SBML Model Report

Model name: "Lei2001_Yeast_Aerobic_Metabolism"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Lukas Endler[1] at March 25th 2010 at 2:28 a. m. and last time modified at June third 2010 at 10:40 a. m. Table 1 shows 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	2
species types	0	species	11
events	0	constraints	0
reactions	20	function definitions	0
global parameters	42	unit definitions	8
rules	6	initial assignments	0

Model Notes

This the model from the article:
A biochemically structured model for Saccharomyces cerevisiae.
Lei F, Rotbll M, Jrgensen SB. J Biotechnol. 2001 Jul 12;88(3):205-21. PMID: 11434967 ,DOI: 10.1016/S0168-1656(01)00269-3

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Abstract:
A biochemically structured model for the aerobic growth of Saccharomyces cerevisiae on glucose and ethanol is presented. The model focuses on the pyruvate and acetaldehyde branch points where overflow metabolism occurs when the growth changes from oxidative to oxido-reductive. The model is designed to describe the onset of aerobic alcoholic fermentation during steady-state as well as under dynamical conditions, by triggering an increase in the glycolytic flux using a key signalling component which is assumed to be closely related to acetaldehyde. An investigation of the modelled process dynamics in a continuous cultivation revealed multiple steady states in a region of dilution rates around the transition between oxidative and oxido-reductive growth. A bifurcation analysis using the two external variables, the dilution rate, D, and the inlet concentration of glucose, S(f), as parameters, showed that a fold bifurcation occurs close to the critical dilution rate resulting in multiple steady-states. The region of dilution rates within which multiple steady states may occur depends strongly on the substrate feed concentration. Consequently a single steady state may prevail at low feed concentrations, whereas multiple steady states may occur over a relatively wide range of dilution rates at higher feed concentrations.

2 Unit Definitions

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

2.1 Unit `substance`

Name gram

Definition g

2.2 Unit `time`

Name hours

Definition 3600 s

2.3 Unit `volume`

Name liter

Definition l

2.4 Unit per_h

Name per hour

Definition $(3600\ \mathrm{s})^{-1}$

2.5 Unit g_per_l

Name gram per liter

Definition $\mathrm{g} \cdot \mathrm{l}^{-1}$

2.6 Unit l_per_g

Name liter per gram

Definition $\mathrm{g}^{-1} \cdot \mathrm{l}$

2.7 Unit g_per_l_per_h

Name gram per liter per hour

Definition $\mathrm{g} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$

2.8 Unit mmole_per_g_per_h

Name mmole per gram BM per hour

Definition $\mathrm{mmol} \cdot (3600\ \mathrm{s})^{-1} \cdot \mathrm{g}^{-1}$

2.9 Unit area

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

Definition m^2

2.10 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`env`	environment	0000290	3	1	litre	☑	
`cell`		0000290	3	1	litre	☑	

3.1 Compartment `env`

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

Name environment

SBO:0000290 physical compartment

3.2 Compartment `cell`

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

SBO:0000290 physical compartment

4 Species

This model contains eleven species. The boundary condition of five of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 8 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
s_glu	Glucose	env	$g \cdot l^{-1}$	⊟	⊟
s_pyr	Pyruvate	env	$g \cdot l^{-1}$	⊟	⊟
s_acetate	Acetate	env	$g \cdot l^{-1}$	⊟	⊟
s_acetald	Acetaldehyde	env	$g \cdot l^{-1}$	⊟	⊟
s_EtOH	EtOH	env	$g \cdot l^{-1}$	⊟	⊟
x	BM	env	$g \cdot l^{-1}$	⊟	⊟
a	BM(active)	env	$g \cdot l^{-1}$	⊟	☑
AcDH	BM(AcDH)	env	$g \cdot l^{-1}$	⊟	☑
CO2	CO2	env	$g \cdot l^{-1}$	⊟	☑
Red	Red. Equ. (NADH)	env	$g \cdot l^{-1}$	⊟	☑
S_f	Glucose(feed)	env	$g \cdot l^{-1}$	⊟	☑

