**SBML Model Report**

# Model name: "Conant2007_WGD_glycolysis_2A3AB"

May 5, 2016

## 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following three authors: Gavin Conant[1], Lukas Endler[2] and Kenneth Wolfe[3] at August sixth 2008 at 10:23 a. m. and last time modified at May 16th 2012 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 | 25 |
| events | 0 | constraints | 0 |
| reactions | 19 | function definitions | 0 |
| global parameters | 11 | unit definitions | 8 |
| rules | 0 | initial assignments | 0 |

### Model Notes

This a model from the article:
**Increased glycolytic flux as an outcome of whole-genome duplication in yeast.**
Conant GC, Wolfe KH Mol. Syst. Biol. [2007 ; Volume: 3 (Issue: )]: 129 17667951 ,

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**Abstract:**
After whole-genome duplication (WGD), deletions return most loci to single copy. However, duplicate loci may survive through selection for increased dosage. Here, we show how the WGD increased copy number of some glycolytic genes could have conferred an almost immediate selective advantage to an ancestor of Saccharomyces cerevisiae, providing a rationale for the success of the WGD. We propose that the loss of other redundant genes throughout the genome resulted in incremental dosage increases for the surviving duplicated glycolytic genes. This increase gave post-WGD yeasts a growth advantage through rapid glucose fermentation; one of this lineage's many adaptations to glucose-rich environments. Our hypothesis is supported by data from enzyme kinetics and comparative genomics. Because changes in gene dosage follow directly from post-WGD deletions, dosage selection can confer an almost instantaneous benefit after WGD, unlike neofunctionalization or subfunctionalization, which require specific mutations. We also show theoretically that increased fermentative capacity is of greatest advantage when glucose resources are both large and dense, an observation potentially related to the appearance of angiosperms around the time of WGD.

The original model submitted by the authors was slightly altered and now comprises the models originally submitted as MODEL2426780967, MODEL2427021978, MODEL2427095802. It reproduces figures 2A,3A and 3B from the publication.

This model uses the glycolysis model from Pritchard and Kell (2002) with an additional parameter, **WGD_E** , to adjust for the differing enzyme conzentrations before the whole genome duplication (WGD) and parameters **fV_xxx** that adjust the **Vmax** of the different reactions (xxx eg. HXT or PYK).
Figure 3A from the article can be reproduced by changing the value of the parameters **fV_xxx** to 0.9 indiviually, with xxx signifying the different enzymes (HXT, HXK ...)
Figure 3B from the publication can be reproduced by setting the parameter **WGD_E** to 0.75 and individually setting the parameters **fV_xxx** to 1.333.
To reproduce figure 2A from the article change the parameter **WGD_E** in the range between 0.65 and 1.0.



## 2 Unit Definitions

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

### 2.1 Unit time

**Name** minute

**Definition** $60\ \mathrm{s}$

### 2.2 Unit substance

**Name** mmol

**Definition** mmol

### 2.3 Unit mM

**Name** mM

**Definition** $\mathrm{l}^{-1} \cdot \mathrm{mmol}$

### 2.4 Unit mmpmin

**Name** mmolepermin

**Definition** $\mathrm{mmol} \cdot (60\ \mathrm{s})^{-1}$

### 2.5 Unit mMpmin

**Name** mMpermin

**Definition** $\mathrm{mmol} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$

### 2.6 Unit pmin

**Name** permin

**Definition** $(60\ \mathrm{s})^{-1}$

### 2.7 Unit lpmin

**Name** permin

**Definition** $\mathrm{l} \cdot (60\ \mathrm{s})^{-1}$

### 2.8 Unit pmMpmin

**Name** permMpermin

**Definition** $\mathrm{mmol}^{-1} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}$

### 2.9 Unit volume

**Notes** Litre is the predefined SBML unit for volume.

**Definition** l

### 2.10 Unit area

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

**Definition** $m^2$

### 2.11 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 |
|---|---|---|---|---|---|---|---|
| cyto | cytoplasm | | 3 | 1 | litre | ☑ | |

### 3.1 Compartment cyto

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

**Name** cytoplasm

## 4 Species

This model contains 25 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 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 Condition |
|---|---|---|---|---|---|
| GLCi | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| ATP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| G6P | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| ADP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| F6P | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| F16bP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| F26bP | Fru2,6-P2 | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |
| AMP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| DHAP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| GAP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| NAD | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| BPG | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| NADH | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| P3G | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| P2G | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| PEP | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| PYR | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| AcAld | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ⊟ |
| GLCo | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |
| CO2 | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |
| EtOH | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |

| Id | Name | Compartment | Derived Unit | Constant | Boundary Condition |
|---|---|---|---|---|---|
| Glycerol | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |
| Glycogen | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |
| Trehalose | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |
| Succinate | | cyto | $\mathrm{mmol} \cdot \mathrm{l}^{-1}$ | ⊟ | ☑ |

