Supplemental Material

Diffusion Coefficients and Boundary Conditions

Name	$D_{aq} \cdot 10^{10}$ (m^2/s)	SA	SE	HHW Media [6] BC (mmol)		References
Aspartate	8.2	−		X	1.13	[13]
Biotin	7.5	−	−	X	0.0041	Wilke-Chang
Cl^-	20	−	−	X	0.09	[2, 4, 5, 16]
CO_2	19					[5]
HCO_3^-	12	+	+			[4]
Cysteine	6.7	−	−	X	0.41	[7]
4,5-dihydroxy-2,3-pentanedione	8.2	+	+			Wilke-Chang
Ethanol	12	+	+			[2, 5]
Fe^{2+}	7.2	−	−	X	0.02	[4]
Glucose	6.7	−	−	X	55.5	[8]
Glutamate	7.5	−		X	1.02	[14] glutamine
Glycine	10	−	−	X	1.33	[8, 9]
Glycolate	8.8	+	+			Wilke-Chang
Guanine	8.7	−	−	X	0.13	Wilke-Chang
K^+	20	−	−	X	22.05	[2, 4, 5, 16]
Mg^{2+}	7.1	−	−	X	2.04	[4]
Mn^{2+}	7.1	−	−	X	0.03	[4]
Molybdate	10	−	−		1.0	[3]
Na^+	13	−	−	X	154	[2, 4, 5, 16]
NH_4^+	20	−	−	X	0.016	[4, 5]
Nicotinate	12	−	−	X	0.017	[15]
O_2	23	−	−		0.4	[5]
PO_4^{3-}	6.1					[4]
HPO_4^{2-}	7.6	−	−	X	99.0	[11]
$H_2PO_4^-$	9.6					[11]
Proline	8.8	−		X	1.3	[2, 8]
Putrescine	7.5		−		1.0	Wilke-Chang
Riboflavin	6.5	−	−	X	0.0053	[10]
Serine	9.2		−	X	0.95	[9]
SO_4^{2-}	11	−	−	X	3.74	[4, 16]
Thiamin	8.3	−	−	X	0.0075	Wilke-Chang
Thymine	11		+			[15]
Tryptophan	6.6	−	−	X	0.49	[2, 8]
Tyrosine	6.7	−	−	X	0.55	[18]
Uracil	12	+	+			[15]
Zn^{2+}	7.0	−	−		1.0	[4]

Measurements at $T = 298$ or $T = 303$ K in water at low dilutions (value for cysteine reported at $T = 288$ K), neutral pH. (−) uptake; (+) product; (X) present in HHW media with boundary concentration (mmol) at non-zero boundary ($z = 0$ for all except O_2, which has non-zero boundary concentration at $z = L$). For some metabolites, the Wilke-Chang formula [12, 19] was used. The value for riboflavin diffusivity was measured in a transepithelial environment.

Notes: reported glutamate diffusivity is actually that of glutamine, which has a similar structure but is uncharged, see [14]. Also, three chemical concentrations (molybdate, putrescine, zinc ion) were absent from HHW but were found necessary for growth in at least one species, and were introduced at the lower boundary with concentration 1 mmol.

Diffusion coefficients in the above table are for pure water solvent, and will generally be smaller in biofilms. Measuring diffusivities in biofilms is problematic even without consideration of variability between different biofilm communities [1]. To convert from aqueous to biofilm diffusivities, we utilize the rule of thumb suggested in reference [17], namely to multiply aqueous diffusivities for light gases by a conversion factor of 0.6 and to multiply other diffusivities by conversion factor 0.25.

In computations, the diffusion coefficient for HCO_3^- is used (rather that that for CO_2), and, similarly, the diffusion coefficient for HPO_4^{2-} was used.

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