5 Parameters

This model contains 42 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
q02			0.000	$\text{mmol} \cdot (3600\ \text{s})^{-1} \cdot \text{g}^{-1}$	⊟
qCO2			0.000	$\text{mmol} \cdot (3600\ \text{s})^{-1} \cdot \text{g}^{-1}$	⊟
X_a	X_a		0.100	dimensionless	⊟
X_AcDH	X_AcDH		0.008	dimensionless	⊟
k_1h			0.584	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_1h			0.012	$\text{g} \cdot \text{l}^{-1}$	☑
k_1l			1.430	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_1l			0.940	$\text{g} \cdot \text{l}^{-1}$	☑
k_1e			47.100	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_1e			0.120	$\text{g} \cdot \text{l}^{-1}$	☑
K_1i			14.200	$\text{g}^{-1} \cdot 1$	☑
k_2			0.501	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_2			$2 \cdot 10^{-5}$	$\text{g} \cdot \text{l}^{-1}$	☑
K_2i			0.101	$\text{g}^{-1} \cdot 1$	☑
k_3			5.810	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_3			$5 \cdot 10^{-7}$	$\text{g} \cdot \text{l}^{-1}$	☑
k_4			4.800	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_4			$2.64 \cdot 10^{-4}$	$\text{g} \cdot \text{l}^{-1}$	☑
k_5			0.010	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_5			0.010	$\text{g} \cdot \text{l}^{-1}$	☑
k_5e			0.775	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_5e			0.100	$\text{g} \cdot \text{l}^{-1}$	☑
K_5i			440.000	$\text{g}^{-1} \cdot 1$	☑
k_6			2.820	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_6			0.034	$\text{g} \cdot \text{l}^{-1}$	☑
k_6r			0.013	dimensionless	☑
K_6e			0.057	$\text{g} \cdot \text{l}^{-1}$	☑
k_7			1.203	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_7			0.010	$\text{g} \cdot \text{l}^{-1}$	☑
k_8			0.589	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
k_9			0.008	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
K_9			10^{-6}	$\text{g} \cdot \text{l}^{-1}$	☑
k_9e			0.075	$\text{g} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
K_9e			13.000	$\mathrm{g}\cdot\mathrm{l}^{-1}$	☑
K_9i			25.000	$\mathrm{g}^{-1}\cdot\mathrm{l}$	☑
k_9c			0.004	$\mathrm{g}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
k_10			0.392	$\mathrm{g}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
K_10			0.002	$\mathrm{g}\cdot\mathrm{l}^{-1}$	☑
k_10e			0.003	$\mathrm{g}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
K_10e			0.002	$\mathrm{g}\cdot\mathrm{l}^{-1}$	☑
k_11			0.020	$\mathrm{g}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
D	Dilutionrate		0.100	$(3600\ \mathrm{s})^{-1}$	☑

6 Rules

This is an overview of six rules.

6.1 Rule a

Rule a is an assignment rule for species a:

$$\mathrm{a} = [\mathrm{x}]\cdot \mathrm{X\_a} \tag{1}$$

Derived unit $\mathrm{g}\cdot\mathrm{l}^{-1}$

6.2 Rule AcDH

Rule AcDH is an assignment rule for species AcDH:

$$\mathrm{AcDH} = [\mathrm{x}]\cdot \mathrm{X\_AcDH} \tag{2}$$

Derived unit $\mathrm{g}\cdot\mathrm{l}^{-1}$

6.3 Rule X_a

Rule X_a is a rate rule for parameter X_a:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X\_a} = \frac{(0.732\cdot \mathrm{r7} + 0.619\cdot \mathrm{r8})\cdot(1-\mathrm{X\_a}) - \mathrm{r9} - \mathrm{r10}}{[\mathrm{x}]\cdot \mathrm{vol}\,(\mathrm{env})} \tag{3}$$

6.4 Rule X_AcDH

Rule X_AcDH is a rate rule for parameter X_AcDH:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X\_AcDH} = \frac{\mathrm{r9} - \mathrm{r11} - (0.732\cdot \mathrm{r7} + 0.619\cdot \mathrm{r8})\cdot \mathrm{X\_AcDH}}{[\mathrm{x}]\cdot \mathrm{vol}\,(\mathrm{env})} \tag{4}$$

6.5 Rule qO2

Rule qO2 is an assignment rule for parameter qO2:

$$\mathrm{qO2} = \frac{\frac{1000}{32} \cdot (0.178 \cdot \mathrm{r1} + 0.908 \cdot \mathrm{r2} + 0.363 \cdot \mathrm{r4} + 1.066 \cdot \mathrm{r5} - 0.363 \cdot \mathrm{r6} + 0.063 \cdot \mathrm{r7} + 0.214 \cdot \mathrm{r8})}{[\mathrm{x}] \cdot \mathrm{vol}\,(\mathrm{env})} \tag{5}$$

