

SBML Model Report

Model name: “Rohwer2001_Sucrose”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Jacky L Snoep¹ at May third 2005 at 1:08 p. m. and last time modified at May 20th 2012 at 12:43 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	13
events	0	constraints	0
reactions	11	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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To cite BioModels Database, please use [Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. \(2006\) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.](#)

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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 millimole (default)

Definition mmol

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 m²

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	<input checked="" type="checkbox"/>	

3.1 Compartment `compartment`

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

Name cell

4 Species

This model contains 13 species. The boundary condition of eight 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 Condi- tion
Fru		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Glc		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
HexP		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Suc6P		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Suc		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Sucvac		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
glycolysis		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
phos		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
UDP		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
ADP		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
ATP		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Glcex		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Fruex		compartment	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

5 Reactions

This model contains eleven 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

Nº	Id	Name	Reaction Equation	SBO
1	v1		$\text{Fruex} \rightleftharpoons \text{Fru}$	
2	v2		$\text{Glcex} \rightleftharpoons \text{Glc}$	
3	v3		$\text{ATP} + \text{Glc} \xrightleftharpoons{\text{Fru}} \text{HexP} + \text{ADP}$	
4	v4		$\text{Fru} + \text{ATP} \xrightleftharpoons{\text{Glc}} \text{HexP} + \text{ADP}$	
5	v5		$\text{Fru} + \text{ATP} \rightleftharpoons \text{HexP} + \text{ADP}$	
6	v6		$2 \text{HexP} \xrightleftharpoons{\text{phos}} \text{UDP} + \text{Suc6P}$	
7	v7		$\text{Suc6P} \rightleftharpoons \text{Suc} + \text{phos}$	
8	v8		$\text{HexP} + \text{Fru} \rightleftharpoons \text{Suc} + \text{UDP}$	
9	v9		$\text{Suc} \rightleftharpoons \text{Fru} + \text{Glc}$	
10	v10		$\text{HexP} \rightleftharpoons \text{glycolysis}$	
11	v11		$\text{Suc} \rightleftharpoons \text{Sucvac}$	

5.1 Reaction v1

This is a reversible reaction of one reactant forming one product.

Reaction equation



Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
Fruex		

Product

Table 6: Properties of each product.

Id	Name	SBO
Fru		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment}) \cdot \frac{V_{\max 1} \cdot [\text{Fruex}]}{K_{m1\text{Fruex}} \cdot \left(1 + \frac{[\text{Fru}]}{K_{i1\text{Fru}}}\right) + [\text{Fruex}]} \quad (2)$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax1			0.286		✓
Km1Fruex			0.200		✓
Ki1Fru			1.000		✓

5.2 Reaction v2

This is a reversible reaction of one reactant forming one product.

Reaction equation



Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Glcex		

Product

Table 9: Properties of each product.

Id	Name	SBO
Glc		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{compartment}) \cdot \frac{V_{\max 2} \cdot [\text{Glcex}]}{K_{m2\text{Glcex}} \cdot \left(1 + \frac{[\text{Glc}]}{K_{i2\text{Glc}}}\right) + [\text{Glcex}]} \quad (4)$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax2			0.286		✓
Km2Glcex			0.200		✓
Ki2Glc			1.000		✓

5.3 Reaction v3

This is a reversible reaction of two reactants forming two products influenced by one modifier.

Reaction equation



Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
ATP		
Glc		

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
Fru		

Products

Table 13: Properties of each product.

Id	Name	SBO
HexP		
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment}) \cdot \frac{V_{\max 3} \cdot \frac{[\text{Glc}]}{K_{m3\text{Glc}}} \cdot \frac{[\text{ATP}]}{K_{m3\text{ATP}}}}{\left(1 + \frac{[\text{ATP}]}{K_{m3\text{ATP}}}\right) \cdot \left(1 + \frac{[\text{Glc}]}{K_{m3\text{Glc}}} + \frac{[\text{Fru}]}{K_{m4\text{Fru}}} + \frac{0.113 \cdot [\text{HexP}]}{K_{i3\text{G6P}}} + \frac{0.0575 \cdot [\text{HexP}]}{K_{i4\text{F6P}}}\right)} \quad (6)$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax3			0.197		✓
Km3Glc			0.070		✓
Km3ATP			0.250		✓
Km4Fru			10.000		✓
Ki3G6P			0.100		✓
Ki4F6P			10.000		✓

5.4 Reaction v4

This is a reversible reaction of two reactants forming two products influenced by one modifier.

Reaction equation



Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
Fru		
ATP		

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
Glc		

Products

Table 17: Properties of each product.

