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

Shadi Zaheria, Fatemeh Hassanipoura,\*

<sup>a</sup>Department of Mechanical Engineering, The University of Texas at Dallas, Richardson, TX, 75080, USA

- 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.

<sup>\*</sup>This document is the result of the research project funded by the National Science Foundation.

<sup>\*</sup>Corresponding author

$ \begin{bmatrix} I_{Na,Na_{v}} = g_{Na_{v}}^{max} m_{Na_{v}}^{3} h_{Na_{v}} j_{Na_{v}} \left(V_{m} - V_{Na,rev}^{M-N}\right) \\ \frac{dm_{Na_{v}}}{dt} = \frac{\bar{m}_{Na_{v}} - m_{Na_{v}}}{\tau_{m}} \tag{39} \\ \frac{dh_{Na_{v}}}{dt} = \frac{\bar{h}_{Na_{v}} - h_{Na_{v}}}{\tau_{h}} \tag{40} \\ \frac{dj_{Na_{v}}}{dt} = \frac{\bar{j}_{Na_{v}} - j_{Na_{v}}}{\tau_{j}} \tag{41} \\ \bar{m}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{-(V_{m}^{M-N} - V_{1/2,m}^{M-N})}{k_{m}Na_{v}}\right)\right)^{2}}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,n}^{M-N})}{k_{h}Na_{v}}\right)\right)^{2}} \tag{43} \\ \bar{b}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,n}^{M-N})}{k_{h}Na_{v}}\right)\right)^{2}} \tag{44} \\ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,n}^{M-N})}{k_{h}Na_{v}}\right)\right)^{2}} \tag{45} \\ \bar{\tau}_{m} = \alpha_{m} \beta_{m} \tag{45} \\ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} \tag{46} \\ \tau_{j} = \frac{1}{\alpha_{j} + \beta_{j}} \tag{47} $	<b>Voltage Gated Sodium Channel</b> (VGSC, Na <sub>v</sub> , VONa)	Ref
$ \frac{dm_{Na_{v}}}{dt} = \frac{\bar{m}_{Na_{v}} - m_{Na_{v}}}{\tau_{m}} \tag{39} $ $ \frac{dh_{Na_{v}}}{dt} = \frac{\bar{h}_{Na_{v}} - h_{Na_{v}}}{\tau_{h}} \tag{40} $ $ \frac{dj_{Na_{v}}}{dt} = \frac{\bar{j}_{Na_{v}} - j_{Na_{v}}}{\tau_{j}} \tag{41} $ $ \bar{m}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{-(V_{m}^{M-N} - V_{1/2,m}^{M-N} Na_{v}})}{k_{m} Na_{v}}\right)\right)^{2}} \tag{42} $ $ \bar{h}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,h}^{M-N} Na_{v}})}{k_{h} Na_{v}}\right)\right)^{2}} \tag{43} $ $ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,j}^{M-N} Na_{v}})}{k_{j} Na_{v}}\right)\right)^{2}} \tag{44} $ $ \tau_{m} = \alpha_{m} \beta_{m} \tag{45} $ $ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} \tag{46} $		[14–16]
$ \frac{dh_{Na_{v}}}{dt} = \frac{\bar{h}_{Na_{v}} - h_{Na_{v}}}{\tau_{h}} \tag{40} $ $ \frac{dj_{Na_{v}}}{dt} = \frac{\bar{j}_{Na_{v}} - j_{Na_{v}}}{\tau_{j}} \tag{41} $ $ \bar{m}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{-(V_{m}^{M-N} - V_{1/2,m}^{M-N}}{k_{m}Na_{v}})\right)\right)^{2}} \tag{42} $ $ \bar{h}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,h}^{M-N}}{k_{h}Na_{v}}\right)\right)\right)^{2}} \tag{43} $ $ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,j}^{M-N}}{k_{j}Na_{v}}\right)\right)\right)^{2}} \tag{44} $ $ \tau_{m} = \alpha_{m} \beta_{m} \tag{45} $ $ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} \tag{46} $	$I_{Na,Na_{v}} = g_{Na_{v}}^{max} m_{Na_{v}}^{3} h_{Na_{v}} j_{Na_{v}} \left( V_{m} - V_{Na,rev}^{M-N} \right) $ (38)	3)
$ \frac{dj_{Na_{v}}}{dt} = \frac{\bar{j}_{Na_{v}} - j_{Na_{v}}}{\tau_{j}} \tag{41} $ $ \bar{m}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{-(V_{m}^{M-N} - V_{1/2, m Na_{v}}^{M-N})}{k_{m Na_{v}}}\right)\right)^{2}} \tag{42} $ $ \bar{h}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2, h Na_{v}}^{M-N})}{k_{h Na_{v}}}\right)\right)^{2}} \tag{43} $ $ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2, j Na_{v}}^{M-N})}{k_{j Na_{v}}}\right)\right)^{2}} \tag{44} $ $ \tau_{m} = \alpha_{m} \beta_{m} \tag{45} $ $ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} \tag{46} $	$\frac{dm_{Na_v}}{dt} = \frac{\bar{m}_{Na_v} - m_{Na_v}}{\tau_m} \tag{39}$	9)
$ \bar{m}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{-(V_{m}^{M-N} - V_{1/2,m Na_{v}}^{M-N})}{k_{m Na_{v}}}\right)\right)^{2}} $ $ \bar{h}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,h Na_{v}}^{M-N})}{k_{h Na_{v}}}\right)\right)^{2}} $ $ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,j Na_{v}}^{M-N})}{k_{j Na_{v}}}\right)\right)^{2}} $ $ \tau_{m} = \alpha_{m} \beta_{m} $ $ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} $ (45)	$\frac{dh_{Na_{\nu}}}{dt} = \frac{\bar{h}_{Na_{\nu}} - h_{Na_{\nu}}}{\tau_h} \tag{40}$	))
$ \bar{h}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,h}^{M-N})}{k_{hNa_{v}}}\right)\right)^{2}} $ $ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,j}^{M-N})}{k_{jNa_{v}}}\right)\right)^{2}} $ $ \tau_{m} = \alpha_{m} \beta_{m} $ $ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} $ (43) $(44)$ $(45)$	$\frac{dj_{Na_{\nu}}}{dt} = \frac{\bar{j}_{Na_{\nu}} - j_{Na_{\nu}}}{\tau_{j}} \tag{4}$	
$ \bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2, j Na_{v}}^{M-N})}{k_{j Na_{v}}}\right)\right)^{2}} $ $ \tau_{m} = \alpha_{m} \beta_{m} $ $ \tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} $ (45)	$\bar{m}_{Na_v} = \frac{1}{\left(1 + exp\left(\frac{-(V_m^{M-N} - V_{1/2, m Na_v}^{M-N})}{k_{m Na_v}}\right)\right)^2} $ (42)	2)
$\tau_{m} = \alpha_{m} \beta_{m} \tag{45}$ $\tau_{h} = \frac{1}{\alpha_{h} + \beta_{h}} \tag{46}$	$\bar{h}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,h Na_{v}}^{M-N})}{k_{h Na_{v}}}\right)\right)^{2}} $ (43)	3)
$\tau_h = \frac{1}{\alpha_h + \beta_h} \tag{46}$	$\bar{j}_{Na_{v}} = \frac{1}{\left(1 + exp\left(\frac{(V_{m}^{M-N} + V_{1/2,j}^{M-N})}{k_{jNa_{v}}}\right)\right)^{2}} $ (44)	4)
$\tau_h = \frac{1}{\alpha_h + \beta_h} $ $\tau_j = \frac{1}{\alpha_j + \beta_j} $ (46) $(47)$		5)
$\tau_j = \frac{1}{\alpha_j + \beta_j} \tag{47}$	$\tau_h = \frac{1}{\alpha_h + \beta_h} \tag{46}$	6)
	$\tau_j = \frac{1}{\alpha_j + \beta_j} \tag{47}$	7)

