SBML Model Report

Model name: "Nielsen1998_Glycolysis"



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Nicolas Le Novre¹, Christoph Flamm² and Lukas Endler³ at June 30th 2005 at 2:08 p. m. and last time modified at April eighth 2016 at 3:21 p. 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	15
events	0	constraints	0
reactions	25	function definitions	0
global parameters	25	unit definitions	2
rules	0	initial assignments	0

Model Notes

This model was automatically converted from model BIOMD000000042 by using libSBML . According to the BioModels Database terms of use , this generated model is not related with model BIOMD0000000042 any more.

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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

Definition mmol

2.2 Unit time

Name minute

Definition 60 s

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.4 Unit area

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

 $\textbf{Definition}\ m^2$

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			3	1	litre	Ø	

3.1 Compartment compartment

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

4 Species

This model contains 15 species. Section 7 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
ATP		compartment	$\operatorname{mmol} \cdot l^{-1}$		
ADP		compartment	$\operatorname{mmol} \cdot 1^{-1}$	\Box	
AMP		compartment	$\operatorname{mmol} \cdot 1^{-1}$	\Box	\Box
GLC		compartment	$mmol \cdot l^{-1}$		
F6P		compartment	$mmol \cdot l^{-1}$		
FBP		compartment	$mmol \cdot l^{-1}$		
GAP		compartment	$\operatorname{mmol} \cdot 1^{-1}$		
NAD		compartment	$\operatorname{mmol} \cdot 1^{-1}$	\Box	
NADH		compartment	$\operatorname{mmol} \cdot 1^{-1}$	\Box	\Box
DPG		compartment	$mmol \cdot l^{-1}$		
PEP		compartment	$mmol \cdot l^{-1}$		
PYR		compartment	$mmol \cdot l^{-1}$		
ACA		compartment	$\operatorname{mmol} \cdot 1^{-1}$	\Box	\Box
EtOH		compartment	$\operatorname{mmol} \cdot 1^{-1}$	\Box	\Box
P		compartment	$\operatorname{mmol} \cdot 1^{-1}$		\Box

5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V1			0.500		✓
K1GLC			0.100		$\overline{\mathbf{Z}}$
K1ATP			0.063		$\overline{\mathbf{Z}}$
V2			1.500		$ \overline{\mathbf{Z}} $
K2			0.002		$ \overline{\mathbf{Z}} $
k2			0.017		$ \overline{\mathbf{Z}} $
K2ATP			0.010		$ \overline{\mathbf{Z}} $
k3f			1.000		$\overline{\mathbf{Z}}$
k3b			50.000		$\overline{\mathbf{Z}}$
V4			10.000		$\overline{\mathbf{Z}}$
K4GAP			1.000		$\overline{\mathbf{Z}}$
K4NAD			1.000		$\overline{\mathbf{Z}}$
k5f			1.000		$\overline{\mathbf{Z}}$
k5b			0.500		$\overline{\mathbf{Z}}$
V6			10.000		$\overline{\mathbf{Z}}$
K6PEP			0.200		$\overline{\mathbf{Z}}$
K6ADP			0.300		$\overline{\mathbf{Z}}$
٧7			2.000		$\overline{\mathbf{Z}}$
K7PYR			0.300		$\overline{\mathbf{Z}}$
k8f			1.000		$\overline{\mathbf{Z}}$
k8b		1	$1.43 \cdot 10^{-4}$		$\overline{\mathbf{Z}}$
k9f			10.000		$\overline{\mathbf{Z}}$
k9b			10.000		$\overline{\mathbf{Z}}$
k10			0.050		$\overline{\mathbf{Z}}$
flow			0.011		$\overline{\mathbf{Z}}$

6 Reactions

This model contains 25 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 5: Overview of all reactions

