1.
Graphs showing H_{21}, $P_{v,1}$, ϕ_1 and ϕ_2 plotted against Temperature for $T \in [10,80]$ °C

And to note, the number behind H_{21} is $\times 10^8$ and the number behind $P_{v,1}$ is $\times 10^5$.

To do this, I first inputted all the variables into MATLAB and programmed the necessary equations. Then, I got a list of values for $P_{v,1}$ and H_{21} for integer values of temperature. After that, I used the roots function to find the relevant max and min real roots then used that to solve for ϕ_1 and ϕ_2. Lastly, I plotted all 4 variables against temperature.

2.B Validation Task

	P = 50 kPa		P = 101.325 kPa		P = 200 kPa	
Temperature	Achieved	Expected	Achieved	Expected	Achieved	Expected
10°C	0.658	0.670	0.948	0.962	1.886	1.900
20°C	0.455	0.479	0.688	0.704	1.372	1.398
30°C	0.221	0.251	0.512	0.531	0.957	1.065
40°C	0.169	0.186	0.389	0.409	0.813	0.835
50°C	0.122	0.135	0.257	0.319	0.645	0.669
60°C	0.082	0.091	0.225	0.247	0.532	0.544
70°C	0.039	0.047	0.164	0.185	0.421	0.444
80°C	0.015	0.006	0.113	0.127	0.319	0.357

From the solubilities that I calculated, most of the data points seem to be as expected except for some anomalies. This could be due to discrepancies during the methodology when the solubilities were worked out in the research paper. However, as the code simulates an ideal environment with the given assumptions that there is only CO_2 in the atmosphere, this could mean that my results are only applicable in ideal environments. Also, my constant values (e.g. H_{21}) might be slightly different.

2.C Modelling Task

To first model the equilibrium concentration of CO_2 in water over time, I first had to clean the data. I did this by finding anomalies in the temperature, pressure and CO_2 concentration columns. I then deleted each row that had an anomaly in either one of those variables. First, I would have to rearrange equation 1.2 for x_2 ($x_2 = \frac{(y_2 \phi_2 P)}{H_{21}}$) and

then after calculating $P_{v,1}$ and H_{21}, substitute those values to find x_2 as y_2 is already given in the dataset.

3 Task 3

3.A Coding Task

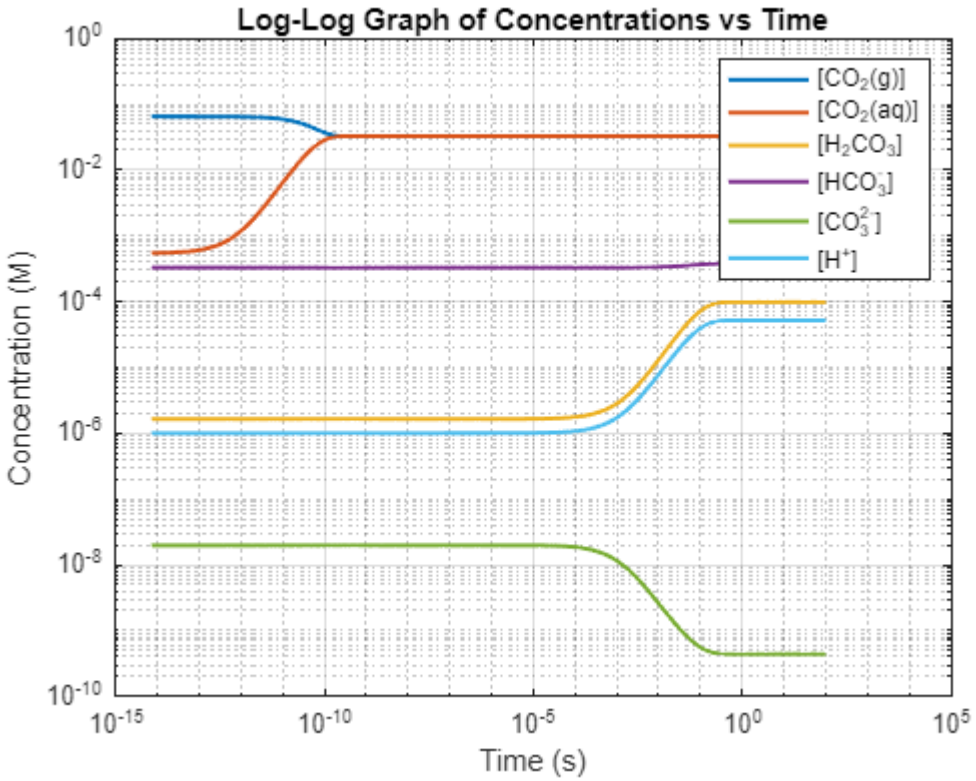

Figure 2: Graphs showing all chemicals involved in equations 6.1 to 6.6 and how they vary with time.

3.B Analysis Task

If we look at the reactions that take place, in R1, there are 2 variables involved: gaseous carbon dioxide and aqueous carbon dioxide. They are also linked by the constants k_1 and k_{-1} where k_1 is the rate of the forward reaction and k_{-1} is the rate of the backward reaction. Looking at table 3, we can see that the rate of the forward reaction is equal to the rate of the backward reaction and they are both very large. Since all k constants are measured in s^{-1}, this means that the reaction in fact occurs very quickly – almost instantaneously. Coming to R2, we can see that equation 6.2 is involved and links aqueous carbon dioxide, gaseous carbon dioxide and carbonic acid. The constants in the reaction are k_1, k_{-1}, k_2 and k_{-2}. Since we have already seen k_1 and k_{-1}, if we focus on k_2 and k_{-2}, we can see that k_2 is relatively smaller which means that the rate of the backward reaction is greater than the rate of the forward reaction. So, it is still quite fast but not as fast as R1. This also means that more CO_2 and H_2O is produced per second than carbonic acid. Coming to R3, this links equation 6.3 and constants k_2, k_{-2}, k_3 and k_{-3}. Now both k_3 and k_{-3} have high orders of magnitude which means that they both occur very quickly. But if we were to compare, we can see that k_3 is larger so the forward reaction occurs more which means more H^+ and HCO_3^- is produced per second. Lastly, looking at R4, this links equation 6.4 and constants k_3, k_{-3}, k_4 and k_{-4}. As k_4 is significantly lower than k_{-4}, this means that the backwards reaction occurs much quicker so more

HCO_3^- is produced per second. However, the orders of magnitude aren't as big as for other constants so the reaction occurs moderately fast. When I used my programme, I found that the time taken for the system to reach steady-state equilibrium was around 0.018 seconds. Another way to check this is by manually measuring the time difference on the x-axis between the start of the experiment and when the last chemical reaches equilibrium (in this case CO_3^{2-}). Doing this, I got a rough estimate of 0.01 seconds using 10^{-1} and 10^{-14}. This is quite close to my answer in MATLAB so it seems acceptable.

3.C Summary Task

The models mentioned in the phase equilibrium and reaction kinetics sections both describe the behaviour of carbon dioxide in water but they both differ slightly from one another. The phase equilibrium model focuses on the system at a fixed moment in time an only focuses on the balance between gaseous CO_2 and dissolved CO_2 at equilibrium. The model also requires the use of Henry's Law and assumes constant temperature and pressure. It assumes an ideal environment and requires specific conditions for it to work. This can be seen in the assumptions where we treat seawater as pure water and ignore other atmospheric gases or impurities. This approach allows us to predict solubility under equilibrium conditions but only for a fixed moment in time.

On the other hand, the reaction kinetics model uses a model that changes with time – as it does in the real world. It uses a range of reversible reactions and involves many more chemicals including carbonic acid and carbonate ions. The model also uses a system of ordinary differential equations along with constants that describe rates of reactions. This makes it ideal for analysing how each chemical's concentrations change over time. However, unlike the phase equilibrium model, it doesn't need many unknowns as solely the k values and initial conditions were enough.

However, I believe that both models can still be connected. Instead of thinking of the phase equilibrium model as a final or initial state, we can think of it as the range of states of equilibrium that the system goes through by following the reaction kinetics model – much like a quasi-static process (5). Therefore, the reaction kinetics model can be seen as only describing the same process but continuously rather than being done discretely in the phase equilibrium model. Additionally looking solely at the final and initial states, the phase equilibrium model can be used to predict the final state of the reaction kinetics model.

Coming to phenomena, the phase equilibrium model describes the connection of CO_2 between gas and liquid phases at equilibrium and uses Henry's Law, assuming constant conditions. The reaction kinetics model can be used to find out how the chemical reactions vary with time and what occurs, chemically, when CO_2 dissolves in water, producing carbonic acid and carbonate ions, for example. Both models, however, can be used to predict the behaviour of the dissolution of CO_2 in water.

4 Appendix

4.A References

[1] Avishay DM, Tenny KM. Henry's Law [Internet]. PubMed. Treasure Island (FL): StatPearls Publishing; 2023. Available from: https://pubmed.ncbi.nlm.nih.gov/31335021/ (Accessed on: 31/12/2024)

[2] Henry's Law Constants [Internet]. Henrys-law.org. 2023. Available from: https://henrys-law.org/henry/index.html (Accessed on: 31/12/2024)