6.6 Rule qCO2

Rule qCO2 is an assignment rule for parameter qCO2:

$$\mathrm{qCO2} = \frac{\frac{1000}{44.01} \cdot (1.499 \cdot \mathrm{r2} + 0.5 \cdot \mathrm{r3} + 1.466 \cdot \mathrm{r5} + 0.127 \cdot \mathrm{r7} + 0.325 \cdot \mathrm{r8})}{[\mathrm{x}] \cdot \mathrm{vol}\,(\mathrm{env})} \tag{6}$$

7 Reactions

This model contains 20 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
1	r1	glycolysis	$\text{s\_glu} \xrightarrow{\text{s\_acetald, x}} 0 \cdot 978\,\text{s\_pyr} + 0 \cdot 178\,\text{Red}$	0000205
2	r2	TCA (pyruvate)	$\text{s\_pyr} \xrightarrow{\text{x, s\_glu}} 1 \cdot 499\,\text{CO2} + 0 \cdot 908\,\text{Red}$	0000205
3	r3	Pyruvate Dehydrogenase	$\text{s\_pyr} \xrightarrow{\text{x}} 0 \cdot 5\,\text{s\_acetald} + 0 \cdot 33\,\text{CO2}$	0000200
4	r4	Acetald. dehydrogenase	$\text{s\_acetald} \xrightarrow{\text{x, s\_EtOH}} 1 \cdot 363\,\text{s\_acetate} + 0 \cdot 363\,\text{Red}$	0000200
5	r5	TCA (acetate)	$\text{s\_acetate} \xrightarrow{\text{x, s\_glu}} 1 \cdot 446\,\text{CO2} + 1 \cdot 066\,\text{Red}$	0000205
6	r6	ADH	$\text{s\_acetald} + 0 \cdot 363\,\text{Red} \overset{\text{x}}{\rightleftharpoons} 1 \cdot 045\,\text{s\_EtOH}$	0000200
7	r7	BM growth (gluc)	$\text{s\_glu} \xrightarrow{\text{x}} 0 \cdot 732\,\text{x} + 0 \cdot 127\,\text{CO2} + 0 \cdot 063\,\text{Red}$	0000205
8	r8	BM growth (acetate)	$\text{s\_acetate} \xrightarrow{\text{x, s\_glu}} 0 \cdot 619\,\text{x} + 0 \cdot 325\,\text{CO2} + 0 \cdot 214\,\text{Red}$	0000205
9	r9	Acdh production	$\text{a} \xrightarrow{\text{x, s\_glu, s\_EtOH}} \text{AcDH}$	0000184
10	r10	active BM degradation	$\text{a} \xrightarrow{\text{x, s\_glu, s\_EtOH}} \emptyset$	0000179
11	r11	Acdh degradation	$\text{AcDH} \xrightarrow{\text{x}} \emptyset$	0000179
12	s_glu_in	Glucose inflow	$\text{S\_f} \longrightarrow \text{s\_glu}$	0000185
13	s_glu_out	Glucose outflow	$\text{s\_glu} \longrightarrow \emptyset$	0000185
14	s_pyr_out	Pyruvate outflow	$\text{s\_pyr} \longrightarrow \emptyset$	0000185
15	s_acetate_out	Acetate outflow	$\text{s\_acetate} \longrightarrow \emptyset$	0000185
16	s_acetald_out	Acetaldehyde outflow	$\text{s\_acetald} \longrightarrow \emptyset$	0000185
17	s_EtOH_out	EtOH outflow	$\text{s\_EtOH} \longrightarrow \emptyset$	0000185
18	a_out	active BM outflow	$\text{a} \longrightarrow \emptyset$	0000185

№	Id	Name	Reaction Equation	SBO
19	x_out	BM outflow	x $\longrightarrow \emptyset$	0000185
20	AcDH_out	AcDH BM outflow	AcDH $\longrightarrow \emptyset$	0000185

7.1 Reaction r1

This is an irreversible reaction of one reactant forming two products influenced by two modifiers.

