SBML Model Report

Model name: "Hoefnagel2002_PyruvateBranches"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Nicolas Le Novre[1] and Maria Schilstra[2] at March sixth 2005 at 8:03 p. m. and last time modified at April eighth 2016 at 2:25 p. 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	19
events	0	constraints	0
reactions	14	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

This a model from the article:
Metabolic engineering of lactic acid bacteria, the combined approach: kinetic modelling, metabolic control and experimental analysis.

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Hoefnagel MH, Starrenburg MJ, Martens DE, Hugenholtz J, Kleerebezem M, Van Swam II, Bongers R, Westerhoff HV, Snoep JL Microbiology2002 Apr; 148(4):1003-13 11932446,

Abstract:
Everyone who has ever tried to radically change metabolic fluxes knows that it is often harder to determine which enzymes have to be modified than it is to actually implement these changes. In the more traditional genetic engineering approaches bottle-necks are pinpointed using qualitative, intuitive approaches, but the alleviation of suspected rate-limiting steps has not often been successful. Here the authors demonstrate that a model of pyruvate distribution in Lactococcus lactis based on enzyme kinetics in combination with metabolic control analysis clearly indicates the key control points in the flux to acetoin and diacetyl, important flavour compounds. The model presented here (available at http://jjj.biochem.sun.ac.za/wcfs.html) showed that the enzymes with the greatest effect on this flux resided outside the acetolactate synthase branch itself. Experiments confirmed the predictions of the model, i.e. knocking out lactate dehydrogenase and overexpressing NADH oxidase increased the flux through the acetolactate synthase branch from 0 to 75% of measured product formation rates.

The paper does not have any figure to be put as a curation figure in the BioModels database. The model does reproduce the fluxes and control-coefficients given in Figure 2 and Table 4. To reproduce the results, the model was changed from the description in the article according to the model on JWS: the parameter Kmpyr was changed to 2.5 from 25. The equillibrium constant for PTA reaction (R4) was changed from 0.0281 to 0.0065. The Km for oxygen in the NOX reaction (R13) was changed from 0.01 to 0.2. Slight deviations between the values in the article and the model results may stem from different algorithms used for finding the steady state.

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 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	☑	

3.1 Compartment `compartment`

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

4 Species

This model contains 19 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 Condition
ADP		compartment	mmol	☐	☐
NAD		compartment	mmol	☐	☐
ATP		compartment	mmol	☐	☐
NADH		compartment	mmol	☐	☐
pyruvate		compartment	mmol	☐	☐
lactate		compartment	mmol	☐	☑
CoA		compartment	mmol	☐	☐
halfglucose		compartment	mmol	☐	☑
AcCoA		compartment	mmol	☐	☐
AcP		compartment	mmol	☐	☐
Ac		compartment	mmol	☐	☑
AcO		compartment	mmol	☐	☐
EtOH		compartment	mmol	☐	☑
AcLac		compartment	mmol	☐	☐
AcetoinIn		compartment	mmol	☐	☐
AcetoinOut		compartment	mmol	☐	☑
Butanediol		compartment	mmol	☐	☑
O2		compartment	mmol	☐	☑
PO4		compartment	$\text{mmol} \cdot \text{l}^{-1}$	☑	☑

5 Reactions

This model contains 14 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	R1		ADP + NAD + halfglucose ⟶ ATP + NADH + pyruvate	
2	R2		NADH + pyruvate ⟶ NAD + lactate	
3	R3		NAD + pyruvate + CoA ⟶ NADH + AcCoA	
4	R4		AcCoA + PO4 ⟶ CoA + AcP	
5	R5		ADP + AcP ⟶ ATP + Ac	
6	R6		NADH + AcCoA ⟶ NAD + CoA + AcO	
7	R7		NADH + AcO ⟶ NAD + EtOH	
8	R8		2 pyruvate ⟶ AcLac	
9	R9		AcLac ⟶ AcetoinIn	
10	R10		AcetoinIn ⟶ AcetoinOut	
11	R11		NADH + AcetoinIn ⟶ NAD + Butanediol	
12	R12		ATP ⟶ ADP	
13	R13		NADH + O2 ⟶ NAD	
14	R14		AcLac ⟶ AcetoinIn	

5.1 Reaction R1

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

Reaction equation

$$\mathrm{ADP} + \mathrm{NAD} + \mathrm{halfglucose} \longrightarrow \mathrm{ATP} + \mathrm{NADH} + \mathrm{pyruvate} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
ADP		
NAD		
halfglucose		

Products

Table 6: Properties of each product.