Id Name	Reaction Equation	SBO
ATPflow	$\emptyset \Longrightarrow ATP$	
ADPflow	$\emptyset \Longrightarrow ADP$	
NADHflow	$\emptyset \Longrightarrow NADH$	
NADflow	$\emptyset \Longrightarrow NAD$	
GLCflow	$\emptyset \Longrightarrow GLC$	
F6Pflow	$F6P \longrightarrow \emptyset$	
FBPflow	$FBP \longrightarrow \emptyset$	
GAPflow	$GAP \longrightarrow \emptyset$	
DPGflow	$DPG \longrightarrow \emptyset$	
PEPflow	$PEP \longrightarrow \emptyset$	
PYRflow	$PYR \longrightarrow \emptyset$	
ACAflow	$ACA \longrightarrow \emptyset$	
EtOHflow	EtOH $\longrightarrow \emptyset$	
AMPflow	$AMP \longrightarrow \emptyset$	
Pflow	$P \longrightarrow \emptyset$	
reaction_1	$GLC + ATP \longrightarrow F6P + ADP$	
reaction_2	$F6P + ATP \xrightarrow{AMP} FBP + ADP$	
reaction_3	$FBP \Longrightarrow 2 GAP$	
reaction_4	$GAP + NAD \longrightarrow DPG + NADH$	
reaction_5	$DPG + ADP \Longrightarrow PEP + ATP$	
reaction_6	$PEP + ADP \longrightarrow PYR + ATP$	
reaction_7	$PYR \longrightarrow ACA$	
	ADPflow NADHflow NADflow GLCflow F6Pflow F8Pflow GAPflow DPGflow PEPflow PYRflow ACAflow EtOHflow AMPflow Pflow reaction_1 reaction_2 reaction_3 reaction_4 reaction_5 reaction_6	ADPflow $\emptyset \rightleftharpoons ADP$ NADHflow $\emptyset \rightleftharpoons NADH$ NADflow $\emptyset \rightleftharpoons NAD$ GLCflow $\emptyset \rightleftharpoons GLC$ F6Pflow F6P $\to \emptyset$ FBFlow F8PP $\to \emptyset$ GAPflow Θ PPEPflow Θ PPEPflow Θ PPEPflow Θ ACA $\to \emptyset$ EtOHflow Θ FIDHOW Θ POPGFlow Θ POPGFlow Θ POPGFlow Θ POPGFlow Θ POPGFlow Θ PEP $\to \emptyset$ POPGFlow Θ POPGFlow

Nº	Id	Name	Reaction Equation	SBO
23	reaction_8		$ACA + NADH \Longrightarrow EtOH + NAD$	
24	reaction_9 $AMP + ATP \rightleftharpoons 2ADP$			
25	${\tt reaction_10}$		$F6P \longrightarrow P$	

6.1 Reaction ATPflow

This is a reversible reaction of no reactant forming one product.

Reaction equation

$$\emptyset \Longrightarrow ATP$$
 (1)

Product

Table 6: Properties of each product.

Id	Name	SBO
ATP		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment}\right) \cdot (3.5 - [\text{ATP}]) \cdot \text{flow}$$
 (2)

6.2 Reaction ADPflow

This is a reversible reaction of no reactant forming one product.

Reaction equation

$$\emptyset \Longrightarrow ADP$$
 (3)

Product

Table 7: Properties of each product.

Id	Name	SBO
ADP		

Kinetic Law

$$v_2 = \text{vol}(\text{compartment}) \cdot (1.1 - [\text{ADP}]) \cdot \text{flow}$$
 (4)

6.3 Reaction NADHflow

This is a reversible reaction of no reactant forming one product.

Reaction equation

$$\emptyset \Longrightarrow NADH$$
 (5)

Product

Table 8: Properties of each product.

Id	Name	SBO
NADH		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\left(\text{compartment}\right) \cdot \left(0.24 - [\text{NADH}]\right) \cdot \text{flow}$$
 (6)

6.4 Reaction NADflow

This is a reversible reaction of no reactant forming one product.

Reaction equation

$$\emptyset \rightleftharpoons NAD$$
 (7)

Product

Table 9: Properties of each product.

Id	Name	SBO
NAD		

Kinetic Law

$$v_4 = \text{vol}\left(\text{compartment}\right) \cdot \left(4 - [\text{NAD}]\right) \cdot \text{flow}$$
 (8)

6.5 Reaction GLCflow

This is a reversible reaction of no reactant forming one product.

