Table S2. Optimized respiration parameters. Parameters were allowed to vary between "Min." and "Max." values obtained or approximated from literature. "Reaction #s" are the reactions associated with each rate parameter, with numbering corresponding to that in Table S1, which is continued from the previous model [1]. "Optimal" are the optimized parameter values that best reproduce O_2 consumption dynamics of aerobic, exponential phase *E. coli* measured in this study.

#	Parameter	Parameter description/reaction involved	Reaction #s	Min.	Max.	Optimal	Units	Ref.
1	k _{Cyo,cat}	Cytochrome bo terminal oxidase	180	18.3	150	126	s^{-1}	[2-4]
2	k _{Cyd,cat}	Cytochrome bd terminal oxidase	181	12	469	393	s^{-1}	[2,4,5]
3	$k_{\rm NDH1,cat}$	NADH dehydrogenase I	182	50	600	492	s^{-1}	[6,7]
4	$k_{\rm NDH2,cat}$	NADH dehydrogenase II	183	17.1	474	218	s^{-1}	[8,9]
5	[Cyo] ₀	Initial concentration of cytochrome bo		$1.58 imes 10^{-8}$	$1.58 imes 10^{-6}$	5.89×10^{-7}	М	$[10]^{a}$
6	$[Cyd]_0$	Initial concentration of cytochrome bd		$1.06 imes 10^{-8}$	$1.06 imes 10^{-6}$	$9.54 imes 10^{-7}$	М	$[10]^{a}$
7	$[Q_8]_0$	Initial concentration of ubiquinone-8		4.48×10^{-5}	4.48×10^{-3}	4.24×10^{-3}	М	$[11]^{a,b}$
8	$[Q_8H_2]_0$	Initial concentration of ubiquinol-8		4.48×10^{-5}	4.48×10^{-3}	9.26×10^{-5}	М	$[11]^{a,b}$
9	[NDH1] ₀	Initial concentration of NADH dehydrogenase I		$2.70 imes 10^{-8}$	$2.70 imes 10^{-6}$	1.87×10^{-6}	М	$[12]^{a}$
10	[NDH2] ₀	Initial concentration of NADH dehydrogenase II		3.05×10^{-9}	3.05×10^{-7}	2.95×10^{-7}	М	$[13]^{a}$

a. Species concentrations were allowed to vary within one order of magnitude in either direction of the value calculated from literature, as the concentrations were typically reported in molecules/cell, and were converted to intracellular concentrations assuming a cell volume of 3.2×10^{-15} L [14].

b. The concentrations of ubiquinone-8 and ubiquinol-8 were reported to be approximately 1 µmol/g dry cell weight [11], which was converted to an intracellular concentration by assuming a cell density of 448 gDW/L [12].

References

- 1. Robinson JL, Brynildsen MP: A Kinetic Platform to Determine the Fate of Nitric Oxide in *Escherichia coli*. *PloS Comput Biol* 2013, **9**:e1003049.
- Mason MG, Shepherd M, Nicholls P, Dobbin PS, Dodsworth KS, Poole RK, Cooper CE: Cytochrome bd confers nitric oxide resistance to *Escherichia coli*. Nat Chem Biol 2009, 5:94-96.
- 3. Bolgiano B, Salmon I, Poole RK: **Reactions of the membrane-bound cytochrome bo** terminal oxidase of *Escherichia coli* with carbon monoxide and oxygen. *Biochim Biophys Acta* 1993, **1141**:95-104.
- 4. Rice CW, Hempfling WP: Oxygen-limited continuous culture and respiratory energy conservation in *Escherichia coli*. J Bacteriol 1978, **134**:115-124.
- Junemann S, Butterworth PJ, Wrigglesworth JM: A suggested mechanism for the catalytic cycle of cytochrome bd terminal oxidase based on kinetic analysis. *Biochemistry* 1995, 34:14861-14867.
- 6. Verkhovskaya ML, Belevich N, Euro L, Wikstrom M, Verkhovsky MI: **Real-time electron** transfer in respiratory complex I. *Proc Natl Acad Sci U S A* 2008, **105**:3763-3767.
- 7. Leif H, Sled VD, Ohnishi T, Weiss H, Friedrich T: Isolation and characterization of the proton-translocating NADH: ubiquinone oxidoreductase from *Escherichia coli*. Eur J Biochem 1995, 230:538-548.
- Jaworowski A, Campbell HD, Poulis MI, Young IG: Genetic identification and purification of the respiratory NADH dehydrogenase of *Escherichia coli*. *Biochemistry* 1981, 20:2041-2047.
- 9. Villegas JM, Volentini SI, Rintoul MR, Rapisarda VA: Amphipathic C-terminal region of *Escherichia coli* NADH dehydrogenase-2 mediates membrane localization. Arch Biochem Biophys 2011, 505:155-159.
- 10. Cotter PA, Chepuri V, Gennis RB, Gunsalus RP: Cytochrome-O (CyoABCDE) and D (CydAB) Oxidase Gene Expression in *Escherichia coli* Is Regulated by Oxygen, pH, and the Fnr Gene Product. *J Bacteriol* 1990, **172**:6333-6338.
- 11. Bekker M, Kramer G, Hartog AF, Wagner MJ, de Koster CG, Hellingwerf KJ, de Mattos MJT: Changes in the redox state and composition of the quinone pool of *Escherichia coli* during aerobic batch-culture growth. *Microbiol* 2007, **153**:1974-1980.
- 12. Sundararaj S, Guo A, Habibi-Nazhad B, Rouani M, Stothard P, Ellison M, Wishart DS: The CyberCell Database (CCDB): a comprehensive, self-updating, relational database to coordinate and facilitate in silico modeling of *Escherichia coli*. Nucleic Acids Res 2004, **32**:D293-D295.
- 13. Taniguchi Y, Choi PJ, Li GW, Chen H, Babu M, Hearn J, Emili A, Xie XS: Quantifying E. coli proteome and transcriptome with single-molecule sensitivity in single cells. Science 2010, 329:533-538.
- Volkmer B, Heinemann M: Condition-dependent cell volume and concentration of *Escherichia coli* to facilitate data conversion for systems biology modeling. *PLoS One* 2011, 6:e23126.