

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 Novre¹ and Maria Schilstra² 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 *Microbiology* 2002 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 equilibrium constant for PTA reaction (R4) was changed from 0.0281 to 0.0065. The *K_m* 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.

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To cite BioModels Database, please use: [Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C \(2010\) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.](#)

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 1

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			3	1	litre	<input checked="" type="checkbox"/>	

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	<input type="checkbox"/>	<input type="checkbox"/>
NAD		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
ATP		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
NADH		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
pyruvate		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
lactate		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
CoA		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
halfglucose		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
AcCoA		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
AcP		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
Ac		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
AcO		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
EtOH		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
AcLac		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
AcetoinIn		compartment	mmol	<input type="checkbox"/>	<input type="checkbox"/>
AcetoinOut		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Butanediol		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
O2		compartment	mmol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
P04		compartment	mmol · l ⁻¹	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

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.

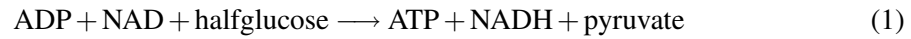
Table 4: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	R1		$\text{ADP} + \text{NAD} + \text{halfglucose} \longrightarrow \text{ATP} + \text{NADH} + \text{pyruvate}$	
2	R2		$\text{NADH} + \text{pyruvate} \longrightarrow \text{NAD} + \text{lactate}$	
3	R3		$\text{NAD} + \text{pyruvate} + \text{CoA} \longrightarrow \text{NADH} + \text{AcCoA}$	
4	R4		$\text{AcCoA} + \text{PO4} \longrightarrow \text{CoA} + \text{AcP}$	
5	R5		$\text{ADP} + \text{AcP} \longrightarrow \text{ATP} + \text{Ac}$	
6	R6		$\text{NADH} + \text{AcCoA} \longrightarrow \text{NAD} + \text{CoA} + \text{AcO}$	
7	R7		$\text{NADH} + \text{AcO} \longrightarrow \text{NAD} + \text{EtOH}$	
8	R8		$2 \text{ pyruvate} \longrightarrow \text{AcLac}$	
9	R9		$\text{AcLac} \longrightarrow \text{AcetoinIn}$	
10	R10		$\text{AcetoinIn} \longrightarrow \text{AcetoinOut}$	
11	R11		$\text{NADH} + \text{AcetoinIn} \longrightarrow \text{NAD} + \text{Butanediol}$	
12	R12		$\text{ATP} \longrightarrow \text{ADP}$	
13	R13		$\text{NADH} + \text{O2} \longrightarrow \text{NAD}$	
14	R14		$\text{AcLac} \longrightarrow \text{AcetoinIn}$	

5.1 Reaction R1

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

Reaction equation



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

$$v_1 = \frac{2 \cdot V_1 \cdot \frac{\text{halfglucose}}{2 \cdot K_{\text{glc}_1}} \cdot \frac{\text{NAD}}{K_{\text{nad}_1}} \cdot \frac{\text{ADP}}{K_{\text{adp}_1}}}{\left(1 + \frac{\text{halfglucose}}{2 \cdot K_{\text{glc}_1}} + \frac{\text{pyruvate}}{K_{\text{pyr}_1}}\right) \cdot \left(1 + \frac{\text{NAD}}{K_{\text{nad}_1}} + \frac{\text{NADH}}{K_{\text{nadh}_1}}\right) \cdot \left(1 + \frac{\text{ADP}}{K_{\text{adp}_1}} + \frac{\text{ATP}}{K_{\text{atp}_1}}\right)} \quad (2)$$

Table 7: Properties of each parameter.

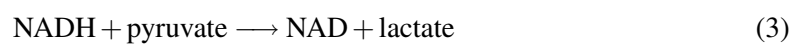
Id	Name	SBO	Value	Unit	Constant
V_1			2397.000		✓
K _{glc_1}			0.100		✓
K _{nad_1}			0.141		✓
K _{adp_1}			0.047		✓
K _{pyr_1}			2.500		✓

Id	Name	SBO	Value	Unit	Constant
Knadh_1			0.090		<input checked="" type="checkbox"/>
Katp_1			0.019		<input checked="" type="checkbox"/>

5.2 Reaction R2

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

Reaction equation



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

$$v_2 = \frac{V_2 \cdot \frac{\text{pyruvate} \cdot \text{NADH} - \frac{\text{lactate} \cdot \text{NAD}}{\text{Keq}_2}}{K_{\text{pyr}_2} \cdot K_{\text{nadh}_2}}}{\left(1 + \frac{\text{pyruvate}}{K_{\text{pyr}_2}} + \frac{\text{lactate}}{K_{\text{lac}_2}}\right) \cdot \left(1 + \frac{\text{NADH}}{K_{\text{nadh}_2}} + \frac{\text{NAD}}{K_{\text{nad}_2}}\right)} \quad (4)$$

Table 10: Properties of each parameter.

