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

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

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

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3. Symporter model

3.1. Sodium Potassium Chloride Symporter (NKCC):

Sodium Potassium Chloride Symporter (NKCC)	Ref
NKCC1 $J^{M,N(net)}_{Cl,NKCC} = [E]_{NKCC}\left(\frac{R_{NN}\big(g^{M}_{ECl}Cl^{M} + g^{M}_{EClNa}Cl^{M}Na^{M} + g^{M}_{EClNaCl}Cl^{M}Na^{M}Cl''^{M}}{R_{M}R_{NN} + R_{N}R_{MM}} \frac{+g^{M}_{EClNaClK}Cl^{M}Na^{M}Cl''^{M}K^{M}\big)}{R_{M}R_{NN} + R_{N}R_{MM}}\right) - [E]_{NKCC}\left(\frac{R_{MM}\big(g^{N}_{ECl}Cl^{N} + g^{N}_{EClNa}Cl^{N}Na^{N} + g^{N}_{EClNaCl}Cl^{N}Na^{N}Cl''^{N}}{R_{M}R_{NN} + R_{N}R_{MM}} \frac{+g^{N}_{EClNaClK}Cl^{N}Na^{N}Cl''^{N}K^{N}\big)}{R_{M}R_{NN} + R_{N}R_{MM}}\right) \quad (124a)$ $J^{M,N(net)}_{Na,NKCC} = [E]_{NKCC}\left(\frac{R_{NN}\left(g^{M}_{EClNa}Cl^{M}Na^{M} + g^{M}_{EClNaCl}Cl^{M}Na^{M}Cl''^{M} + g^{M}_{EClNaClK}Cl^{M}Na^{M}Cl''^{M}K^{M}\right)}{R_{M}R_{NN} + R_{N}R_{MM}} - \frac{R_{MM}\left(g^{N}_{EClNa}Cl^{N}Na^{N} + g^{N}_{EClNaCl}Cl^{N}Na^{N}Cl''^{N} + g^{N}_{EClNaClK}Cl^{N}Na^{N}Cl''^{N}K^{M}\right)}{R_{M}R_{NN} + R_{N}R_{MM}}\right) \quad (124b)$ $J^{M,N(net)}_{K,NKCC} = [E]_{NKCC}\left(\frac{R_{NN}(g^{M}_{EClNaClK}Cl^{M}Na^{M}Cl''^{M}K^{M}) - R_{MM}(g^{N}_{EClNaClK}Cl^{N}Na^{N}Cl''^{N}K^{N})}{R_{M}R_{NN} + R_{N}R_{MM}}\right) \quad (124c)$	[34, 46–48]

Table 15: The corresponding equations describing the flux transported via sodium potassium chloride symporter (NKCC) across the cell membrane (part 1/2 continued on the next page)

Sodium Potassium Chloride Symporter (NKCC)	**Ref**
NKCC1-Continued from previous page Where $[E]_t = [E]_M + [ECl]_M + [EClNa]_M + [EClNaCl]_M + [EClNaClK]_M + [EClNaClK]_N + [EClNaCl]_N + [EClNa]_N + [ECl]_N + [E]_N$ $Cl^M = \frac{[Cl]_M}{K^M_{Cl}}$, $Na^M = \frac{[Na]_M}{K^M_{ClNa}}$, $Cl'^M = \frac{[Cl]_M}{K^M_{ClNaCl}}$, $K^M = \frac{[K]_M}{K^M_{ClNaClK}}$ $Cl^N = \frac{[A]_N}{K^N_A}$, $Na^N = \frac{[B]_N}{K^N_{ClNa}}$, $Cl'^N = \frac{[A]_N}{K^N_{ABA}}$, $K^N = \frac{[C]_N}{K^N_{ClNaClK}}$ $R_M = 1 + Cl^M + Cl^M Na^M + Cl^M Na^M Cl'^M + Cl^M Na^M Cl'^M K^M$ $R_N = 1 + Cl^N + Cl^N Na^N + Cl^N Na^N Cl'^N + Cl^N Na^N Cl'^N K^N$ $R_{MM} = g^M_E + g^M_{ECl} Cl^M + g^M_{EClNa} Cl^M Na^M + g^M_{EABA} Cl^M Na^M Cl'^M + g^M_{EClNaClK} Cl^M Na^M Cl'^M K^M$ $R_{NN} = g^N_E + g^N_{ECl} Cl^N + g^N_{EClNa} Cl^N Na^N + g^N_{EClNaCl} Cl^N Na^N Cl'^N + g^N_{EClNaClK} Cl^N Na^N Cl'^N K^N$	[34, 46–48]

Table 16: The corresponding equations describing the flux transported via sodium potassium chloride symporter (NKCC) across the cell membrane (part 2/2 continued from the previous page)

