Table 1. List of reactions of the non-compartmented model of the central carbon metabolism of CHO-K1

Flux	*Reaction*
v1	GLC_{ex} *(abcdef) → G6P (abcdef)*
v2	*G6P (abcdef) → PG (abc) + PG (def)*
v3	*3 G6P (abcdef) → 5 PG (def) + 3* CO_2 *(a)*
v4	*G6P (abcdef) → Biomass*
v5	*PG (abc) → PEP (abc)*
v6	*PEP (abc) → PYR (abc)*
v7	*PYR (abc) → AcoA (bc) +*CO_2 *(a)*
v8	*OAA (abcd) + AcoA (ef) → CIT (efbcda)*
v9	*CIT (abcdef)→ AKG (abcde)+* CO_2 *(f)*
v10	*AKG (abcde)→ 0.5 MAL (abcd) + 0.5 MAL (dcba) +* CO_2 *(e)*
v11	*MAL (abcd) ↔ OAA (abcd)*
v12	*PYR (abc) ↔ LAC (abc)*
v13	*LAC (abc) ↔* LAC_{ex} *(abc)*
v14	*OAA (abcd) → PEP (abc) +* CO_2 *(d)*
v15	*MAL (abcd) → PYR (abc) +* CO_2 *(d)*
v16	*PYR (abc) +* CO_2 *(d) → OAA (abcd)*
v17	*PG (abc) → SER (abc)*
v18	*SER (abc) ↔ GLY (ab) + MTHF (c)*
v19	SER_{ex} *(abc) ↔ SER (abc)*
v20	*SER (abc)→ Biomass*
v21	*GLY (abc) ↔* GLY_{ex} *(abc)*
v22	*GLY (abc) → Biomass*
v23	*SER (abc) → PYR (abc)*
v24	*PYR (abc) + GLU (defgh) ↔ ALA (abc)+ AKG (defgh)*
v25	*ALA (abc) ↔* ALA_{ex} *(abc)*
v26	*ALA (abc)→ Biomass*
v27	*PYR (abc) ↔* PYR_{ex} *(abc)*
v28	*ASP (abcd) + AKG (efghi) ↔ OAA (abcd) + GLU (efghi)*
v29	*ASN (abcd) → ASP (abcd)*
v30	ASP_{ex} *(abcd) ↔ ASP (abcd)*
v31	*ASP (abcd) → Biomass*
v32	*AKG (abcde) ↔ GLU (abcde)*
v33	*GLU (abcde) ↔* GLU_{ex} *(abcde)*
v34	*GLU (abcde) → Biomass*
v35	*GLN (abcde) → GLU (abcde)*
v36	GLN_{ex} *(abcde) ↔ GLN (abcde)*
v37	*AcoA (ab) → Biomass*
v38	AA_{ex} *(ILE, VAL, MET, THR, TYR, PHE) → MAL (AA catabolism)*
v39	AA_{ex} *(LEU, ILE, LYS, TYR, PHE) → ACOA (AA catabolism)*
v40	*AKG (abcde) → GLU (abcde) (AA catabolism)*
v41	*AA(PRO, HIS, ARG) → GLU (AA catabolism)*
v42	*G6P (abcdef) → carbohydrates*

Table 2. List of reactions of the compartmented model of CHO-K1 central carbon metabolism, including carbon transfer rules, and computed fluxes and reaction reversibilities

