SBML Model Report

Model name: "Rohwer2000_Phosphotransferase_System"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Harish Dharuri[1] and Jacky L Snoep[2] at July 28th 2005 at 9:39 a. m. and last time modified at April thirteenth 2015 at 10:26 a. m. Table 1 provides 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	17
events	0	constraints	0
reactions	10	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS
Run this model online at http://jjj.biochem.sun.ac.za
To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online, Bioinformatics, 20:2143-2144

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2 Unit Definitions

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

2.1 Unit `substance`

Name micromole (default)

Definition µmol

2.2 Unit `time`

Name minute (default)

Definition 60 s

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `compartment`

This is a three dimensional compartment with a constant size of one litre.

Name cell

4 Species

This model contains 17 species. The boundary condition of four of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 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 Condition
EI		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
PyrPI		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIP		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
HPr		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIPHPr		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
HPrP		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIIA		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
HPrPIIA		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIIAP		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIICB		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIIAPIICB		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIICBP		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
EIICBPGlc		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
PEP		compartment	$\mu mol \cdot l^{-1}$	⊟	☑
Pyr		compartment	$\mu mol \cdot l^{-1}$	⊟	☑
GlcP		compartment	$\mu mol \cdot l^{-1}$	⊟	☑
Glc		compartment	$\mu mol \cdot l^{-1}$	⊟	☑

5 Reactions

This model contains ten reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	v1		$PEP + EI \rightleftharpoons PyrPI$	
2	v2		$PyrPI \rightleftharpoons EIP + Pyr$	
3	v3		$HPr + EIP \rightleftharpoons EIPHPr$	
4	v4		$EIPHPr \rightleftharpoons HPrP + EI$	
5	v5		$HPrP + EIIA \rightleftharpoons HPrPIIA$	
6	v6		$HPrPIIA \rightleftharpoons EIIAP + HPr$	
7	v7		$EIICB + EIIAP \rightleftharpoons EIIAPIICB$	
8	v8		$EIIAPIICB \rightleftharpoons EIICBP + EIIA$	
9	v9		$EIICBP + Glc \rightleftharpoons EIICBPGlc$	
10	v10		$EIICBPGlc \rightleftharpoons EIICB + GlcP$	

5.1 Reaction v1

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{PEP} + \mathrm{EI} \rightleftharpoons \mathrm{PyrPI} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
PEP		
EI		

Product

Table 6: Properties of each product.

Id	Name	SBO
PyrPI		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1f} \cdot [\mathrm{PEP}] \cdot [\mathrm{EI}] - \mathrm{k1r} \cdot [\mathrm{PyrPI}]) \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1f			1960.0		☑
k1r			480000.0		☑

5.2 Reaction v2

This is a reversible reaction of one reactant forming two products.

Reaction equation

$$\mathrm{PyrPI} \rightleftharpoons \mathrm{EIP} + \mathrm{Pyr} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
PyrPI		

Products

Table 9: Properties of each product.

Id	Name	SBO
EIP		
Pyr		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k2f} \cdot [\mathrm{PyrPI}] - \mathrm{k2r} \cdot [\mathrm{Pyr}] \cdot [\mathrm{EIP}]) \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2f			108000.0		☑
k2r			294.0		☑

5.3 Reaction v3

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{HPr} + \mathrm{EIP} \rightleftharpoons \mathrm{EIPHPr} \tag{5}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
HPr		
EIP		

Product

Table 12: Properties of each product.

Id	Name	SBO
EIPHPr		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k3f} \cdot [\mathrm{EIP}] \cdot [\mathrm{HPr}] - \mathrm{k3r} \cdot [\mathrm{EIPHPr}]) \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3f			14000.0		☑
k3r			14000.0		☑

5.4 Reaction v4

This is a reversible reaction of one reactant forming two products.

Reaction equation

$$\mathrm{EIPHPr} \rightleftharpoons \mathrm{HPrP} + \mathrm{EI} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
EIPHPr		

Products

Table 15: Properties of each product.

Id	Name	SBO
HPrP		
EI		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k4f} \cdot [\mathrm{EIPHPr}] - \mathrm{k4r} \cdot [\mathrm{EI}] \cdot [\mathrm{HPrP}]) \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4f			84000.0		☑
k4r			3360.0		☑

5.5 Reaction v5

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{HPrP} + \mathrm{EIIA} \rightleftharpoons \mathrm{HPrPIIA} \tag{9}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
HPrP		
EIIA		

Product

Table 18: Properties of each product.

Id	Name	SBO
HPrPIIA		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k5f} \cdot [\mathrm{HPrP}] \cdot [\mathrm{EIIA}] - \mathrm{k5r} \cdot [\mathrm{HPrPIIA}]) \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5f			21960.0		☑
k5r			21960.0		☑

5.6 Reaction v6

This is a reversible reaction of one reactant forming two products.

Reaction equation

$$\mathrm{HPrPIIA} \rightleftharpoons \mathrm{EIIAP} + \mathrm{HPr} \tag{11}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
HPrPIIA		

Products

Table 21: Properties of each product.

Id	Name	SBO
EIIAP		
HPr		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k6f} \cdot [\mathrm{HPrPIIA}] - \mathrm{k6r} \cdot [\mathrm{HPr}] \cdot [\mathrm{EIIAP}]) \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6f			4392.0		☑
k6r			3384.0		☑

5.7 Reaction v7

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{EIICB} + \mathrm{EIIAP} \rightleftharpoons \mathrm{EIIAPIICB} \tag{13}$$

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
EIICB		
EIIAP		

Product

Table 24: Properties of each product.

