A mathematical modeling toolbox for ion channels and transporters across cell membranes

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- 1 The following supplementary material is from " A mathematical modeling toolbox for ion channels
- 2 and transporters across cell membranes" manuscript. It contains an overview of all equations
- 3 related to Ion channels, Pumps, Cotransporters, and Symporters, organized in a table form. The
- 4 detailed transporters along with the descriptions of their equatuons can be found from here.

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22 **2. ATPase model**

23 2.1. Sodium Potassium ATPase pump (Na-K ATPase)

Sodium Potassium ATPase pump (Na-K ATPase)	Ref
	[29–34]
$ATP + 3 Na_{M}^{+} + 2 K_{N}^{+} \Longrightarrow ADP + Pi + 3 Na_{N}^{+} + 2 K_{M}^{+}$ (100)	1
$J_{Na^{+}}^{NakATpase} = J_{Na^{+}}^{NakATpase,max} \left(\frac{[Na]_{M(i)}}{[Na]_{M(i)} + K_{Na_{M}}}\right)^{3} \left(\frac{[K]_{N(e)}}{[K]_{N(e)} + K_{K_{N}}}\right)^{2} $ (101)	
$J_{K^{+}}^{NakATpase} = \left(\frac{-2}{3}\right)J_{Na^{+}}^{NakATpase} \tag{102}$	
where:	[31]
$K_{Nai} = K_{Na}^{NaK} \left(1 + \frac{[K]_i}{a_{NaK}}\right) \tag{103}$	
$K_{Ki} = K_K^{NaK} \left(1 + \frac{[Na]_e}{b_{NaK}}\right) $ (104)	
	[35, 36]
$J_{Na}^{Pump} = J_{Na}^{NaKATPase,max} \left(\frac{[Na]_c}{[Na]_c + K_{Na}} \right)^3 \left(\frac{[K]_{bl}}{[K]_{bl} + K_K} \right)^2 $ (105)	
$J_K^{pump} + J_{NH4}^{pump} = -\frac{2}{3} J_{Na}^{pump} $ (106)	
$ \frac{J_{NH4}^{pump}}{J_{K}^{pump}} = \frac{[NH4]_{e}}{K_{NH4}} \cdot \frac{K_{K}}{[K]_{e}} $ (107)	

Table 9: The corresponding equations describing the flux and current transported via sodium potassium ATPase pumps across the cell membrane

Sodium Potassium ATPase pump (Na-K ATPase)		Ref
		[2, 37]
$I_{NaK}^{M-N} = I_{NaK}^{max} \psi_{NaK}^{cyt} \left(\frac{[Na]_{cyt}^{1.5}}{[Na]_{cyt}^{1.5} + K_{m,Na,\alpha1}^{1.5}} \right) \left(\frac{[K]_{out}}{[K]_{out} + K_{m,K}} \right)$	(108)	
$\psi_{NaK}^{cyt} = \frac{1}{1 + 0.1245 exp\left(-0.1\frac{V_m^{M-N}F}{RT}\right) + 0.365 \ \sigma \ exp\left(\frac{-V_m^{M-N}F}{RT}\right)}$	(109a)	
$\sigma = \frac{1}{7} \left(\frac{[Na]_{out}}{67.3} - 1 \right)$	(109b)	
$J_{pump} = P_{pump} \left(\frac{[Na]_c}{[Na]_c + K_{Na}} \right)^3 \left(\frac{[K]_{bl}}{[K]_{bl} + K_K} \right)^2 (a \times V_m^b + b)$	(110)	[8, 38]
$J_{NaKATPase} = P_{pump} \left(\frac{[Na]_i}{[Na]_i + K_{Na}^{NaK}} \right)^3 \left(\frac{[K]_{bl}}{[K]_{bl} + K_K^{NaK}} \right)^2 (V_m^{i-bl} - V_{rev})$	(111)	[38]

Table 10: The corresponding equations describing the flux and current transported via Sodium Potassium ATPase pumps across the cell membrane