Reaction equation

$$\emptyset \rightleftharpoons GLC$$
 (9)

Product

Table 10: Properties of each product.

Id	Name	SBO
GLC		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\left(\text{compartment}\right) \cdot \left(50 - [\text{GLC}]\right) \cdot \text{flow}$$
 (10)

6.6 Reaction F6Pflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$F6P \longrightarrow \emptyset \tag{11}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
F6P		

Kinetic Law

$$v_6 = \text{vol}(\text{compartment}) \cdot [\text{F6P}] \cdot \text{flow}$$
 (12)

6.7 Reaction FBPflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$FBP \longrightarrow \emptyset \tag{13}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
FBP		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\left(\text{compartment}\right) \cdot [\text{FBP}] \cdot \text{flow}$$
 (14)

6.8 Reaction GAPflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$GAP \longrightarrow \emptyset \tag{15}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
GAP		

Kinetic Law

$$v_8 = \text{vol}\left(\text{compartment}\right) \cdot [\text{GAP}] \cdot \text{flow}$$
 (16)

6.9 Reaction DPGflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$DPG \longrightarrow \emptyset \tag{17}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
DPG		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\left(\text{compartment}\right) \cdot [\text{DPG}] \cdot \text{flow}$$
 (18)

6.10 Reaction PEPflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$PEP \longrightarrow \emptyset \tag{19}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
PEP		

Kinetic Law

$$v_{10} = \text{vol}\left(\text{compartment}\right) \cdot [\text{PEP}] \cdot \text{flow}$$
 (20)

6.11 Reaction PYRflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$PYR \longrightarrow \emptyset \tag{21}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
PYR		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}\left(\text{compartment}\right) \cdot [\text{PYR}] \cdot \text{flow}$$
 (22)

6.12 Reaction ACAflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$ACA \longrightarrow \emptyset$$
 (23)

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
ACA		

Kinetic Law

$$v_{12} = \text{vol}\left(\text{compartment}\right) \cdot [\text{ACA}] \cdot \text{flow}$$
 (24)

6.13 Reaction EtOHflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

EtOH
$$\longrightarrow \emptyset$$
 (25)

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
EtOH		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol} (\text{compartment}) \cdot [\text{EtOH}] \cdot \text{flow}$$
 (26)

6.14 Reaction AMPflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$AMP \longrightarrow \emptyset \tag{27}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
AMP		

Kinetic Law

$$v_{14} = \text{vol}\left(\text{compartment}\right) \cdot [\text{AMP}] \cdot \text{flow}$$
 (28)

6.15 Reaction Pflow

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$P \longrightarrow \emptyset$$
 (29)

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
Р		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}\left(\text{compartment}\right) \cdot [P] \cdot \text{flow}$$
 (30)

6.16 Reaction reaction_1

This is an irreversible reaction of two reactants forming two products.

Reaction equation

$$GLC + ATP \longrightarrow F6P + ADP$$
 (31)

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
GLC		
ATP		

Products

Table 22: Properties of each product.

Id	Name	SBO
F6P		

Id	Name	SBO
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = vol\left(compartment\right) \cdot \frac{V1 \cdot [ATP] \cdot [GLC]}{(K1GLC + [GLC]) \cdot (K1ATP + [ATP])} \tag{32}$$

6.17 Reaction reaction_2

This is an irreversible reaction of two reactants forming two products influenced by one modifier.

Reaction equation

$$F6P + ATP \xrightarrow{AMP} FBP + ADP$$
 (33)

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
F6P		
ATP		

Modifier

Table 24: Properties of each modifier.

Id	Name	SBO
AMP		

Products

Table 25: Properties of each product.

Id	Name	SBO
FBP		
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}\left(\text{compartment}\right) \cdot \frac{\text{V2} \cdot [\text{ATP}] \cdot [\text{F6P}]^2}{\left(\text{K2} \cdot \left(1 + \text{k2} \cdot \left(\frac{[\text{ATP}]}{[\text{AMP}]}\right)^2\right) + [\text{F6P}]^2\right) \cdot \left(\text{K2ATP} + [\text{ATP}]\right)} \tag{34}$$

6.18 Reaction reaction_3

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

Reaction equation

$$FBP \Longrightarrow 2GAP$$
 (35)

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
FBP		

Product

Table 27: Properties of each product.