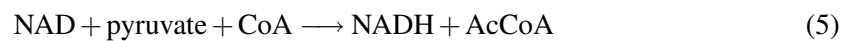
Id	Name	SBO	Value	Unit	Constant
V_2			5118.00		<input checked="" type="checkbox"/>

Id	Name	SBO	Value	Unit	Constant
Keq_2			21120.69		<input checked="" type="checkbox"/>
Kpyr_2			1.50		<input checked="" type="checkbox"/>
Knadh_2			0.08		<input checked="" type="checkbox"/>
Klac_2			100.00		<input checked="" type="checkbox"/>
Knad_2			2.40		<input checked="" type="checkbox"/>

5.3 Reaction R3

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

Reaction equation



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

$$v_3 = \frac{V_{-3} \cdot \frac{\text{pyruvate}}{K_{\text{pyr}_3}} \cdot \frac{\text{NAD}}{K_{\text{nad}_3}} \cdot \frac{\text{CoA}}{K_{\text{coa}_3}} \cdot \frac{\text{NAD}}{\text{NAD} + K_{i_3} \cdot \text{NADH}}}{\left(1 + \frac{\text{pyruvate}}{K_{\text{pyr}_3}}\right) \cdot \left(1 + \frac{\text{NAD}}{K_{\text{nad}_3}} + \frac{\text{NADH}}{K_{\text{nadh}_3}}\right) \cdot \left(1 + \frac{\text{CoA}}{K_{\text{coa}_3}} + \frac{\text{AcCoA}}{K_{\text{accoa}_3}}\right)} \quad (6)$$

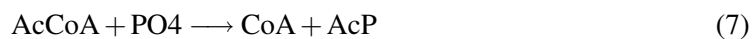
Table 13: Properties of each parameter.

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



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

$$v_4 = \frac{V_4 \cdot \frac{\text{AcCoA} \cdot [\text{PO4}] - \frac{\text{AcP} \cdot \text{CoA}}{K_{eq,4}}}{K_{i\text{accoa},4} \cdot K_{pi,4}}}{1 + \frac{\text{AcCoA}}{K_{i\text{accoa},4}} + \frac{[\text{PO4}]}{K_{pi,4}} + \frac{\text{AcP}}{K_{i\text{acp},4}} + \frac{\text{CoA}}{K_{i\text{coa},4}} + \frac{\text{AcCoA} \cdot [\text{PO4}]}{K_{i\text{accoa},4} \cdot K_{pi,4}} + \frac{\text{AcP} \cdot \text{CoA}}{K_{i\text{acp},4} \cdot K_{i\text{coa},4}}} \quad (8)$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_4			42.000		<input checked="" type="checkbox"/>
Keq_4			0.007		<input checked="" type="checkbox"/>
Kiacc_4			0.200		<input checked="" type="checkbox"/>
Kpi_4			2.600		<input checked="" type="checkbox"/>
Kipi_4			2.600		<input checked="" type="checkbox"/>
Kiacp_4			0.200		<input checked="" type="checkbox"/>
Kicoa_4			0.029		<input checked="" type="checkbox"/>
Kacp_4			0.700		<input checked="" type="checkbox"/>

5.5 Reaction R5

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

Reaction equation



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

$$v_5 = \frac{V_5 \cdot \frac{AcP \cdot ADP - \frac{Ac \cdot ATP}{K_{eq_5}}}{K_{adp_5} \cdot K_{acp_5}}}{\left(1 + \frac{AcP}{K_{acp_5}} + \frac{Ac}{K_{ac_5}}\right) \cdot \left(1 + \frac{ADP}{K_{adp_5}} + \frac{ATP}{K_{atp_5}}\right)} \quad (10)$$

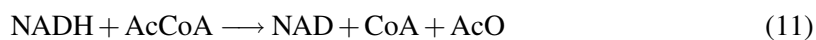
Table 19: Properties of each parameter.

