# APPENDIX B

## Calculation functions of selected thermodynamics properties of the ammonia-water system

A set of equations for calculation of ammonia-water solution properties used in the study was obtained from Patek and Klomfar [1995]. Five functions for calculations of the selected properties are,

$$T(p,x) = T_0 \sum_i a_i (1-x)^{m_i} \left[ \ln\left(\frac{p_0}{p}\right) \right]^{n_i} \tag{b-1}$$

$$T(p,y) = T_0 \sum_i a_i (1-y)^{m_i/4} \left[ \ln\left(\frac{p_0}{p}\right) \right]^{n_i} \tag{b-2}$$

$$y(p,x) = 1 - \exp\left[ \ln(1-x) \sum_i a_i \left(\frac{p}{p_0}\right)^{m_i} x^{n_i/3} \right] \tag{b-3}$$

$$h_l(T,x) = h_0 \sum_i a_i \left(\frac{T}{T_0} - 1\right)^{m_i} x^{n_i} \tag{b-4}$$

$$h_g(T,y) = h_0 \sum_i a_i \left(1 - \frac{T}{T_0}\right)^{m_i} (1-y)^{n_i/4} \tag{b-5}$$

Coefficients and exponents for function specified in equation (b-1) to (b-5) are listed in table b.1 to table b.5 respectively. In the calculations, these functions are used to calculate in reverse manner e.g. concentration of liquid, x, could be calculated with the specified T and p by iteration of equation (b-1). However, concentrations are specified in mole fraction, which could be converted into mass basis by,

$$w = \frac{yM_A}{yM_A + (1-y)M_w} \tag{b-6}$$

**Table B.1 $T_0$=100K $p_0$=2MPa**

| i | $m_i$ | $n_i$ | $a_i$ |
|---|---|---|---|
| 1 | 0 | 0 | $+0.322302 \times 10^{1}$ |
| 2 | 0 | 1 | $-0.384206 \times 10^{0}$ |
| 3 | 0 | 2 | $+0.460965 \times 10^{-1}$ |
| 4 | 0 | 3 | $-0.378945 \times 10^{-2}$ |
| 5 | 0 | 4 | $+0.135610 \times 10^{-3}$ |
| 6 | 1 | 0 | $+0.487755 \times 10^{0}$ |
| 7 | 1 | 1 | $-0.120108 \times 10^{0}$ |
| 8 | 1 | 2 | $+0.106154 \times 10^{-1}$ |
| 9 | 2 | 3 | $-0.533589 \times 10^{-3}$ |
| 10 | 4 | 0 | $+0.785041 \times 10^{1}$ |
| 11 | 5 | 0 | $-0.115941 \times 10^{2}$ |
| 12 | 5 | 1 | $-0.523159 \times 10^{-1}$ |
| 13 | 6 | 0 | $+0.489596 \times 10^{1}$ |
| 14 | 13 | 1 | $+0.421059 \times 10^{-1}$ |

**Table B.2 $T_0$=100K $p_0$=2MPa**

| i | $m_i$ | $n_i$ | $a_i$ |
|---|---|---|---|
| 1 | 0 | 0 | $+0.324004 \times 10^{1}$ |
| 2 | 0 | 1 | $-0.395920 \times 10^{0}$ |
| 3 | 0 | 2 | $+0.435624 \times 10^{-1}$ |
| 4 | 0 | 3 | $-0.218943 \times 10^{-2}$ |
| 5 | 1 | 0 | $-0.143526 \times 10^{1}$ |
| 6 | 1 | 1 | $+0.105256 \times 10^{1}$ |
| 7 | 1 | 2 | $-0.719281 \times 10^{-1}$ |
| 8 | 2 | 0 | $+0.122362 \times 10^{2}$ |
| 9 | 2 | 1 | $-0.224368 \times 10^{1}$ |
| 10 | 3 | 0 | $-0.201780 \times 10^{2}$ |
| 11 | 3 | 1 | $+0.110834 \times 10^{1}$ |
| 12 | 4 | 0 | $+0.145399 \times 10^{2}$ |
| 13 | 4 | 2 | $+0.644312 \times 10^{0}$ |
| 14 | 5 | 0 | $-0.221246 \times 10^{1}$ |
| 15 | 5 | 2 | $-0.756266 \times 10^{0}$ |
| 16 | 6 | 0 | $-0.135529 \times 10^{1}$ |
| 17 | 7 | 2 | $+0.183541 \times 10^{0}$ |