## 5 Parameters

This model contains eleven global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| WGD_E | WGD enzyme conc change | | 1.0 | dimensionless | ☑ |
| fV_HXT | | | 1.0 | dimensionless | ☑ |
| fV_HXK | | | 1.0 | dimensionless | ☑ |
| fV_TDH | | | 1.0 | dimensionless | ☑ |
| fV_ENO | | | 1.0 | dimensionless | ☑ |
| fV_PFK | | | 1.0 | dimensionless | ☑ |
| fV_FBA | | | 1.0 | dimensionless | ☑ |
| fV_PYK | | | 1.0 | dimensionless | ☑ |
| fV_PGK | | | 1.0 | dimensionless | ☑ |
| fV_GPM | | | 1.0 | dimensionless | ☑ |
| fV_PGI | | | 1.0 | dimensionless | ☑ |

## 6 Reactions

This model contains 19 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 | HXT | HXT | $\mathrm{GLCo} \rightleftharpoons \mathrm{GLCi}$ | |
| 2 | HXK | HXK | $\mathrm{GLCi} + \mathrm{ATP} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP}$ | |
| 3 | PGI | PGI | $\mathrm{G6P} \rightleftharpoons \mathrm{F6P}$ | |
| 4 | PFK | PFK | $\mathrm{ATP} + \mathrm{F6P} \xrightarrow{\mathrm{AMP,\ F26bP}} \mathrm{ADP} + \mathrm{F16bP}$ | |
| 5 | FBA | FBA | $\mathrm{F16bP} \rightleftharpoons \mathrm{DHAP} + \mathrm{GAP}$ | |
| 6 | TPI | TPI | $\mathrm{DHAP} \rightleftharpoons \mathrm{GAP}$ | |
| 7 | TDH | TDH | $\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{BPG} + \mathrm{NADH}$ | |
| 8 | PGK | PGK | $\mathrm{ADP} + \mathrm{BPG} \rightleftharpoons \mathrm{ATP} + \mathrm{P3G}$ | |
| 9 | GPM | GPM | $\mathrm{P3G} \rightleftharpoons \mathrm{P2G}$ | |
| 10 | ENO | ENO | $\mathrm{P2G} \rightleftharpoons \mathrm{PEP}$ | |
| 11 | PYK | PYK | $\mathrm{ADP} + \mathrm{PEP} \rightleftharpoons \mathrm{ATP} + \mathrm{PYR}$ | |
| 12 | PDC | PDC | $\mathrm{PYR} \longrightarrow \mathrm{AcAld} + \mathrm{CO2}$ | |
| 13 | ADH | ADH | $\mathrm{NAD} + \mathrm{EtOH} \rightleftharpoons \mathrm{NADH} + \mathrm{AcAld}$ | |
| 14 | ATPase | | $\mathrm{ATP} \longrightarrow \mathrm{ADP}$ | |
| 15 | AK | adenylate kinase | $2\,\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{AMP}$ | |
| 16 | G3PDH | G3PDH | $\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{NAD} + \mathrm{Glycerol}$ | |
| 17 | glycogen_branch | glycogenbranch | $\mathrm{ATP} + \mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Glycogen}$ | |
| 18 | trehalose_synth | trehalose_synthesis | $\mathrm{ATP} + 2\,\mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Trehalose}$ | |
| 19 | succinate_syn | succinate_synthesis | $3\,\mathrm{NAD} + 2\,\mathrm{AcAld} \longrightarrow 3\,\mathrm{NADH} + \mathrm{Succinate}$ | |

## 6.1 Reaction HXT

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

**Name** HXT

### Reaction equation

$$\mathrm{GLCo} \rightleftharpoons \mathrm{GLCi} \tag{1}$$

### Reactant

Table 6: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| GLCo | | |

### Product

Table 7: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| GLCi | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = \frac{\frac{\mathrm{Vmax\_1} \cdot \mathrm{fV\_HXT} \cdot \mathrm{WGD\_E} \cdot (\mathrm{[GLCo]} - \mathrm{[GLCi]})}{\mathrm{Kglc\_1}}}{1 + \frac{\mathrm{[GLCo]} + \mathrm{[GLCi]}}{\mathrm{Kglc\_1}} + \frac{\mathrm{Ki\_1} \cdot \mathrm{[GLCo]} \cdot \mathrm{[GLCi]}}{\mathrm{Kglc\_1}^2}} \tag{2}$$