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4.B MATLAB Code

```
% Defining known variables
T_Celsius = linspace(10,80,71) % Temperature in Celsius
```

```
T_Celsius = 1×71
    10    11    12    13    14    15    16    17    18    19    20    21 ⋯
```

```
T_Kelvin = T_Celsius + 273.15 % Convert to Kelvin
```

```
T_Kelvin = 1×71
  283.1500  284.1500  285.1500  286.1500  287.1500  288.1500  289.1500 ⋯
```

```
P = 101325 % Pressure in Pa
```

```
P = 101325
```

```
Tc_water = 647.096 % Critical temperature of water (K)
```

```
Tc_water = 647.0960
```

```
Pc_water = 22064000 % Critical pressure of water (Pa)
```

```
Pc_water = 22064000
```

```
R = 8.314 % Units of J/(mol K)
```

```
R = 8.3140
```

```
Tc_carbon = 304.18 % Kelvin
```

```
Tc_carbon = 304.1800
```

```
Pc_carbon = 7380000 % Pa
```

```
Pc_carbon = 7380000
```

```
Tr_water = T_Kelvin/Tc_water
```

```
Tr_water = 1×71
    0.4376    0.4391    0.4407    0.4422    0.4438    0.4453    0.4468 ⋯
```

```
x = 1-Tr_water
```

```
x = 1×71
    0.5624    0.5609    0.5593    0.5578    0.5562    0.5547    0.5532 ⋯
```

```
Tr_carbon = T_Kelvin/Tc_carbon
```

```
Tr_carbon = 1×71
    0.9309    0.9342    0.9374    0.9407    0.9440    0.9473    0.9506 ⋯
```

```
% Coefficients for Eq. (3)
alpha1 = -7.85951783
```

```
alpha1 = -7.8595
```

```
alpha2 = 1.84408259
```

```
alpha2 = 1.8441
```

```
alpha3 = -11.7866497
```

```
alpha3 = -11.7866
```

```
alpha4 = 22.6807411
```

```
alpha4 = 22.6807
```

```
alpha5 = -15.9618719
```

```
alpha5 = -15.9619
```

```
alpha6 = 1.80122502
```

```
alpha6 = 1.8012
```

```
Pv1 = Pc_water.*(exp((alpha1.*x)+(alpha2.*x.^(1.5))+(alpha3.*x.^(3))+(alpha4.*x.^(3.5))+(alpha5.*x.^(4))+(alpha6.*x.^(7.5)))./Tr_water)
```

```
Pv1 = 1×71
10^6 ×
    0.6935    0.7009    0.7084    0.7159    0.7236    0.7313    0.7390 ⋯
```

```
% Coefficients for Eq. (4)
h1 = -6.8346
```

```
h1 = -6.8346
```

```
h2 = 1.2817*(10^4)
```

```
h2 = 12817
```

```
h3 = -3.7668*(10^6)
```

```
h3 = -3766800
```

```
h4 = 2.9970*(10^8)
```

```
h4 = 299700000
```

```
H21 = 10.^6.*exp(h1+(h2./T_Kelvin)+(h3./(T_Kelvin.^2))+(h4./(T_Kelvin.^3)))
```

```
H21 = 1×71
10^8 ×
    1.0461    1.0800    1.1146    1.1498    1.1856    1.2221    1.2592 ⋯
```

```
% H2O Cubic
a_water = (0.45724.*(R.*Tc_water).^2)./Pc_water
```

```
a_water = 0.5998
```

```
w_water = 0.348
```

```
w_water = 0.3480
```

```
alpha_water = (1+(0.37464+1.54226.*w_water-0.2699.*w_water.^2).*(1-
sqrt(Tr_water))).^2
```

```
alpha_water = 1×71
    1.6833    1.6807    1.6780    1.6754    1.6727    1.6701    1.6675 ⋯
```

```
a_star_water = a_water.*alpha_water
```

```
a_star_water = 1×71
    1.0097    1.0081    1.0065    1.0049    1.0033    1.0018    1.0002 ⋯
```

```
A_water = (a_star_water.*P)./((R.*T_Kelvin).^2)
```

```
A_water = 1×71
    0.0185    0.0183    0.0181    0.0180    0.0178    0.0177    0.0175 ⋯
```

```
b_water = (0.0778.*R.*Tc_water)./Pc_water
```

```
b_water = 1.8970e-05
```

```
B_water = (b_water.*P)./(R.*T_Kelvin)
```

```
B_water = 1×71
10^-3 ×
    0.8165    0.8136    0.8108    0.8080    0.8051    0.8023    0.7996 ⋯
```

```
H2O_coeff_1 = ones(1,71)
```

```
H2O_coeff_1 = 1×71
     1     1     1     1     1     1     1     1     1     1     1     1 ⋯
```

```
H2O_coeff_2 = B_water-1
```

```
H2O_coeff_2 = 1×71
   -0.9992   -0.9992   -0.9992   -0.9992   -0.9992   -0.9992   -0.9992 ⋯
```

```
H2O_coeff_3 = A_water-(3.*(B_water).^2)-(2.*B_water)
```

```
H2O_coeff_3 = 1×71
    0.0168    0.0167    0.0165    0.0164    0.0162    0.0161    0.0159 ⋯
```

```
H2O_coeff_4 = ((B_water).^3)+(B_water).^2-(A_water.*B_water)
```

```
H2O_coeff_4 = 1×71
10^-4 ×
   -0.1441   -0.1423   -0.1405   -0.1388   -0.1371   -0.1355   -0.1338 ⋯
```

```
Zv_water = zeros(1, 71)
```

```
Zv_water = 1×71
```

```
     0     0     0     0     0     0     0     0     0     0     0     0 ⋯
```

```
Zl_water = zeros(1, 71)
```

```
Zl_water = 1×71
     0     0     0     0     0     0     0     0     0     0     0     0 ⋯
```

```
for n = 1:71
    cubic_coeffs_H2O = [H2O_coeff_1(n), H2O_coeff_2(n), H2O_coeff_3(n),
H2O_coeff_4(n)]
    roots_H2O = roots(cubic_coeffs_H2O)
    Zv_water(n) = max(roots_H2O)
    Zl_water(n) = min(roots_H2O)
end
```

```
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0168   -0.0000
roots_H2O = 3×1
    0.9821
    0.0162
    0.0009
Zv_water = 1×71
    0.9821         0         0         0         0         0         0 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048         0         0         0         0         0         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0167   -0.0000
roots_H2O = 3×1
    0.9822
    0.0161
    0.0009
Zv_water = 1×71
    0.9821    0.9822         0         0         0         0         0 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048    0.9021         0         0         0         0         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0165   -0.0000
roots_H2O = 3×1
    0.9824
    0.0159
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824         0         0         0         0 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048    0.9021    0.8995         0         0         0         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0164   -0.0000
roots_H2O = 3×1
    0.9825
    0.0158
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825         0         0         0 ⋯
Zl_water = 1×71
10^-3 ×
```

```
    0.9048    0.9021    0.8995    0.8969         0         0         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0162   -0.0000
roots_H2O = 3×1
    0.9827
    0.0156
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827         0         0 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048    0.9021    0.8995    0.8969    0.8944         0         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0161   -0.0000
roots_H2O = 3×1
    0.9829
    0.0155
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829         0 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0159   -0.0000
roots_H2O = 3×1
    0.9830
    0.0153
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829    0.9830 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918    0.8893 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0158   -0.0000
roots_H2O = 3×1
    0.9832
    0.0152
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829    0.9830 ⋯
Zl_water = 1×71
10^-3 ×
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918    0.8893 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0157   -0.0000
roots_H2O = 3×1
    0.9833
    0.0150
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *
```

```
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0155   -0.0000
roots_H2O = 3×1
    0.9834
    0.0149
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0154   -0.0000
roots_H2O = 3×1
    0.9836
    0.0147
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0152   -0.0000
roots_H2O = 3×1
```

```
    0.9837
    0.0146
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0151   -0.0000
roots_H2O = 3×1
    0.9839
    0.0145
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0150   -0.0000
roots_H2O = 3×1
    0.9840
    0.0143
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
```

```
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0148   -0.0000
roots_H2O = 3×1
    0.9842
    0.0142
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0147   -0.0000
roots_H2O = 3×1
    0.9843
    0.0141
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843         0         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
```

```
    1.0000   -0.9992    0.0146   -0.0000
roots_H2O = 3×1
    0.9844
    0.0139
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844         0         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0145   -0.0000
roots_H2O = 3×1
    0.9846
    0.0138
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846         0         0
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0143   -0.0000
roots_H2O = 3×1
    0.9847
    0.0137
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847         0
```

```
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0142   -0.0000
roots_H2O = 3×1
    0.9848
    0.0136
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0141   -0.0000
roots_H2O = 3×1
    0.9850
    0.0134
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850         0         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
```

```
0.8560         0         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0140   -0.0000
roots_H2O = 3×1
    0.9851
    0.0133
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851         0         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537         0         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0138   -0.0000
roots_H2O = 3×1
    0.9852
    0.0132
    0.0009
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852         0         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515         0         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0137   -0.0000
roots_H2O = 3×1
    0.9853
    0.0131
    0.0008
Zv_water = 1×71
```

```
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853         0         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493         0         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0136   -0.0000
roots_H2O = 3×1
    0.9855
    0.0129
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855         0         0
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471         0         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9992    0.0135   -0.0000
roots_H2O = 3×1
    0.9856
    0.0128
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856         0
0         0         0
Zl_water = 1×71
1.0e-03 *
```

```
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449         0
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0134   -0.0000
roots_H2O = 3×1
    0.9857
    0.0127
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0133   -0.0000
roots_H2O = 3×1
    0.9858
    0.0126
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858         0         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406         0         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0131   -0.0000
roots_H2O = 3×1
    0.9859
```

```
    0.0125
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859         0
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385         0
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0130   -0.0000
roots_H2O = 3×1
    0.9861
    0.0124
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0129   -0.0000
roots_H2O = 3×1
    0.9862
    0.0123
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
```

```
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0128   -0.0000
roots_H2O = 3×1
    0.9863
    0.0122
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0127   -0.0000
roots_H2O = 3×1
    0.9864
    0.0120
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0126   -0.0000
```

```
roots_H2O = 3×1
    0.9865
    0.0119
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0125   -0.0000
roots_H2O = 3×1
    0.9866
    0.0118
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0124   -0.0000
roots_H2O = 3×1
    0.9867
    0.0117
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
```

```
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0123   -0.0000
roots_H2O = 3×1
    0.9868
    0.0116
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0122   -0.0000
roots_H2O = 3×1
    0.9869
    0.0115
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
```

```
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0121   -0.0000
roots_H2O = 3×1
    0.9870
    0.0114
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0120   -0.0000
roots_H2O = 3×1
    0.9871
    0.0113
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0119   -0.0000
roots_H2O = 3×1
    0.9873
    0.0112
    0.0008
Zv_water = 1×71
```

```
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0118   -0.0000
roots_H2O = 3×1
    0.9874
    0.0111
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0117   -0.0000
roots_H2O = 3×1
    0.9875
    0.0110
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *
```

```
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0116   -0.0000
roots_H2O = 3×1
    0.9876
    0.0109
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0115   -0.0000
roots_H2O = 3×1
    0.9877
    0.0108
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0114   -0.0000
roots_H2O = 3×1
    0.9878
```

```
    0.0107
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0113   -0.0000
roots_H2O = 3×1
    0.9879
    0.0106
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0112   -0.0000
roots_H2O = 3×1
    0.9879
    0.0106
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
```

```
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0111   -0.0000
roots_H2O = 3×1
    0.9880
    0.0105
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0110   -0.0000
roots_H2O = 3×1
    0.9881
    0.0104
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0110   -0.0000
```

```
roots_H2O = 3×1
    0.9882
    0.0103
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0109   -0.0000
roots_H2O = 3×1
    0.9883
    0.0102
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0108   -0.0000
roots_H2O = 3×1
    0.9884
    0.0101
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
```

```
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0107   -0.0000
roots_H2O = 3×1
    0.9885
    0.0100
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0106   -0.0000
roots_H2O = 3×1
    0.9886
    0.0099
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
```

```
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0105   -0.0000
roots_H2O = 3×1
    0.9887
    0.0098
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0104   -0.0000
roots_H2O = 3×1
    0.9888
    0.0098
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0104   -0.0000
roots_H2O = 3×1
    0.9889
    0.0097
    0.0008
Zv_water = 1×71
```

```
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0103   -0.0000
roots_H2O = 3×1
    0.9889
    0.0096
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0102   -0.0000
roots_H2O = 3×1
    0.9890
    0.0095
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *
```

```
    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0101   -0.0000
roots_H2O = 3×1
    0.9891
    0.0094
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0100   -0.0000
roots_H2O = 3×1
    0.9892
    0.0094
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0100   -0.0000
roots_H2O = 3×1
    0.9893
```

```
    0.0093
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0099   -0.0000
roots_H2O = 3×1
    0.9894
    0.0092
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0098   -0.0000
roots_H2O = 3×1
    0.9894
    0.0091
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
```

```
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0097   -0.0000
roots_H2O = 3×1
    0.9895
    0.0090
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0096   -0.0000
roots_H2O = 3×1
    0.9896
    0.0090
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0096   -0.0000
```

```
roots_H2O = 3×1
    0.9897
    0.0089
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0095   -0.0000
roots_H2O = 3×1
    0.9898
    0.0088
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0094   -0.0000
roots_H2O = 3×1
    0.9898
    0.0087
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
```

```
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
cubic_coeffs_H2O = 1×4
    1.0000   -0.9993    0.0093   -0.0000
roots_H2O = 3×1
    0.9899
    0.0087
    0.0008
Zv_water = 1×71
    0.9821    0.9822    0.9824    0.9825    0.9827    0.9829
0.9830    0.9832    0.9833    0.9834    0.9836    0.9837    0.9839
0.9840    0.9842    0.9843    0.9844    0.9846    0.9847    0.9848
0.9850    0.9851    0.9852    0.9853    0.9855    0.9856    0.9857
0.9858    0.9859    0.9861
Zl_water = 1×71
1.0e-03 *

    0.9048    0.9021    0.8995    0.8969    0.8944    0.8918
0.8893    0.8868    0.8843    0.8818    0.8794    0.8770    0.8746
0.8722    0.8698    0.8674    0.8651    0.8628    0.8605    0.8582
0.8560    0.8537    0.8515    0.8493    0.8471    0.8449    0.8428
0.8406    0.8385    0.8364
