SBML Model Report

Model name: "Fridlyand2010_GlucoseSensitivity_A"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Ishan Ajmera¹ at August nineth 2011 at 5:04 p. m. and last time modified at October tenth 2014 at 10:29 a. m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	7
events	0	constraints	0
reactions	0	function definitions	0
global parameters	97	unit definitions	0
rules	35	initial assignments	7

Model Notes

This a model from the article:

Glucose sensing in the pancreatic beta cell: a computational systems analysis. Fridlyand LE, Philipson LH.Theor Biol Med Model.2010 May 24;7:15. 20497556,

Abstract:

BACKGROUND:Pancreatic beta-cells respond to rising blood glucose by increasing oxidative

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metabolism, leading to an increased ATP/ADP ratio in the cytoplasm. This leads to a closure of KATP channels, depolarization of the plasma membrane, influx of calcium and the eventual secretion of insulin. Such mechanism suggests that beta-cell metabolism should have a functional regulation specific to secretion, as opposed to coupling to contraction. The goal of this work is to uncover contributions of the cytoplasmic and mitochondrial processes in this secretory coupling mechanism using mathematical modeling in a systems biology approach.METHODS:We describe a mathematical model of beta-cell sensitivity to glucose. The cytoplasmic part of the model includes equations describing glucokinase, glycolysis, pyruvate reduction, NADH and ATP production and consumption. The mitochondrial part begins with production of NADH, which is regulated by pyruvate dehydrogenase. NADH is used in the electron transport chain to establish a proton motive force, driving the F1F0 ATPase. Redox shuttles and mitochondrial Ca2+ handling were also modeled.RESULTS: The model correctly predicts changes in the ATP/ADP ratio, Ca2+ and other metabolic parameters in response to changes in substrate delivery at steady-state and during cytoplasmic Ca2+ oscillations. Our analysis of the model simulations suggests that the mitochondrial membrane potential should be relatively lower in beta cells compared with other cell types to permit precise mitochondrial regulation of the cytoplasmic ATP/ADP ratio. This key difference may follow from a relative reduction in respiratory activity. The model demonstrates how activity of lactate dehydrogenase, uncoupling proteins and the redox shuttles can regulate beta-cell function in concert; that independent oscillations of cytoplasmic Ca2+ can lead to slow coupled metabolic oscillations; and that the relatively low production rate of reactive oxygen species in beta-cells under physiological conditions is a consequence of the relatively decreased mitochondrial membrane potential.CONCLUSION: This comprehensive model predicts a special role for mitochondrial control mechanisms in insulin secretion and ROS generation in the beta cell. The model can be used for testing and generating control hypotheses and will help to provide a more complete understanding of beta-cell glucose-sensing central to the physiology and pathology of pancreatic beta-cells.

This model was taken from the Vcell MathModel directory and was converted to SBML

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2 Unit Definitions

This is an overview of five unit definitions which are all predefined by SBML and not mentioned in the model.

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.3 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m^2

2.4 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment			3	1	litre		

3.1 Compartment compartment

This is a three dimensional compartment with a constant size given in litre.

4 Species

This model contains seven species. Section 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary
					Condi-
					tion
G3P	G3P	compartment	$\text{mol} \cdot 1^{-1}$		
PYR	PYR	compartment	$\text{mol} \cdot 1^{-1}$		
ATP	ATP	compartment	$\text{mol} \cdot 1^{-1}$		\Box
NADHm	NADHm	compartment	$\text{mol} \cdot 1^{-1}$		
NADHc	NADHc	compartment	$\text{mol} \cdot 1^{-1}$		
Vm	Vm	compartment	$\text{mol} \cdot 1^{-1}$		
Cam	Cam	compartment	$\text{mol} \cdot 1^{-1}$		\Box