Table 8: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_1 | | | 97.240 | $\mathrm{mmol} \cdot (60\ \mathrm{s})^{-1}$ | ☑ |
| Kglc_1 | | | 1.192 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Ki_1 | | | 0.910 | dimensionless | ☑ |

## 6.2 Reaction HXK

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

**Name** HXK

### Reaction equation

$$\mathrm{GLCi} + \mathrm{ATP} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP} \tag{3}$$

### Reactants

Table 9: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| GLCi | | |
| ATP | | |

### Products

Table 10: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| G6P | | |
| ADP | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{WGD\_E} \cdot \mathrm{fV\_HXK} \cdot \mathrm{Vmax\_2} \cdot \left( \frac{[\mathrm{GLCi}] \cdot [\mathrm{ATP}]}{\mathrm{Kglc\_2} \cdot \mathrm{Katp\_2}} - \frac{[\mathrm{G6P}] \cdot [\mathrm{ADP}]}{\mathrm{Kglc\_2} \cdot \mathrm{Katp\_2} \cdot \mathrm{Keq\_2}} \right)}{\left(1 + \frac{[\mathrm{GLCi}]}{\mathrm{Kglc\_2}} + \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_2}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_2}} + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_2}}\right)} \tag{4}$$

Table 11: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_2 | | | 236.70 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kglc_2 | | | 0.08 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Katp_2 | | | 0.15 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Keq_2 | | | 2000.00 | dimensionless | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kg6p_2 | | | 30.00 | $l^{-1} \cdot mmol$ | ☑ |
| Kadp_2 | | | 0.23 | $l^{-1} \cdot mmol$ | ☑ |

## 6.3 Reaction PGI

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

**Name** PGI

### Reaction equation

$$G6P \rightleftharpoons F6P \tag{5}$$

### Reactant

Table 12: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| G6P | | |

### Product

Table 13: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| F6P | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = \frac{\mathrm{vol}(\mathrm{cyto}) \cdot \mathrm{Vmax\_3} \cdot \mathrm{fV\_PGI} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_3}} - \frac{[\mathrm{F6P}]}{\mathrm{Kg6p\_3} \cdot \mathrm{Keq\_3}} \right)}{1 + \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_3}} + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_3}}} \tag{6}$$

Table 14: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_3 | | | 1056.00 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot l^{-1}$ | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Kg6p_3 | | | 1.40 | $l^{-1} \cdot mmol$ | ☑ |
| Keq_3 | | | 0.29 | dimensionless | ☑ |
| Kf6p_3 | | | 0.30 | $l^{-1} \cdot mmol$ | ☑ |

## 6.4 Reaction PFK

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

**Name** PFK

### Reaction equation

$$\mathrm{ATP} + \mathrm{F6P} \xrightarrow{\text{AMP, F26bP}} \mathrm{ADP} + \mathrm{F16bP} \tag{7}$$

### Reactants

Table 15: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ATP | | |
| F6P | | |

### Modifiers

Table 16: Properties of each modifier.

| Id | Name | SBO |
|---|---|---|
| AMP | | |
| F26bP | Fru2,6-P2 | |

### Products

Table 17: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ADP | | |
| F16bP | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_4} \cdot \mathrm{fV\_PFK} \cdot \mathrm{WGD\_E} \cdot \frac{\mathrm{gR\_4} \cdot \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} \cdot \left(1 + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} + \frac{\frac{\mathrm{gR\_4} \cdot [\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot [\mathrm{ATP}]}{\mathrm{Katp\_4}}\right)}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} + \frac{\frac{\mathrm{gR\_4} \cdot [\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot [\mathrm{ATP}]}{\mathrm{Katp\_4}}\right)^2 + \mathrm{L0\_4} \cdot \left(\frac{1 + \frac{\mathrm{Ciatp\_4} \cdot [\mathrm{ATP}]}{\mathrm{Kiatp\_4}}}{1 + \frac{[\mathrm{ATP}]}{\mathrm{Kiatp\_4}}}\right)^2 \cdot \left(\frac{1 + \frac{\mathrm{Camp\_4} \cdot [\mathrm{AMP}]}{\mathrm{Kamp\_4}}}{1 + \frac{[\mathrm{AMP}]}{\mathrm{Kamp\_4}}}\right)^2 \cdot \left(\frac{1 + \frac{\mathrm{Cf26\_4} \cdot [\mathrm{F26bP}]}{\mathrm{Kf26\_4}} + \frac{\mathrm{Cf16\_4} \cdot [\mathrm{F16bP}]}{\mathrm{Kf16\_4}}}{1 + \frac{[\mathrm{F26bP}]}{\mathrm{Kf26\_4}} + \frac{[\mathrm{F16bP}]}{\mathrm{Kf16\_4}}}\right)^2} \tag{8}$$

