Appendix B

Parameters for Modelling of Uptake Coupled with Reaction and Diffusion in Aqueous Droplets

Table B.1. Diffusion Constants for Species in Reaction-Diffusion Model

Molecule	D x 10^5, $cm^2\ s^{-1}$	Reference
CO_2	1.9	355
HCO_3^-	1.0	355
CO_3^{2-}	0.8	355
H_2CO_3	1.0	Assumed equivalent to HCO_3^-
NH_3	1.9	356
NH_4^+	1.9	357
H^+	8.8	358
OH^-	5.0	358

Table B.2. Reaction Kinetic Parameters for Reaction-Diffusion Model

Reaction #	Reaction	Rate	Units	Reference
3f	$NH_3 + H_2O \rightarrow NH_4^+ + OH^-$	5.0×10^5	s^{-1}	121
3r	$NH_4^+ + OH^- \rightarrow NH_3 + H_2O$	3.4×10^{10}	$M^{-1}\ s^{-1}$	121
4f	$NH_3 + H_3O^+ \rightarrow NH_4^+ + H_2O$	4.3×10^{10}	$M^{-1}\ s^{-1}$	120,121
4r	$NH_4^+ + H_2O \rightarrow NH_3 + H_3O^+$	24.6	s^{-1}	120,121
5f	$2\ H_2O \rightarrow H_3O^+ + OH^-$	1.4×10^{-3}	$M^{-1}\ s^{-1}$	121
5r	$H_3O^+ + OH^- \rightarrow 2\ H_2O$	1.4×10^{11}	$M^{-1}\ s^{-1}$	121
6f	$CO_2 + H_2O \rightarrow H_2CO_3$	0.04	s^{-1}	122
6r	$H_2CO_3 \rightarrow CO_2 + H_2O$	18	s^{-1}	122
7f	$CO_2 + OH^- \rightarrow HCO_3^-$	8.5×10^3	$M^{-1}\ s^{-1}$	359, 360
7r	$HCO_3^- \rightarrow CO_2 + OH^-$	2×10^4	s^{-1}	360
8f	$H_2CO_3 + H_2O \rightarrow HCO_3^- + H_3O^+$	1.0×10^7	s^{-1}	121
8r	$HCO_3^- + H_3O^+ \rightarrow H_2CO_3 + H_2O$	5.0×10^{10}	$M^{-1}\ s^{-1}$	121
9f	$HCO_3^- + OH^- \rightarrow CO_2 + H_2O$	6×10^9	$M^{-1}\ s^{-1}$	121
9r	$CO_2 + H_2O \rightarrow HCO_3^- + OH^-$	1.3×10^6	s^{-1}	121

Table B.3. Henry's Law Constants and Mass Accommodation Coefficients for Reaction-Diffusion Model

Constant	Value	Units	Reference
H_{CO2}	3.3×10^{-4}	mol Pa m^{-3}	361
H_{NH3}	3.1×10^{-1}	mol Pa m^{-3}	103
α_{CO2}	0.0001	Unitless	20
α_{NH3}	0.08	Unitless	103

Table B.4. Initial Conditions for Reaction-Diffusion Model

Condition	Value	Units
T	295	K
$[CO_2]$ (g)	40.5	Pa
$[CO_2]$ (aq)	1.35×10^{-5}	M
$[H_2CO_3]$	3.00×10^{-7}	M
$[HCO_3^-]$	2.45×10^{-6}	M
$[CO_3^{2-}]$	4.69×10^{-11}	M
$[H_3O^+]$	2.45×10^{-6}	M
$[OH^-]$	4.08×10^{-9}	M