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



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

$$v_6 = \frac{V_6 \cdot \frac{AcCoA \cdot NADH - \frac{CoA \cdot NAD \cdot AcO}{K_{eq_6}}}{K_{accoa_6} \cdot K_{nadh_6}}}{\left(1 + \frac{NAD}{K_{nad_6}} + \frac{NADH}{K_{nadh_6}}\right) \cdot \left(1 + \frac{AcCoA}{K_{accoa_6}} + \frac{CoA}{K_{coa_6}}\right) \cdot \left(1 + \frac{AcO}{K_{aco_6}}\right)} \quad (12)$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_6			97.000		<input checked="" type="checkbox"/>
Keq_6			1.000		<input checked="" type="checkbox"/>
Kaccoa_6			0.007		<input checked="" type="checkbox"/>
Knadh_6			0.025		<input checked="" type="checkbox"/>
Knad_6			0.080		<input checked="" type="checkbox"/>
Kcoa_6			0.008		<input checked="" type="checkbox"/>
Kaco_6			10.000		<input checked="" type="checkbox"/>

5.7 Reaction R7

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

Reaction equation



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
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Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{V_7 \cdot \frac{\text{AcO} \cdot \text{NADH} - \frac{\text{EtOH} \cdot \text{NAD}}{\text{Keq}_7}}{\text{Kaco}_7 \cdot \text{Knadh}_7}}{\left(1 + \frac{\text{NAD}}{\text{Knad}_7} + \frac{\text{NADH}}{\text{Knadh}_7}\right) \cdot \left(1 + \frac{\text{AcO}}{\text{Kaco}_7} + \frac{\text{EtOH}}{\text{Ketoh}_7}\right)} \quad (14)$$

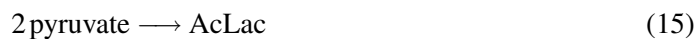
Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_7			162.00		<input checked="" type="checkbox"/>
Keq_7			12354.90		<input checked="" type="checkbox"/>
Kaco_7			0.03		<input checked="" type="checkbox"/>
Knadh_7			0.05		<input checked="" type="checkbox"/>
Knad_7			0.08		<input checked="" type="checkbox"/>
Ketoh_7			1.00		<input checked="" type="checkbox"/>

5.8 Reaction R8

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

Reaction equation



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
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Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{V_8 \cdot \frac{\text{pyruvate}}{K_{\text{pyr}.8}} \cdot \left(1 - \frac{\text{AcLac}}{\text{pyruvate} \cdot K_{\text{eq}.8}}\right) \cdot \left(\frac{\text{pyruvate}}{K_{\text{pyr}.8}} + \frac{\text{AcLac}}{K_{\text{aclac}.8}}\right)^{n_8-1}}{1 + \left(\frac{\text{pyruvate}}{K_{\text{pyr}.8}} + \frac{\text{AcLac}}{K_{\text{aclac}.8}}\right)^{n_8}} \quad (16)$$

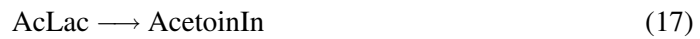
Table 28: Properties of each parameter.

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



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
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Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{V_9 \cdot \frac{AcLac}{Kaclac_9}}{1 + \frac{AcLac}{Kaclac_9} + \frac{AcetoinIn}{Kacet_9}} \quad (18)$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_9			106.0		<input checked="" type="checkbox"/>
Kaclac_9			10.0		<input checked="" type="checkbox"/>
Kacet_9			100.0		<input checked="" type="checkbox"/>

5.10 Reaction R10

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

Reaction equation



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

$$v_{10} = \frac{V_{10} \cdot \frac{\text{AcetoinIn}}{\text{Kacet}_{10}}}{1 + \frac{\text{AcetoinIn}}{\text{Kacet}_{10}}} \quad (20)$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_10			200.0		<input checked="" type="checkbox"/>
Kacet_10			5.0		<input checked="" type="checkbox"/>