Id	Name	SBO
EIIAPIICB		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k7f} \cdot [\mathrm{EIIAP}] \cdot [\mathrm{EIICB}] - \mathrm{k7r} \cdot [\mathrm{EIIAPIICB}]) \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7f			880.0		☑
k7r			880.0		☑

5.8 Reaction v8

This is a reversible reaction of one reactant forming two products.

Reaction equation

$$\mathrm{EIIAPIICB} \rightleftharpoons \mathrm{EIICBP} + \mathrm{EIIA} \tag{15}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
EIIAPIICB		

Products

Table 27: Properties of each product.

Id	Name	SBO
EIICBP		
EIIA		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k8f} \cdot [\mathrm{EIIAPIICB}] - \mathrm{k8r} \cdot [\mathrm{EIIA}] \cdot [\mathrm{EIICBP}]) \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8f			2640.0		☑
k8r			960.0		☑

5.9 Reaction v9

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{EIICBP} + \mathrm{Glc} \rightleftharpoons \mathrm{EIICBPGlc} \tag{17}$$

Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
EIICBP		
Glc		

Product

Table 30: Properties of each product.

Id	Name	SBO
EIICBPGlc		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k9f} \cdot [\mathrm{EIICBP}] \cdot [\mathrm{Glc}] - \mathrm{k9r} \cdot [\mathrm{EIICBPGlc}]) \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9f			260.0		☑
k9r			389.0		☑

5.10 Reaction v10

This is a reversible reaction of one reactant forming two products.

Reaction equation

$$\text{EIICBPGlc} \rightleftharpoons \text{EIICB} + \text{GlcP} \tag{19}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
EIICBPGlc		

Products

Table 33: Properties of each product.

Id	Name	SBO
EIICB		
GlcP		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\,(\text{compartment}) \cdot (\text{k10f} \cdot [\text{EIICBPGlc}] - \text{k10r} \cdot [\text{EIICB}] \cdot [\text{GlcP}]) \tag{20}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k10f			4800.000		☑
k10r			0.005		☑

6 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.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or

- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.

6.1 Species `EI`

Initial concentration $3\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v1` and as a product in `v4`).

$$\frac{\text{d}}{\text{d}t}\text{EI} = v_4 - v_1 \tag{21}$$

6.2 Species `PyrPI`

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v2` and as a product in `v1`).

$$\frac{\text{d}}{\text{d}t}\text{PyrPI} = v_1 - v_2 \tag{22}$$

6.3 Species `EIP`

Initial concentration $2\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v3` and as a product in `v2`).

$$\frac{\text{d}}{\text{d}t}\text{EIP} = v_2 - v_3 \tag{23}$$

6.4 Species `HPr`

Initial concentration $25\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v3` and as a product in `v6`).

$$\frac{\text{d}}{\text{d}t}\text{HPr} = v_6 - v_3 \tag{24}$$

6.5 Species `EIPHPr`

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v4` and as a product in `v3`).

$$\frac{\text{d}}{\text{d}t}\text{EIPHPr} = v_3 - v_4 \tag{25}$$

6.6 Species HPrP

Initial concentration 25 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v5 and as a product in v4).

$$\frac{\text{d}}{\text{d}t}\text{HPrP} = v_4 - v_5 \tag{26}$$

6.7 Species EIIA

Initial concentration 20 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v5 and as a product in v8).

$$\frac{\text{d}}{\text{d}t}\text{EIIA} = v_8 - v_5 \tag{27}$$

6.8 Species HPrPIIA

Initial concentration 0 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v6 and as a product in v5).

$$\frac{\text{d}}{\text{d}t}\text{HPrPIIA} = v_5 - v_6 \tag{28}$$

6.9 Species EIIAP

Initial concentration 20 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v7 and as a product in v6).

$$\frac{\text{d}}{\text{d}t}\text{EIIAP} = v_6 - v_7 \tag{29}$$

6.10 Species EIICB

Initial concentration 5 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v7 and as a product in v10).

$$\frac{\text{d}}{\text{d}t}\text{EIICB} = v_{10} - v_7 \tag{30}$$

6.11 Species EIIAPIICB

Initial concentration 0 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v8 and as a product in v7).

$$\frac{\text{d}}{\text{d}t}\text{EIIAPIICB} = v_7 - v_8 \tag{31}$$

6.12 Species EIICBP

Initial concentration $5\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v9 and as a product in v8).

$$\frac{\text{d}}{\text{d}t}\text{EIICBP} = v_8 - v_9 \tag{32}$$

6.13 Species EIICBPGlc

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in v10 and as a product in v9).

$$\frac{\text{d}}{\text{d}t}\text{EIICBPGlc} = v_9 - v_{10} \tag{33}$$

6.14 Species PEP

Initial concentration $2800\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in v1), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{PEP} = 0 \tag{34}$$

6.15 Species Pyr

Initial concentration $900\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in v2), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{Pyr} = 0 \tag{35}$$

6.16 Species GlcP

Initial concentration $50\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in v10), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{GlcP} = 0 \tag{36}$$

6.17 Species Glc

Initial concentration $500\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in v9), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc} = 0 \tag{37}$$

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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