Table 18: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_4 | | | 110.000 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| gR_4 | | | 5.120 | dimensionless | ☑ |
| Kf6p_4 | | | 0.100 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Katp_4 | | | 0.710 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| L0_4 | | | 0.660 | dimensionless | ☑ |
| Ciatp_4 | | | 100.000 | dimensionless | ☑ |
| Kiatp_4 | | | 0.650 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Camp_4 | | | 0.085 | dimensionless | ☑ |
| Kamp_4 | | | 0.100 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Cf26_4 | | | 0.017 | dimensionless | ☑ |
| Kf26_4 | | | $6.82 \cdot 10^{-4}$ | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Cf16_4 | | | 0.397 | dimensionless | ☑ |
| Kf16_4 | | | 0.111 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Catp_4 | | | 3.000 | dimensionless | ☑ |

## 6.5 Reaction FBA

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

**Name** FBA

### Reaction equation

$$\mathrm{F16bP} \rightleftharpoons \mathrm{DHAP} + \mathrm{GAP} \tag{9}$$

### Reactant

Table 19: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| F16bP | | |

### Products

Table 20: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| DHAP | | |
| GAP | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_5} \cdot \mathrm{fV\_FBA} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{F16bP}]}{\mathrm{Kf16bp\_5}} - \frac{[\mathrm{DHAP}] \cdot [\mathrm{GAP}]}{\mathrm{Kf16bp\_5} \cdot \mathrm{Keq\_5}} \right)}{1 + \frac{[\mathrm{F16bP}]}{\mathrm{Kf16bp\_5}} + \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_5}} + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_5}} + \frac{[\mathrm{F16bP}] \cdot [\mathrm{GAP}]}{\mathrm{Kf16bp\_5} \cdot \mathrm{Kigap\_5}} + \frac{[\mathrm{DHAP}] \cdot [\mathrm{GAP}]}{\mathrm{Kdhap\_5} \cdot \mathrm{Kgap\_5}}} \tag{10}$$

Table 21: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_5 | | | 94.690 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kf16bp_5 | | | 0.300 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Keq_5 | | | 0.069 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Kdhap_5 | | | 2.000 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Kgap_5 | | | 2.400 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Kigap_5 | | | 10.000 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |

## 6.6 Reaction TPI

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

**Name** TPI

### Reaction equation

$$\mathrm{DHAP} \rightleftharpoons \mathrm{GAP} \tag{11}$$

### Reactant

Table 22: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| DHAP | | |

### Product

Table 23: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| GAP | | |

### Kinetic Law

**Derived unit** $(60\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_6 = \mathrm{vol}\,(\mathrm{cyto}) \cdot (\mathrm{k1\_6} \cdot [\mathrm{DHAP}] - \mathrm{k2\_6} \cdot [\mathrm{GAP}]) \tag{12}$$

Table 24: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k1_6 | | | 450000.000 | $(60\ \mathrm{s})^{-1}$ | ☑ |
| k2_6 | | | $10^7$ | $(60\ \mathrm{s})^{-1}$ | ☑ |

## 6.7 Reaction TDH

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

**Name** TDH

### Reaction equation

$$\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{BPG} + \mathrm{NADH} \tag{13}$$

### Reactants

Table 25: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| GAP | | |
| NAD | | |

### Products

Table 26: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| BPG | | |
| NADH | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_7 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{C\_7} \cdot \left( \frac{\mathrm{Vmaxf\_7} \cdot \mathrm{fV\_TDH} \cdot \mathrm{WGD\_E} \cdot [\mathrm{GAP}] \cdot [\mathrm{NAD}]}{\mathrm{Kgap\_7} \cdot \mathrm{Knad\_7}} - \frac{\mathrm{Vmaxr\_7} \cdot \mathrm{fV\_TDH} \cdot \mathrm{WGD\_E} \cdot [\mathrm{BPG}] \cdot [\mathrm{NADH}]}{\mathrm{Kbpg\_7} \cdot \mathrm{Knadh\_7}} \right)}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_7}} + \frac{[\mathrm{BPG}]}{\mathrm{Kbpg\_7}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{Knad\_7}} + \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_7}}\right)} \tag{14}$$