Id	Name	SBO
HexP		
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{compartment}) \cdot \frac{V_{\max 4} \cdot \frac{[\text{Fru}]}{K_{m4\text{Fru}}} \cdot \frac{[\text{ATP}]}{K_{m4\text{ATP}}}}{\left(1 + \frac{[\text{ATP}]}{K_{m4\text{ATP}}}\right) \cdot \left(1 + \frac{[\text{Glc}]}{K_{m3\text{Glc}}} + \frac{[\text{Fru}]}{K_{m4\text{Fru}}} + \frac{0.113 \cdot [\text{HexP}]}{K_{i3\text{G6P}}} + \frac{0.0575 \cdot [\text{HexP}]}{K_{i4\text{F6P}}}\right)} \quad (8)$$

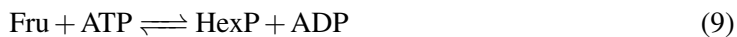
Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax4			0.197		<input checked="" type="checkbox"/>
Km4Fru			10.000		<input checked="" type="checkbox"/>
Km4ATP			0.250		<input checked="" type="checkbox"/>
Km3Glc			0.070		<input checked="" type="checkbox"/>
Ki3G6P			0.100		<input checked="" type="checkbox"/>
Ki4F6P			10.000		<input checked="" type="checkbox"/>

5.5 Reaction v5

This is a reversible reaction of two reactants forming two products.

Reaction equation



Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
	Fru	
	ATP	

Products

Table 20: Properties of each product.

Id	Name	SBO
	HexP	
	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{compartment}) \cdot \frac{\frac{V_{\max 5}}{1 + \frac{[\text{Fru}]}{K_{i5}\text{Fru}}} \cdot \frac{[\text{Fru}]}{K_{m5}\text{Fru}} \cdot \frac{[\text{ATP}]}{K_{m5}\text{ATP}}}{1 + \frac{[\text{Fru}]}{K_{m5}\text{Fru}} + \frac{[\text{ATP}]}{K_{m5}\text{ATP}} + \frac{[\text{Fru}] \cdot [\text{ATP}]}{K_{m5}\text{Fru} \cdot K_{m5}\text{ATP}} + \frac{[\text{ADP}]}{K_{i5}\text{ADP}}} \quad (10)$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax5			0.164		<input checked="" type="checkbox"/>
Ki5Fru			12.000		<input checked="" type="checkbox"/>
Km5Fru			0.100		<input checked="" type="checkbox"/>
Km5ATP			0.085		<input checked="" type="checkbox"/>
Ki5ADP			2.000		<input checked="" type="checkbox"/>

5.6 Reaction v6

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

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
HexP		

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
phos		

Products

Table 24: Properties of each product.

Id	Name	SBO
UDP		
Suc6P		

Kinetic Law

Derived unit contains undeclared units

$v_6 = \text{vol}(\text{compartment})$ (12)

$$0.0575 \cdot [\text{HexP}] \cdot 0.8231 \cdot [\text{HexP}] \cdot \left(1 + \frac{[\text{Suc6P}]}{\text{Ki6Suc6P}}\right) + \text{Km6F6P} \cdot \left(1 + \frac{[\text{phos}]}{\text{Ki6Pi}}\right) \cdot (0.8231 \cdot [\text{HexP}] + \text{Ki6UDPGlc}) -$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax6f			0.379		✓
Keq6			10.000		✓
Ki6Suc6P			0.070		✓
Km6F6P			0.600		✓
Ki6Pi			3.000		✓
Ki6UDPGlc			1.400		✓
Km6UDPGlc			1.800		✓
Vmax6r			0.200		✓
Km6UDP			0.300		✓
Km6Suc6P			0.100		✓
Ki6F6P			0.400		✓

5.7 Reaction v7

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

Reaction equation



Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Suc6P		

Products

Table 27: Properties of each product.

Id	Name	SBO
Suc		
phos		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment}) \cdot \frac{V_{\max 7} \cdot [\text{Suc6P}]}{K_{m7} \text{Suc6P} + [\text{Suc6P}]} \quad (14)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _{max7}			0.5		<input checked="" type="checkbox"/>
K _{m7} Suc6P			0.1		<input checked="" type="checkbox"/>

5.8 Reaction v8

This is a reversible reaction of two reactants forming two products.

Reaction equation



Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
HexP		
Fru		

Products

Table 30: Properties of each product.

Id	Name	SBO
Suc		

Id	Name	SBO
UDP		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{compartment}) \quad (16)$$

$$\frac{V_{\max 8f} \cdot ([\text{Suc}] \cdot [\text{UDP}] - [\text{Suc}] \cdot [\text{UDP}] \cdot \left(1 + \frac{[\text{Fru}]}{K_{i8\text{Fru}}}\right) + K_{m8\text{Suc}} \cdot ([\text{UDP}] + K_{i8\text{UDP}}) + K_{m8\text{UDP}} \cdot [\text{Suc}] + \frac{V_{\max 8f}}{V_{\max 8r} \cdot K_{eq8}} \cdot (K_{m8\text{UDPGlc}} \cdot [\text{Glc}] + K_{m8\text{Fru}} \cdot [\text{Fru}] + K_{i8\text{Suc}} \cdot [\text{Suc}])}{K_{m8\text{UDP}} \cdot [\text{Suc}] + \frac{V_{\max 8f}}{V_{\max 8r} \cdot K_{eq8}} \cdot (K_{m8\text{UDPGlc}} \cdot [\text{Glc}] + K_{m8\text{Fru}} \cdot [\text{Fru}] + K_{i8\text{Suc}} \cdot [\text{Suc}])}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax8f			0.677		✓
Keq8			5.000		✓
Ki8Fru			4.000		✓
Km8Suc			50.000		✓
Ki8UDP			0.300		✓
Km8UDP			0.300		✓
Vmax8r			0.300		✓
Km8UDPGlc			0.300		✓
Km8Fru			4.000		✓
Ki8Suc			40.000		✓

5.9 Reaction v9

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

Reaction equation



Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
Suc		

Products

Table 33: Properties of each product.

