

Table S1: Modified parameters in the binary K₂CO₃-H₂O

Modified parameters	Parameter name	Specie i	Specie j	Original value	Modified value
Electrolyte-molecule pair parameters	GMELCC	H2O	(K+, CO3--)	8.045	7.678220
	GMELCC	(K+, CO3--)	H2O	-5.652	-7.292450
	GMELCD	H2O	(K+, CO3--)	0	-0.001347
	GMELCD	(K+, CO3--)	H2O	440	1000

Table S2: Modified parameters in the binary MEA-H₂O

Modified parameters	Parameter name	Specie i	Specie j	Original Value	Modified Value
DIPPR equation parameters for ideal gas heat capacity (cal/mol*K)	CPIGDP/1	MEA	-	17.2303	16.928726
	CPIGDP/2	MEA	-	43.3505	160
	CPIGDP/3	MEA	-	2030	2253.291750
	CPIGDP/4	MEA	-	31.3844	280.278000
	CPIGDP/5	MEA	-	860	983.913958
DIPPR equation parameters for heat of vaporization (cal/mol)	DHVLDP/1	MEA	-	19679.2	19672.6
	DHVLDP/2	MEA	-	0.59045	0.907689
	DHVLDP/3	MEA	-	-0.43602	-0.689079
	DHVLDP/4	MEA	-	0.37843	0.477909
	DHVLDP/5	MEA	-	0	-1.691447
NRTL activity coefficient model paramaters	NRTL/1	H2O	MEA	1.438498	0.809196
	NRTL/2	H2O	MEA	99.02104	733.067637
	NRTL/1	MEA	H2O	-1.046602	-0.227256
	NRTL/2	MEA	H2O	-337.5456	-637.600337

Table S3: Modified parameters in the ternary CO₂-MEA-H₂O

Modified parameters	Parameter name	Specie i	Specie j	Original Value	Modified Value
Enthalpy of formation (cal/mol)	DHAQFM	MEA+		-80610.5	-79705
	DHAQFM	MEACOO-			-166826
Gibbs free energy (cal/mol)	DGAQFM	MEA+		-164207	-45311
	DGAQFM	MEACOO-			-117650
Coefficients for the equation of aqueous phase heat capacity at infinite dilution (cal/mol*K)	CPAQ0/1	MEA+	-	19.2539	74.04223
	CPAQ0/2	MEA+	-	0.0705	-0.03583
	CPAQ0/3	MEA+	-	0	0
	CPAQ0/4	MEA+	-	0	0
	CPAQ0/5	MEA+	-	0	0
	CPAQ0/6	MEA+	-	0	0
	CPAQ0/1	MEACOO-	-	19.4744	-5.66E-05
	CPAQ0/2	MEACOO-	-	0.0713	-3.54E-06
	CPAQ0/3	MEACOO-	-	0	1.59E-06
	CPAQ0/4	MEACOO-	-	0	-5.66E-05
	CPAQ0/5	MEACOO-	-	0	-5.62E-05
	CPAQ0/6	MEACOO-	-	0	-5.51E-05
Electrolyte-molecule parameters	GMELCC/1	MEA	(MEA+,OH-)	15	8
	GMELCC/1	(MEA+,OH-)	MEA	-8	-4
	GMELCC/1	H2O	(MEA+,OH-)	0	8
	GMELCC/1	(MEA+,OH-)	H2O	0	-4
	GMELCC/1	MEA	(MEA+,MEACOO-)	15	8
	GMELCC/1	(MEA+,MEACOO-)	MEA	-8	-4
	GMELCC/1	H2O	(MEA+,MEACOO-)	9.8877	7
	GMELCC/1	(MEA+,MEACOO-)	H2O	-4.9511	-3
	GMELCC/1	MEA	(MEA+,HCO3-)	15	8
	GMELCC/1	(MEA+,HCO3-)	MEA	-8	-4
	GMELCC/1	H2O	(MEA+,HCO3-)	5.3541	1.5
	GMELCC/1	(MEA+,HCO3-)	H2O	-4.0705	-1.5
	GMELCD/1	H2O	(MEA+,HCO3-)	965.24	500
	GMELCD/1	(MEA+,HCO3-)	H2O	-11.067	0