Name glycolysis

SBO:0000205 composite biochemical process

Reaction equation

$$\text{s\_glu} \xrightarrow{\text{s\_acetald, x}} 0{\cdot}978\,\text{s\_pyr} + 0{\cdot}178\,\text{Red} \tag{7}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s_glu	Glucose	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
s_acetald	Acetaldehyde	
x	BM	

Products

Table 8: Properties of each product.

Id	Name	SBO
s_pyr	Pyruvate	
Red	Red. Equ. (NADH)	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \left(\frac{\text{k\_1l} \cdot [\text{s\_glu}]}{[\text{s\_glu}] + \text{K\_1l}} + \frac{\text{k\_1h} \cdot [\text{s\_glu}]}{[\text{s\_glu}] + \text{K\_1h}} + \frac{\text{k\_1e} \cdot [\text{s\_acetald}] \cdot [\text{s\_glu}]}{[\text{s\_glu}] \cdot (\text{K\_1i} \cdot [\text{s\_acetald}] + 1) + \text{K\_1e}} \right) \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{vol}\,(\text{env}) \tag{8}$$

7.2 Reaction r2

This is an irreversible reaction of one reactant forming two products influenced by two modifiers.

Name TCA (pyruvate)

SBO:0000205 composite biochemical process

Reaction equation

$$\text{s\_pyr} \xrightarrow{\text{x, s\_glu}} 1 \cdot 499\,\text{CO2} + 0 \cdot 908\,\text{Red} \tag{9}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s_pyr	Pyruvate	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
x	BM	
s_glu	Glucose	

Products

Table 11: Properties of each product.

Id	Name	SBO
CO2	CO2	
Red	Red. Equ. (NADH)	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\text{k\_2} \cdot [\text{s\_pyr}]}{([\text{s\_pyr}] + \text{K\_2}) \cdot (\text{K\_2i} \cdot [\text{s\_glu}] + 1)} \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{vol}\,(\text{env}) \tag{10}$$

7.3 Reaction r3

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

Name Pyruvate Dehydrogenase

SBO:0000200 redox reaction

Reaction equation

$$\text{s\_pyr} \xrightarrow{\text{x}} 0{\cdot}5\,\text{s\_acetald} + 0{\cdot}33\,\text{CO2} \tag{11}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s_pyr	Pyruvate	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
x	BM	

Products

Table 14: Properties of each product.

Id	Name	SBO
s_acetald	Acetaldehyde	
CO2	CO2	

Kinetic Law

Derived unit $\text{g}^2 \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$

$$v_3 = \frac{\text{k\_3} \cdot [\text{s\_pyr}]^4}{[\text{s\_pyr}]^4 + \text{K\_3}} \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{vol}\,(\text{env}) \tag{12}$$

7.4 Reaction r4

This is an irreversible reaction of one reactant forming two products influenced by two modifiers.

Name Acetald. dehydrogenase

SBO:0000200 redox reaction

Reaction equation

$$\text{s\_acetald} \xrightarrow{\text{x, s\_EtOH}} 1 \cdot 363\,\text{s\_acetate} + 0 \cdot 363\,\text{Red} \tag{13}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
s_acetald	Acetaldehyde	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
x	BM	
s_EtOH	EtOH	

Products

Table 17: Properties of each product.

Id	Name	SBO
s_acetate	Acetate	
Red	Red. Equ. (NADH)	

Kinetic Law

Derived unit $\text{g}^2 \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$

$$v_4 = \frac{\text{k\_4} \cdot [\text{s\_acetald}]}{[\text{s\_acetald}] + \text{K\_4}} \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{X\_AcDH} \cdot \text{vol}\,(\text{env}) \tag{14}$$

7.5 Reaction r5

This is an irreversible reaction of one reactant forming two products influenced by two modifiers.

Name TCA (acetate)

SBO:0000205 composite biochemical process

Reaction equation

$$\text{s\_acetate} \xrightarrow{\text{x, s\_glu}} 1{\cdot}446\,\text{CO2} + 1{\cdot}066\,\text{Red} \tag{15}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s_acetate	Acetate	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
x	BM	
s_glu	Glucose	

Products

Table 20: Properties of each product.