Table 27: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| C_7 | | | 1.000 | dimensionless | ☑ |
| Vmaxf_7 | | | 1152.000 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kgap_7 | | | 0.210 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Knad_7 | | | 0.090 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Vmaxr_7 | | | 6719.000 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kbpg_7 | | | 0.010 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Knadh_7 | | | 0.060 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |

## 6.8 Reaction PGK

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

**Name** PGK

### Reaction equation

$$\mathrm{ADP} + \mathrm{BPG} \rightleftharpoons \mathrm{ATP} + \mathrm{P3G} \tag{15}$$

### Reactants

Table 28: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ADP | | |
| BPG | | |

### Products

Table 29: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ATP | | |
| P3G | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_8 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{fV\_PGK} \cdot \mathrm{Vmax\_8} \cdot \mathrm{WGD\_E} \cdot \frac{\mathrm{Keq\_8} \cdot [\mathrm{BPG}] \cdot [\mathrm{ADP}] - [\mathrm{P3G}] \cdot [\mathrm{ATP}]}{\mathrm{Kp3g\_8} \cdot \mathrm{Katp\_8}}}{\left(1 + \frac{[\mathrm{BPG}]}{\mathrm{Kbpg\_8}} + \frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_8}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_8}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_8}}\right)} \tag{16}$$

Table 30: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_8 | | | 1288.000 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Keq_8 | | | 3200.000 | dimensionless | ☑ |
| Kp3g_8 | | | 0.530 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Katp_8 | | | 0.300 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Kbpg_8 | | | 0.003 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Kadp_8 | | | 0.200 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |

## 6.9 Reaction GPM

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

**Name** GPM

### Reaction equation

$$\mathrm{P3G} \rightleftharpoons \mathrm{P2G} \tag{17}$$

### Reactant

Table 31: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| P3G | | |

### Product

Table 32: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| P2G | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_9 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_9} \cdot \mathrm{fV\_GPM} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_9}} - \frac{[\mathrm{P2G}]}{\mathrm{Kp3g\_9} \cdot \mathrm{Keq\_9}} \right)}{1 + \frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_9}} + \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_9}}} \tag{18}$$

Table 33: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_9 | | | 2585.00 | $\mathrm{mmol} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kp3g_9 | | | 1.20 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Keq_9 | | | 0.19 | dimensionless | ☑ |
| Kp2g_9 | | | 0.08 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |

## 6.10 Reaction ENO

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

**Name** ENO

### Reaction equation

$$\mathrm{P2G} \rightleftharpoons \mathrm{PEP} \tag{19}$$

### Reactant

Table 34: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| P2G | | |

### Product

Table 35: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| PEP | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{10} = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_10} \cdot \mathrm{fV\_ENO} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_10}} - \frac{[\mathrm{PEP}]}{\mathrm{Kp2g\_10} \cdot \mathrm{Keq\_10}} \right)}{1 + \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_10}} + \frac{[\mathrm{PEP}]}{\mathrm{Kpep\_10}}} \tag{20}$$

Table 36: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_10 | | | 201.60 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kp2g_10 | | | 0.04 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Keq_10 | | | 6.70 | dimensionless | ☑ |
| Kpep_10 | | | 0.50 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |

## 6.11 Reaction PYK

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

**Name** PYK

### Reaction equation

$$\mathrm{ADP} + \mathrm{PEP} \rightleftharpoons \mathrm{ATP} + \mathrm{PYR} \tag{21}$$

### Reactants

Table 37: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ADP | | |
| PEP | | |

### Products

Table 38: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ATP | | |
| PYR | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{11} = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_11} \cdot \mathrm{fV\_PYK} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{PEP}] \cdot [\mathrm{ADP}]}{\mathrm{Kpep\_11} \cdot \mathrm{Kadp\_11}} - \frac{[\mathrm{PYR}] \cdot [\mathrm{ATP}]}{\mathrm{Kpep\_11} \cdot \mathrm{Kadp\_11} \cdot \mathrm{Keq\_11}} \right)}{\left( 1 + \frac{[\mathrm{PEP}]}{\mathrm{Kpep\_11}} + \frac{[\mathrm{PYR}]}{\mathrm{Kpyr\_11}} \right) \cdot \left( 1 + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_11}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_11}} \right)} \tag{22}$$

