

Table 3. Definitions and values of parameters for the simulation described

Parameters	Definitions	Values	Ref.
k^*	Acetate production rate of the cells	3 mM/min	
V_{max1}	Specific activity of acetate kinase from AcP to acetate	$2.6 \text{ mM} \cdot \text{min}^{-1} \cdot \text{mg}^{-1}$	1
$Km1$	Km value of acetate kinase for AcP	5 mM	1
V_{max2}	Specific activity of acetate kinase from acetate to AcP	$2.0 \text{ mM} \cdot \text{min}^{-1} \cdot \text{mg}^{-1}$	1
$Km2$	Km value of acetate kinase for acetate	300 mM	2
ack^\dagger	Concentration of acetate kinase	$6.642 \times 10^{-15} \text{ mM}$ (100 molecules)	
Vc	Volume of individual <i>E. coli</i> cells	8×10^{-16} liters	3
μ^\ddagger	<i>E. coli</i> growth rate. (function of pH)		
k_f^\S	Rate constant of reaction from acetate to acetic acid	10^6 min^{-1}	
k_{rev}^\S	Rate constant of reaction from acetic acid to acetate	17.7 min^{-1}	
H_i^+	Concentration of intracellular H^+ , calculated from intracellular pH		
H_e^+	Concentration of extracellular H^+ , calculated from extracellular pH		
a_s^\P	Surface area of individual <i>E. coli</i> cells	$3.14 \mu\text{m}^2$	
g_m	Mass transfer coefficient of acetic acid through the membrane	$60 \mu\text{m/s}$	4
V_t	Total culture volume	3 ml	
k_d^\parallel	Degradation rate of AcP	0.0693 min^{-1} (half-life of 10 min)	
γ	Degradation rate of gfp mRNA	0.0693 min^{-1} (half-life of 10 min).	5
α	Maximum gene expression rate of glnAp ₂ promoter.	$0.5 \times 10^{-5} \text{ mM/min}$	5
K_i^{**}	Concentration of AcP to half-maximally induce glnAp ₂ promoter.		
h	Hill coefficient of glnAp ₂ promoter	2	5
α_o	Basal expression rate of glnAp ₂ promoter	$\alpha/1000$	5
θ	Number of protein produced from each mRNA molecule per minute.	10 min^{-1}	5
$\beta^{\dagger\dagger}$	Degradation rate of GFP protein.	$4.81 \times 10^{-4} \text{ min}^{-1}$ (half-life of 24 h)	6

*This parameter is estimated from the extracellular acetate production from experimental data.

†The intracellular concentration of acetate kinase was unknown and was estimated to be ~100 molecules per cell.

‡The growth rate of BW18793 at different pH values was obtained from experimental data.

§The rate of equilibrium reactions is known to be very high, especially compared with gene expression. Therefore we set the reaction rate constant for the conversion of acetate to acetic acid, k_f , to an arbitrarily high number, 10^6 min^{-1} , then calculated the reverse reaction, the conversion of acetic acid to acetate, from the pK_a value of acetic acid (4.75) and the k_f with: $k_{rev} = k_f 10^{-pK_a}$.

[¶]The surface area of a single *E. coli* is estimated by assuming a cylinder geometry with 0.5- μm diameter and 1- μm length.

^{||}Acetyl phosphate is a labile compound, but the intracellular degradation rate is unknown. We chose the value to be the same as the degradation rate of the mRNA.

^{**}This is an adjustable parameter range. This value depends on the strength of the promoter. In the model, it ranges from 0.12 to 10 mM.

^{††}The half-life of $\text{gfp}_{\text{mut3.1}}$ is longer than 24 h, but the exact value is not known (6). We chose 24 h as the half-life. The system is not sensitive to the value of this parameter.

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