5 Parameters

This model contains 97 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ai		0000009	0.341		
am		0000009	0.200		Z
Ao		0000196	4000.000		\mathbf{Z}
$\mathtt{ATP_init}$		0000196	3700.000		\mathbf{Z}
$\mathtt{Cac_init}$		0000196	0.100		$\overline{\mathscr{L}}$
Cam_init		0000196	0.200		$\overline{\mathbf{Z}}$
CaR		0000196	0.090		$\overline{\mathscr{L}}$
Cmit		0000258	5200.000		\mathbf{Z}
F		0000568	96480.000		\mathbf{Z}
fi		0000540	0.010		$\overline{\mathbf{Z}}$
fm		0000540	$3 \cdot 10^{-4}$		$\overline{\mathbf{Z}}$
${\tt G3P_init}$		0000196	30.000		$\overline{\mathbf{Z}}$
Glu		0000196	8.000		$\overline{\mathbf{Z}}$
hCa		0000190	4.000		$\overline{\mathbf{Z}}$
hgl		0000190	1.700		$\overline{\mathbf{Z}}$
hp		0000190	8.000		$\overline{\mathbf{Z}}$
kACa		0000380	0.250		$\overline{\mathbf{Z}}$
KAD		0000009	25.000		$ \overline{\mathbf{Z}} $
kat		0000009	-0.005		$ \overline{\mathbf{Z}} $
kATP		0000009	$4 \cdot 10^{-5}$		$ \overline{\mathbf{A}} $
kATPCa		0000009	$9 \cdot 10^{-5}$		$ \overline{\mathbf{Z}} $
kbt		0000009	-0.004		$ \overline{\mathbf{Z}} $
kCaA		0000009	30.000		$ \overline{\mathbf{Z}} $
KCaj		0000009	8.000		$ \mathbf{Z} $
KCam		0000009	0.050		$ \overline{\mathbf{Z}} $
KgNc		0000540	0.090		
kgpd		0000009	10^{-5}		
Klnc		0000540	1.000		
klp		0000009	0.031		
Kmadp		0000027	20.000		$ \overline{\mathbf{Z}} $
KmATP		0000027	500.000		$ \overline{\checkmark} $
Kmg3p		0000027	200.000		$ \overline{\checkmark} $
Kmgl		0000027	7.000		$ \overline{\mathbf{Z}} $
KmLD		0000027	47.500		$\overline{m{arphi}}$
KmNh		0000027	3000.000		$\overline{\mathbf{Z}}$
Kmph		0000027	131.400		$\overline{\mathbf{Z}}$
Kmpyr		0000027	47.500		$\overline{\mathbf{Z}}$

Id	Name	SBO	Value	Unit	Constant
knadhc		0000009	10^{-4}		Ø
knadhm		0000009	10^{-4}		$\overline{\mathbf{Z}}$
KNaj		0000009	8000.000		$\overline{\mathscr{A}}$
KpCam		0000009	0.165		$\overline{\mathbf{Z}}$
KPNm		0000540	81.000		$\overline{\mathbf{Z}}$
KTNc		0000231	0.002		$\overline{\mathbf{Z}}$
KTNm		0000231	16.780		$\overline{\mathbf{Z}}$
$NADHc_init$		0000196	10.000		$\overline{\mathbf{Z}}$
${\tt NADHm_init}$		0000196	50.000		$\overline{\mathbf{Z}}$
Nam		0000196	5000.000		$\overline{\mathbf{Z}}$
Ni		0000196	10000.000		$\overline{\mathscr{A}}$
Ntc		0000196	2000.000		$\overline{\mathbf{Z}}$
Ntm		0000196	2200.000		$\overline{\mathbf{Z}}$
PCa		0000538	0.004		$\overline{\mathbf{Z}}$
Plb		0000380	0.001		$\overline{\mathbf{Z}}$
Plr		0000380	0.001		$\overline{\mathbf{Z}}$
PYR_{-} init		0000196	10.000		$\overline{\mathbf{Z}}$
Tnadh		0000009	0.050		$\overline{\mathbf{Z}}$
Tv		0000259	26.730		$\overline{\mathbf{Z}}$
u1		0000009	1.500		$\overline{\mathbf{Z}}$
u2		0000009	1.100		$\overline{\mathbf{Z}}$
Vi		0000468	0.530		$\overline{\mathbf{Z}}$
${\tt Vm_init}$		0000196	100.000		$\overline{\mathbf{Z}}$
Vme		0000009	22.000		$ \mathbf{Z} $
Vmglu		0000009	0.011		$ \mathbf{Z} $
Vmgpd		0000009	0.500		
Vmldh		0000009	1.200		
Vmmit		0000468	0.014		
Vmnc		0000009	0.025		
Vmpdh		0000009	0.300		
Vmph		0000009	8.000		
ZCa		0000545	2.000		\square
ACa			0.000		
AD			0.000		
ADP			0.000		
AT			0.000		
Cac			0.000		
DelJNCa			0.000		
FDe			0.000		
FLNADc			0.000		
FNADc			0.000		
FPCa			0.000		