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol} \left(\text{compartment} \right) \cdot \left(\text{k3f} \cdot [\text{FBP}] - \text{k3b} \cdot [\text{GAP}]^2 \right)$$
 (36)

6.19 Reaction reaction_4

This is an irreversible reaction of two reactants forming two products.

Reaction equation

$$GAP + NAD \longrightarrow DPG + NADH \tag{37}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
GAP		
NAD		

Products

Table 29: Properties of each product.

Id	Name	SBO
DPG		
NADH		

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = vol\left(compartment\right) \cdot \frac{V4 \cdot [NAD] \cdot [GAP]}{(K4GAP + [GAP]) \cdot (K4NAD + [NAD])} \tag{38}$$

6.20 Reaction reaction_5

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

Reaction equation

$$DPG + ADP \Longrightarrow PEP + ATP \tag{39}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
DPG		
ADP		

Products

Table 31: Properties of each product.

Id	Name	SBO
PEP		
ATP		

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}\left(\text{compartment}\right) \cdot \left(\text{k5f} \cdot \left[\text{DPG}\right] \cdot \left[\text{ADP}\right] - \text{k5b} \cdot \left[\text{PEP}\right] \cdot \left[\text{ATP}\right]\right) \tag{40}$$

6.21 Reaction reaction_6

This is an irreversible reaction of two reactants forming two products.

Reaction equation

$$PEP + ADP \longrightarrow PYR + ATP \tag{41}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
PEP		
ADP		

Products

Table 33: Properties of each product.

Id	Name	SBO
PYR		
ATP		

Kinetic Law

$$v_{21} = \text{vol}\left(\text{compartment}\right) \cdot \frac{\text{V6} \cdot [\text{ADP}] \cdot [\text{PEP}]}{(\text{K6PEP} + [\text{PEP}]) \cdot (\text{K6ADP} + [\text{ADP}])} \tag{42}$$

6.22 Reaction reaction_7

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$PYR \longrightarrow ACA \tag{43}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
PYR		

Product

Table 35: Properties of each product.

Id	Name	SBO
ACA		

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}\left(\text{compartment}\right) \cdot \frac{\text{V7} \cdot [\text{PYR}]}{\text{K7PYR} + [\text{PYR}]}$$
 (44)

6.23 Reaction reaction_8

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

Reaction equation

$$ACA + NADH \Longrightarrow EtOH + NAD$$
 (45)

Reactants

Table 36: Properties of each reactant.

Id	Name	SBO
ACA		

Id	Name	SBO
NADH		

Products

Table 37: Properties of each product.

Id	Name	SBO
EtOH		
NAD		

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{compartment}) \cdot (\text{k8f} \cdot [\text{NADH}] \cdot [\text{ACA}] - \text{k8b} \cdot [\text{NAD}] \cdot [\text{EtOH}])$$
 (46)

6.24 Reaction reaction_9

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

Reaction equation

$$AMP + ATP \Longrightarrow 2ADP \tag{47}$$

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
AMP		
ATP		

Product

Table 39: Properties of each product.

Id	Name	SBO
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}\left(\text{compartment}\right) \cdot \left(\text{k9f} \cdot [\text{AMP}] \cdot [\text{ATP}] - \text{k9b} \cdot [\text{ADP}]^2\right) \tag{48}$$

6.25 Reaction reaction_10

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$F6P \longrightarrow P \tag{49}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
F6P		

Product

Table 41: Properties of each product.

Id	Name	SBO
P		

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol}\left(\text{compartment}\right) \cdot \text{k10} \cdot [\text{F6P}]$$
 (50)

7 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.