Id	Name	SBO
CO2	CO2	
Red	Red. Equ. (NADH)	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \left(\frac{\text{k\_5} \cdot [\text{s\_acetate}]}{[\text{s\_acetate}] + \text{K\_5}} + \frac{\text{k\_5e} \cdot [\text{s\_acetate}]}{([\text{s\_acetate}] + \text{K\_5e}) \cdot (1 + \text{K\_5i} \cdot [\text{s\_glu}])} \right) \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{vol}\,(\text{env}) \tag{16}$$

7.6 Reaction r6

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

Name ADH

SBO:0000200 redox reaction

Reaction equation

$$\text{s\_acetald} + 0.363\,\text{Red} \overset{\text{x}}{\rightleftharpoons} 1.045\,\text{s\_EtOH} \tag{17}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
s_acetald	Acetaldehyde	
Red	Red. Equ. (NADH)	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
x	BM	

Product

Table 23: Properties of each product.

Id	Name	SBO
s_EtOH	EtOH	

Kinetic Law

Derived unit $\text{g}^2 \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$

$$v_6 = \frac{\text{k\_6} \cdot (\text{[s\_acetald]} - \text{k\_6r} \cdot \text{[s\_EtOH]})}{\text{[s\_acetald]} + \text{K\_6} + \text{K\_6e} \cdot \text{[s\_EtOH]}} \cdot \text{[x]} \cdot \text{X\_a} \cdot \text{vol(env)} \tag{18}$$

7.7 Reaction r7

This is an irreversible reaction of one reactant forming three products influenced by one modifier.

Name BM growth (gluc)

SBO:0000205 composite biochemical process

Reaction equation

$$\text{s\_glu} \xrightarrow{\text{x}} 0{\cdot}732\,\text{x} + 0{\cdot}127\,\text{CO2} + 0{\cdot}063\,\text{Red} \tag{19}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
s_glu	Glucose	

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
x	BM	

Products

Table 26: Properties of each product.

Id	Name	SBO
x	BM	
CO2	CO2	
Red	Red. Equ. (NADH)	

Kinetic Law

Derived unit $\text{g}^2 \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$

$$v_7 = \frac{\text{k\_7} \cdot [\text{s\_glu}]}{[\text{s\_glu}] + \text{K\_7}} \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{vol}\,(\text{env}) \tag{20}$$

7.8 Reaction r8

This is an irreversible reaction of one reactant forming three products influenced by two modifiers.

Name BM growth (acetate)

SBO:0000205 composite biochemical process

Reaction equation

$$\text{s\_acetate} \xrightarrow{\text{x, s\_glu}} 0{\cdot}619\,\text{x} + 0{\cdot}325\,\text{CO2} + 0{\cdot}214\,\text{Red} \tag{21}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s_acetate	Acetate	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
x	BM	
s_glu	Glucose	

Products

Table 29: Properties of each product.

Id	Name	SBO
x	BM	
CO2	CO2	
Red	Red. Equ. (NADH)	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\text{k\_8} \cdot [\text{s\_acetate}]}{([\text{s\_acetate}] + \text{K\_5e}) \cdot (1 + \text{K\_5i} \cdot [\text{s\_glu}])} \cdot [\text{x}] \cdot \text{X\_a} \cdot \text{vol}\,(\text{env}) \tag{22}$$

7.9 Reaction r9

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name Acdh production

SBO:0000184 translation

Reaction equation

$$\mathrm{a} \xrightarrow{\mathrm{x},\ \mathrm{s\_glu},\ \mathrm{s\_EtOH}} \mathrm{AcDH} \tag{23}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
a	BM(active)	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
x	BM	
s_glu	Glucose	
s_EtOH	EtOH	

Product

Table 32: Properties of each product.

Id	Name	SBO
AcDH	BM(AcDH)	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \left(\frac{\frac{\mathrm{k\_9} \cdot [\mathrm{s\_glu}]}{[\mathrm{s\_glu}] + \mathrm{K\_9}} + \frac{\mathrm{k\_9e} \cdot [\mathrm{s\_EtOH}]}{[\mathrm{s\_EtOH}] + \mathrm{K\_9e}}}{\mathrm{K\_9i} \cdot [\mathrm{s\_glu}] + 1} + \frac{\mathrm{k\_9c} \cdot [\mathrm{s\_glu}]}{[\mathrm{s\_glu}] + \mathrm{K\_9}} \right) \cdot \mathrm{X\_a} \cdot [\mathrm{x}] \cdot \mathrm{vol}\,(\mathrm{env}) \tag{24}$$

7.10 Reaction r10

This is an irreversible reaction of one reactant forming no product influenced by three modifiers.