Id	Name	SBO	Value	Unit	Constant
FPNAD			0.000		
FPYR			0.000		
FTe			0.000		
JGlu			0.000		
Jgpd			0.000		
Jhl			0.000		
Jhres			0.000		
JLDH			0.000		
JNCa			0.000		
J02			0.000		
Jph			0.000		
JPYR			0.000		
Jtnadh			0.000		
Juni			0.000		
MgADP			0.000		
NADc			0.000		
NADm			0.000		
ID	ID		0.000		

6 Initialassignments

This is an overview of seven initial assignments.

6.1 Initialassignment G3P

Derived unit contains undeclared units

Math G3P_init

6.2 Initialassignment PYR

Derived unit contains undeclared units

Math PYR_init

6.3 Initialassignment ATP

Derived unit contains undeclared units

Math ATP_init

6.4 Initialassignment NADHm

Derived unit contains undeclared units

Math NADHm_init

6.5 Initialassignment NADHc

Derived unit contains undeclared units

Math NADHc_init

6.6 Initialassignment Vm

Derived unit contains undeclared units

Math Vm_init

6.7 Initialassignment Cam

Derived unit contains undeclared units

Math Cam_init

7 Rules

This is an overview of 35 rules.

7.1 Rule ACa

Rule ACa is an assignment rule for parameter ACa:

$$ACa = 1 + \left(\left(1 \cdot \frac{1}{\exp\left([Cam] \cdot \frac{1}{KpCam} \right)} \right) \right)$$
 (1)

7.2 Rule AD

Rule AD is an assignment rule for parameter AD:

$$AD = MgADP \cdot MgADP \cdot \frac{1}{MgADP \cdot MgADP + Kmadp \cdot Kmadp} \tag{2}$$

7.3 Rule ADP

Rule ADP is an assignment rule for parameter ADP:

$$ADP = Ao + ([ATP]) \tag{3}$$

7.4 Rule AT

Rule AT is an assignment rule for parameter AT:

$$AT = [Vm]^{hp} \cdot \frac{1}{Kmph^{hp} + [Vm]^{hp}}$$

$$\tag{4}$$

7.5 Rule Cac

Rule Cac is an assignment rule for parameter Cac:

$$Cac = CaR + kACa \cdot \left([ATP] \cdot \frac{1}{ADP} \right)^{hCa} \cdot \frac{1}{KAD^{hCa} + \left([ATP] \cdot \frac{1}{ADP} \right)^{hCa}}$$
(5)

7.6 Rule DelJNCa

Rule DelJNCa is an assignment rule for parameter DelJNCa:

$$\begin{aligned} \text{DelJNCa} &= 1 + \text{Ni}^3 \cdot \frac{1}{\text{KNaj}^3} + [\text{Cam}] \cdot \frac{1}{\text{KCaj}} + \text{Ni}^3 \cdot [\text{Cam}] \cdot \frac{1}{\text{KNaj}^3 \cdot \text{KCaj}} \\ &+ \text{Nam}^3 \cdot \frac{1}{\text{KNaj}^3} + \text{Cac} \cdot \frac{1}{\text{KCaj}} + \text{Nam}^3 \cdot \text{Cac} \cdot \frac{1}{\text{KNaj}^3 \cdot \text{KCaj}} \end{aligned} \tag{6}$$