Table 39: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_11 | | | 1000.00 | $\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$ | ☑ |
| Kpep_11 | | | 0.14 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| Kadp_11 | | | 0.53 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Keq_11 | | | 6500.00 | dimensionless | ☑ |
| Kpyr_11 | | | 21.00 | $l^{-1} \cdot mmol$ | ☑ |
| Katp_11 | | | 1.50 | $l^{-1} \cdot mmol$ | ☑ |

## 6.12 Reaction PDC

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

**Name** PDC

### Reaction equation

$$PYR \longrightarrow AcAld + CO2 \tag{23}$$

### Reactant

Table 40: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| PYR | | |

### Products

Table 41: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| AcAld | | |
| CO2 | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{12} = \frac{\text{vol}(\text{cyto}) \cdot \text{Vmax\_12} \cdot \text{WGD\_E} \cdot \left(\frac{[\text{PYR}]}{\text{Kpyr\_12}}\right)^{\text{nH\_12}}}{1 + \left(\frac{[\text{PYR}]}{\text{Kpyr\_12}}\right)^{\text{nH\_12}}} \tag{24}$$

Table 42: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_12 | | | 857.80 | mmol · $(60\,\mathrm{s})^{-1}$ · $\mathrm{l}^{-1}$ | ☑ |
| Kpyr_12 | | | 4.33 | $\mathrm{l}^{-1} \cdot \mathrm{mmol}$ | ☑ |
| nH_12 | | | 1.90 | dimensionless | ☑ |

## 6.13 Reaction ADH

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

**Name** ADH

### Reaction equation

$$\mathrm{NAD} + \mathrm{EtOH} \rightleftharpoons \mathrm{NADH} + \mathrm{AcAld} \tag{25}$$

### Reactants

Table 43: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| NAD | | |
| EtOH | | |

### Products

Table 44: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| NADH | | |
| AcAld | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{13} = \frac{\mathrm{vol}(\mathrm{cyto}) \cdot \mathrm{Vmax\_13} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{EtOH}] \cdot [\mathrm{NAD}]}{\mathrm{Ketoh\_13} \cdot \mathrm{Kinad\_1}} \right.}{1 + \frac{[\mathrm{NAD}]}{\mathrm{Kinad\_13}} + \frac{[\mathrm{EtOH}] \cdot \mathrm{Knad\_13}}{\mathrm{Kinad\_13} \cdot \mathrm{Ketoh\_13}} + \frac{[\mathrm{AcAld}] \cdot \mathrm{Knadh\_13}}{\mathrm{Kinadh\_13} \cdot \mathrm{Kacald\_13}} + \frac{[\mathrm{NADH}]}{\mathrm{Kinadh\_13}} + \frac{[\mathrm{EtOH}] \cdot [\mathrm{NAD}]}{\mathrm{Kinad\_13} \cdot \mathrm{Ketoh\_13}} + \frac{[\mathrm{NAD}] \cdot [\mathrm{AcAld}] \cdot \mathrm{Knadh\_13}}{\mathrm{Kinad\_13} \cdot \mathrm{Kinadh\_13} \cdot \mathrm{Kacald\_13}} + \frac{[\mathrm{Et}}{\mathrm{Kinac}}} \tag{26}$$

Table 45: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_13 | | | 209.500 | mmol · $(60\,\mathrm{s})^{-1}$ · $\mathrm{l}^{-1}$ | ☑ |
| Ketoh_13 | | | 17.000 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Kinad_13 | | | 0.920 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Keq_13 | | | $6.9 \cdot 10^{-5}$ | dimensionless | ☑ |
| Knad_13 | | | 0.170 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Knadh_13 | | | 0.110 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Kinadh_13 | | | 0.031 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Kacald_13 | | | 1.110 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Kiacald_13 | | | 1.100 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |
| Kietoh_13 | | | 90.000 | $\mathrm{l}^{-1} \cdot$ mmol | ☑ |

## 6.14 Reaction ATPase

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

### Reaction equation

$$\mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{27}$$

### Reactant

Table 46: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ATP | | |

### Product

Table 47: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ADP | | |

### Kinetic Law

**Derived unit** $(60\,\mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{14} = \mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Katpase\_14} \cdot [\mathrm{ATP}] \tag{28}$$

Table 48: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Katpase_14 | | | 39.5 | $(60\ \mathrm{s})^{-1}$ | ☑ |

## 6.15 Reaction AK

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

**Name** adenylate kinase

### Reaction equation

$$2\,\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{AMP} \tag{29}$$

### Reactant

Table 49: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ADP | | |

### Products

Table 50: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ATP | | |
| AMP | | |