Table 3: The corresponding equations describing the ionic current transported via voltage gated sodium channels  $(VGSCs, Na_vs, VONas)$  across the cell membrane (part 2/3 continued from previous page)

<b>Voltage Gated Sodium Channel</b> (VGSC, Na <sub>v</sub> , VONa)		Ref
For all range of $V_m$ : $\begin{cases} \alpha_m = \frac{1}{1 + exp\left(\frac{-(V_m^{M-N} + V_{1\alpha_m})}{k_{\alpha_m}}\right)} \\ \beta_m = \frac{A_{\beta_m}}{1 + exp\left(\frac{(V_m^{M-N} + V_{1\beta_m})}{k_{\beta_m}}\right)} + \frac{B_{\beta_m}}{1 + exp\left(\frac{(V_m^{M-N} - V_{2\beta_m})}{k_{2\beta_m}}\right)} \end{cases}$	(48)	
For $V_m \ge -40$ : $\begin{cases} \alpha_h = 0 \\ \beta_h = \frac{A_{\beta_h}}{1 + exp\left(\frac{-(V_m^{M-N} + V_{1\beta_h})}{k_{\beta_h}}\right)} \end{cases}$	(49)	
For $V_m < -40$ : $\begin{cases} \alpha_h = A_{\alpha_h} exp\left(\frac{-(V_m + V_{\alpha_h}^{Na_v})}{k_{\alpha_h}^{Na_v}}\right) \\ \beta_h = A_{\beta_h} exp(a_{\beta_h} V_m) + B_{\beta_h} exp(b_{\beta_h} V_m) \end{cases}$	(50)	
	(51)	
$For \ V_{m} < -40: \begin{cases} \alpha_{j} = \frac{\left(A_{\alpha_{j}} exp(a_{\alpha_{j}} V_{m}) - B_{\alpha_{j}} exp(b_{\alpha_{j}} V_{m})\right) (V_{m} + V_{1\alpha_{j}})}{1 + exp(\frac{V + V_{2\alpha_{j}}}{k_{\alpha_{j}}})} \\ \beta_{j} = \frac{A_{\beta_{j}} exp(a_{\beta_{j}} V_{m})}{1 + exp\left(\frac{-(V_{m}^{M - N} + V_{2\beta_{j}})}{k_{\beta_{j}}}\right)} \end{cases}$	(52)	
$V_{Na,rev}^{M-N(a)} = \frac{RT}{z_{Na}F} ln\left(\frac{[Na]_{M(l)}}{[Na]_{N(i)}}\right)$	(53)	[14–16]

Table 3: The corresponding equations describing the ionic current transported via voltage gated sodium channels  $(VGSCs, Na_vs, VONas)$  across the cell membrane (part 3/3 continued from previous page)