Sodium Potassium Chloride Symporter (NKCC)	Ref
$$\boxed{J^{M,N(net)}_{symporter} = [E]_t\left(\frac{\left(g^M_{ENaClKCl}Na^M Cl^M K^M Cl''^M\right) g^N_E - \left(g^N_{ENaClKCl}Na^N Cl^N K^N Cl''^N\right) g^M_E}{R_M R_{NN} + R_N R_{MM}}\right)} \quad (125a)$$ $$\boxed{J^{M,N(net)}_{Na,symporter} = J^{M,N(net)}_{symporter}} \quad (125b)$$ $$\boxed{J^{M,N(net)}_{Cl,symporter} = 2J^{M,N(net)}_{symporter}} \quad (125c)$$ $$\boxed{J^{M,N(net)}_{K,symporter} = J^{M,N(net)}_{symporter}} \quad (125d)$$ Where $[E]_t = [E]_M + [ENa]_M + [ENaCl]_M + [ENaClK]_M + [ENaClKCl]_M + [ENaClKCl]_N + [ENaClK]_N + [ENaCl]_N + [ENa]_N + [E]_N$. $Na^M = \frac{[Na]_M}{K^M_{Na}}$, $Cl^M = \frac{[Cl]_M}{K^M_{NaCl}}$, $K^M = \frac{[K]_M}{K^M_{NaClK}}$, $Cl''^M = \frac{[Cl]_M}{K^M_{NaClKCl}}$, $Na^N = \frac{[Na]_N}{K^N_{NaClKCl}}$, $Cl^N = \frac{[Cl]_N}{K^N_{BCB}}$ $K^N = \frac{[K]_N}{K^N_{ABC}}$, $Na''^N = \frac{[Cl]_N}{K^N_{NaClKCl}}$. $R_M = 1 + Na^M + Na^M Cl^M + Na^M Cl^M K^M + Na^M Cl^M K^M Cl''^M$ $R_N = 1 + Cl''^N + K^N Cl''^N + Cl^N K^N Cl''^N + Na^N Cl^N K^N Cl''^N$ $R_{MM} = g^M_E + g^M_{ENaClKCl} Na^M Cl^M K^M Cl''^M$ $R_{NN} = g^N_E + g^N_{ENaClKCl} Na^N Cl^N K^N Cl''^N$	[34, 49]
$$\boxed{J^{M,N(net)}_{Na,NKCC} = [E]_t\left(\frac{g^N_E R_{MM} - g^M_E R_{NN}}{R_M R_{NN} + R_N R_{MM}}\right)} \quad (126a)$$ $$\boxed{J^{M,N(net)}_{K,NKCC} = [E]_t\left(\frac{\left(g^M_{ENKCC} Na^M K^M (Cl^M)^2\right) R_{NN} - \left(g^N_{ENKCC} Na^N K^N (Cl^N)^2\right) R_{MM}}{R_M R_{NN} + R_N R_{MM}}\right)} \quad (126b)$$ Where $[E]_t = R_M[E]_M + R_N[E]_N$ $Na^M = \frac{[Na]_M}{K_{Na}}$, $K^M = \frac{[K]_M}{K_K}$, $Cl^M = \frac{[Cl]_M}{K_{Cl}}$, $NH_4{}^M = \frac{[NH_4]_M}{K_{NH_4}}$ $Na^N = \frac{[Na]_N}{K_{Na}}$, $K^N = \frac{[K]_N}{K_K}$, $Cl^N = \frac{[Cl]_N}{K_{Cl}}$, $NH_4{}^N = \frac{[NH_4]_N}{K_{NH_4}}$ $R_M = 1 + Na^M + Na^M Cl^M + Na^M K^M Cl^M + Na^M K^M (Cl^M)^2 + Na^M NH_4{}^M Cl^M + Na^M NH^M_4 (Cl^M)^2$ $R_N = 1 + Cl^N + K^N Cl^N + K^N (Cl^N)^2 + Na^N K^N (Cl^N)^2 + NH^N_4 Cl^N + NH_4{}^N (Cl^N)^2 + Na^N NH^N_4 + (Cl^N)^2$ $R_{MM} = g^M_E + g^M_{ENKCC} Na^M K^M (Cl^M)^2 + g^M_{ENNH_4CC} Na^M NH_4{}^M (Cl^M)^2$ $R_{NN} = g^N_E + g^N_{ENKCC} Na^N K^N (Cl^N)^2 + g^N_{ENNH_4CC} Na^N NH_4{}^N (Cl^N)^2$	[50]

Table 17: The corresponding equations describing the flux transported via sodium potassium chloride symporter (NKCC) across the cell membrane

Sodium Potassium Chloride Symporter (NKCC)	**Ref**
$$\boxed{J^{M-N}_{NKCC2} = P^{symporter}_{NKCC2} \frac{[Na]_{M(e)}[K]_{M(e)}[Cl]^2_{M(e)} - [Na]_{N(i)}[K]_{N(i)}[Cl]^2_{N(i)}}{\left[\frac{[Na]_{N(i)}}{K_{Na}} + 1\right]\left[\frac{[K]_{N(i)}}{K_K} + 1\right]\left[\frac{[Cl]_{N(i)}}{K_{Cl}} + 1\right]^2}} \quad (127)$$ $$\boxed{J^{M,N(net)}_{Na,NKCC2} = J^{M,N(net)}_{NKCC2}} \quad (128)$$ $$\boxed{J^{M,N(net)}_{K,NKCC2} = J^{M,N(net)}_{NKCC2}} \quad (129)$$ $$\boxed{J^{M,N(net)}_{Cl,NKCC2} = 2J^{M,N}_{NKCC2}} \quad (130)$$	[8, 51]
$$\boxed{J_{NKCC} = [E]_{NKCC}\left(r_{NKCC}\frac{1 - \alpha_1[Na]_i[K]_i[Cl]^2_i}{K_{NKCC} + \alpha_2[Na]_i[K]_i[Cl]_i{}^2}\right)} \quad (131)$$	[7, 52]

Table 18: The corresponding equations describing the flux transported via sodium potassium chloride symporter (NKCC) across the cell membrane