```

```
 phi_v_H2O = exp((Zv_water-1)-(log(Zv_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zv_water+(1+sqrt(2)).*B_water)./(Zv_wat
er+(1-sqrt(2))*B_water)))
```

```
phi_v_H2O = 1×71
    0.9824    0.9825    0.9827    0.9828    0.9830    0.9831
0.9833    0.9834    0.9836    0.9837    0.9838    0.9840    0.9841
0.9843    0.9844    0.9845    0.9847    0.9848    0.9849    0.9850
0.9852    0.9853    0.9854    0.9855    0.9857    0.9858    0.9859
0.9860    0.9861    0.9862
```

```
 phi_l_H2O = exp((Zl_water-1)-(log(Zl_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zl_water+(1+sqrt(2)).*B_water)./(Zl_wat
er+(1-sqrt(2))*B_water)))
```

```
phi_l_H2O = 1×71
```

```
    0.0096    0.0103    0.0110    0.0118    0.0126    0.0135
0.0144    0.0154    0.0164    0.0175    0.0187    0.0200    0.0213
0.0227    0.0241    0.0257    0.0273    0.0291    0.0309    0.0328
0.0348    0.0370    0.0392    0.0416    0.0441    0.0467    0.0495
0.0524    0.0554    0.0586
```

```
phi_1 = phi_v_H2O./phi_l_H2O
```

```
phi_1 = 1×71
  102.7474   95.8492   89.4641   83.5504   78.0702   72.9889
68.2747   63.8988   59.8347   56.0579   52.5465   49.2799   46.2396
43.4083   40.7704   38.3113   36.0179   33.8778   31.8799   30.0137
28.2698   26.6393   25.1142   23.6870   22.3508   21.0992   19.9262
18.8266   17.7951   16.8273
```

```
% CO2 Cubic
a_carbon = (0.45724.*(R.*Tc_carbon).^2)./Pc_carbon
```

```
a_carbon = 0.3962
```

```
w_carbon = 0.225
```

```
w_carbon = 0.2250
```

```
alpha_carbon = (1+(0.37464+1.54226.*w_carbon-0.2699.*w_carbon.^2).*(1-
sqrt(Tr_carbon))).^2
```

```
alpha_carbon = 1×71
    1.0504    1.0480    1.0455    1.0431    1.0406    1.0382
1.0357    1.0333    1.0309    1.0285    1.0261    1.0237    1.0213
1.0189    1.0165    1.0142    1.0118    1.0094    1.0071    1.0047
1.0024    1.0001    0.9977    0.9954    0.9931    0.9908    0.9885
0.9862    0.9839    0.9817
```

```
a_star_carbon = a_carbon.*alpha_carbon
```

```
a_star_carbon = 1×71
    0.4162    0.4153    0.4143    0.4133    0.4123    0.4114
0.4104    0.4095    0.4085    0.4075    0.4066    0.4056    0.4047
0.4037    0.4028    0.4019    0.4009    0.4000    0.3991    0.3981
0.3972    0.3963    0.3954    0.3944    0.3935    0.3926    0.3917
0.3908    0.3899    0.3890
```

```
A_carbon = (a_star_carbon.*P)./((R.*T_Kelvin).^2)
```

```
A_carbon = 1×71
    0.0076    0.0075    0.0075    0.0074    0.0073    0.0073
0.0072    0.0071    0.0071    0.0070    0.0069    0.0069    0.0068
```

```
0.0067    0.0067    0.0066    0.0066    0.0065    0.0065    0.0064
0.0063    0.0063    0.0062    0.0062    0.0061    0.0061    0.0060
0.0060    0.0059    0.0059
```

```
b_carbon = (0.0778.*R.*Tc_carbon)./Pc_carbon
```

```
b_carbon = 2.6660e-05
```

```
B_carbon = (b_carbon.*P)./(R.*T_Kelvin)
```

```
B_carbon = 1×71
    0.0011    0.0011    0.0011    0.0011    0.0011    0.0011
0.0011    0.0011    0.0011    0.0011    0.0011    0.0011    0.0011
0.0011    0.0011    0.0011    0.0011    0.0011    0.0011    0.0011
0.0011    0.0011    0.0011    0.0011    0.0011    0.0011    0.0011
0.0010    0.0010    0.0010
```

```
CO2_coeff_1 = ones(1,71)
```

```
CO2_coeff_1 = 1×71
     1     1     1     1     1     1     1     1     1     1     1
1     1     1     1     1     1     1     1     1     1     1     1
1     1     1     1     1     1     1
```

```
CO2_coeff_2 = B_carbon-1
```

```
CO2_coeff_2 = 1×71
   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -
0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989
-0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989
-0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989   -0.9989
-0.9990   -0.9990   -0.9990
```

```
CO2_coeff_3 = A_carbon-(3.*(B_carbon).^2)-(2.*B_carbon)
```

```
CO2_coeff_3 = 1×71
    0.0053    0.0052    0.0052    0.0051    0.0051    0.0050
0.0049    0.0049    0.0048    0.0048    0.0047    0.0047    0.0046
0.0046    0.0045    0.0044    0.0044    0.0043    0.0043    0.0042
0.0042    0.0041    0.0041    0.0040    0.0040    0.0039    0.0039
0.0039    0.0038    0.0038
```

```
CO2_coeff_4 = ((B_carbon).^3)+(B_carbon).^2-(A_carbon.*B_carbon)
```

```
CO2_coeff_4 = 1×71
```

```
1.0e-05 *

   -0.7415   -0.7312   -0.7210   -0.7111   -0.7013   -0.6916   -
0.6822   -0.6728   -0.6636   -0.6546   -0.6457   -0.6369   -0.6283
-0.6198   -0.6115   -0.6033   -0.5952   -0.5872   -0.5794   -0.5717
-0.5641   -0.5566   -0.5492   -0.5419   -0.5348   -0.5278   -0.5208
-0.5140   -0.5073   -0.5007
```

```
Zv_carbon = zeros(1, 71)
```

```
Zv_carbon = 1×71
     0     0     0     0     0     0     0     0     0     0     0
0     0     0     0     0     0     0     0     0     0     0     0
0     0     0     0     0     0     0
```

```
for n = 1:71
    cubic_coeffs_CO2 = [CO2_coeff_1(n), CO2_coeff_2(n), CO2_coeff_3(n),
CO2_coeff_4(n)]
    roots_CO2 = roots(cubic_coeffs_CO2)
    Zv_carbon(n) = max(real(roots_CO2))
end
```

```
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0053   -0.0000
roots_CO2 = 3×1
   0.9935 + 0.0000i
   0.0027 + 0.0006i
   0.0027 - 0.0006i
Zv_carbon = 1×71
    0.9935         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0052   -0.0000
roots_CO2 = 3×1
   0.9936 + 0.0000i
   0.0026 + 0.0006i
   0.0026 - 0.0006i
Zv_carbon = 1×71
    0.9935    0.9936         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
```

```
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0052   -0.0000
roots_CO2 = 3×1
   0.9936 + 0.0000i
   0.0026 + 0.0007i
   0.0026 - 0.0007i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0051   -0.0000
roots_CO2 = 3×1
   0.9937 + 0.0000i
   0.0026 + 0.0007i
   0.0026 - 0.0007i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0051   -0.0000
roots_CO2 = 3×1
   0.9938 + 0.0000i
   0.0025 + 0.0008i
   0.0025 - 0.0008i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0050   -0.0000
roots_CO2 = 3×1
   0.9938 + 0.0000i
   0.0025 + 0.0008i
   0.0025 - 0.0008i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
```

```
    1.0000   -0.9989    0.0049   -0.0000
roots_CO2 = 3×1
   0.9939 + 0.0000i
   0.0025 + 0.0008i
   0.0025 - 0.0008i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0049   -0.0000
roots_CO2 = 3×1
   0.9940 + 0.0000i
   0.0025 + 0.0009i
   0.0025 - 0.0009i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0048   -0.0000
roots_CO2 = 3×1
   0.9940 + 0.0000i
   0.0024 + 0.0009i
   0.0024 - 0.0009i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940         0         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0048   -0.0000
roots_CO2 = 3×1
   0.9941 + 0.0000i
   0.0024 + 0.0009i
   0.0024 - 0.0009i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941         0         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0047   -0.0000
```

```
roots_CO2 = 3×1
   0.9942 + 0.0000i
   0.0024 + 0.0009i
   0.0024 - 0.0009i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942         0         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0047   -0.0000
roots_CO2 = 3×1
   0.9942 + 0.0000i
   0.0023 + 0.0010i
   0.0023 - 0.0010i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942         0
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0046   -0.0000
roots_CO2 = 3×1
   0.9943 + 0.0000i
   0.0023 + 0.0010i
   0.0023 - 0.0010i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0046   -0.0000
roots_CO2 = 3×1
   0.9943 + 0.0000i
   0.0023 + 0.0010i
   0.0023 - 0.0010i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943         0         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0045   -0.0000
roots_CO2 = 3×1
```

```
   0.9944 + 0.0000i
   0.0023 + 0.0010i
   0.0023 - 0.0010i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944         0         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0044   -0.0000
roots_CO2 = 3×1
   0.9944 + 0.0000i
   0.0022 + 0.0010i
   0.0022 - 0.0010i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944         0         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0044   -0.0000
roots_CO2 = 3×1
   0.9945 + 0.0000i
   0.0022 + 0.0011i
   0.0022 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945         0         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0043   -0.0000
roots_CO2 = 3×1
   0.9946 + 0.0000i
   0.0022 + 0.0011i
   0.0022 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946         0         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0043   -0.0000
roots_CO2 = 3×1
   0.9946 + 0.0000i
```

```
   0.0022 + 0.0011i
   0.0022 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946         0
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0042   -0.0000
roots_CO2 = 3×1
   0.9947 + 0.0000i
   0.0021 + 0.0011i
   0.0021 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0042   -0.0000
roots_CO2 = 3×1
   0.9947 + 0.0000i
   0.0021 + 0.0011i
   0.0021 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947         0         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0041   -0.0000
roots_CO2 = 3×1
   0.9948 + 0.0000i
   0.0021 + 0.0011i
   0.0021 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948         0         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0041   -0.0000
roots_CO2 = 3×1
   0.9948 + 0.0000i
   0.0021 + 0.0011i
```

```
   0.0021 - 0.0011i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948         0         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0040   -0.0000
roots_CO2 = 3×1
   0.9949 + 0.0000i
   0.0020 + 0.0012i
   0.0020 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949         0         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0040   -0.0000
roots_CO2 = 3×1
   0.9949 + 0.0000i
   0.0020 + 0.0012i
   0.0020 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949         0         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0039   -0.0000
roots_CO2 = 3×1
   0.9950 + 0.0000i
   0.0020 + 0.0012i
   0.0020 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950         0
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9989    0.0039   -0.0000
roots_CO2 = 3×1
   0.9950 + 0.0000i
   0.0020 + 0.0012i
   0.0020 - 0.0012i
```

```
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0039   -0.0000
roots_CO2 = 3×1
   0.9951 + 0.0000i
   0.0019 + 0.0012i
   0.0019 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951         0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0038   -0.0000
roots_CO2 = 3×1
   0.9951 + 0.0000i
   0.0019 + 0.0012i
   0.0019 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0038   -0.0000
roots_CO2 = 3×1
   0.9952 + 0.0000i
   0.0019 + 0.0012i
   0.0019 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0037   -0.0000
roots_CO2 = 3×1
   0.9952 + 0.0000i
   0.0019 + 0.0012i
   0.0019 - 0.0012i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0037   -0.0000
roots_CO2 = 3×1
   0.9953 + 0.0000i
   0.0018 + 0.0012i
   0.0018 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0036   -0.0000
roots_CO2 = 3×1
   0.9953 + 0.0000i
   0.0018 + 0.0012i
   0.0018 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0036   -0.0000
roots_CO2 = 3×1
   0.9954 + 0.0000i
   0.0018 + 0.0012i
   0.0018 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0036   -0.0000
roots_CO2 = 3×1
   0.9954 + 0.0000i
   0.0018 + 0.0012i
   0.0018 - 0.0012i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0035   -0.0000
roots_CO2 = 3×1
   0.9955 + 0.0000i
   0.0018 + 0.0012i
   0.0018 - 0.0012i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0035   -0.0000
roots_CO2 = 3×1
   0.9955 + 0.0000i
   0.0017 + 0.0013i
   0.0017 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0034   -0.0000
roots_CO2 = 3×1
   0.9955 + 0.0000i
   0.0017 + 0.0013i
   0.0017 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0034   -0.0000
roots_CO2 = 3×1
   0.9956 + 0.0000i
   0.0017 + 0.0013i
   0.0017 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0033   -0.0000
roots_CO2 = 3×1
   0.9956 + 0.0000i
   0.0017 + 0.0013i
   0.0017 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0033   -0.0000
roots_CO2 = 3×1
   0.9957 + 0.0000i
   0.0017 + 0.0013i
   0.0017 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0033   -0.0000
roots_CO2 = 3×1
   0.9957 + 0.0000i
   0.0016 + 0.0013i
   0.0016 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0032   -0.0000
roots_CO2 = 3×1
   0.9958 + 0.0000i
   0.0016 + 0.0013i
   0.0016 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0032   -0.0000
roots_CO2 = 3×1
   0.9958 + 0.0000i
   0.0016 + 0.0013i
   0.0016 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0032   -0.0000
roots_CO2 = 3×1
   0.9958 + 0.0000i
   0.0016 + 0.0013i
   0.0016 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0031   -0.0000
roots_CO2 = 3×1
   0.9959 + 0.0000i
   0.0016 + 0.0013i
   0.0016 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0031   -0.0000
roots_CO2 = 3×1
   0.9959 + 0.0000i
   0.0015 + 0.0013i
   0.0015 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0030   -0.0000
roots_CO2 = 3×1
   0.9960 + 0.0000i
   0.0015 + 0.0013i
   0.0015 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0030   -0.0000
roots_CO2 = 3×1
   0.9960 + 0.0000i
   0.0015 + 0.0013i
   0.0015 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0030   -0.0000
roots_CO2 = 3×1
   0.9960 + 0.0000i
   0.0015 + 0.0013i
   0.0015 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0029   -0.0000
roots_CO2 = 3×1
   0.9961 + 0.0000i
   0.0015 + 0.0013i
   0.0015 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0029   -0.0000
roots_CO2 = 3×1
   0.9961 + 0.0000i
   0.0015 + 0.0013i
   0.0015 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0029   -0.0000
roots_CO2 = 3×1
   0.9962 + 0.0000i
   0.0014 + 0.0013i
   0.0014 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0028   -0.0000
roots_CO2 = 3×1
   0.9962 + 0.0000i
   0.0014 + 0.0013i
   0.0014 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0028   -0.0000
roots_CO2 = 3×1
   0.9962 + 0.0000i
   0.0014 + 0.0013i
   0.0014 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0028   -0.0000
roots_CO2 = 3×1
   0.9963 + 0.0000i
   0.0014 + 0.0013i
   0.0014 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0027   -0.0000
roots_CO2 = 3×1
   0.9963 + 0.0000i
   0.0014 + 0.0013i
   0.0014 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0027   -0.0000
roots_CO2 = 3×1
   0.9963 + 0.0000i
   0.0014 + 0.0013i
   0.0014 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9990    0.0027   -0.0000
roots_CO2 = 3×1
   0.9964 + 0.0000i
   0.0013 + 0.0013i
   0.0013 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0026   -0.0000
roots_CO2 = 3×1
   0.9964 + 0.0000i
   0.0013 + 0.0013i
   0.0013 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0026   -0.0000
roots_CO2 = 3×1
   0.9964 + 0.0000i
   0.0013 + 0.0013i
   0.0013 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0026   -0.0000
roots_CO2 = 3×1
   0.9965 + 0.0000i
   0.0013 + 0.0013i
   0.0013 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0026   -0.0000
roots_CO2 = 3×1
   0.9965 + 0.0000i
   0.0013 + 0.0013i
   0.0013 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0025   -0.0000
roots_CO2 = 3×1
   0.9965 + 0.0000i
   0.0013 + 0.0013i
   0.0013 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0025   -0.0000
roots_CO2 = 3×1
   0.9966 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0025   -0.0000
roots_CO2 = 3×1
   0.9966 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0024   -0.0000
roots_CO2 = 3×1
   0.9966 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0024   -0.0000
roots_CO2 = 3×1
   0.9967 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0024   -0.0000
roots_CO2 = 3×1
   0.9967 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0023   -0.0000
roots_CO2 = 3×1
   0.9967 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9991    0.0023   -0.0000
roots_CO2 = 3×1
   0.9968 + 0.0000i
   0.0012 + 0.0013i
   0.0012 - 0.0013i
Zv_carbon = 1×71
```

```
    0.9935    0.9936    0.9936    0.9937    0.9938    0.9938
0.9939    0.9940    0.9940    0.9941    0.9942    0.9942    0.9943
0.9943    0.9944    0.9944    0.9945    0.9946    0.9946    0.9947
0.9947    0.9948    0.9948    0.9949    0.9949    0.9950    0.9950
0.9951    0.9951    0.9952
```

```
phi_v_CO2 = exp((Zv_carbon-1)-(log(Zv_carbon-B_carbon))-
(A_carbon./(2*sqrt(2).*B_water)).*log((Zv_carbon+(1+sqrt(2)).*B_carbon)./(Zv_
carbon+(1-sqrt(2))*B_carbon)))
```

