APPENDIX B

B.1 Reaction chemistry of CO₂-DEEA-AEEA system

When CO₂ absorbed in an aqueous DEEA+AEEA solution, the following set of chemical reactions occur in the liquid phase and chemical equilibrium is represented by the equilibrium constants. The reaction mechanisms are also described in details by the authors (Luo et al., 2016b; Wezland and Trass 1971).

Physical solubility:
$$CO_2(g) \xleftarrow{H_{CO2}} CO_2(aq)$$
 R6.1

Dissociation of water:
$$H_2O \leftarrow H^+ + OH^-$$

Formation of bicarbonate ion:
$$CO_2 + H_2O \xleftarrow{K_2} HCO_3^- + H^+$$

Formation of carbonate ion:
$$HCO_3^- \leftarrow \stackrel{K_3}{\leftarrow} CO_3^{2-} + H^+$$

Dissociation of protonated AEEA: AEEA
$$^+ \leftarrow \stackrel{K_4}{\longleftarrow} AEEA + H^+$$
 R6.5

Formation of carbamate:
$$AEEA + CO_2 \leftarrow K_5 \rightarrow AEEACOO^- + H^+$$

Dissociation of carbamate:
$$AEEACOO^-H^+ \leftarrow \stackrel{K_6}{\longleftarrow} AEEACOO^- + H^+$$
 R6.7

Formation of dicarbamate:
$$AEEACOO^- \leftarrow \stackrel{K_7}{\longleftarrow} AEEA(COO^-)_2 + H^+$$
 R6.8

Dissociation of protonated DEEA:
$$DEEAH^+ \leftarrow \stackrel{K_8}{\longleftarrow} DEEA + H^+$$
 R6.9

Where, H_{CO_2} , K_1 - K_8 , R6.1-R6.9 represent the Henry's law constant, equilibrium constants and equations of respective chemical reactions.

B.2 Reaction chemistry of CO₂-DEEA-HMDA system

When CO₂ absorbed in an aqueous mixture of DEEA and HMDA solution, the following set of chemical reactions occur in the liquid phase and chemical equilibrium is represented by the equilibrium constants and main reaction mechanisms are also described in details by the authors (Luo et al., 2016b; Vaidya and Kenig, 2007).

Physical solubility:
$$CO_2(g) \leftarrow {}^{H_{CO2}} \rightarrow CO_2(aq)$$
 R6.1

Dissociation of water:
$$H_2O \leftarrow \stackrel{K_1}{\longleftrightarrow} H^+ + OH^-$$

Formation of bicarbonate ion:
$$CO_2 + H_2O \xleftarrow{K_2} HCO_3^- + H^+$$

Formation of carbonate ion:
$$HCO_3^- \leftarrow \stackrel{K_3}{\leftarrow} CO_3^{2-} + H^+$$

Dissociation of protonated HMDA: HMDA⁺
$$\leftarrow$$
 $\stackrel{K_4}{\leftarrow}$ HMDA + H^+

Formation of carbamate:
$$HMDA + CO_2 \leftarrow \stackrel{K_5}{\longleftrightarrow} HMDACOO^- + H^+$$

Dissociation of carbamate:
$$HMDACOO^-H^+ \leftarrow \stackrel{K_6}{\longleftrightarrow} HMDACOO^- + H^+$$
 R6.7

Formation of dicarbamate:
$$\text{HMDA}COO^- \leftarrow \stackrel{K_7}{\longleftrightarrow} \text{HMDA}(COO^-)_2 + H^+$$
 R6.8

Dissociation of protonated DEEA:
$$DEEAH^+ \leftarrow \stackrel{K_8}{\longleftarrow} DEEA + H^+$$
 R6.9

Where, H_{CO_2} , K_1 - K_8 , R6.1-R6.9 represent the Henry's law constant, equilibrium constants and equations of respective chemical reactions.