7.7 Rule FDe

Rule FDe is an assignment rule for parameter FDe:

$$FDe = [NADHm] \cdot \frac{1}{KmNh + [NADHm]}$$
 (7)

7.8 Rule FLNADc

Rule FLNADc is an assignment rule for parameter FLNADc:

$$FLNADc = [NADHc] \cdot \frac{1}{Klnc + [NADHc] \cdot \frac{1}{NADc}} \cdot \frac{1}{NADc}$$
 (8)

7.9 Rule FNADc

Rule FNADc is an assignment rule for parameter FNADc:

$$FNADc = [NADHc] \cdot \frac{1}{KTNc + [NADHc] \cdot \frac{1}{NADc}} \cdot \frac{1}{NADc}$$
 (9)

7.10 Rule FPCa

Rule FPCa is an assignment rule for parameter FPCa:

$$FPCa = 1 \cdot \frac{1}{1 + u2 \cdot \left(1 + u1 \cdot \frac{1}{\left(1 + [Cam] \cdot \frac{1}{KCam}\right)^2}\right)}$$
(10)

7.11 Rule FPNAD

Rule FPNAD is an assignment rule for parameter FPNAD:

$$FPNAD = NADm \cdot \frac{1}{KPNm + NADm \cdot \frac{1}{[NADHm]}} \cdot \frac{1}{[NADHm]}$$
 (11)

7.12 Rule FPYR

Rule FPYR is an assignment rule for parameter FPYR:

$$FPYR = [PYR] \cdot \frac{1}{Kmpyr + [PYR]}$$
 (12)

7.13 Rule FTe

Rule FTe is an assignment rule for parameter FTe:

$$FTe = (1 + kat \cdot [Vm]) \cdot \frac{1}{1 + kbt \cdot [Vm]}$$
(13)

7.14 Rule JGlu

Rule JGlu is an assignment rule for parameter JGlu:

$$JGlu = Vmglu \cdot Glu^{hgl} \cdot [ATP] \cdot \frac{1}{Kmgl^{hgl} + Glu^{hgl}} \cdot \frac{1}{KmATP + [ATP]}$$
 (14)

7.15 Rule Jgpd

Rule Jgpd is an assignment rule for parameter Jgpd:

$$Jgpd = Vmgpd \cdot [G3P] \cdot NADc \cdot \frac{1}{[G3P] + Kmg3p} \cdot \frac{1}{KgNc + NADc \cdot \frac{1}{[NADHc]}} \cdot \frac{1}{[NADHc]}$$
(15)

7.16 Rule Jhl

Rule Jhl is an assignment rule for parameter Jhl:

$$Jhl = (Plb + Plr) \cdot exp(klp \cdot [Vm])$$
(16)

7.17 Rule Jhres

Rule Jhres is an assignment rule for parameter Jhres:

$$Jhres = Vme \cdot FTe \cdot FDe \tag{17}$$

7.18 Rule JLDH

Rule JLDH is an assignment rule for parameter JLDH:

$$JLDH = Vmldh \cdot FLNADc \cdot [PYR] \cdot \frac{1}{KmLD + [PYR]}$$
(18)

7.19 Rule JNCa

Rule JNCa is an assignment rule for parameter JNCa:

$$\begin{split} JNCa &= Vmnc \cdot \left(exp \left(0.5 \cdot [Vm] \cdot Ni^3 \cdot [Cam] \cdot \frac{1}{Tv \cdot KNaj^3 \cdot KCaj} \right) \\ &+ \left(\left(exp \left(\left(0.5 \cdot [Vm] \cdot Nam^3 \cdot Cac \cdot \frac{1}{Tv \cdot KNaj^3 \cdot KCaj} \right) \right) \right) \right) \cdot \frac{1}{DelJNCa} \end{split} \tag{19}$$