### Kinetic Law

**Derived unit** $(60\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{15} = \mathrm{vol}\,(\mathrm{cyto}) \cdot (\mathrm{k1\_15} \cdot [\mathrm{ADP}] \cdot [\mathrm{ADP}] - \mathrm{k2\_15} \cdot [\mathrm{ATP}] \cdot [\mathrm{AMP}]) \tag{30}$$

Table 51: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k1_15 | | | 45.0 | $\mathrm{mmol}^{-1} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}$ | ☑ |

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k2_15 | | | 100.0 | $\mathrm{mmol}^{-1} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}$ | ☑ |

## 6.16 Reaction G3PDH

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

**Name** G3PDH

### Reaction equation

$$\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{NAD} + \mathrm{Glycerol} \tag{31}$$

### Reactants

Table 52: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| DHAP | | |
| NADH | | |

### Products

Table 53: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| NAD | | |
| Glycerol | | |

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{16} = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_16} \cdot \mathrm{WGD\_E} \cdot \left( \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_16}} \cdot \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_16}} - \frac{[\mathrm{Glycerol}]}{\mathrm{Kdhap\_16}} \cdot \frac{[\mathrm{NAD}]}{\mathrm{Knadh\_16}} \cdot \frac{1}{\mathrm{Keq\_16}} \right)}{\left(1 + \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_16}} + \frac{[\mathrm{Glycerol}]}{\mathrm{Kglycerol\_16}}\right) \cdot \left(1 + \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_16}} + \frac{[\mathrm{NAD}]}{\mathrm{Knad\_16}}\right)} \tag{32}$$

Table 54: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Vmax_16 | | | 47.110 | mmol · $(60\,\mathrm{s})^{-1}$ · $\mathrm{l}^{-1}$ | ☑ |
| Kdhap_16 | | | 0.400 | $\mathrm{l}^{-1}\cdot$mmol | ☑ |
| Knadh_16 | | | 0.023 | $\mathrm{l}^{-1}\cdot$mmol | ☑ |
| Keq_16 | | | 4300.000 | dimensionless | ☑ |
| Kglycerol_16 | | | 1.000 | $\mathrm{l}^{-1}\cdot$mmol | ☑ |
| Knad_16 | | | 0.930 | $\mathrm{l}^{-1}\cdot$mmol | ☑ |

## 6.17 Reaction glycogen_branch

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

**Name** glycogenbranch

### Reaction equation

$$\mathrm{ATP} + \mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Glycogen} \tag{33}$$

### Reactants

Table 55: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ATP | | |
| G6P | | |

### Products

Table 56: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ADP | | |
| Glycogen | | |

### Kinetic Law

**Derived unit** $\mathrm{mmol}\cdot(60\,\mathrm{s})^{-1}$

$$v_{17} = \mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{KGLYCOGEN\_17} \tag{34}$$

Table 57: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| KGLYCOGEN_17 | | | 6.0 | $\text{mmol} \cdot (60\,\text{s})^{-1} \cdot \text{l}^{-1}$ | ☑ |

## 6.18 Reaction trehalose_synth

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

**Name** trehalose_synthesis

### Reaction equation

$$\text{ATP} + 2\,\text{G6P} \longrightarrow \text{ADP} + \text{Trehalose} \tag{35}$$

### Reactants

Table 58: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| ATP | | |
| G6P | | |

### Products

Table 59: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| ADP | | |
| Trehalose | | |

### Kinetic Law

**Derived unit** $\text{mmol} \cdot (60\,\text{s})^{-1}$

$$v_{18} = \text{vol}\,(\text{cyto}) \cdot \text{Ktrehalose\_18} \tag{36}$$

Table 60: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| Ktrehalose_18 | | | 2.4 | $\text{mmol} \cdot (60\,\text{s})^{-1} \cdot \text{l}^{-1}$ | ☑ |

## 6.19 Reaction succinate_syn

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

**Name** succinate_synthesis

### Reaction equation

$$3\,\text{NAD} + 2\,\text{AcAld} \longrightarrow 3\,\text{NADH} + \text{Succinate} \tag{37}$$

### Reactants

Table 61: Properties of each reactant.

| Id | Name | SBO |
|---|---|---|
| NAD | | |
| AcAld | | |

### Products

Table 62: Properties of each product.

| Id | Name | SBO |
|---|---|---|
| NADH | | |
| Succinate | | |

### Kinetic Law

**Derived unit** $(60\,\text{s})^{-1} \cdot \text{mmol}$

$$v_{19} = \text{vol}\,(\text{cyto}) \cdot \text{k\_19} \cdot [\text{AcAld}] \tag{38}$$