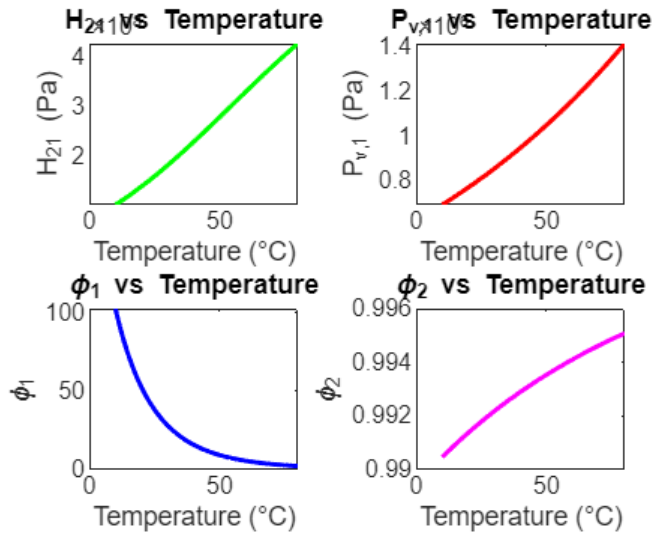
```
phi_v_CO2 = 1×71
    0.9905    0.9906    0.9907    0.9908    0.9908    0.9909
0.9910    0.9911    0.9912    0.9913    0.9914    0.9915    0.9915
0.9916    0.9917    0.9918    0.9919    0.9919    0.9920    0.9921
0.9922    0.9923    0.9923    0.9924    0.9925    0.9925    0.9926
0.9927    0.9928    0.9928
```

```
phi_2 = phi_v_CO2
```

```
phi_2 = 1×71
    0.9905    0.9906    0.9907    0.9908    0.9908    0.9909
0.9910    0.9911    0.9912    0.9913    0.9914    0.9915    0.9915
0.9916    0.9917    0.9918    0.9919    0.9919    0.9920    0.9921
0.9922    0.9923    0.9923    0.9924    0.9925    0.9925    0.9926
0.9927    0.9928    0.9928
```

```
% Plotting 4 graphs
figure;

% H21 Subplot
subplot(2, 2, 1);
plot(T_Celsius, H21, 'g', 'LineWidth', 1.5);
title('H_2_1 vs Temperature');
xlabel('Temperature (°C)');
ylabel('H_2_1 (Pa)');

% Pv1 Subplot
subplot(2, 2, 2);
plot(T_Celsius, Pv1, 'r', 'LineWidth', 1.5);
title('P_v_,_1 vs Temperature');
xlabel('Temperature (°C)');
ylabel('P_v_,_1 (Pa)');

% phi1 Subplot
subplot(2, 2, 3);
plot(T_Celsius, phi_1, 'b', 'LineWidth', 1.5);
```

```
title('\phi_1 vs Temperature');
xlabel('Temperature (°C)');
ylabel('\phi_1');

% phi2 Subplot
subplot(2, 2, 4);
plot(T_Celsius, phi_2, 'm', 'LineWidth', 1.5);
title('\phi_2 vs Temperature');
xlabel('Temperature (°C)');
ylabel('\phi_2');
```




```
%%%%%% TASK 2B %%%%%%

T_Celsius_split = 10:10:80
```

```
T_Celsius_split = 1×8
    10    20    30    40    50    60    70    80
```

```
T_Kelvin_split = T_Celsius_split + 273.15
P1 = 50000
P2 = 101325
P3 = 200000

Tr_water_new = T_Kelvin_split/Tc_water
x_new = 1-Tr_water
Tr_carbon_new = T_Kelvin_split/Tc_carbon
% Coefficients for Eq. (3)
Pv1_new =
Pc_water.*(exp((alpha1.*x)+(alpha2.*x.^(1.5))+(alpha3.*x.^(3))+(alpha4.*x.^(3
.5))+(alpha5.*x.^(4))+(alpha6.*x.^(7.5)))./Tr_water_new)
% Coefficients for Eq. (4)
H21 =
10.^6.*exp(h1+(h2./T_Kelvin_split)+(h3./(T_Kelvin_split.^2))+(h4./(T_Kelvin_s
plit.^3)))
% H2O Cubic
```

```
 a_water = (0.45724.*(R.*Tc_water).^2)./Pc_water
 w_water = 0.348
 alpha_water = (1+(0.37464+1.54226.*w_water-0.2699.*w_water.^2).*(1-
sqrt(Tr_water_new))).^2
 a_star_water = a_water.*alpha_water
 A_water = (a_star_water.*P1)./((R.*T_Kelvin_split).^2)

 b_water = (0.0778.*R.*Tc_water)./Pc_water
 B_water = (b_water.*P1)./(R.*T_Kelvin_split)

 H2O_coeff_1 = ones(1,71)
 H2O_coeff_2 = B_water-1
 H2O_coeff_3 = A_water-(3.*(B_water).^2)-(2.*B_water)
 H2O_coeff_4 = ((B_water).^3)+(B_water).^2-(A_water.*B_water)

 Zv_water = zeros(1, 71)
 Zl_water = zeros(1, 71)

 for n = 1:71
     cubic_coeffs_H2O = [H2O_coeff_1(n), H2O_coeff_2(n), H2O_coeff_3(n),
H2O_coeff_4(n)]
     roots_H2O = roots(cubic_coeffs_H2O)
     Zv_water(n) = max(roots_H2O)
     Zl_water(n) = min(roots_H2O)
 end

 phi_v_H2O = exp((Zv_water-1)-(log(Zv_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zv_water+(1+sqrt(2)).*B_water)./(Zv_wat
er+(1-sqrt(2))*B_water)))
 phi_l_H2O = exp((Zl_water-1)-(log(Zl_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zl_water+(1+sqrt(2)).*B_water)./(Zl_wat
er+(1-sqrt(2))*B_water)))
 phi_1 = phi_v_H2O./phi_l_H2O

 % CO2 Cubic
 a_carbon = (0.45724.*(R.*Tc_carbon).^2)./Pc_carbon
 w_carbon = 0.225
 alpha_carbon = (1+(0.37464+1.54226.*w_carbon-0.2699.*w_carbon.^2).*(1-
sqrt(Tr_carbon))).^2
 a_star_carbon = a_carbon.*alpha_carbon
 A_carbon = (a_star_carbon.*P)./((R.*T_Kelvin).^2)

 b_carbon = (0.0778.*R.*Tc_carbon)./Pc_carbon
 B_carbon = (b_carbon.*P)./(R.*T_Kelvin)

 CO2_coeff_1 = ones(1,71)
 CO2_coeff_2 = B_carbon-1
 CO2_coeff_3 = A_carbon-(3.*(B_carbon).^2)-(2.*B_carbon)
 CO2_coeff_4 = ((B_carbon).^3)+(B_carbon).^2-(A_carbon.*B_carbon)
```

```
 Zv_carbon = zeros(1, 71)

 for n = 1:71
     cubic_coeffs_CO2 = [CO2_coeff_1(n), CO2_coeff_2(n), CO2_coeff_3(n),
CO2_coeff_4(n)]
     roots_CO2 = roots(cubic_coeffs_CO2)
     Zv_carbon(n) = max(real(roots_CO2))
 end

 phi_v_CO2 = exp((Zv_carbon-1)-(log(Zv_carbon-B_carbon))-
(A_carbon./(2*sqrt(2).*B_water)).*log((Zv_carbon+(1+sqrt(2)).*B_carbon)./(Zv_
carbon+(1-sqrt(2))*B_carbon)))
 phi_2 = phi_v_CO2
 % Defining known variables
 T_Celsius = 10:10:80 % Temperature in Celsius
```

```
T_Celsius = 1×8
    10    20    30    40    50    60    70    80
```

```
 T_Kelvin = T_Celsius + 273.15 % Convert to Kelvin
```

```
T_Kelvin = 1×8
  283.1500  293.1500  303.1500  313.1500  323.1500  333.1500  343.1500 ⋯
```

```
 Tc_water = 647.096 % Critical temperature of water (K)
```

```
Tc_water = 647.0960
```

```
 Pc_water = 22064000 % Critical pressure of water (Pa)
```

```
Pc_water = 22064000
```

```
 R = 8.314 % Units of J/(mol K)
```

```
R = 8.3140
```

```
 Tc_carbon = 304.18 % Kelvin
```

```
Tc_carbon = 304.1800
```

```
 Pc_carbon = 7380000 % Pa
```

```
Pc_carbon = 7380000
```

```
 P1 = 50000
```

```
P1 = 50000
```

```
 P2 = 101325
```

```
P2 = 101325
```

```
 P3 = 200000
```

```
P3 = 200000
```

```
%%%%%% TASK 2B %%%%%%
Tr_water = T_Kelvin/Tc_water
```

```
Tr_water = 1×8
    0.4376    0.4530    0.4685    0.4839    0.4994    0.5148    0.5303 ⋯
```

```
x = 1-Tr_water
```

```
x = 1×8
    0.5624    0.5470    0.5315    0.5161    0.5006    0.4852    0.4697 ⋯
```

```
Tr_carbon = T_Kelvin/Tc_carbon
```

```
Tr_carbon = 1×8
    0.9309    0.9637    0.9966    1.0295    1.0624    1.0952    1.1281 ⋯
```

```
% Coefficients for Eq. (3)
alpha1 = -7.85951783
```

```
alpha1 = -7.8595
```

```
alpha2 = 1.84408259
```

```
alpha2 = 1.8441
```

```
alpha3 = -11.7866497
```

```
alpha3 = -11.7866
```

```
alpha4 = 22.6807411
```

```
alpha4 = 22.6807
```

```
alpha5 = -15.9618719
```

```
alpha5 = -15.9619
```

```
alpha6 = 1.80122502
```

```
alpha6 = 1.8012
```

```
Pv1 =
Pc_water.*(exp((alpha1.*x)+(alpha2.*x.^(1.5))+(alpha3.*x.^(3))+(alpha4.*x.^(3
.5))+(alpha5.*x.^(4))+(alpha6.*x.^(7.5)))./Tr_water)
```

```
Pv1 = 1×8
10^6 ×
    0.6935    0.7708    0.8557    0.9486    1.0502    1.1613    1.2826 ⋯
```

```
% Coefficients for Eq. (4)
h1 = -6.8346
```

```
h1 = -6.8346
```

```
h2 = 1.2817*(10^4)
```

```
h2 = 12817
```

```
h3 = -3.7668*(10^6)
```

```
h3 = -3766800
```

```
h4 = 2.9970*(10^8)
```

```
h4 = 299700000
```

```
H21 = 10.^6.*exp(h1+(h2./T_Kelvin)+(h3./(T_Kelvin.^2))+(h4./(T_Kelvin.^3)))
```

```
H21 = 1×8
10^8 ×
    1.0461    1.4136    1.8388    2.3094    2.8086    3.3172    3.8155 ⋯
```

```
% H2O Cubic
a_water = (0.45724.*(R.*Tc_water).^2)./Pc_water
```

```
a_water = 0.5998
```

```
w_water = 0.348
```

```
w_water = 0.3480
```

```
alpha_water = (1+(0.37464+1.54226.*w_water-0.2699.*w_water.^2).*(1-
sqrt(Tr_water))).^2
```

```
alpha_water = 1×8
    1.6833    1.6570    1.6314    1.6064    1.5819    1.5580    1.5346 ⋯
```

```
a_star_water = a_water.*alpha_water
```

```
a_star_water = 1×8
    1.0097    0.9939    0.9785    0.9635    0.9488    0.9345    0.9205 ⋯
```

```
A_water = (a_star_water.*P1)./((R.*T_Kelvin).^2)
```

```
A_water = 1×8
    0.0091    0.0084    0.0077    0.0071    0.0066    0.0061    0.0057 ⋯
```

```
b_water = (0.0778.*R.*Tc_water)./Pc_water
```

```
b_water = 1.8970e-05
```

```
B_water = (b_water.*P1)./(R.*T_Kelvin)
```

```
B_water = 1×8
10^-3 ×
    0.4029    0.3892    0.3763    0.3643    0.3530    0.3424    0.3325 ⋯
```

```
H2O_coeff_1 = ones(1,8)
```

```
H2O_coeff_1 = 1×8
     1     1     1     1     1     1     1     1
```

```
H2O_coeff_2 = B_water-1
```

```
H2O_coeff_2 = 1×8
   -0.9996   -0.9996   -0.9996   -0.9996   -0.9996   -0.9997   -0.9997 ⋯
```

```
H2O_coeff_3 = A_water-(3.*(B_water).^2)-(2.*B_water)
```

```
H2O_coeff_3 = 1×8
    0.0083    0.0076    0.0069    0.0064    0.0059    0.0054    0.0050 ⋯
```

```
H2O_coeff_4 = ((B_water).^3)+(B_water).^2-(A_water.*B_water)
```

```
H2O_coeff_4 = 1×8
10^-5 ×
   -0.3508   -0.3104   -0.2757   -0.2457   -0.2196   -0.1968   -0.1769 ⋯
```

```
Zv_water = zeros(1, 8)
```

```
Zv_water = 1×8
     0     0     0     0     0     0     0     0
```

```
Zl_water = zeros(1, 8)
```

```
Zl_water = 1×8
     0     0     0     0     0     0     0     0
```

```
for n = 1:8
    cubic_coeffs_H2O = [H2O_coeff_1(n), H2O_coeff_2(n), H2O_coeff_3(n),
H2O_coeff_4(n)]
    roots_H2O = roots(cubic_coeffs_H2O)
    Zv_water(n) = max(roots_H2O)
    Zl_water(n) = min(roots_H2O)
end
```

```
cubic_coeffs_H2O = 1×4
    1.0000   -0.9996    0.0083   -0.0000
roots_H2O = 3×1
    0.9912
    0.0079
    0.0004
Zv_water = 1×8
    0.9912         0         0         0         0         0         0 ⋯
Zl_water = 1×8
10^-3 ×
    0.4465         0         0         0         0         0         0 ⋯
cubic_coeffs_H2O = 1×4
    1.0000   -0.9996    0.0076   -0.0000
roots_H2O = 3×1
    0.9920
    0.0072
    0.0004
Zv_water = 1×8
    0.9912    0.9920         0         0         0         0         0 ⋯
```

```
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340         0         0         0         0         0 …
cubic_coeffs_H2O = 1×4
    1.0000   -0.9996    0.0069   -0.0000
roots_H2O = 3×1
    0.9926
    0.0066
    0.0004
Zv_water = 1×8
    0.9912    0.9920    0.9926         0         0         0         0 …
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340    0.4224         0         0         0         0 …
cubic_coeffs_H2O = 1×4
    1.0000   -0.9996    0.0064   -0.0000
roots_H2O = 3×1
    0.9932
    0.0060
    0.0004
Zv_water = 1×8
    0.9912    0.9920    0.9926    0.9932         0         0         0 …
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340    0.4224    0.4117         0         0         0 …