7.1 Species ATP

Initial amount 4.49064 mmol

This species takes part in six reactions (as a reactant in reaction_1, reaction_2, reaction_9 and as a product in ATPflow, reaction_5, reaction_6).

$$\frac{d}{dt}ATP = v_1 + v_{20} + v_{21} - v_{16} - v_{17} - v_{24}$$
(51)

7.2 Species ADP

Initial amount 0.108367 mmol

This species takes part in six reactions (as a reactant in reaction_5, reaction_6 and as a product in ADPflow, reaction_1, reaction_2, reaction_9).

$$\frac{\mathrm{d}}{\mathrm{d}t} ADP = |v_2| + |v_{16}| + |v_{17}| + 2|v_{24}| - |v_{20}| - |v_{21}|$$
(52)

7.3 Species AMP

Initial amount 0.00261149 mmol

This species takes part in three reactions (as a reactant in AMPflow, reaction_9 and as a modifier in reaction_2).

$$\frac{d}{dt}AMP = -v_{14} - v_{24} \tag{53}$$

7.4 Species GLC

Initial amount 0.0112817 mmol

This species takes part in two reactions (as a reactant in reaction_1 and as a product in GLCflow).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLC} = |v_5| - |v_{16}| \tag{54}$$

7.5 Species F6P

Initial amount 0.65939 mmol

This species takes part in four reactions (as a reactant in F6Pflow, reaction_2, reaction_10 and as a product in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t} F6P = |v_{16}| - |v_{6}| - |v_{17}| - |v_{25}| \tag{55}$$

7.6 Species FBP

Initial amount 0.00770135 mmol

This species takes part in three reactions (as a reactant in FBPflow, reaction_3 and as a product in reaction_2).

$$\frac{d}{dt}FBP = |v_{17}| - |v_{7}| - |v_{18}| \tag{56}$$

7.7 Species GAP

Initial amount 0.00190919 mmol

This species takes part in three reactions (as a reactant in GAPflow, reaction_4 and as a product in reaction_3).

$$\frac{d}{dt}GAP = 2|v_{18}| - |v_8| - |v_{19}| \tag{57}$$

7.8 Species NAD

Initial amount 3.62057 mmol

This species takes part in three reactions (as a reactant in reaction_4 and as a product in NADflow, reaction_8).

$$\frac{d}{dt}NAD = v_4 + v_{23} - v_{19} \tag{58}$$

7.9 Species NADH

Initial amount 0.616118 mmol

This species takes part in three reactions (as a reactant in reaction_8 and as a product in NADHflow, reaction_4).

$$\frac{d}{dt}NADH = |v_3| + |v_{19}| - |v_{23}| \tag{59}$$

7.10 Species DPG

Initial amount 0.299109 mmol

This species takes part in three reactions (as a reactant in DPGflow, reaction_5 and as a product in reaction_4).

$$\frac{d}{dt}DPG = |v_{19}| - |v_{9}| - |v_{20}| \tag{60}$$

7.11 Species PEP

Initial amount 0.0021125 mmol

This species takes part in three reactions (as a reactant in PEPflow, reaction_6 and as a product in reaction_5).

$$\frac{d}{dt}PEP = |v_{20} - v_{10}| - |v_{21}| \tag{61}$$

7.12 Species PYR

Initial amount 0.00422702 mmol

This species takes part in three reactions (as a reactant in PYRflow, reaction_7 and as a product in reaction_6).

$$\frac{d}{dt}PYR = |v_{21}| - |v_{11}| - |v_{22}| \tag{62}$$

7.13 Species ACA

Initial amount 0.0738334 mmol

This species takes part in three reactions (as a reactant in ACAflow, reaction_8 and as a product in reaction_7).

$$\frac{d}{dt}ACA = v_{22} - |v_{12}| - |v_{23}| \tag{63}$$

7.14 Species Et OH

Initial amount 0.33981 mmol

This species takes part in two reactions (as a reactant in EtOHflow and as a product in reaction—8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOH} = |v_{23}| - |v_{13}| \tag{64}$$

7.15 Species P

Initial amount 0 mmol

This species takes part in two reactions (as a reactant in Pflow and as a product in reaction—10).

$$\frac{d}{dt}P = v_{25} - v_{15} \tag{65}$$

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