

# Appendix A

## Activities calculation

Solution activities are computed with the help of the Debye-Huckel theory [1]:

$$\ln(a) = M_{m_{sol}} \nu M_{AB} \left( 1 - \frac{\alpha(T)}{3} |z^+ z^-| \sqrt{I} \sigma(B\sqrt{I}) + \frac{\delta I}{2} \right) \quad (1)$$

In this equation,  $M_{m_{sol}}$  is the molar mass of solvent (in  $\frac{kg}{mol}$ ). It is  $0.018 \frac{kg}{mol}$  in the case of water.  $\nu$  is the number of ions present after dissociation of the compounds and  $z^+$  and  $z^-$  their valence. For example,  $NaCl$  dissolution generates two ions ( $Na^+$  and  $Cl^-$ ) and  $\nu = 2$ ,  $z^+ = 1$  and  $z^- = -1$ . For  $Na_2CO_3$ ,  $\nu = 3$ ,  $z^+ = 1$  and  $z^- = -2$  as it liberates 2  $Na^+$  and 1  $CO_3^{2-}$ .  $M_{AB}$  is the molality of the solution, the number of moles of solute by kg of solvent (in  $\frac{mol}{kg}$ ).  $I$  is the ionic strength given by the relationship:

$$I = \frac{1}{2} M_{AB} \sum_{ions} \nu_i z_i^2 \quad (2)$$

with  $\nu_i$  the number ion species  $i$  (for example,  $\nu_{Na^+} = 2$  in  $Na_2CO_3$ ).

$\alpha(T)$  is the first Debye-Huckel coefficient. It depends on temperature. A linear approximation has been made to estimate its evolution (see Figure 1).

$$\alpha(T) = 0.0025 \cdot T + 1.1149 \quad (3)$$

$B$  and  $\delta$  are two other Debye-Huckel coefficients. Their value is given in the Table 1. Finally,  $\sigma(y)$  is the following function:

$$\sigma(y) = \frac{3}{y} \left( 1 + y - 2 \ln(1 + y) - \frac{1}{1 + y} \right) \quad (4)$$

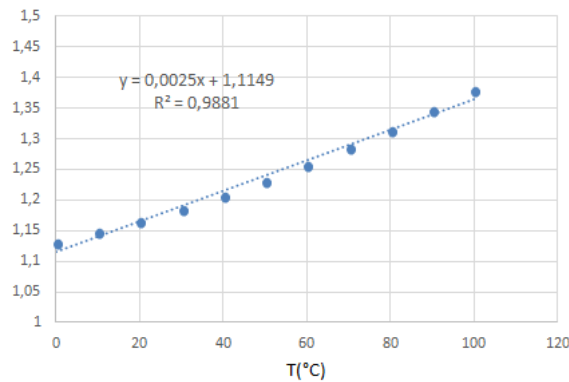


Figure 1: Linear regression of the first Debye-Huckel coefficient.

	$B$	$\delta$	References
$Na_2CO_3$	0.8953	0.0150	[1]
$NaCl$	1.0000	0.1370	[2]

Table 1: Debye-Huckel coefficients

Finally, the water vapor pressure  $p^{vap}(T)$  is given by the Antoine relation [3]:

$$p^{vap}(T) = 133.32 \exp\left(8.07131 - \frac{1730.63}{233.426 + T}\right) \quad (5)$$

with  $p^{vap}$  in *bar* and  $T$  in °C.

# Bibliography

- [1] S. I. Sandler, *Chemical, biochemical and engineering thermodynamics*. John Wiley & Sons, 6th ed., 2006.
- [2] D. W. Green and R. H. Perry, *Perry's chemical engineer's handbook*. McGraw Hill, 8th ed., 2008.
- [3] W. Ye, J. Lin, J. Shen, P. Luis, and B. Van der Bruggen, "Membrane crystallization of sodium carbonate for carbon dioxide recovery: Effect of impurities on the crystal morphology," *Crystal Growth and Design*, vol. 13, pp. 2363–2372, 2013.