cubic_coeffs_H2O = 1×4
    1.0000   -0.9996    0.0059   -0.0000
roots_H2O = 3×1
    0.9937
    0.0055
    0.0004
Zv_water = 1×8
    0.9912    0.9920    0.9926    0.9932    0.9937         0         0 …
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340    0.4224    0.4117    0.4018         0         0 …
cubic_coeffs_H2O = 1×4
    1.0000   -0.9997    0.0054   -0.0000
roots_H2O = 3×1
    0.9942
    0.0050
    0.0004
Zv_water = 1×8
    0.9912    0.9920    0.9926    0.9932    0.9937    0.9942         0 …
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340    0.4224    0.4117    0.4018    0.3927         0 …
cubic_coeffs_H2O = 1×4
    1.0000   -0.9997    0.0050   -0.0000
roots_H2O = 3×1
    0.9947
    0.0046
    0.0004
Zv_water = 1×8
    0.9912    0.9920    0.9926    0.9932    0.9937    0.9942    0.9947 …
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340    0.4224    0.4117    0.4018    0.3927    0.3842 …
cubic_coeffs_H2O = 1×4
    1.0000   -0.9997    0.0046   -0.0000
roots_H2O = 3×1
    0.9950
```

```
    0.0043
    0.0004
Zv_water = 1×8
    0.9912    0.9920    0.9926    0.9932    0.9937    0.9942    0.9947 ⋯
Zl_water = 1×8
10^-3 ×
    0.4465    0.4340    0.4224    0.4117    0.4018    0.3927    0.3842 ⋯
```

```
 phi_v_H2O = exp((Zv_water-1)-(log(Zv_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zv_water+(1+sqrt(2)).*B_water)./(Zv_wat
er+(1-sqrt(2))*B_water)))
```

```
phi_v_H2O = 1×8
    0.9913    0.9920    0.9927    0.9933    0.9938    0.9943    0.9947 ⋯
```

```
 phi_l_H2O = exp((Zl_water-1)-(log(Zl_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zl_water+(1+sqrt(2)).*B_water)./(Zl_wat
er+(1-sqrt(2))*B_water)))
```

```
phi_l_H2O = 1×8
    0.0194    0.0379    0.0706    0.1255    0.2141    0.3519
0.5590    0.8609
```

```
 phi_1 = phi_v_H2O./phi_l_H2O
```

```
phi_1 = 1×8
   51.1861   26.1569   14.0625    7.9137    4.6409    2.8253
1.7793    1.1558
```

```
 % CO2 Cubic
 a_carbon = (0.45724.*(R.*Tc_carbon).^2)./Pc_carbon
```

```
a_carbon = 0.3962
```

```
 w_carbon = 0.225
```

```
w_carbon = 0.2250
```

```
 alpha_carbon = (1+(0.37464+1.54226.*w_carbon-0.2699.*w_carbon.^2).*(1-
sqrt(Tr_carbon))).^2
```

```
alpha_carbon = 1×8
    1.0504    1.0261    1.0024    0.9794    0.9570    0.9352
0.9140    0.8933
```

```
 a_star_carbon = a_carbon.*alpha_carbon
```

```
a_star_carbon = 1×8
    0.4162    0.4066    0.3972    0.3881    0.3792    0.3706
0.3622    0.3540
```

```
A_carbon = (a_star_carbon.*P1)./((R.*T_Kelvin).^2)
```

```
A_carbon = 1×8
    0.0038    0.0034    0.0031    0.0029    0.0026    0.0024
0.0022    0.0021
```

```
b_carbon = (0.0778.*R.*Tc_carbon)./Pc_carbon
```

```
b_carbon = 2.6660e-05
```

```
B_carbon = (b_carbon.*P1)./(R.*T_Kelvin)
```

```
B_carbon = 1×8
1.0e-03 *

    0.5662    0.5469    0.5289    0.5120    0.4962    0.4813
0.4672    0.4540
```

```
CO2_coeff_1 = ones(1,8)
```

```
CO2_coeff_1 = 1×8
     1     1     1     1     1     1     1     1
```

```
CO2_coeff_2 = B_carbon-1
```

```
CO2_coeff_2 = 1×8
   -0.9994   -0.9995   -0.9995   -0.9995   -0.9995   -0.9995   -
0.9995   -0.9995
```

```
CO2_coeff_3 = A_carbon-(3.*(B_carbon).^2)-(2.*B_carbon)
```

```
CO2_coeff_3 = 1×8
    0.0026    0.0023    0.0021    0.0018    0.0016    0.0015
0.0013    0.0011
```

```
CO2_coeff_4 = ((B_carbon).^3)+(B_carbon).^2-(A_carbon.*B_carbon)
```

```
CO2_coeff_4 = 1×8
1.0e-05 *

   -0.1806   -0.1572   -0.1374   -0.1203   -0.1057   -0.0931   -
0.0821   -0.0726
```

```
 Zv_carbon = zeros(1, 8)
```

```
Zv_carbon = 1×8
     0     0     0     0     0     0     0     0
```

```
 for n = 1:8
     cubic_coeffs_CO2 = [CO2_coeff_1(n), CO2_coeff_2(n), CO2_coeff_3(n),
CO2_coeff_4(n)]
     roots_CO2 = roots(cubic_coeffs_CO2)
     Zv_carbon(n) = max(real(roots_CO2))
 end
```

```
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9994    0.0026   -0.0000
roots_CO2 = 3×1
   0.9968 + 0.0000i
   0.0013 + 0.0003i
   0.0013 - 0.0003i
Zv_carbon = 1×8
    0.9968         0         0         0         0         0
0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0023   -0.0000
roots_CO2 = 3×1
   0.9971 + 0.0000i
   0.0012 + 0.0005i
   0.0012 - 0.0005i
Zv_carbon = 1×8
    0.9968    0.9971         0         0         0         0
0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0021   -0.0000
roots_CO2 = 3×1
   0.9974 + 0.0000i
   0.0010 + 0.0006i
   0.0010 - 0.0006i
Zv_carbon = 1×8
    0.9968    0.9971    0.9974         0         0         0
0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0018   -0.0000
roots_CO2 = 3×1
   0.9976 + 0.0000i
   0.0009 + 0.0006i
   0.0009 - 0.0006i
Zv_carbon = 1×8
```

```
    0.9968    0.9971    0.9974    0.9976         0         0
0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0016   -0.0000
roots_CO2 = 3×1
   0.9979 + 0.0000i
   0.0008 + 0.0006i
   0.0008 - 0.0006i
Zv_carbon = 1×8
    0.9968    0.9971    0.9974    0.9976    0.9979         0
0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0015   -0.0000
roots_CO2 = 3×1
   0.9981 + 0.0000i
   0.0007 + 0.0006i
   0.0007 - 0.0006i
Zv_carbon = 1×8
    0.9968    0.9971    0.9974    0.9976    0.9979    0.9981
0         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0013   -0.0000
roots_CO2 = 3×1
   0.9982 + 0.0000i
   0.0006 + 0.0006i
   0.0006 - 0.0006i
Zv_carbon = 1×8
    0.9968    0.9971    0.9974    0.9976    0.9979    0.9981
0.9982         0
cubic_coeffs_CO2 = 1×4
    1.0000   -0.9995    0.0011   -0.0000
roots_CO2 = 3×1
   0.9984 + 0.0000i
   0.0006 + 0.0006i
   0.0006 - 0.0006i
Zv_carbon = 1×8
    0.9968    0.9971    0.9974    0.9976    0.9979    0.9981
0.9982    0.9984
```

```
 phi_v_CO2 = exp((Zv_carbon-1)-(log(Zv_carbon-B_carbon))-
(A_carbon./(2*sqrt(2).*B_water)).*log((Zv_carbon+(1+sqrt(2)).*B_carbon)./(Zv_
carbon+(1-sqrt(2))*B_carbon)))
```

```
phi_v_CO2 = 1×8
    0.9953    0.9957    0.9961    0.9965    0.9968    0.9971
0.9973    0.9976
```

```
 phi_2 = phi_v_CO2
```

```
phi_2 = 1×8
    0.9953    0.9957    0.9961    0.9965    0.9968    0.9971
0.9973    0.9976
```

```
 val1 = Pv1./1000
```

```
val1 = 1×8
1.0e+03 *

    0.6935    0.7708    0.8557    0.9486    1.0502    1.1613
1.2826    1.4151
```

```
 val2 = (-phi_1.*P1)./1000
```

```
val2 = 1×8
1.0e+03 *

   -2.5593   -1.3078   -0.7031   -0.3957   -0.2320   -0.1413   -
0.0890   -0.0578
```

```
 val3 = H21./1000
```

```
val3 = 1×8
1.0e+05 *

    1.0461    1.4136    1.8388    2.3094    2.8086    3.3172
3.8155    4.2845
```

```
 val4 = (-phi_2.*P1)./1000
```

```
val4 = 1×8
  -49.7646  -49.7871  -49.8069  -49.8246  -49.8404  -49.8545  -
49.8671  -49.8785
```

```
 matrix1 = [val1(1), 0, val2(1), 0; 0, val3(1), 0, val4(1); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix2 = [0;0;1;1];
 matrix3 = inv(matrix1)*matrix2;
 result1 = (matrix3(2,1)*1000);

 matrix4 = [val1(2), 0, val2(2), 0; 0, val3(2), 0, val4(2); 0, 0, 1, 1; 1, 1,
0, 0];
```

```
 matrix5 = inv(matrix4)*matrix2;
 result2 = (matrix5(2,1)*1000);

 matrix6 = [val1(3), 0, val2(3), 0; 0, val3(3), 0, val4(3); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix7 = inv(matrix6)*matrix2;
 result3 = (matrix7(2,1)*1000);

 matrix8 = [val1(4), 0, val2(4), 0; 0, val3(4), 0, val4(4); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix9 = inv(matrix8)*matrix2;
 result4 = (matrix9(2,1)*1000);

 matrix10 = [val1(5), 0, val2(5), 0; 0, val3(5), 0, val4(5); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix11 = inv(matrix10)*matrix2;
 result5 = (matrix11(2,1)*1000);

 matrix12 = [val1(6), 0, val2(6), 0; 0, val3(6), 0, val4(6); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix13 = inv(matrix12)*matrix2;
 result6 = (matrix13(2,1)*1000);

 matrix14 = [val1(7), 0, val2(7), 0; 0, val3(7), 0, val4(7); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix15 = inv(matrix14)*matrix2;
 result7 = (matrix15(2,1)*1000);

 matrix16 = [val1(8), 0, val2(8), 0; 0, val3(8), 0, val4(8); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix17 = inv(matrix16)*matrix2;
 result8 = (matrix17(2,1)*1000);

 allresults = [result1; result2; result3; result4; result5; result6; result7;
result8]
```

```
allresults = 8×1
    0.3469
    0.1446
   -0.0588
   -0.3016
   -0.6262
   -1.0866
   -1.7569
   -2.7419
```

```
 % Defining known variables
```

```
 T_Celsius = 10:10:80 % Temperature in Celsius
 T_Kelvin = T_Celsius + 273.15 % Convert to Kelvin
 Tc_water = 647.096 % Critical temperature of water (K)
 Pc_water = 22064000 % Critical pressure of water (Pa)
 R = 8.314 % Units of J/(mol K)
 Tc_carbon = 304.18 % Kelvin
 Pc_carbon = 7380000 % Pa
 P1 = 50000
 P2 = 101325
 P3 = 200000
 %%%%%% TASK 2B %%%%%%
 Tr_water = T_Kelvin/Tc_water
 x = 1-Tr_water

 Tr_carbon = T_Kelvin/Tc_carbon
 % Coefficients for Eq. (3)
 alpha1 = -7.85951783
 alpha2 = 1.84408259
 alpha3 = -11.7866497
 alpha4 = 22.6807411
 alpha5 = -15.9618719
 alpha6 = 1.80122502

 Pv1 =
Pc_water.*(exp((alpha1.*x)+(alpha2.*x.^(1.5))+(alpha3.*x.^(3))+(alpha4.*x.^(3
.5))+(alpha5.*x.^(4))+(alpha6.*x.^(7.5)))./Tr_water)
 % Coefficients for Eq. (4)
 h1 = -6.8346
 h2 = 1.2817*(10^4)
 h3 = -3.7668*(10^6)
 h4 = 2.9970*(10^8)

 H21 = 10.^6.*exp(h1+(h2./T_Kelvin)+(h3./(T_Kelvin.^2))+(h4./(T_Kelvin.^3)))
 % H2O Cubic
 a_water = (0.45724.*(R.*Tc_water).^2)./Pc_water
 w_water = 0.348
 alpha_water = (1+(0.37464+1.54226.*w_water-0.2699.*w_water.^2).*(1-
sqrt(Tr_water))).^2
 a_star_water = a_water.*alpha_water
 A_water = (a_star_water.*P2)./((R.*T_Kelvin).^2)

 b_water = (0.0778.*R.*Tc_water)./Pc_water