Name active BM degradation

SBO:0000179 degradation

Reaction equation

$$\mathrm{a} \xrightarrow{\mathrm{x},\ \mathrm{s\_glu},\ \mathrm{s\_EtOH}} \emptyset \tag{25}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
a	BM(active)	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
x	BM	
s_glu	Glucose	
s_EtOH	EtOH	

Kinetic Law

Derived unit $\mathrm{g}^2 \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{10} = \left(\frac{\mathrm{k\_10} \cdot [\mathrm{s\_glu}]}{[\mathrm{s\_glu}] + \mathrm{K\_10}} + \frac{\mathrm{k\_10e} \cdot [\mathrm{s\_EtOH}]}{[\mathrm{s\_EtOH}] + \mathrm{K\_10e}} \right) \cdot \mathrm{X\_a} \cdot [\mathrm{x}] \cdot \mathrm{vol}\,(\mathrm{env}) \tag{26}$$

7.11 Reaction r11

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

Name Acdh degradation

SBO:0000179 degradation

Reaction equation

$$\mathrm{AcDH} \xrightarrow{\mathrm{x}} \emptyset \tag{27}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
AcDH	BM(AcDH)	

Modifier

Table 36: Properties of each modifier.

Id	Name	SBO
x	BM	

Kinetic Law

Derived unit $\mathrm{g}^2 \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{11} = \mathrm{k\_11} \cdot \mathrm{X\_AcDH} \cdot [\mathrm{x}] \cdot \mathrm{vol}\,(\mathrm{env}) \tag{28}$$

7.12 Reaction s_glu_in

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

Name Glucose inflow

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{S\_f} \longrightarrow \mathrm{s\_glu} \tag{29}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
S_f	Glucose(feed)	

Product

Table 38: Properties of each product.

Id	Name	SBO
s_glu	Glucose	

Kinetic Law

Derived unit $\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{12} = [\mathrm{S\_f}] \cdot \mathrm{D} \cdot \mathrm{vol}\,(\mathrm{env}) \tag{30}$$

7.13 Reaction s_glu_out

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

Name Glucose outflow

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{s\_glu} \longrightarrow \emptyset \tag{31}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
s_glu	Glucose	

Kinetic Law

Derived unit $\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{13} = [\mathrm{s\_glu}] \cdot \mathrm{D} \cdot \mathrm{vol}\,(\mathrm{env}) \tag{32}$$

7.14 Reaction s_pyr_out

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

Name Pyruvate outflow

SBO:0000185 transport reaction

Reaction equation

$$\text{s\_pyr} \longrightarrow \emptyset \tag{33}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
s_pyr	Pyruvate	

Kinetic Law

Derived unit $\text{g} \cdot (3600\ \text{s})^{-1}$

$$v_{14} = [\text{s\_pyr}] \cdot \text{D} \cdot \text{vol}(\text{env}) \tag{34}$$

7.15 Reaction s_acetate_out

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

Name Acetate outflow

SBO:0000185 transport reaction

Reaction equation

$$\text{s\_acetate} \longrightarrow \emptyset \tag{35}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
s_acetate	Acetate	

Kinetic Law

Derived unit $\text{g} \cdot (3600\ \text{s})^{-1}$

$$v_{15} = [\text{s\_acetate}] \cdot \text{D} \cdot \text{vol}(\text{env}) \tag{36}$$

7.16 Reaction s_acetald_out

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

Name Acetaldehyde outflow

SBO:0000185 transport reaction

Reaction equation

$$\text{s\_acetald} \longrightarrow \emptyset \tag{37}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
s_acetald	Acetaldehyde	

Kinetic Law

Derived unit $\text{g} \cdot (3600\ \text{s})^{-1}$

$$v_{16} = [\text{s\_acetald}] \cdot \text{D} \cdot \text{vol}(\text{env}) \tag{38}$$

7.17 Reaction s_EtOH_out

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

Name EtOH outflow

SBO:0000185 transport reaction

Reaction equation

$$\text{s\_EtOH} \longrightarrow \emptyset \tag{39}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
s_EtOH	EtOH	

Kinetic Law

Derived unit $\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{17} = [\mathrm{s\_EtOH}] \cdot \mathrm{D} \cdot \mathrm{vol}\,(\mathrm{env}) \tag{40}$$

7.18 Reaction a_out

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

Name active BM outflow

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{a} \longrightarrow \emptyset \tag{41}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
a	BM(active)	