5.11 Reaction R11

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

Reaction equation



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

$$v_{11} = \frac{V_{11} \cdot \frac{\text{AcetoinIn} \cdot \text{NADH} - \frac{\text{Butanediol} \cdot \text{NAD}}{\text{Keq}_{11}}}{K_{\text{acet}_{11}} \cdot K_{\text{nadh}_{11}}}}{\left(1 + \frac{\text{AcetoinIn}}{K_{\text{acet}_{11}}} + \frac{\text{Butanediol}}{K_{\text{but}_{11}}}\right) \cdot \left(1 + \frac{\text{NADH}}{K_{\text{nadh}_{11}}} + \frac{\text{NAD}}{K_{\text{nad}_{11}}}\right)} \quad (22)$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_11			105.00		<input checked="" type="checkbox"/>
Keq_11			1400.00		<input checked="" type="checkbox"/>
Kacet_11			0.06		<input checked="" type="checkbox"/>
Knadh_11			0.02		<input checked="" type="checkbox"/>
Kbut_11			2.60		<input checked="" type="checkbox"/>
Knad_11			0.16		<input checked="" type="checkbox"/>

5.12 Reaction R12

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

Reaction equation



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

$$v_{12} = \frac{V_{12} \cdot \left(\frac{ATP}{ADP \cdot Katp_{12}} \right)^{n_{12}}}{1 + \left(\frac{ATP}{ADP \cdot Katp_{12}} \right)^{n_{12}}} \quad (24)$$

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



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

$$v_{13} = \frac{V_{13} \cdot \frac{NADH \cdot O_2}{K_{nadh_13} \cdot K_{o_13}}}{\left(1 + \frac{NADH}{K_{nadh_13}} + \frac{NAD}{K_{nad_13}} \right) \cdot \left(1 + \frac{O_2}{K_{o_13}} \right)} \quad (26)$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_13			118.000		<input checked="" type="checkbox"/>
Knadh_13			0.041		<input checked="" type="checkbox"/>
Ko_13			0.200		<input checked="" type="checkbox"/>
Knad_13			1.000		<input checked="" type="checkbox"/>

5.14 Reaction R14

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

Reaction equation



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

$$v_{14} = k_{14} \cdot \text{AcLac} \quad (28)$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_14			$3 \cdot 10^{-4}$		<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 `spatialDimensions` > 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).

$$\frac{d}{dt}\text{ADP} = v_{12} - v_1 - v_5 \quad (29)$$

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).

$$\frac{d}{dt}\text{NAD} = v_2 + v_6 + v_7 + v_{11} + v_{13} - v_1 - v_3 \quad (30)$$

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).

$$\frac{d}{dt}\text{ATP} = v_1 + v_5 - v_{12} \quad (31)$$

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).

$$\frac{d}{dt}\text{NADH} = v_1 + v_3 - v_2 - v_6 - v_7 - v_{11} - v_{13} \quad (32)$$

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](#)).

$$\frac{d}{dt}\text{pyruvate} = v_1 - v_2 - v_3 - 2 v_8 \quad (33)$$

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:

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

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](#)).

$$\frac{d}{dt}\text{CoA} = v_4 + v_6 - v_3 \quad (35)$$

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:

$$\frac{d}{dt}\text{halfglucose} = 0 \quad (36)$$

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](#)).

$$\frac{d}{dt}\text{AcCoA} = v_3 - v_4 - v_6 \quad (37)$$

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).

$$\frac{d}{dt}\text{AcP} = v_4 - v_5 \quad (38)$$

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:

$$\frac{d}{dt}\text{Ac} = 0 \quad (39)$$

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).

$$\frac{d}{dt}\text{AcO} = v_6 - v_7 \quad (40)$$

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:

$$\frac{d}{dt}\text{EtOH} = 0 \quad (41)$$

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).

$$\frac{d}{dt}\text{AcLac} = v_8 - v_9 - v_{14} \quad (42)$$

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).

$$\frac{d}{dt}\text{AcetoinIn} = v_9 + v_{14} - v_{10} - v_{11} \quad (43)$$

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:

$$\frac{d}{dt}\text{AcetoinOut} = 0 \quad (44)$$

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:

$$\frac{d}{dt}\text{Butanediol} = 0 \quad (45)$$

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:

$$\frac{d}{dt}\text{O2} = 0 \quad (46)$$

6.19 Species P04

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:

$$\frac{d}{dt}\text{P04} = 0 \quad (47)$$

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