 B_water = (b_water.*P2)./(R.*T_Kelvin)

 H2O_coeff_1 = ones(1,8)
 H2O_coeff_2 = B_water-1
 H2O_coeff_3 = A_water-(3.*(B_water).^2)-(2.*B_water)
 H2O_coeff_4 = ((B_water).^3)+(B_water).^2-(A_water.*B_water)
```

```
 Zv_water = zeros(1, 8)
 Zl_water = zeros(1, 8)

 for n = 1:8
     cubic_coeffs_H2O = [H2O_coeff_1(n), H2O_coeff_2(n), H2O_coeff_3(n),
H2O_coeff_4(n)]
     roots_H2O = roots(cubic_coeffs_H2O)
     Zv_water(n) = max(roots_H2O)
     Zl_water(n) = min(roots_H2O)
 end

 phi_v_H2O = exp((Zv_water-1)-(log(Zv_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zv_water+(1+sqrt(2)).*B_water)./(Zv_wat
er+(1-sqrt(2))*B_water)))
 phi_l_H2O = exp((Zl_water-1)-(log(Zl_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zl_water+(1+sqrt(2)).*B_water)./(Zl_wat
er+(1-sqrt(2))*B_water)))
 phi_1 = phi_v_H2O./phi_l_H2O
 % CO2 Cubic
 a_carbon = (0.45724.*(R.*Tc_carbon).^2)./Pc_carbon
 w_carbon = 0.225
 alpha_carbon = (1+(0.37464+1.54226.*w_carbon-0.2699.*w_carbon.^2).*(1-
sqrt(Tr_carbon))).^2
 a_star_carbon = a_carbon.*alpha_carbon
 A_carbon = (a_star_carbon.*P2)./((R.*T_Kelvin).^2)

 b_carbon = (0.0778.*R.*Tc_carbon)./Pc_carbon
 B_carbon = (b_carbon.*P2)./(R.*T_Kelvin)

 CO2_coeff_1 = ones(1,8)
 CO2_coeff_2 = B_carbon-1
 CO2_coeff_3 = A_carbon-(3.*(B_carbon).^2)-(2.*B_carbon)
 CO2_coeff_4 = ((B_carbon).^3)+(B_carbon).^2-(A_carbon.*B_carbon)

 Zv_carbon = zeros(1, 8)

 for n = 1:8
     cubic_coeffs_CO2 = [CO2_coeff_1(n), CO2_coeff_2(n), CO2_coeff_3(n),
CO2_coeff_4(n)]
     roots_CO2 = roots(cubic_coeffs_CO2)
     Zv_carbon(n) = max(real(roots_CO2))
 end

 phi_v_CO2 = exp((Zv_carbon-1)-(log(Zv_carbon-B_carbon))-
(A_carbon./(2*sqrt(2).*B_water)).*log((Zv_carbon+(1+sqrt(2)).*B_carbon)./(Zv_
carbon+(1-sqrt(2))*B_carbon)))
 phi_2 = phi_v_CO2

 val1 = Pv1./1000
```

```
 val2 = (-phi_1.*P2)./1000
 val3 = H21./1000
 val4 = (-phi_2.*P2)./1000

 matrix1 = [val1(1), 0, val2(1), 0; 0, val3(1), 0, val4(1); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix2 = [0;0;1;1];
 matrix3 = inv(matrix1)*matrix2;
 result1 = (matrix3(2,1)*1000);

 matrix4 = [val1(2), 0, val2(2), 0; 0, val3(2), 0, val4(2); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix5 = inv(matrix4)*matrix2;
 result2 = (matrix5(2,1)*1000);

 matrix6 = [val1(3), 0, val2(3), 0; 0, val3(3), 0, val4(3); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix7 = inv(matrix6)*matrix2;
 result3 = (matrix7(2,1)*1000);

 matrix8 = [val1(4), 0, val2(4), 0; 0, val3(4), 0, val4(4); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix9 = inv(matrix8)*matrix2;
 result4 = (matrix9(2,1)*1000);

 matrix10 = [val1(5), 0, val2(5), 0; 0, val3(5), 0, val4(5); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix11 = inv(matrix10)*matrix2;
 result5 = (matrix11(2,1)*1000);

 matrix12 = [val1(6), 0, val2(6), 0; 0, val3(6), 0, val4(6); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix13 = inv(matrix12)*matrix2;
 result6 = (matrix13(2,1)*1000);

 matrix14 = [val1(7), 0, val2(7), 0; 0, val3(7), 0, val4(7); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix15 = inv(matrix14)*matrix2;
 result7 = (matrix15(2,1)*1000);

 matrix16 = [val1(8), 0, val2(8), 0; 0, val3(8), 0, val4(8); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix17 = inv(matrix16)*matrix2;
 result8 = (matrix17(2,1)*1000);

 allresults = [result1; result2; result3; result4; result5; result6; result7;
result8]
```

```
% Defining known variables
T_Celsius = 10:10:80 % Temperature in Celsius
T_Kelvin = T_Celsius + 273.15 % Convert to Kelvin
Tc_water = 647.096 % Critical temperature of water (K)
Pc_water = 22064000 % Critical pressure of water (Pa)
R = 8.314 % Units of J/(mol K)
Tc_carbon = 304.18 % Kelvin
Pc_carbon = 7380000 % Pa
P1 = 50000
P2 = 101325
P3 = 200000
%%%%%% TASK 2B %%%%%%
Tr_water = T_Kelvin/Tc_water
x = 1-Tr_water

Tr_carbon = T_Kelvin/Tc_carbon
% Coefficients for Eq. (3)
alpha1 = -7.85951783
alpha2 = 1.84408259
alpha3 = -11.7866497
alpha4 = 22.6807411
alpha5 = -15.9618719
alpha6 = 1.80122502

Pv1 =
Pc_water.*(exp((alpha1.*x)+(alpha2.*x.^(1.5))+(alpha3.*x.^(3))+(alpha4.*x.^(3
.5))+(alpha5.*x.^(4))+(alpha6.*x.^(7.5)))./Tr_water)
% Coefficients for Eq. (4)
h1 = -6.8346
h2 = 1.2817*(10^4)
h3 = -3.7668*(10^6)
h4 = 2.9970*(10^8)

H21 = 10.^6.*exp(h1+(h2./T_Kelvin)+(h3./(T_Kelvin.^2))+(h4./(T_Kelvin.^3)))
% H2O Cubic
a_water = (0.45724.*(R.*Tc_water).^2)./Pc_water
w_water = 0.348
alpha_water = (1+(0.37464+1.54226.*w_water-0.2699.*w_water.^2).*(1-
sqrt(Tr_water))).^2
a_star_water = a_water.*alpha_water
A_water = (a_star_water.*P3)./((R.*T_Kelvin).^2)

b_water = (0.0778.*R.*Tc_water)./Pc_water
B_water = (b_water.*P3)./(R.*T_Kelvin)

H2O_coeff_1 = ones(1,8)
H2O_coeff_2 = B_water-1
H2O_coeff_3 = A_water-(3.*(B_water).^2)-(2.*B_water)
```

```
 H2O_coeff_4 = ((B_water).^3)+(B_water).^2-(A_water.*B_water)

 Zv_water = zeros(1, 8)
 Zl_water = zeros(1, 8)

 for n = 1:8
     cubic_coeffs_H2O = [H2O_coeff_1(n), H2O_coeff_2(n), H2O_coeff_3(n),
H2O_coeff_4(n)]
     roots_H2O = roots(cubic_coeffs_H2O)
     Zv_water(n) = max(roots_H2O)
     Zl_water(n) = min(roots_H2O)
 end

 phi_v_H2O = exp((Zv_water-1)-(log(Zv_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zv_water+(1+sqrt(2)).*B_water)./(Zv_wat
er+(1-sqrt(2))*B_water)))
 phi_l_H2O = exp((Zl_water-1)-(log(Zl_water-B_water))-
(A_water./(2*sqrt(2).*B_water)).*log((Zl_water+(1+sqrt(2)).*B_water)./(Zl_wat
er+(1-sqrt(2))*B_water)))
 phi_1 = phi_v_H2O./phi_l_H2O
 % CO2 Cubic
 a_carbon = (0.45724.*(R.*Tc_carbon).^2)./Pc_carbon
 w_carbon = 0.225
 alpha_carbon = (1+(0.37464+1.54226.*w_carbon-0.2699.*w_carbon.^2).*(1-
sqrt(Tr_carbon))).^2
 a_star_carbon = a_carbon.*alpha_carbon
 A_carbon = (a_star_carbon.*P3)./((R.*T_Kelvin).^2)

 b_carbon = (0.0778.*R.*Tc_carbon)./Pc_carbon
 B_carbon = (b_carbon.*P3)./(R.*T_Kelvin)

 CO2_coeff_1 = ones(1,8)
 CO2_coeff_2 = B_carbon-1
 CO2_coeff_3 = A_carbon-(3.*(B_carbon).^2)-(2.*B_carbon)
 CO2_coeff_4 = ((B_carbon).^3)+(B_carbon).^2-(A_carbon.*B_carbon)

 Zv_carbon = zeros(1, 8)

 for n = 1:8
     cubic_coeffs_CO2 = [CO2_coeff_1(n), CO2_coeff_2(n), CO2_coeff_3(n),
CO2_coeff_4(n)]
     roots_CO2 = roots(cubic_coeffs_CO2)
     Zv_carbon(n) = max(real(roots_CO2))
 end

 phi_v_CO2 = exp((Zv_carbon-1)-(log(Zv_carbon-B_carbon))-
(A_carbon./(2*sqrt(2).*B_water)).*log((Zv_carbon+(1+sqrt(2)).*B_carbon)./(Zv_
carbon+(1-sqrt(2))*B_carbon)))
 phi_2 = phi_v_CO2
```

```
 val1 = Pv1./1000
 val2 = (-phi_1.*P3)./1000
 val3 = H21./1000
 val4 = (-phi_2.*P3)./1000

 matrix1 = [val1(1), 0, val2(1), 0; 0, val3(1), 0, val4(1); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix2 = [0;0;1;1];
 matrix3 = inv(matrix1)*matrix2;
 result1 = (matrix3(2,1)*1000);

 matrix4 = [val1(2), 0, val2(2), 0; 0, val3(2), 0, val4(2); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix5 = inv(matrix4)*matrix2;
 result2 = (matrix5(2,1)*1000);

 matrix6 = [val1(3), 0, val2(3), 0; 0, val3(3), 0, val4(3); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix7 = inv(matrix6)*matrix2;
 result3 = (matrix7(2,1)*1000);

 matrix8 = [val1(4), 0, val2(4), 0; 0, val3(4), 0, val4(4); 0, 0, 1, 1; 1, 1,
0, 0];
 matrix9 = inv(matrix8)*matrix2;
 result4 = (matrix9(2,1)*1000);

 matrix10 = [val1(5), 0, val2(5), 0; 0, val3(5), 0, val4(5); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix11 = inv(matrix10)*matrix2;
 result5 = (matrix11(2,1)*1000);

 matrix12 = [val1(6), 0, val2(6), 0; 0, val3(6), 0, val4(6); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix13 = inv(matrix12)*matrix2;
 result6 = (matrix13(2,1)*1000);

 matrix14 = [val1(7), 0, val2(7), 0; 0, val3(7), 0, val4(7); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix15 = inv(matrix14)*matrix2;
 result7 = (matrix15(2,1)*1000);

 matrix16 = [val1(8), 0, val2(8), 0; 0, val3(8), 0, val4(8); 0, 0, 1, 1; 1,
1, 0, 0];
 matrix17 = inv(matrix16)*matrix2;
 result8 = (matrix17(2,1)*1000);

 allresults = [result1; result2; result3; result4; result5; result6; result7;
result8]
```

```
% Import the dataset
data = ProjectData; % Replace 'your_dataset.csv' with the actual file name

% Initial table containing all data points
initialTable = table(data.site_code, data.measurement_id, data.TIME, ...
                     data.TEMP, data.Press_ATM, data.CO2EQ_PPM, ...
                     'VariableNames', {'SiteCode', 'Measurement', 'Time',
...
                                       'Temperature', 'Pressure',
'CO2ConcWater'});

% Remove duplicate rows
uniqueTable = unique(initialTable, "rows");

% Clipping data columns for easier handling
TempClipped = uniqueTable.Temperature;
PressureClipped = uniqueTable.Pressure;
CO2WaterClipped = uniqueTable.CO2ConcWater;

% Detecting outliers in specified variables
detection_Pressure = isoutlier(PressureClipped, "quartiles");
detection_Temperature = isoutlier(TempClipped, "quartiles");
detection_CO2Water = isoutlier(CO2WaterClipped, "quartiles");

% Removing rows with outliers
% Create logical index to remove rows where any of the selected variables
have outliers
outlierIndex = detection_Pressure | detection_Temperature |
detection_CO2Water;

% Create a cleaned table by removing rows with outliers
cleanTable = uniqueTable(~outlierIndex, :);

% Adding a 'Year' column for easier analysis
cleanTable.Year = year(datetime(cleanTable.Time, 'InputFormat', 'yyyy-MM-
dd''T''HH:mm:ss''Z'''));



% Save the cleaned dataset
writetable(cleanTable, 'cleaned_dataset.csv');
disp(size(cleanTable))
```

```
    154437           7
```

```
data = cleanTable
```