Kinetic Law

Derived unit $\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{18} = [\mathrm{a}] \cdot \mathrm{D} \cdot \mathrm{vol}\,(\mathrm{env}) \tag{42}$$

7.19 Reaction x_out

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

Name BM outflow

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{x} \longrightarrow \emptyset \tag{43}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
x	BM	

Kinetic Law

Derived unit $\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{19} = [\mathrm{x}] \cdot \mathrm{D} \cdot \mathrm{vol}(\mathrm{env}) \tag{44}$$

7.20 Reaction AcDH_out

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

Name AcDH BM outflow

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{AcDH} \longrightarrow \emptyset \tag{45}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
AcDH	BM(AcDH)	

Kinetic Law

Derived unit $\mathrm{g} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{20} = [\mathrm{AcDH}] \cdot \mathrm{D} \cdot \mathrm{vol}(\mathrm{env}) \tag{46}$$

8 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.

8.1 Species `s_glu`

Name Glucose

SBO:0000247 simple chemical

Initial concentration $15\ \mathrm{g} \cdot \mathrm{l}^{-1}$

This species takes part in nine reactions (as a reactant in `r1`, `r7`, `s_glu_out` and as a product in `s_glu_in` and as a modifier in `r2`, `r5`, `r8`, `r9`, `r10`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s\_glu} = v_{12} - v_1 - v_7 - v_{13} \tag{47}$$

8.2 Species `s_pyr`

Name Pyruvate

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{g} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in `r2`, `r3`, `s_pyr_out` and as a product in `r1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s\_pyr} = 0.978\, v_1 - v_2 - v_3 - v_{14} \tag{48}$$

8.3 Species `s_acetate`

Name Acetate

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{g} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in `r5`, `r8`, `s_acetate_out` and as a product in `r4`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s\_acetate} = 1.363\, v_4 - v_5 - v_8 - v_{15} \tag{49}$$

8.4 Species s_acetald

Name Acetaldehyde

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{g}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in r4, r6, s_acetald_out and as a product in r3 and as a modifier in r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s\_acetald} = 0.5\,v_3 - v_4 - v_6 - v_{16} \tag{50}$$

8.5 Species s_EtOH

Name EtOH

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{g}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in s_EtOH_out and as a product in r6 and as a modifier in r4, r9, r10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s\_EtOH} = 1.045\,v_6 - v_{17} \tag{51}$$

8.6 Species x

Name BM

SBO:0000240 material entity

Initial concentration $0.0020\ \mathrm{g}\cdot\mathrm{l}^{-1}$

This species takes part in 14 reactions (as a reactant in x_out and as a product in r7, r8 and as a modifier in r1, r2, r3, r4, r5, r6, r7, r8, r9, r10, r11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x} = 0.732\,v_7 + 0.619\,v_8 - v_{19} \tag{52}$$

8.7 Species a

Name BM(active)

SBO:0000241 functional entity

Initial concentration $0\ \mathrm{g}\cdot\mathrm{l}^{-1}$

Involved in rule a

This species takes part in three reactions (as a reactant in r9, r10, a_out). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.8 Species AcDH

Name BM(AcDH)

SBO:0000241 functional entity

Initial concentration $0\ \mathrm{g}\cdot\mathrm{l}^{-1}$

Involved in rule AcDH

This species takes part in three reactions (as a reactant in r11, AcDH_out and as a product in r9). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.9 Species CO2

Name CO2

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{g}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a product in r2, r3, r5, r7, r8), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{53}$$

8.10 Species Red

Name Red. Equ. (NADH)

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{g}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in r6 and as a product in r1, r2, r4, r5, r7, r8), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Red} = 0 \tag{54}$$

8.11 Species S_f

Name Glucose(feed)

SBO:0000247 simple chemical

Initial concentration $15\ \mathrm{g}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S\_f} = 0 \tag{55}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000179 degradation: Complete disappearance of a physical entity

SBO:0000184 translation: Process in which a polypeptide chain is produced from a messenger RNA

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

SBO:0000200 redox reaction: Chemical process in which atoms have their oxidation number (oxidation state) changed

SBO:0000205 composite biochemical process: Process that involves the participation of chemical or biological entities and is composed of several elementary steps or reactions.

SBO:0000240 material entity: A real thing that is defined by its physico-chemical structure.

SBO:0000241 functional entity: A real thing, defined by its properties or the actions it performs, rather than it physico-chemical structure

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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