Id	Name	SBO
Fru		
Glc		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{compartment}) \cdot \frac{\frac{V_{\max 9}}{1 + \frac{[\text{Glc}]}{K_{i9\text{Glc}}}} \cdot [\text{Suc}]}{K_{m9\text{Suc}} \cdot \left(1 + \frac{[\text{Fru}]}{K_{i9\text{Fru}}}\right) + [\text{Suc}]} \quad (18)$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax9			0.372		<input checked="" type="checkbox"/>
Ki9Glc			15.000		<input checked="" type="checkbox"/>
Km9Suc			10.000		<input checked="" type="checkbox"/>
Ki9Fru			15.000		<input checked="" type="checkbox"/>

5.10 Reaction v10

This is a reversible reaction of one reactant forming one product.

Reaction equation



Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
HexP		

Product

Table 36: Properties of each product.

Id	Name	SBO
	glycolysis	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{compartment}) \cdot \frac{V_{\max 10} \cdot 0.0575 \cdot [\text{HexP}]}{K_{m10F6P} + 0.0575 \cdot [\text{HexP}]} \quad (20)$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax10			0.1		<input checked="" type="checkbox"/>
Km10F6P			0.2		<input checked="" type="checkbox"/>

5.11 Reaction v11

This is a reversible reaction of one reactant forming one product.

Reaction equation



Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
	Suc	

Product

Table 39: Properties of each product.

Id	Name	SBO
	Sucvac	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{compartment}) \cdot \frac{V_{\text{max}11} \cdot [\text{Suc}]}{K_{\text{m}11\text{Suc}} + [\text{Suc}]} \quad (22)$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
$V_{\text{max}11}$			1.0		<input checked="" type="checkbox"/>
$K_{\text{m}11\text{Suc}}$			100.0		<input checked="" type="checkbox"/>

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 Fru

Initial concentration 1 mmol · l⁻¹

This species takes part in six reactions (as a reactant in [v4](#), [v5](#), [v8](#) and as a product in [v1](#), [v9](#) and as a modifier in [v3](#)).

$$\frac{d}{dt}\text{Fru} = v_1 + v_9 - v_4 - v_5 - v_8 \quad (23)$$

6.2 Species Glc

Initial concentration 1 mmol · l⁻¹

This species takes part in four reactions (as a reactant in [v3](#) and as a product in [v2](#), [v9](#) and as a modifier in [v4](#)).

$$\frac{d}{dt}\text{Glc} = v_2 + v_9 - v_3 \quad (24)$$

6.3 Species HexP

Initial concentration 1 mmol · l⁻¹

This species takes part in six reactions (as a reactant in v6, v8, v10 and as a product in v3, v4, v5).

$$\frac{d}{dt}\text{HexP} = v_3 + v_4 + v_5 - 2v_6 - v_8 - v_{10} \quad (25)$$

6.4 Species Suc6P

Initial concentration 1 mmol · l⁻¹

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

$$\frac{d}{dt}\text{Suc6P} = v_6 - v_7 \quad (26)$$

6.5 Species Suc

Initial concentration 1 mmol · l⁻¹

This species takes part in four reactions (as a reactant in v9, v11 and as a product in v7, v8).

$$\frac{d}{dt}\text{Suc} = v_7 + v_8 - v_9 - v_{11} \quad (27)$$

6.6 Species Sucvac

Initial concentration 0 mmol · l⁻¹

This species takes part in one reaction (as a product in v11), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Sucvac} = 0 \quad (28)$$

6.7 Species glycolysis

Initial concentration 0 mmol · 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:

$$\frac{d}{dt}\text{glycolysis} = 0 \quad (29)$$

6.8 Species `phos`

Initial concentration $5.1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in `v7` and as a modifier in `v6`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{phos} = 0 \quad (30)$$

6.9 Species `UDP`

Initial concentration $0.2 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in `v6`, `v8`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{UDP} = 0 \quad (31)$$

6.10 Species `ADP`

Initial concentration $0.2 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a product in `v3`, `v4`, `v5`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{ADP} = 0 \quad (32)$$

6.11 Species `ATP`

Initial concentration $1 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in `v3`, `v4`, `v5`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{ATP} = 0 \quad (33)$$

6.12 Species `Glcex`

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

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

$$\frac{d}{dt}\text{Glcex} = 0 \quad (34)$$

6.13 Species Fruex

Initial concentration 5 mmol · 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:

$$\frac{d}{dt}\text{Fruex} = 0 \quad (35)$$

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