data = 154437×7 table

	SiteCode	Measurement	Time	Temperature	...
1	GBRWIS	1	"2020-10-31T10:00:00Z"	24.3132	
2	GBRWIS	1	"2021-03-27T10:00:00Z"	26.9895	
3	GBRWIS	1	"2021-09-21T10:00:00Z"	22.4750	
4	GBRWIS	1	"2022-05-16T12:00:00Z"	24.8867	
5	GBRWIS	1	"2022-11-02T04:00:00Z"	24.4562	
6	GBRWIS	1	"2023-05-01T10:00:00Z"	25.6385	
7	GBRWIS	1	"2023-10-11T06:00:00Z"	23.0590	
8	GBRWIS	2	"2020-10-31T12:00:00Z"	24.1960	
9	GBRWIS	2	"2021-03-27T12:00:00Z"	27.0938	
10	GBRWIS	2	"2021-09-21T12:00:00Z"	22.3367	
11	GBRWIS	2	"2022-05-16T14:00:00Z"	24.8710	
12	GBRWIS	2	"2022-11-02T06:00:00Z"	24.4706	
13	GBRWIS	2	"2023-05-01T12:00:00Z"	25.6113	
14	GBRWIS	2	"2023-10-11T08:00:00Z"	22.8557	
15	GBRWIS	3	"2020-10-31T14:00:00Z"	24.1836	
16	GBRWIS	3	"2021-03-27T14:00:00Z"	27.0388	
17	GBRWIS	3	"2021-09-21T14:00:00Z"	22.1666	
18	GBRWIS	3	"2022-05-16T16:00:00Z"	24.8712	
19	GBRWIS	3	"2022-11-02T08:00:00Z"	24.2090	
20	GBRWIS	3	"2023-05-01T14:00:00Z"	25.5656	
21	GBRWIS	3	"2023-10-11T10:00:00Z"	22.8102	
22	GBRWIS	4	"2020-10-31T16:00:00Z"	24.1438	
23	GBRWIS	4	"2021-03-27T16:00:00Z"	27.1254	
24	GBRWIS	4	"2021-09-21T16:00:00Z"	21.9194	
25	GBRWIS	4	"2022-05-16T18:00:00Z"	24.8447	
26	GBRWIS	4	"2022-11-02T10:00:00Z"	24.1262	
27	GBRWIS	4	"2023-05-01T16:00:00Z"	25.5886	
28	GBRWIS	4	"2023-10-11T12:00:00Z"	22.9046	
29	GBRWIS	5	"2020-10-31T18:00:00Z"	24.1152	
30	GBRWIS	5	"2021-03-27T18:00:00Z"	27.1007	
31	GBRWIS	5	"2021-09-21T18:00:00Z"	21.9535	
32	GBRWIS	5	"2022-05-16T20:00:00Z"	24.8342	
33	GBRWIS	5	"2022-11-02T12:00:00Z"	24.0226	
34	GBRWIS	5	"2023-05-01T18:00:00Z"	25.5826	
35	GBRWIS	5	"2023-10-11T14:00:00Z"	23.3348	
36	GBRWIS	6	"2020-10-31T20:00:00Z"	24.0574	
37	GBRWIS	6	"2021-03-27T20:00:00Z"	26.9823	
38	GBRWIS	6	"2021-09-21T20:00:00Z"	21.9551	

	SiteCode	Measurement	Time	Temperature	…
39	GBRWIS	6	"2022-05-16T22:00:00Z"	24.8936	
40	GBRWIS	6	"2022-11-02T14:00:00Z"	24.2494	
41	GBRWIS	6	"2023-05-01T20:00:00Z"	25.5685	
42	GBRWIS	6	"2023-10-11T16:00:00Z"	22.9298	
43	GBRWIS	7	"2020-10-31T22:00:00Z"	24.1220	
44	GBRWIS	7	"2021-03-27T22:00:00Z"	26.9796	
45	GBRWIS	7	"2021-09-21T22:00:00Z"	21.9069	
46	GBRWIS	7	"2022-05-17T00:00:00Z"	24.9454	
47	GBRWIS	7	"2022-11-02T16:00:00Z"	24.2046	
48	GBRWIS	7	"2023-05-01T22:00:00Z"	25.5693	
49	GBRWIS	7	"2023-10-11T18:00:00Z"	22.8290	
50	GBRWIS	8	"2020-11-01T00:00:00Z"	24.2227	
51	GBRWIS	8	"2021-03-28T00:00:00Z"	27.0428	
52	GBRWIS	8	"2021-09-22T00:00:00Z"	21.9473	
53	GBRWIS	8	"2022-05-17T02:00:00Z"	24.9087	
54	GBRWIS	8	"2022-11-02T18:00:00Z"	24.1167	
55	GBRWIS	8	"2023-05-02T00:00:00Z"	25.5798	
56	GBRWIS	8	"2023-10-11T20:00:00Z"	22.7747	
57	GBRWIS	9	"2020-11-01T02:00:00Z"	24.9186	
58	GBRWIS	9	"2021-03-28T02:00:00Z"	27.4048	
59	GBRWIS	9	"2021-09-22T02:00:00Z"	22.0762	
60	GBRWIS	9	"2022-05-17T04:00:00Z"	25.1657	
61	GBRWIS	9	"2022-11-02T20:00:00Z"	24.0587	
62	GBRWIS	9	"2023-05-02T02:00:00Z"	25.6358	
63	GBRWIS	9	"2023-10-11T22:00:00Z"	22.8217	
64	GBRWIS	10	"2020-11-01T04:00:00Z"	25.4500	
65	GBRWIS	10	"2021-03-28T04:00:00Z"	28.2432	
66	GBRWIS	10	"2021-09-22T04:00:00Z"	22.3441	
67	GBRWIS	10	"2022-05-17T06:00:00Z"	24.9786	
68	GBRWIS	10	"2022-11-02T22:00:00Z"	24.0738	
69	GBRWIS	10	"2023-05-02T04:00:00Z"	25.7073	
70	GBRWIS	10	"2023-10-12T00:00:00Z"	22.9473	
71	GBRWIS	11	"2020-11-01T06:00:00Z"	24.6910	
72	GBRWIS	11	"2021-03-28T06:00:00Z"	27.2303	
73	GBRWIS	11	"2021-09-22T06:00:00Z"	22.1390	
74	GBRWIS	11	"2022-05-17T08:00:00Z"	24.9591	
75	GBRWIS	11	"2022-11-03T00:00:00Z"	24.0673	
76	GBRWIS	11	"2023-05-02T06:00:00Z"	25.5942	

	SiteCode	Measurement	Time	Temperature	⋯
77	GBRWIS	11	"2023-10-12T02:00:00Z"	24.2813	
78	GBRWIS	12	"2020-11-01T08:00:00Z"	24.6383	
79	GBRWIS	12	"2021-03-28T08:00:00Z"	27.2084	
80	GBRWIS	12	"2021-09-22T08:00:00Z"	22.0102	
81	GBRWIS	12	"2022-05-17T10:00:00Z"	24.9529	
82	GBRWIS	12	"2022-11-03T02:00:00Z"	24.2072	
83	GBRWIS	12	"2023-05-02T08:00:00Z"	25.6123	
84	GBRWIS	12	"2023-10-12T04:00:00Z"	23.4801	
85	GBRWIS	13	"2020-11-01T10:00:00Z"	24.4941	
86	GBRWIS	13	"2021-03-28T10:00:00Z"	27.1524	
87	GBRWIS	13	"2021-09-22T10:00:00Z"	22.0491	
88	GBRWIS	13	"2022-05-17T12:00:00Z"	24.9093	
89	GBRWIS	13	"2022-11-03T04:00:00Z"	24.2029	
90	GBRWIS	13	"2023-05-02T10:00:00Z"	25.5825	
91	GBRWIS	13	"2023-10-12T06:00:00Z"	23.0891	
92	GBRWIS	14	"2020-11-01T12:00:00Z"	24.4879	
93	GBRWIS	14	"2021-03-28T12:00:00Z"	27.1884	
94	GBRWIS	14	"2021-09-22T12:00:00Z"	22.0046	
95	GBRWIS	14	"2022-05-17T14:00:00Z"	24.8798	
96	GBRWIS	14	"2022-11-03T06:00:00Z"	24.1388	
97	GBRWIS	14	"2023-05-02T12:00:00Z"	25.5450	
98	GBRWIS	14	"2023-10-12T08:00:00Z"	22.9383	
99	GBRWIS	15	"2020-11-01T14:00:00Z"	24.3364	
100	GBRWIS	15	"2021-09-22T14:00:00Z"	21.9002	

⋮

```
T_Celsius = data.Temperature % Temperature in Celsius
```

```
T_Celsius = 154437×1
   24.3132
   26.9895
   22.4750
   24.8867
   24.4562
   25.6385
   23.0590
   24.1960
   27.0938
   22.3367
      ⋮
```

```
T_Kelvin = T_Celsius + 273.15 % Convert to Kelvin
```

```
T_Kelvin = 154437×1
   297.4632
   300.1395
   295.6250
   298.0367
   297.6062
   298.7885
   296.2090
   297.3460
   300.2438
   295.4867
      ⋮
```

```
 P = data.Pressure * 100; % Pressure in Pa (assuming Pressure in atmosphere,
so multiply by 100)
 y2 = data.CO2ConcWater; % The equilibrium CO2 concentration in water (ppm)
 Tc_water = 647.096 % Critical temperature of water (K)
```

```
Tc_water = 647.0960
```

```
 Pc_water = 22064000 % Critical pressure of water (Pa)
```

```
Pc_water = 22064000
```

```
 R = 8.314 % Units of J/(mol K)
```

```
R = 8.3140
```

```
 Tc_carbon = 304.18 % Kelvin
```

```
Tc_carbon = 304.1800
```

```
 Pc_carbon = 7380000 % Pa
```

```
Pc_carbon = 7380000
```

```
 Tr_water = T_Kelvin/Tc_water
```

```
Tr_water = 154437×1
    0.4597
    0.4638
    0.4568
    0.4606
    0.4599
    0.4617
    0.4578
    0.4595
    0.4640
    0.4566
      ⋮
```

```
 x = 1-Tr_water
```

```
x = 154437×1
    0.5403
    0.5362
    0.5432
    0.5394
```

```
    0.5401
    0.5383
    0.5422
    0.5405
    0.5360
    0.5434
      ⋮
```

```
Tr_carbon = T_Kelvin/Tc_carbon
```

```
Tr_carbon = 154437×1
    0.9779
    0.9867
    0.9719
    0.9798
    0.9784
    0.9823
    0.9738
    0.9775
    0.9871
    0.9714
      ⋮
```

```
% Coefficients for Eq. (3)
alpha1 = -7.85951783
```

```
alpha1 = -7.8595
```

```
alpha2 = 1.84408259
```

```
alpha2 = 1.8441
```

```
alpha3 = -11.7866497
```

```
alpha3 = -11.7866
```

```
alpha4 = 22.6807411
```

```
alpha4 = 22.6807
```

```
alpha5 = -15.9618719
```

```
alpha5 = -15.9619
```

```
alpha6 = 1.80122502
```

```
alpha6 = 1.8012
```

```
Pv1 =
Pc_water.*(exp((alpha1.*x)+(alpha2.*x.^(1.5))+(alpha3.*x.^(3))+(alpha4.*x.^(3
.5))+(alpha5.*x.^(4))+(alpha6.*x.^(7.5)))./Tr_water)
```

```
Pv1 = 154437×1
10^5 ×
    8.0649
    8.2933
    7.9112
```

```
    8.1134
    8.0770
    8.1773
    7.9598
    8.0550
    8.3023
    7.8998
      ⋮
```

```
% Coefficients for Eq. (4)
h1 = -6.8346
```

```
h1 = -6.8346
```

```
h2 = 1.2817*(10^4)
```

```
h2 = 12817
```

```
h3 = -3.7668*(10^6)
```

```
h3 = -3766800
```

```
h4 = 2.9970*(10^8)
```

```
h4 = 299700000
```

```
H21 = 10.^6.*exp(h1+(h2./T_Kelvin)+(h3./(T_Kelvin.^2))+(h4./(T_Kelvin.^3)))
```

```
H21 = 154437×1
10^8 ×
    1.5906
    1.7054
    1.5139
    1.6149
    1.5966
    1.6470
    1.5381
    1.5856
    1.7099
    1.5082
      ⋮
```

```
% CO2 Cubic
a_carbon = (0.45724.*(R.*Tc_carbon).^2)./Pc_carbon
```

```
a_carbon = 0.3962
```

```
w_carbon = 0.225
```

```
w_carbon = 0.2250
```

```
alpha_carbon = (1+(0.37464+1.54226.*w_carbon-0.2699.*w_carbon.^2).*(1-
sqrt(Tr_carbon))).^2
```

```
alpha_carbon = 154437×1
    1.0158
    1.0095
```

```
    1.0202
    1.0144
    1.0154
    1.0126
    1.0188
    1.0161
    1.0092
    1.0205
      ⋮
```

```
a_star_carbon = a_carbon.*alpha_carbon
```

```
a_star_carbon = 154437×1
    0.4025
    0.4000
    0.4042
    0.4020
    0.4024
    0.4013
    0.4037
    0.4026
    0.3999
    0.4044
      ⋮
```

```
A_carbon = (a_star_carbon.*P)./((R.*T_Kelvin).^2)
```

```
A_carbon = 154437×1
10^-3 ×
    0.6638
    0.6508
    0.6778
    0.6609
    0.6631
    0.6585
    0.6765
    0.6651
    0.6505
    0.6798
      ⋮
```

```
b_carbon = (0.0778.*R.*Tc_carbon)./Pc_carbon
```

```
b_carbon = 2.6660e-05
```

```
B_carbon = (b_carbon.*P)./(R.*T_Kelvin)
```

```
B_carbon = 154437×1
10^-3 ×
    0.1087
    0.1082
    0.1099
    0.1086
    0.1087
    0.1087
    0.1100
    0.1089
    0.1083
    0.1101
```

```
⋮
```

```
CO2_coeff_1 = ones(length(T_Kelvin),1)
```

```
CO2_coeff_1 = 154437×1
     1
     1
     1
     1
     1
     1
     1
     1
     1
     1
     ⋮
```

```
CO2_coeff_2 = B_carbon-1
```

```
CO2_coeff_2 = 154437×1
   -0.9999
   -0.9999
   -0.9999
   -0.9999
   -0.9999
   -0.9999
   -0.9999
   -0.9999
   -0.9999
   -0.9999
      ⋮
```

```
CO2_coeff_3 = A_carbon-(3.*(B_carbon).^2)-(2.*B_carbon)
```

```
CO2_coeff_3 = 154437×1
10^-3 ×
    0.4463
    0.4343
    0.4580
    0.4436
    0.4456
    0.4411
    0.4564
    0.4473
    0.4340
    0.4596
      ⋮
```

```
CO2_coeff_4 = ((B_carbon).^3)+(B_carbon).^2-(A_carbon.*B_carbon)
```

```
CO2_coeff_4 = 154437×1
10^-7 ×
   -0.6036
   -0.5873
   -0.6240
   -0.5999
   -0.6026
   -0.5975
   -0.6232
```

```
   -0.6055
   -0.5870
   -0.6273
      ⋮
```

```
Zv_carbon = zeros(length(T_Kelvin),1)
```