Flux	*Reaction*	Flux [mmol/L cell·h]	Lower boundary [mmol/L cell·h]	Upper boundary [mmol/L cell·h]	Reversibility [reverse flux/net flux]	Reversibility lower boundary	Reversibility upper boundary
v1	GLC_{ex} *(abcdef) → G6P (abcdef)*	371.0	326.7	415.3	0	0	0
v2	*G6P (abcdef) → PG (abc) + PG (def)*	65.8	25.2	96.5	0	0	0
v3	*3 G6P (abcdef) → 5 PG (def) + 3* CO_2*(a)*	97.5	87.6	111.0	0	0	0
v4	*G6P (abcdef) → Biomass*	3.9	-	-	0	-	-
v5	*PG (abc) →* PEP_c *(abc)*	597.9	585.7	607.5	0	0	0
v6	PEP_c *(abc) →* PYR_{c1} *(abc)*	540.3	528.1	549.8	0	0	0
v7	PYR_{c1} *(abc)→* PYR_m *(abc)*	375.2	363.0	384.7	0	0	0
v8	PYR_m *(abc) →* $AcoA_m$ *(bc) +*CO_2 *(a)*	455.8	442.4	466.9	0	0	0
v9	OAA_m *(abcd) +* $AcoA_m$ *(ef) →* CIT_m *(efbcda)*	548.7	529.5	556.9	0	0	0
v10	CIT_m *(abcdef)→* AKG_m *(abcde)+* CO_2 *(f)*	441.7	422.8	450.2	0	0	0
v11	AKG_m *(abcde)→ 0.5* MAL_m *(abcd) + 0.5* MAL_m*(dcba) +* CO_2 *(e)*	571.3	555.8	581.1	0	0	0
v12	MAL_m *(abcd) ↔* OAA_m *(abcd)*	474.4	473.0	486.0	14.3	0.16	>100
v13	PYR_{c2} *(abc) ↔* LAC_c *(abc)*	290.8	261.1	320.4	15.3	0	>100
v14	LAC_c *(abc) ↔* LAC_{ex} *(abc)*	290.8	261.1	320.4	n.d.	n.d.	n.d.
v15	OAA_c *(abcd) →* PEP_c *(abc) +* CO_2 *(d)*	65.0	35.5	72.2	0	0	0
v16	MAL_c *(abcd) →* PYR_{c1} *(abc) +* CO_2 *(d)*	16.4	9.4	45.8	0	0	0
v17	OAA_c *(abcd) ↔* MAL_c *(abcd)*	19.3	10.9	50.7	n.d.	n.d.	n.d.
v18	PYR_m *(abc) +* CO_2 *(d) →* OAA_m *(abcd)*	59.6	52.9	64.1	0	0	0
v19	MAL_m *(abcd) →* PYR_m *(abc) +* CO_2 *(d)*	149.4	142.8	154.0	0	0	0
v20	*PG (abc) → SER (abc)*	21.2	19.9	21.9	0	0	0
v21	*SER (abc)↔ GLY (ab) + MTHF (c)*	34.5	33.3	35.2	4.03	3.43	4.75
v22	SER_{ex} *(abc) ↔ SER (abc)*	48.3	39.2	57.4	33.5	14.0	98.5
v23	*SER (abc)→ Biomass*	4.9	-	-	0	-	-
v24	*GLY (abc) ↔* GLY_{ex} *(abc)*	25.5	22.0	29.0	4.6	2.2	6.9
v25	*GLY (abc) → Biomass*	9.0	-	-	0	-	-
v26	*SER (abc) →* PYR_{c1} *(abc)*	30.0	28.8	30.8	0	0	0
v27	PYR_{c1} *(abc) +* GLU_c *(defgh) ↔* ALA_c *(abc)+* AKG_c *(defgh)*	40.1	38.3	129.2	36.6	17.3	>100
v28	ALA_c *(abc) ↔* ALA_{ex} *(abc)*	42.7	39.9	45.5	0.154· ·$e^{(t*0.036)}$	0.142 (0.038)	0.169 (0.042)
v29	ALA_c *(abc)→ Biomass*	6.7	-	-	0	-	-
v30	ALA_m *(abc)↔* ALA_c *(abc)*	9.5	-10.6	13.6	0.15	0	1.15
v31	PYR_m *(abc) +* GLU_m *(defgh) ↔* ALA_m *(abc)+* AKG_m *(defgh)*	9.5	-10.6	13.6	n.d.	-	-
v32	PYR_{c1} *(abc) ↔* PYR_{ex} *(abc)*	3.3	2.1	4.56	2700/t	2055/t	2808/t
v33	ASP_c *(abcd) +* AKG_c *(efghi) ↔* OAA_c *(abcd) +* GLU_c *(efghi)*	45.3	31.9	48.3	19.3	1.3	>100
v34	ASP_c *(abcd) +* AKG_m *(edghi) →* OAA_m *(abcd) +* GLU_m *(efghi)*	14.5	11.4	27.9	0	0	0
v35	*ASN (abcd) →* ASP_c *(abcd)*	47.2	31.1	63.2	0	0	0
v36	ASP_{ex} *(abcd) ↔* ASP_c *(abcd)*	20.9	1.1	40.7	0.7	0.34	0.84
v37	ASP_c *(abcd) → Biomass*	8.4	-	-	0	-	-

v38	MAL_c (abcd) ↔ MAL_m (abcd)	2.9	0.9	5.0	6.9	0.8	15.1
v39	CIT_m (abcdef) → CIT_c (abcdef)	106.6	40.1	n.d.	0	0	0
v40	CIT_c (abcdef) → AKG_c (abcde)+ CO_2 (e)	67.6	1	n.d.	0	0	0
v41	AKG_m (abcde) ↔ AKG_c (abcde)	26.3	-62.8	53.5	8.2	2.15	>100
v42	AKG_c (abcde) ↔ GLU_c (abcde)	71.2	62.7	78.8	n.d.	-	-
v43	GLU_c (abcde) → GLU_m (abcde)	74.8	66.4	82.5	0	0	0
v44	GLU_m (abcde) ↔ AKG_m (abcde)	161.0	158.5	179.8	n.d.	-	-
v45	GLU_c (abcde) ↔ GLU_{ex} (abcde)	6.3	3.4	9.3	1.3	1.2	1.6
v46	GLU_c (abcde) → Biomass	9.7	-	-	0	-	-
v47	GLN_c (abcde) → GLU_c (abcde)	14.6	13.3	15.8	0	0	0
v48	GLN_c (abcde) → GLU_m (abcde)	81.0	80.1	82.4	0	0	0
v49	GLN_{ex} (abcde) ↔ GLN_c (abcde)	66.4	50.3	82.4	1.28	1.02	1.78
v50	CIT_c (abcdef) → OAA_c (fcde) + $AcoA_c$ (ab)	39.1	-	-	0	-	-
v51	$AcoA_c$ (ab) → Biomass	39.1	-	-	0	-	-
v52	AA_{ex} (ILE, VAL, MET, THR, TYR, PHE) → MAL_m (AA catabolism)	49.6	5.1	99.9	0	-	-
v53	AAex (LEU, ILE, LYS, TYR, PHE) → $ACOA_m$ (AA catabolism)	92.6	27.9	161.4	0	-	-
v54	AKG_c (abcde) → GLU_c (abcde) (AA catabolism)	38.7	5.2	75.6	0	-	-
v55	AA(PRO, HIS, ARG) → GLU_c (AA catabolism)	11.6	0.8	25.3	0	-	-
v56	PYR_{c1} (abcd) ↔ ALA_c (abcd)	0	-	-	0	-	-
v57	PYR_m (abc) ↔ LAC (abc)	0	-	-	0	-	-
v58	PYR_{c1} (abc) ↔ PYR_{c2} (abc)	168.1	149.2	174.8	0.13	0	0.41
v59	PEP (abc) → PYR_{c2} (abc)	122.7	103.8	129.4	0	0	0
v60	G6P (abcdef) → carbohydrates	8.9	-	-	0	0	0