Id	Name	SBO
ATP		
NADH		
pyruvate		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{2 \cdot \mathrm{V\_1} \cdot \frac{\mathrm{halfglucose}}{2 \cdot \mathrm{Kglc\_1}} \cdot \frac{\mathrm{NAD}}{\mathrm{Knad\_1}} \cdot \frac{\mathrm{ADP}}{\mathrm{Kadp\_1}}}{\left(1 + \frac{\mathrm{halfglucose}}{2 \cdot \mathrm{Kglc\_1}} + \frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_1}}\right) \cdot \left(1 + \frac{\mathrm{NAD}}{\mathrm{Knad\_1}} + \frac{\mathrm{NADH}}{\mathrm{Knadh\_1}}\right) \cdot \left(1 + \frac{\mathrm{ADP}}{\mathrm{Kadp\_1}} + \frac{\mathrm{ATP}}{\mathrm{Katp\_1}}\right)} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_1			2397.000		☑
Kglc_1			0.100		☑
Knad_1			0.141		☑
Kadp_1			0.047		☑
Kpyr_1			2.500		☑

Id	Name	SBO	Value	Unit	Constant
Knadh_1			0.090		☑
Katp_1			0.019		☑

5.2 Reaction R2

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

Reaction equation

$$\mathrm{NADH} + \mathrm{pyruvate} \longrightarrow \mathrm{NAD} + \mathrm{lactate} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
NADH		
pyruvate		

Products

Table 9: Properties of each product.

Id	Name	SBO
NAD		
lactate		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{V\_2} \cdot \frac{\mathrm{pyruvate} \cdot \mathrm{NADH} - \frac{\mathrm{lactate} \cdot \mathrm{NAD}}{\mathrm{Keq\_2}}}{\mathrm{Kpyr\_2} \cdot \mathrm{Knadh\_2}}}{\left(1 + \frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_2}} + \frac{\mathrm{lactate}}{\mathrm{Klac\_2}}\right) \cdot \left(1 + \frac{\mathrm{NADH}}{\mathrm{Knadh\_2}} + \frac{\mathrm{NAD}}{\mathrm{Knad\_2}}\right)} \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_2			5118.00		☑

Id	Name	SBO	Value	Unit	Constant
Keq_2			21120.69		☑
Kpyr_2			1.50		☑
Knadh_2			0.08		☑
Klac_2			100.00		☑
Knad_2			2.40		☑

5.3 Reaction R3

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

Reaction equation

$$\mathrm{NAD} + \mathrm{pyruvate} + \mathrm{CoA} \longrightarrow \mathrm{NADH} + \mathrm{AcCoA} \tag{5}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
NAD		
pyruvate		
CoA		

Products

Table 12: Properties of each product.

Id	Name	SBO
NADH		
AcCoA		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{V\_3} \cdot \frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_3}} \cdot \frac{\mathrm{NAD}}{\mathrm{Knad\_3}} \cdot \frac{\mathrm{CoA}}{\mathrm{Kcoa\_3}} \cdot \frac{\mathrm{NAD}}{\mathrm{NAD}+\mathrm{Ki\_3}\cdot\mathrm{NADH}}}{\left(1+\frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_3}}\right)\cdot\left(1+\frac{\mathrm{NAD}}{\mathrm{Knad\_3}}+\frac{\mathrm{NADH}}{\mathrm{Knadh\_3}}\right)\cdot\left(1+\frac{\mathrm{CoA}}{\mathrm{Kcoa\_3}}+\frac{\mathrm{AcCoA}}{\mathrm{Kaccoa\_3}}\right)} \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_3			259.000		☑
Kpyr_3			1.000		☑
Knad_3			0.400		☑
Kcoa_3			0.014		☑
Ki_3			46.416		☑
Knadh_3			0.100		☑
Kaccoa_3			0.008		☑

5.4 Reaction R4

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

Reaction equation

$$\mathrm{AcCoA} + \mathrm{PO4} \longrightarrow \mathrm{CoA} + \mathrm{AcP} \tag{7}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
AcCoA		
PO4		

Products

Table 15: Properties of each product.

