I. ALTERATIONS TO THE ORIGINAL MODEL OF POOLMAN ET AL. (2009)

For reactions taken from AraCyc the database ID is given.

The following transporter reactions of biomass components were set to irreversible (efflux only):

-reac_460: "L-ALPHA-ALANINE = x_ALA"
-AMP_tx: "AMP = x_AMP"
-ARG_tx: "ARG = x_ARG"
-ASN_tx: "ASN = x_ASN"
-reac_466: "ASP = x_ASP"
-Cell_tx: "1-4-beta-D-Glucan = x_Cellulose"
-CMP_tx: "CMP = x_CMP"
-CYS_tx: "CYS = x_CYS"
-dAMP_tx: "DAMP = x_DAMP"
-dCMP_tx: "DCMP = x_DCMP"
-dGMP_tx: "DGMP = x_DGMP"
-GLN_tx: "GLN = x_GLN"
-GLT_tx: "GLT = x_GLT"
-GLY_tx: "GLY = x_GLY"
-GMP_tx: "GMP = x_GMP"
-HIS_tx: "HIS = x_HIS"
-ILE_tx: "ILE = x_ILE"
-LEU_tx: "LEU = x_LEU"
-LYS_tx: "LYS = x_LYS"
-MET_tx: "MET = x_MET"
-PHE_tx: "PHE = x_PHE"
-PRO_tx: "PRO = x_PRO"
-SER_tx: "SER = x_SER"
-Star_tx: "1-4-alpha-D-Glucan = x_Starch"
-THR_tx: "THR = x_THR"
-TMP_tx: "TMP = x_TMP"
-TRP_tx: "TRP = x_TRP"
-TYR_tx: "TYR = x_TYR"
-UMP_tx: "UMP = x_UMP"
-VAL_tx: "VAL = x_VAL"
-ConOL_tx: "CONIFERYL-ALCOHOL = x_ConOL"
-CoumOL_tx: "COUMARYL-ALCOHOL = x_CoumOL"
-Palm_tx: "PALMITATE = x_Palm"
-SinapOL_tx: "SINAPYL-ALCOHOL = x_SinapOL"

The following transporter reactions of precursor metabolites were set to irreversible (influx only):

-GLC_tx: "x_GLC = GLC"
-NH3_tx: "x_NH3 = AMMONIA"
-NO3_tx: "x_NO3 = NITRATE"
-Pi_tx: "x_Pi = Pi"
-SO4_tx: "x_SO4 = SULFATE"

The transporter reactions for bringing amino acids and nucleotides out of the system were corrected to include the energetic costs. Amino acid transporter reactions have been altered in the following way:

$$a + 3ATP = x\_a + 2ADP + 2Pi + 1AMP + 1PPi$$

where a denotes an arbitrary amino acid, x_a the corresponding external metabolite, and PPi denotes pyrophosphate.

Nucleotide transporter reactions have been corrected such:

$$u + 1ATP = x\_u + 1AMP + 1PPi,$$
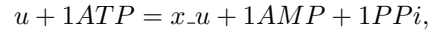
where u denotes an arbitrary nucleotide ($dAMP$, $dGMP$, $dCMP$, TMP, AMP, GMP, CMP, UMP) and x_u its external counterpart.

The reversibilities of the following reactions have been switched:

-reac_343 (ID: GAPOXNPHOSPHN-RXN):
  "GAP + NAD + Pi = DPG + NADH"
  from irreversible to reversible

-reac_558 (ID: PHOSGLYPHOS-RXN):
  "ADP + DPG = ATP + G3P"
  from irreversible to reversible

-reac_551 (ID: PEPDEPHOS-RXN):
  "ATP + PYRUVATE = ADP + PHOSPHO-ENOL-PYRUVATE"
  from reversible to irreversible

-reac_164 (ID: AIRCARBOXY-RXN):
  "PHOSPHORIBOSYL-CARBOXY-AMINOIMIDAZOLE = 5-PHOSPHORIBOSYL-5-AMINOIMIDAZOLE +
  CARBON-DIOXIDE"
  from reversible to irreversible

-reac_677 (ID: RXN-1827):
  "WATER + 2 1-4-alpha-D-Glucan = ALPHA-MALTOSE"
  from reversible to irreversible

The following reactions have been switched from reversible to irreversible to prevent production of lysine and threonine respectively through their degradation pathways:

-reac_1347 (ID: THREONINE-ALDOLASE-RXN):
  "THR = ACETALD + GLY"

-reac_28 (ID: 1.5.1.7-RXN):
  "NAD + SACCHAROPINE = 2-KETOGLUTARATE + LYS + NADH"

-reac_29 (ID: 1.5.1.8-RXN):
  "NADP + SACCHAROPINE = 2-KETOGLUTARATE + LYS + NADPH"