**Table B.3 $p_0$=2MPa**

| i | $m_i$ | $n_i$ | $a_i$ |
|---|---|---|---|
| 1 | 0 | 0 | $+1.98022017 \times 10^{1}$ |
| 2 | 0 | 1 | $-1.18092669 \times 10^{1}$ |
| 3 | 0 | 6 | $+2.77479980 \times 10^{1}$ |
| 4 | 0 | 7 | $-2.88634277 \times 10^{1}$ |
| 5 | 1 | 0 | $-5.91616608 \times 10^{1}$ |
| 6 | 2 | 1 | $+5.78091305 \times 10^{2}$ |
| 7 | 2 | 2 | $-6.21736743 \times 10^{0}$ |
| 8 | 3 | 2 | $-3.42198402 \times 10^{3}$ |
| 9 | 4 | 3 | $+1.19403127 \times 10^{4}$ |
| 10 | 5 | 4 | $-2.45413777 \times 10^{4}$ |
| 11 | 6 | 5 | $+2.91591865 \times 10^{4}$ |
| 12 | 7 | 6 | $-1.84782290 \times 10^{4}$ |
| 13 | 7 | 7 | $+2.34819434 \times 10^{1}$ |
| 14 | 8 | 7 | $+4.80310617 \times 10^{3}$ |

**Table B.4 $T_0$=273.16K $h_0$=100kJ·kg$^{-1}$**

| i | $m_i$ | $n_i$ | $a_i$ |
|---|---|---|---|
| 1 | 0 | 0 | $-0.761080 \times 10^{1}$ |
| 2 | 0 | 1 | $+0.256905 \times 10^{2}$ |
| 3 | 0 | 6 | $-0.247092 \times 10^{3}$ |
| 4 | 0 | 7 | $+0.325952 \times 10^{3}$ |
| 5 | 0 | 0 | $-0.158854 \times 10^{3}$ |
| 6 | 0 | 1 | $+0.619084 \times 10^{2}$ |
| 7 | 1 | 2 | $+0.114314 \times 10^{2}$ |
| 8 | 1 | 2 | $+0.118157 \times 10^{1}$ |
| 9 | 2 | 3 | $+0.284179 \times 10^{1}$ |
| 10 | 3 | 4 | $+0.741609 \times 10^{1}$ |
| 11 | 5 | 5 | $+0.891844 \times 10^{3}$ |
| 12 | 5 | 5 | $-0.161309 \times 10^{4}$ |
| 13 | 5 | 5 | $+0.622106 \times 10^{3}$ |
| 14 | 6 | 6 | $-0.207588 \times 10^{3}$ |
| 15 | 6 | 7 | $-0.687393 \times 10^{1}$ |
| 16 | 8 | 7 | $+0.350716 \times 10^{1}$ |

**Table B.5 $T_0$=324K $h_0$=1000kJ·kg$^{-1}$**

| i | $m_i$ | $n_i$ | $a_i$ |
|---|---|---|---|
| 1 | 0 | 0 | $+0.128827 \times 10^{1}$ |
| 2 | 1 | 0 | $+0.125247 \times 10^{0}$ |
| 3 | 2 | 0 | $-0.208748 \times 10^{1}$ |
| 4 | 3 | 0 | $-0.217696 \times 10^{1}$ |
| 5 | 0 | 2 | $+0.235687 \times 10^{1}$ |
| 6 | 1 | 2 | $-0.886987 \times 10^{1}$ |
| 7 | 2 | 2 | $+0.102635 \times 10^{2}$ |
| 8 | 3 | 2 | $-0.237440 \times 10^{1}$ |
| 9 | 0 | 3 | $-0.670515 \times 10^{1}$ |
| 10 | 1 | 3 | $+0.164508 \times 10^{2}$ |
| 11 | 2 | 3 | $-0.936849 \times 10^{1}$ |
| 12 | 0 | 4 | $+0.842254 \times 10^{1}$ |
| 13 | 1 | 4 | $-0.858807 \times 10^{1}$ |
| 14 | 0 | 5 | $-0.277049 \times 10^{1}$ |
| 15 | 4 | 6 | $-0.961248 \times 10^{0}$ |
| 16 | 2 | 7 | $+0.988009 \times 10^{0}$ |
| 17 | 1 | 10 | $+0.308482 \times 10^{0}$ |

**Nomenclature**

| | |
|---|---|
| h | enthalpy (kJ $kg^{-1}$) |
| M | Molar mass (kg $kmol^{-1}$) |
| p | Pressure (M Pa) |
| T | Temperature (K) |
| x | Ammonia mole fraction in liquid phase |
| y | Ammonia mole fraction in gas phase |
| w | Ammonia mass fraction in gas phase |

Subscripts

| | |
|---|---|
| A | Ammonia |
| g | Gas phase |
| i | term of fitting polynomial |
| l | Liquid phase |
| W | Water |
| 0 | Reference value |