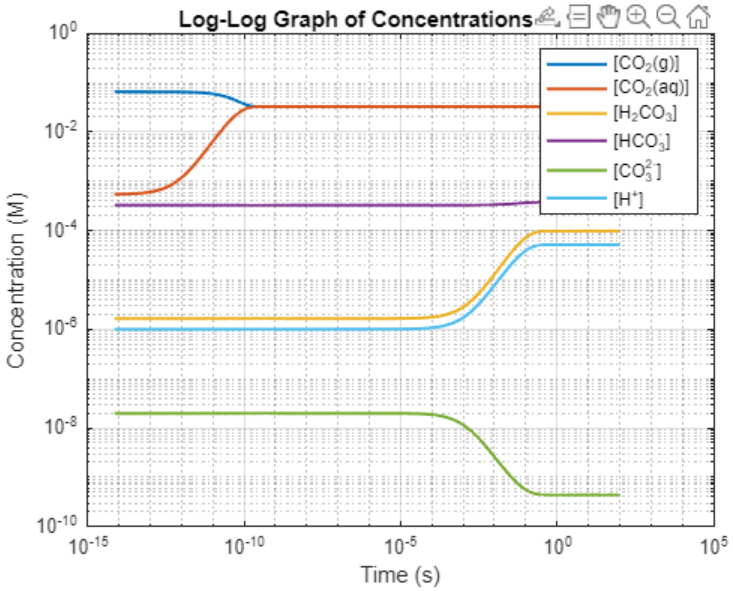
```
Zv_carbon = 154437×1
      0
      0
      0
      0
      0
      0
      0
      0
      0
      0
      ⋮
```

```
for n = 1:length(T_Kelvin);
    cubic_coeffs_CO2 = [CO2_coeff_1(n), CO2_coeff_2(n), CO2_coeff_3(n),
CO2_coeff_4(n)];
    roots_CO2 = roots(cubic_coeffs_CO2);
    Zv_carbon(n) = max(real(roots_CO2));
end


phi_v_CO2 = exp((Zv_carbon-1)-(log(Zv_carbon-B_carbon))-
(A_carbon./(2*sqrt(2).*B_water)).*log((Zv_carbon+(1+sqrt(2)).*B_carbon)./(Zv_
carbon+(1-sqrt(2))*B_carbon)))
phi_2 = phi_v_CO2

% % Extract Temperature, Pressure, and CO2 Equilibrium concentration (y2)
from the dataset
% T_Celsius = data.Temperature; % Temperature in Celsius (from your dataset)
% T_Kelvin = T_Celsius + 273.15; % Convert to Kelvin
% P = data.Pressure * 100; % Pressure in Pa (assuming Pressure in
atmosphere, so multiply by 100)
% y2 = data.CO2ConcWater; % The equilibrium CO2 concentration in water (ppm)
%
% % Constants for CO2 and water
% Tc_water = 647.096; % Critical temperature of water (K)
% Pc_water = 22064000; % Critical pressure of water (Pa)
% Tc_carbon = 304.18; % Critical temperature of CO2 (K)
% Pc_carbon = 7380000; % Critical pressure of CO2 (Pa)
% R = 8.314; % Universal gas constant in J/(mol K)
%
% % Reduced temperature for water and CO2
% Tr_water = T_Kelvin / Tc_water;
% x = 1 - Tr_water; % Deviation from critical temperature
```

```
 %
 % Tr_carbon = T_Kelvin / Tc_carbon; % Reduced temperature for CO2
 %
 % % CO2 Equations
 % h1 = -6.8346;
 % h2 = 1.2817 * 10^4;
 % h3 = -3.7668 * 10^6;
 % h4 = 2.9970 * 10^8;
 %
 % H21 = 10.^6 .* exp(h1 + (h2 ./ T_Kelvin) + (h3 ./ (T_Kelvin .^ 2)) + (h4
./ (T_Kelvin .^ 3)));
 %
 % % CO2 Cubic Equation for Compressibility Factor
 % a_carbon = (0.45724 .* (R .* Tc_carbon) .^ 2) ./ Pc_carbon;
 % w_carbon = 0.225;
 % alpha_carbon = (1 + (0.37464 + 1.54226 .* w_carbon - 0.2699 .* w_carbon .^
2) .* (1 - sqrt(Tr_carbon))) .^ 2;
 % a_star_carbon = a_carbon .* alpha_carbon;
 % A_carbon = (a_star_carbon .* P) ./ ((R .* T_Kelvin) .^ 2);
 %
 % b_carbon = (0.0778 .* R .* Tc_carbon) ./ Pc_carbon;
 % B_carbon = (b_carbon .* P) ./ (R .* T_Kelvin);
 %
 % % Fugacity coefficient for CO2 (phi_2)
 % phi_2 = exp((Pv1 - 1) - (log(Pv1 - B_carbon)) - (A_carbon ./ (2 * sqrt(2)
.* B_carbon)) .* ...
 %     log((Pv1 + (1 + sqrt(2)) * B_carbon) ./ (Pv1 + (1 - sqrt(2)) *
B_carbon)));
 %
 % % Now solve for x_2 using the equation: x_2 = (y_2 * phi_2 * P) / H21
 % x2 = (y2 .* phi_2 .* P) ./ H21;
 %
 % % Plotting the results
 % figure;
 % subplot(3, 1, 1);
 % plot(data.TIME, T_Celsius, 'r');
 % xlabel('Time');
 % ylabel('Temperature (°C)');
 % title('Temperature vs Time');
 %
 % subplot(3, 1, 2);
 % plot(data.TIME, P, 'g');
 % xlabel('Time');
 % ylabel('Pressure (Pa)');
 % title('Pressure vs Time');
 %
 % subplot(3, 1, 3);
 % plot(data.TIME, x2, 'b');
 % xlabel('Time');
```

```
% ylabel('CO₂ Concentration in Water (ppm)');
% title('CO₂ Concentration in Water (x2) vs Time');
%
% % Save the results to a new table
% results = table(data.TIME, T_Celsius, P, x2, 'VariableNames', {'Time',
'Temperature', 'Pressure', 'CO2ConcWater'});
% writetable(results, 'modelled_CO2_concentration.csv');
%
%
% Constants
k1 = 1e10;
k2 = 6e-2;
k3 = 1e7;
k4 = 3;
k_neg1 = 1e10;
k_neg2 = 2e1;
k_neg3 = 5e10;
k_neg4 = 5e10;

% Initial conditions
y0 = [0.065, 5.41e-4, 1.64e-6, 3.28e-4, 1.97e-8, 1e-6];  % [CO2(g)],
[CO2(aq)], [H2CO3], [HCO3^-], [CO3^2-], [H+]

% Time for simulation
tspan = [0 100];

% Combining the equations
carbon_system = @(t, y) [
    -k1*y(1) + k_neg1*y(2); % d[CO2(g)]/dt
    k1*y(1) - (k_neg1 + k2)*y(2) + k_neg2*y(3); % d[CO2(aq)]/dt
    k2*y(2) - (k_neg2 + k3)*y(3) + k_neg3*y(6)*y(4); % d[H2CO3]/dt
    k3*y(3) - k_neg3*y(6)*y(4) - k4*y(4) + k_neg4*y(6)*y(5); % d[HCO3^-]/dt
    k4*y(4) - k_neg4*y(6)*y(5); % d[CO3^2-]/dt
    k3*y(3) - k_neg3*y(6)*y(4) + k4*y(4) - k_neg4*y(6)*y(5); % d[H+]/dt
];

% Set tolerances
options = odeset('AbsTol', 1e-12, 'RelTol', 1e-6);

% Solving the equations
[t, y] = ode15s(@(t, y) carbon_system(t, y), tspan, y0, options);

% Results
CO2_g = y(:,1);    % [CO2(g)]
CO2_aq = y(:,2);   % [CO2(aq)]
H2CO3 = y(:,3);    % [H2CO3]
HCO3_minus = y(:,4); % [HCO3^-]
CO3_2_minus = y(:,5); % [CO3^2-]
H_plus = y(:,6);   % [H+]
```

```
% Plot all chemicals on a log-log graph
figure;
loglog(t, CO2_g,'DisplayName', '[CO_2(g)]', 'LineWidth', 1.5); hold on;
loglog(t, CO2_aq, 'DisplayName', '[CO_2(aq)]', 'LineWidth', 1.5);
loglog(t, H2CO3, 'DisplayName', '[H_2CO_3]', 'LineWidth', 1.5);
loglog(t, HCO3_minus,'DisplayName', '[HCO_3^-]', 'LineWidth', 1.5);
loglog(t, CO3_2_minus,'DisplayName', '[CO_3^2^-]', 'LineWidth', 1.5);
loglog(t, H_plus, 'DisplayName', '[H^+]', 'LineWidth', 1.5);

% Add labels and legend
xlabel('Time (s)');
ylabel('Concentration (M)');
title('Log-Log Graph of Concentrations vs Time');
legend('show'); % Display legend

% Improve plot appearance
grid on;
hold off;
```




```
% Calculate the rate of change for each species
dCO2_g_dt = diff(CO2_g) ./ diff(t);
dCO2_aq_dt = diff(CO2_aq) ./ diff(t);
dH2CO3_dt = diff(H2CO3) ./ diff(t);
dHCO3_minus_dt = diff(HCO3_minus) ./ diff(t);
dCO3_2_minus_dt = diff(CO3_2_minus) ./ diff(t);
dH_plus_dt = diff(H_plus) ./ diff(t);

% Plot the rate of change for each species
figure;
plot(t(2:end), dCO2_g_dt, 'DisplayName', 'd[CO2(g)]/dt');
```

```
hold on;
plot(t(2:end), dCO2_aq_dt, 'DisplayName', 'd[CO2(aq)]/dt');
plot(t(2:end), dH2CO3_dt, 'DisplayName', 'd[H2CO3]/dt');
plot(t(2:end), dHCO3_minus_dt, 'DisplayName', 'd[HCO3^-]/dt');
plot(t(2:end), dCO3_2_minus_dt, 'DisplayName', 'd[CO3^2-]/dt');
plot(t(2:end), dH_plus_dt, 'DisplayName', 'd[H+]/dt');
xlabel('Time (s)');
ylabel('Rate of Change');
title('Rate of Change of Species vs Time');
legend('show');
grid on;
hold off;
```