Id	Name	SBO
CoA		
AcP		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\mathrm{V\_4} \cdot \frac{\mathrm{AcCoA}\cdot[\mathrm{PO4}] - \frac{\mathrm{AcP}\cdot\mathrm{CoA}}{\mathrm{Keq\_4}}}{\mathrm{Kiaccoa\_4}\cdot\mathrm{Kpi\_4}}}{1 + \frac{\mathrm{AcCoA}}{\mathrm{Kiaccoa\_4}} + \frac{[\mathrm{PO4}]}{\mathrm{Kipi\_4}} + \frac{\mathrm{AcP}}{\mathrm{Kiacp\_4}} + \frac{\mathrm{CoA}}{\mathrm{Kicoa\_4}} + \frac{\mathrm{AcCoA}\cdot[\mathrm{PO4}]}{\mathrm{Kiaccoa\_4}\cdot\mathrm{Kpi\_4}} + \frac{\mathrm{AcP}\cdot\mathrm{CoA}}{\mathrm{Kacp\_4}\cdot\mathrm{Kicoa\_4}}} \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_4			42.000		☑
Keq_4			0.007		☑
Kiaccoa_4			0.200		☑
Kpi_4			2.600		☑
Kipi_4			2.600		☑
Kiacp_4			0.200		☑
Kicoa_4			0.029		☑
Kacp_4			0.700		☑

5.5 Reaction R5

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

Reaction equation

$$\mathrm{ADP} + \mathrm{AcP} \longrightarrow \mathrm{ATP} + \mathrm{Ac} \tag{9}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
ADP		
AcP		

Products

Table 18: Properties of each product.

Id	Name	SBO
ATP		
Ac		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{V\_5} \cdot \frac{\mathrm{AcP} \cdot \mathrm{ADP} - \frac{\mathrm{Ac} \cdot \mathrm{ATP}}{\mathrm{Keq\_5}}}{\mathrm{Kadp\_5} \cdot \mathrm{Kacp\_5}}}{\left(1 + \frac{\mathrm{AcP}}{\mathrm{Kacp\_5}} + \frac{\mathrm{Ac}}{\mathrm{Kac\_5}}\right) \cdot \left(1 + \frac{\mathrm{ADP}}{\mathrm{Kadp\_5}} + \frac{\mathrm{ATP}}{\mathrm{Katp\_5}}\right)} \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_5			2700.000		☑
Keq_5			174.217		☑
Kadp_5			0.500		☑
Kacp_5			0.160		☑
Kac_5			7.000		☑
Katp_5			0.070		☑

5.6 Reaction R6

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

Reaction equation

$$\mathrm{NADH} + \mathrm{AcCoA} \longrightarrow \mathrm{NAD} + \mathrm{CoA} + \mathrm{AcO} \tag{11}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
NADH		
AcCoA		

Products

Table 21: Properties of each product.

Id	Name	SBO
NAD		
CoA		
AcO		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\mathrm{V\_6} \cdot \frac{\mathrm{AcCoA} \cdot \mathrm{NADH} - \frac{\mathrm{CoA} \cdot \mathrm{NAD} \cdot \mathrm{AcO}}{\mathrm{Keq\_6}}}{\mathrm{Kaccoa\_6} \cdot \mathrm{Knadh\_6}}}{\left(1 + \frac{\mathrm{NAD}}{\mathrm{Knad\_6}} + \frac{\mathrm{NADH}}{\mathrm{Knadh\_6}}\right) \cdot \left(1 + \frac{\mathrm{AcCoA}}{\mathrm{Kaccoa\_6}} + \frac{\mathrm{CoA}}{\mathrm{Kcoa\_6}}\right) \cdot \left(1 + \frac{\mathrm{AcO}}{\mathrm{Kaco\_6}}\right)} \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_6			97.000		☑
Keq_6			1.000		☑
Kaccoa_6			0.007		☑
Knadh_6			0.025		☑
Knad_6			0.080		☑
Kcoa_6			0.008		☑
Kaco_6			10.000		☑

5.7 Reaction R7

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

Reaction equation

$$\mathrm{NADH} + \mathrm{AcO} \longrightarrow \mathrm{NAD} + \mathrm{EtOH} \tag{13}$$

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
NADH		
AcO		

Products

Table 24: Properties of each product.

Id	Name	SBO
NAD		
EtOH		

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{V\_7} \cdot \frac{\mathrm{AcO} \cdot \mathrm{NADH} - \frac{\mathrm{EtOH} \cdot \mathrm{NAD}}{\mathrm{Keq\_7}}}{\mathrm{Kaco\_7} \cdot \mathrm{Knadh\_7}}}{\left(1 + \frac{\mathrm{NAD}}{\mathrm{Knad\_7}} + \frac{\mathrm{NADH}}{\mathrm{Knadh\_7}}\right) \cdot \left(1 + \frac{\mathrm{AcO}}{\mathrm{Kaco\_7}} + \frac{\mathrm{EtOH}}{\mathrm{Ketoh\_7}}\right)} \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_7			162.00		☑
Keq_7			12354.90		☑
Kaco_7			0.03		☑
Knadh_7			0.05		☑
Knad_7			0.08		☑
Ketoh_7			1.00		☑

5.8 Reaction R8

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

Reaction equation

$$2\,\mathrm{pyruvate} \longrightarrow \mathrm{AcLac} \tag{15}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
pyruvate		

Product

Table 27: Properties of each product.