7.20 Rule J02

Rule J02 is an assignment rule for parameter J02:

$$JO2 = 0.1 \cdot Jhres \tag{20}$$

7.21 Rule Jph

Rule Jph is an assignment rule for parameter Jph:

$$Jph = Vmph \cdot AD \cdot AT \cdot ACa \tag{21}$$

7.22 Rule JPYR

Rule JPYR is an assignment rule for parameter JPYR:

$$JPYR = Vmpdh \cdot FPNAD \cdot FPCa \cdot FPYR \tag{22}$$

7.23 Rule Jtnadh

Rule Jtnadh is an assignment rule for parameter Jtnadh:

$$Jtnadh = Tnadh \cdot FNADc \cdot NADm \cdot \frac{1}{KTNm + NADm \cdot \frac{1}{[NADHm]}} \cdot \frac{1}{[NADHm]} \tag{23}$$

7.24 Rule Juni

Rule Juni is an assignment rule for parameter Juni:

$$\begin{aligned} \text{Juni} &= PCa \cdot ZCa \cdot [Vm] \cdot \left(am \cdot [Cam] \cdot exp \left(\left([Vm] \cdot ZCa \cdot \frac{1}{Tv} \right) \right) + \left((ai \cdot Cac) \right) \right) \\ &\cdot \frac{1}{Tv} \cdot \frac{1}{-1 + exp \left(\left([Vm] \cdot ZCa \cdot \frac{1}{Tv} \right) \right)} \end{aligned} \tag{24}$$

7.25 Rule MgADP

Rule MgADP is an assignment rule for parameter MgADP:

$$MgADP = 0.055 \cdot ADP \tag{25}$$

7.26 Rule NADc

Rule NADc is an assignment rule for parameter NADc:

$$NADc = Ntc + ([NADHc])$$
 (26)

7.27 Rule NADm

Rule NADm is an assignment rule for parameter NADm:

$$NADm = Ntm + ([NADHm])$$
 (27)

7.28 Rule G3P

Rule G3P is a rate rule for species G3P:

$$\frac{\mathrm{d}}{\mathrm{d}t}G3P = (2 \cdot \mathrm{JGlu} + (\mathrm{Jgpd})) \cdot \frac{1}{\mathrm{Vi}} + ((\mathrm{kgpd} \cdot [\mathrm{G3P}])) \tag{28}$$

7.29 Rule PYR

Rule PYR is a rate rule for species PYR:

$$\frac{\mathrm{d}}{\mathrm{d}t} PYR = (Jgpd + (JPYR) + (JLDH)) \cdot \frac{1}{Vi + Vmmit}$$
(29)

7.30 Rule ATP

Rule ATP is a rate rule for species ATP:

$$\frac{d}{dt}ATP = ((kATP + kATPCa \cdot Cac) \cdot [ATP]) + (2 \cdot JGlu + 0.231 \cdot Jph) \cdot \frac{1}{Vi}$$
 (30)

7.31 Rule NADHm

Rule NADHm is a rate rule for species NADHm:

$$\frac{d}{dt}NADHm = (4.6 \cdot JPYR + ((0.1 \cdot Jhres)) + Jtnadh) \cdot \frac{1}{Vmmit} + ((knadhm \cdot [NADHm])) \quad (31)$$

7.32 Rule NADHc

Rule NADHc is a rate rule for species NADHc:

$$\frac{d}{dt}NADHc = (Jgpd + (Jtnadh) + (JLDH)) \cdot \frac{1}{Vi} + ((knadhc \cdot [NADHc]))$$
(32)

7.33 Rule Vm

Rule Vm is a rate rule for species Vm:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Vm} = (\mathrm{Jhres} + (\mathrm{Jph}) + (\mathrm{Jhl}) + ((2 \cdot \mathrm{Juni})) + (\mathrm{JNCa})) \cdot \mathrm{F} \cdot \frac{1}{\mathrm{Cmit}}$$
(33)

