
A basic model of calcium homeostasis in non-excitable cells

Christina H. Selstø, Peter Ruoff*

Department of Chemistry, Bioscience, and Environmental Engineering, University of Stavanger, Stavanger, Norway

Supporting Information S8 Program

Influences of cytosolic calcium and cytosolic inflow rates j_1 on $IP_3R \bullet IP_3$ dissociation and activity

The three folders with names:

```
"i first-order infl of Ca_cyt on j_IP3R diss"  
"ii high Ca_cyt infl on j_IP3R diss"  
"iii no infl of Ca_cyt on j_IP3R diss"
```

contain each a version of CAREG65.f, which considers the following three influences of cytosolic calcium on the dissociation of $IP_3R \bullet IP_3$:

(i) considering a first-order kinetic influence of Ca_{cyt}^{2+} on the $IP_3R \bullet IP_3$ dissociation by using the term $k_{78} \cdot (IP_3R \bullet IP_3) \cdot (Ca_{cyt}^{2+})$

(ii) considering the term $k_{78} \cdot (IP_3R \bullet IP_3) \cdot [1 + (Ca_{cyt}^{2+})]$, when only Ca_{cyt}^{2+} levels $\gg 1 \mu M$ have a significant influence on $IP_3R \bullet IP_3$ dissociation, or finally

(iii) when Ca_{cyt}^{2+} levels have no influence on $IP_3R \bullet IP_3$ dissociation, i.e. using the dissociation term $k_{78} \cdot (IP_3R \bullet IP_3)$.

Each folder contains an Excel file with an overview of the results, i.e. j_1 is varied between $10 \mu M/s$ and $4 \times 10^4 \mu M/s$ and Ca_{cyt} and j_{IP3R} (v_{IP3R}) are calculated. The folders also contain the input files for each run with names CAREG65-runid.INP, where runid is a number identifying each calculation.

In order to recalculate, do the following:

- delete the file CAREG65.INP
- copy the appropriate file CAREG65-runid.INP and rename it to CAREG65.INP
- On a Mac, use the following Terminal command: `./careg65.sh`¹
- On Windows, write into the Command Prompt window: `careg65.cmd`

The results for each calculation can be read from the Terminal or Command Prompt output. For example, when using CAREG65-076.INP from folder "i first-order infl of Ca_cyt on j_IP3R diss" as an input (renaming CAREG65-076.INP to

¹If you should get `Permission denied` give execution rights to `careg65` and `careg65.sh` by executing the two commands: `chmod 755 careg` and `chmod 755 careg.sh`

CAREG65.INP), the values of j_1 , j_{IP3R} , and Ca_{cyt} are outlined in respectively, red, yellow and blue color in the shown copy of the Terminal output (Fig S1):

```

Ca-fluxes at end of phase 1 :
j1 (Leak to cyto) 1.0000E+01
j2 (PMCA outflow) 1.1000E+01
jNCX..... 1.2214E-08
j2+j3..... 1.1008E+01
j23 (ER-filling). 1.8257E+01
j27 (ER-leaking). 1.2000E+01
jARCC..... 0.0000E+00
jIP3R..... 6.2573E+00
jtot..... -4.3751E-06
jSOCC..... 1.0080E+00

NOUT..... 1000

concentrations at end of phase 1 :
8.11091E-04, 3.25944E-01, 1.00000E+03, 1.07015E+02 !Ca_cyt,PMCA.M*,Ca_ext,M
4.33994E-02, 9.98988E+02, 1.01284E+00, 6.16452E-01 !MCA4,B,BCa4,PMCA.M
5.76043E-02, 1.85499E+03, 1.00000E+03, 1.11112E+03 !PMCA,SERCA,Calum,L
1.38889E+03, 0.00000E+00, 1.00000E+02, 0.00000E+00 !LCa30,S,R,R.S
1.00000E+00, 1.22635E+04, 4.99334E+00, 9.91955E-01 !ARCC,IP3R,IP3,IP3,Ind
8.04565E-03, 1.00000E+01, 1.00000E+01, 1.00000E+03 !Cacyt.Ind,S2,Gprot,GS2
1.00000E-01, 1.50588E-08, 9.14533E-03, 8.54584E-04 !PLC,NCX.M*,NCX.M,NCX
1.00798E-01, 1.00798E+02, 1.00000E+00, 1.99334E+00 !STIM,STIM.Ca,SOCC,IP3R

Execution of CAREG65-076 ended at: 15:01:55
Date: 22-Nov-22
=====

```

Figure S1. Example: Terminal output for run CAREG65-076.

If you wish to vary j_1 , this is done by changing k_1 and noting that:

$$j_1 = k_1 \cdot (Ca_{ext}) \quad (S1)$$

where (Ca_{ext}) has been set to 1000 μ M.

Panels A, B, and C in Fig 17 are plots of the data shown in the Excel files for the conditions (i)-(iii).