Id	Name	SBO
AcLac		

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{V\_8} \cdot \frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_8}} \cdot \left(1 - \frac{\mathrm{AcLac}}{\mathrm{pyruvate} \cdot \mathrm{Keq\_8}}\right) \cdot \left(\frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_8}} + \frac{\mathrm{AcLac}}{\mathrm{Kaclac\_8}}\right)^{\mathrm{n\_8}-1}}{1 + \left(\frac{\mathrm{pyruvate}}{\mathrm{Kpyr\_8}} + \frac{\mathrm{AcLac}}{\mathrm{Kaclac\_8}}\right)^{\mathrm{n\_8}}} \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_8			600.000		☑
Kpyr_8			50.000		☑
Keq_8			$9 \cdot 10^{12}$		☑
Kaclac_8			100.000		☑
n_8			2.400		☑

5.9 Reaction R9

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

Reaction equation

$$\mathrm{AcLac} \longrightarrow \mathrm{AcetoinIn} \tag{17}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
AcLac		

Product

Table 30: Properties of each product.

Id	Name	SBO
AcetoinIn		

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\mathrm{V\_9} \cdot \frac{\mathrm{AcLac}}{\mathrm{Kaclac\_9}}}{1 + \frac{\mathrm{AcLac}}{\mathrm{Kaclac\_9}} + \frac{\mathrm{AcetoinIn}}{\mathrm{Kacet\_9}}} \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_9			106.0		☑
Kaclac_9			10.0		☑
Kacet_9			100.0		☑

5.10 Reaction R10

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

Reaction equation

$$\mathrm{AcetoinIn} \longrightarrow \mathrm{AcetoinOut} \tag{19}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
AcetoinIn		

Product

Table 33: Properties of each product.

Id	Name	SBO
AcetoinOut		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\mathrm{V\_10} \cdot \frac{\mathrm{AcetoinIn}}{\mathrm{Kacet\_10}}}{1 + \frac{\mathrm{AcetoinIn}}{\mathrm{Kacet\_10}}} \tag{20}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_10			200.0		☑
Kacet_10			5.0		☑

5.11 Reaction R11

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

Reaction equation

$$\mathrm{NADH} + \mathrm{AcetoinIn} \longrightarrow \mathrm{NAD} + \mathrm{Butanediol} \tag{21}$$

Reactants

Table 35: Properties of each reactant.

Id	Name	SBO
NADH		
AcetoinIn		

Products

Table 36: Properties of each product.

Id	Name	SBO
NAD		
Butanediol		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\mathrm{V\_11} \cdot \frac{\mathrm{AcetoinIn} \cdot \mathrm{NADH} - \frac{\mathrm{Butanediol} \cdot \mathrm{NAD}}{\mathrm{Keq\_11}}}{\mathrm{Kacet\_11} \cdot \mathrm{Knadh\_11}}}{\left(1 + \frac{\mathrm{AcetoinIn}}{\mathrm{Kacet\_11}} + \frac{\mathrm{Butanediol}}{\mathrm{Kbut\_11}}\right) \cdot \left(1 + \frac{\mathrm{NADH}}{\mathrm{Knadh\_11}} + \frac{\mathrm{NAD}}{\mathrm{Knad\_11}}\right)} \tag{22}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_11			105.00		☑
Keq_11			1400.00		☑
Kacet_11			0.06		☑
Knadh_11			0.02		☑
Kbut_11			2.60		☑
Knad_11			0.16		☑

5.12 Reaction R12

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

Reaction equation

$$\mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{23}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
ATP		

Product

Table 39: Properties of each product.

Id	Name	SBO
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\mathrm{V\_12} \cdot \left(\frac{\mathrm{ATP}}{\mathrm{ADP} \cdot \mathrm{Katp\_12}}\right)^{\mathrm{n\_12}}}{1 + \left(\frac{\mathrm{ATP}}{\mathrm{ADP} \cdot \mathrm{Katp\_12}}\right)^{\mathrm{n\_12}}} \tag{24}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_12			900.000		☑
Katp_12			6.196		☑
n_12			2.580		☑

5.13 Reaction R13

This is an irreversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{NADH} + \mathrm{O2} \longrightarrow \mathrm{NAD} \tag{25}$$

Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
NADH		
O2		

Product

Table 42: Properties of each product.