7.34 Rule Cam

Rule Cam is a rate rule for species Cam:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cam} = \mathrm{fm} \cdot (\mathrm{Juni} + (\mathrm{JNCa})) \cdot \frac{1}{\mathrm{Vmmit}}$$
(34)

7.35 Rule ID

Rule ID is an assignment rule for parameter ID:

$$ID = \frac{[ATP]}{ADP} \tag{35}$$

8 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

8.1 Species G3P

Name G3P

SBO:0000247 simple chemical

Initial assignment G3P

Involved in rule G3P

One rule which determines this species' quantity.

8.2 Species PYR

Name PYR

SBO:0000247 simple chemical

Initial assignment PYR

Involved in rule PYR

One rule which determines this species' quantity.

8.3 Species ATP

Name ATP

SBO:0000248 chemical macromolecule

Initial assignment ATP

Involved in rule ATP

One rule which determines this species' quantity.

8.4 Species NADHm

Name NADHm

SBO:0000248 chemical macromolecule

Initial assignment NADHm

Involved in rule NADHm

One rule which determines this species' quantity.

8.5 Species NADHc

Name NADHc

SBO:0000248 chemical macromolecule

Initial assignment NADHc

Involved in rule NADHc

One rule which determines this species' quantity.

8.6 Species Vm

Name Vm

SBO:0000002 quantitative systems description parameter

Initial assignment Vm

Involved in rule Vm

One rule which determines this species' quantity.

8.7 Species Cam

Name Cam

SBO:0000240 material entity

Initial assignment Cam

Involved in rule Cam

One rule which determines this species' quantity.

A Glossary of Systems Biology Ontology Terms

SBO:000002 quantitative systems description parameter: A numerical value that defines certain characteristics of systems or system functions. It may be part of a calculation, but its value is not determined by the form of the equation itself, and may be arbitrarily assigned

SBO:000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

SBO:0000027 Michaelis constant: Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

SBO:0000190 Hill coefficient: Empirical parameter created by Archibald Vivian Hill to describe the cooperative binding of oxygen on hemoglobine (Hill (1910). The possible effects of the aggregation of the molecules of haemoglobin on its dissociation curves. J Physiol 40: iv-vii)

SBO:0000196 concentration of an entity pool: The amount of an entity per unit of volume.

- **SBO:0000231 occurring entity representation:** Representation of an entity that manifests, unfolds or develops through time, such as a discrete event, or a mutual or reciprocal action or influence that happens between participating physical entities, and/or other occurring entities.
- **SBO:0000240** material entity: A real thing that is defined by its physico-chemical structure.
- SBO:0000247 simple chemical: Simple, non-repetitive chemical entity
- **SBO:0000248 chemical macromolecule:** Macromolecule whose sequence is not directly encoded in the genome
- **SBO:0000258 capacitance:** Measure of the amount of electric charge stored (or separated) for a given electric potential. The unit of capacitance id the Farad
- **SBO:0000259 voltage:** Difference of electrical potential between two points of an electrical network, expressed in volts
- **SBO:0000380** biochemical coefficient: number used as a multiplicative or exponential factor for quantities, expressions or function
- **SBO:0000468 volume:** A quantity representing the three-dimensional space occupied by all or part of an object
- **SBO:0000538 ionic permeability:** A parameter that represents the permeability of an ion channel with respect to a particular ion
- **SBO:0000540 fraction of an entity pool:** A ratio that represents the quantity of a defined constituent entity over the total number of all constituent entities present.
- **SBO:0000545** systems description parameter: A value, numerical or symbolic, that defines certain characteristics of systems or system functions, or is necessary in their derivation
- **SBO:0000568 Faraday constant:** Named after Michael Faraday, it is the magnitude of electric charge per mole of electrons. It has the value 96,485.3365 C/mol (Coulombs per Mole), and the symbol F

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