Table 63: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|---|---|---|---|---|---|
| k_19 | | | 21.4 | $(60\ \mathrm{s})^{-1}$ | ☑ |

# 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.

## 7.1 Species GLCi

**Initial concentration** $0.097652231064563\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in HXK and as a product in HXT).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCi} = v_1 - v_2 \tag{39}$$

## 7.2 Species ATP

**Initial concentration** $2.52512746499271\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in HXK, PFK, ATPase, glycogen_branch, trehalose_synth and as a product in PGK, PYK, AK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_8 + v_{11} + v_{15} - v_2 - v_4 - v_{14} - v_{17} - v_{18} \tag{40}$$

## 7.3 Species G6P

**Initial concentration** $2.67504014044787\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PGI, glycogen_branch, trehalose_synth and as a product in HXK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_2 - v_3 - v_{17} - 2v_{18} \tag{41}$$

## 7.4 Species ADP

**Initial concentration** $1.28198768168719\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in PGK, PYK, AK and as a product in HXK, PFK, ATPase, glycogen_branch, trehalose_synth).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_2 + v_4 + v_{14} + v_{17} + v_{18} - v_8 - v_{11} - 2v_{15} \tag{42}$$

## 7.5 Species F6P

**Initial concentration** 0.624976405532373 mmol · l$^{-1}$

This species takes part in two reactions (as a reactant in PFK and as a product in PGI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_3 - v_4 \tag{43}$$

## 7.6 Species F16bP

**Initial concentration** 6.22132076069411 mmol · l$^{-1}$

This species takes part in two reactions (as a reactant in FBA and as a product in PFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F16bP} = v_4 - v_5 \tag{44}$$

## 7.7 Species F26bP

**Name** Fru2,6-P2

**Initial concentration** 0.02 mmol · l$^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F26bP} = 0 \tag{45}$$

## 7.8 Species AMP

**Initial concentration** 0.292884853320091 mmol · l$^{-1}$

This species takes part in two reactions (as a product in AK and as a modifier in PFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = v_{15} \tag{46}$$

## 7.9 Species DHAP

**Initial concentration** 1.00415254899644 mmol · l$^{-1}$

This species takes part in three reactions (as a reactant in TPI, G3PDH and as a product in FBA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_5 - v_6 - v_{16} \tag{47}$$

## 7.10 Species GAP

**Initial concentration** $0.0451809175780963\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in TDH and as a product in FBA, TPI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_5 + v_6 - v_7 \tag{48}$$

## 7.11 Species NAD

**Initial concentration** $1.50329030201531\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in TDH, ADH, succinate_syn and as a product in G3PDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{16} - v_7 - v_{13} - 3v_{19} \tag{49}$$

## 7.12 Species BPG

**Initial concentration** $7.36873499865602\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PGK and as a product in TDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BPG} = v_7 - v_8 \tag{50}$$

## 7.13 Species NADH

**Initial concentration** $0.0867096979846952\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in G3PDH and as a product in TDH, ADH, succinate_syn).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_7 + v_{13} + 3v_{19} - v_{16} \tag{51}$$

## 7.14 Species P3G

**Initial concentration** $0.885688538360659\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in GPM and as a product in PGK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P3G} = v_8 - v_9 \tag{52}$$

## 7.15 Species P2G

**Initial concentration** $0.127695817386632\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in ENO and as a product in GPM).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2G} = v_9 - v_{10} \tag{53}$$

## 7.16 Species PEP

**Initial concentration** $0.0632352144936527\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PYK and as a product in ENO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_{10} - v_{11} \tag{54}$$

## 7.17 Species PYR

**Initial concentration** $1.81531251192736\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PDC and as a product in PYK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYR} = v_{11} - v_{12} \tag{55}$$

## 7.18 Species AcAld

**Initial concentration** $0.178140579850657\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in succinate_syn and as a product in PDC, ADH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcAld} = v_{12} + v_{13} - 2v_{19} \tag{56}$$

## 7.19 Species GLCo

**Initial concentration** $50\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCo} = 0 \tag{57}$$

## 7.20 Species CO2

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{58}$$

## 7.21 Species EtOH

**Initial concentration** $50\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOH} = 0 \tag{59}$$

## 7.22 Species Glycerol

**Initial concentration** $0.15\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in G3PDH), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glycerol} = 0 \tag{60}$$

## 7.23 Species Glycogen

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glycogen} = 0 \tag{61}$$

## 7.24 Species Trehalose

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Trehalose} = 0 \tag{62}$$

## 7.25 Species Succinate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Succinate} = 0 \tag{63}$$

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