Id	Name	SBO
NAD		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{\mathrm{V\_13} \cdot \frac{\mathrm{NADH} \cdot \mathrm{O2}}{\mathrm{Knadh\_13} \cdot \mathrm{Ko\_13}}}{\left(1 + \frac{\mathrm{NADH}}{\mathrm{Knadh\_13}} + \frac{\mathrm{NAD}}{\mathrm{Knad\_13}}\right) \cdot \left(1 + \frac{\mathrm{O2}}{\mathrm{Ko\_13}}\right)} \tag{26}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_13			118.000		☑
Knadh_13			0.041		☑
Ko_13			0.200		☑
Knad_13			1.000		☑

5.14 Reaction R14

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

Reaction equation

$$\text{AcLac} \longrightarrow \text{AcetoinIn} \tag{27}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
AcLac		

Product

Table 45: Properties of each product.

Id	Name	SBO
AcetoinIn		

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{k\_14} \cdot \text{AcLac} \tag{28}$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_14			$3 \cdot 10^{-4}$		☑

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 ADP

Initial amount 4.9 mmol

This species takes part in three reactions (as a reactant in R1, R5 and as a product in R12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_{12} - v_1 - v_5 \tag{29}$$

6.2 Species NAD

Initial amount 6.33 mmol

This species takes part in seven reactions (as a reactant in R1, R3 and as a product in R2, R6, R7, R11, R13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_2 + v_6 + v_7 + v_{11} + v_{13} - v_1 - v_3 \tag{30}$$

6.3 Species ATP

Initial amount 0.1 mmol

This species takes part in three reactions (as a reactant in R12 and as a product in R1, R5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_1 + v_5 - v_{12} \tag{31}$$

6.4 Species NADH

Initial amount 3.67 mmol

This species takes part in seven reactions (as a reactant in R2, R6, R7, R11, R13 and as a product in R1, R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_1 + v_3 - v_2 - v_6 - v_7 - v_{11} - v_{13} \tag{32}$$

6.5 Species pyruvate

Initial amount 1 mmol

This species takes part in four reactions (as a reactant in R2, R3, R8 and as a product in R1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pyruvate} = v_1 - v_2 - v_3 - 2\,v_8 \tag{33}$$

6.6 Species lactate

Initial amount 0.1 mmol

This species takes part in one reaction (as a product in R2), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{lactate} = 0 \tag{34}$$

6.7 Species CoA

Initial amount 1 mmol

This species takes part in three reactions (as a reactant in R3 and as a product in R4, R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoA} = v_4 + v_6 - v_3 \tag{35}$$

6.8 Species halfglucose

Initial amount 30 mmol

This species takes part in one reaction (as a reactant in R1), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{halfglucose} = 0 \tag{36}$$

6.9 Species AcCoA

Initial amount 0 mmol

This species takes part in three reactions (as a reactant in R4, R6 and as a product in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcCoA} = v_3 - v_4 - v_6 \tag{37}$$

6.10 Species AcP

Initial amount 0 mmol

This species takes part in two reactions (as a reactant in R5 and as a product in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcP} = v_4 - v_5 \tag{38}$$

6.11 Species Ac

Initial amount 1 mmol

This species takes part in one reaction (as a product in R5), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ac} = 0 \tag{39}$$

6.12 Species AcO

Initial amount 0 mmol

This species takes part in two reactions (as a reactant in R7 and as a product in R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcO} = v_6 - v_7 \tag{40}$$

6.13 Species EtOH

Initial amount 1 mmol

This species takes part in one reaction (as a product in R7), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOH} = 0 \tag{41}$$

6.14 Species AcLac

Initial amount 0 mmol

This species takes part in three reactions (as a reactant in R9, R14 and as a product in R8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcLac} = v_8 - v_9 - v_{14} \tag{42}$$

6.15 Species AcetoinIn

Initial amount 0 mmol

This species takes part in four reactions (as a reactant in R10, R11 and as a product in R9, R14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcetoinIn} = v_9 + v_{14} - v_{10} - v_{11} \tag{43}$$

6.16 Species AcetoinOut

Initial amount 0 mmol

This species takes part in one reaction (as a product in R10), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcetoinOut} = 0 \tag{44}$$

6.17 Species Butanediol

Initial amount 0.01 mmol

This species takes part in one reaction (as a product in R11), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Butanediol} = 0 \tag{45}$$

6.18 Species O2

Initial amount 0.2 mmol

This species takes part in one reaction (as a reactant in R13), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2} = 0 \tag{46}$$

6.19 Species PO4

Initial amount 10 mmol

This species takes part in one reaction (as a reactant in R4), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PO4} = 0 \tag{47}$$

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