Contents

1. Equations

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\begin{aligned}
EnvZ & \quad \dot{x}_1 = k_{ad}x_2 - k_{ap}x_1RL + k_{d2}x_4 - k_{b2}x_5x_1 - k_{b3} * x_6x_1 + k_{d3}x_7 \\
EnvZ - P & \quad \dot{x}_2 = k_{ap}x_1RL - k_{ad}x_2 + k_{d1}x_3 - k_{b1}x_6x_2 \\
EnvZ - P.OmpR & \quad \dot{x}_3 = -(k_{d1} + k_{pt})x_3 + k_{b1}x_6x_2 \\
EnvZ.OmpR - P & \quad \dot{x}_4 = k_{pt}x_3 - (k_{ph} + k_{d2})x_4 + k_{b2}x_5x_1 \\
OmpR - P & \quad \dot{x}_5 = k_{d2}x_4 - k_{b2}x_5x_1 \\
OmpR & \quad \dot{x}_6 = k_{d1}x_3 + k_{d3}x_7 - k_{b3}x_6x_1 - k_{b1}x_6x_2 \\
EnvZ.OmpR & \quad \dot{x}_7 = k_{ph}x_4 - k_{d3}x_7 + k_{b3}x_6x_1 \\
YcgF_{mRNA} & \quad \dot{x}_8 = k_1 - \gamma_{mRNA}x_8 \\
YcgF_{inactive} & \quad \dot{x}_9 = k_3x_8 - \gamma_2x_9 - 2k_{dim}x_9^2\frac{BL^2}{\left(\frac{1}{2}+BL\right)^2} + 2k_{dis}x_{10} - \gamma_{Protein}x_9 \\
YcgF_{dimer} & \quad \dot{x}_{10} = 2k_{dim}x_9^2\frac{BL^2}{\left(\frac{1}{2}+BL\right)^2} - k_{bind}x_{10}x_{12} - k_{dis}x_{10} + k_{ubind}x_{13} - \gamma_{Protein}x_{10} \\
YcgE_{RNA} & \quad \dot{x}_{11} = k_2 - \gamma_{mRNA}x_{11} \\
YcgE_{Protein} & \quad \dot{x}_{12} = k_4x_{11} - \gamma_2x_{12} - k_{bind}x_{10}x_{12} + k_{ubind}x_{13} - \gamma_{Protein}x_{12} \\
YcgE.YcgF_{complex} & \quad \dot{x}_{13} = -k_{ubind}x_{13} + k_{bind}x_{10}x_{12} \\
tRNA & \quad \dot{x}_{14} = k_t\frac{\left(\frac{x_5}{K1}\right)^2}{\left(1+\frac{x_5}{K1}\right)^2} - (\gamma_1 + k_a)x_{14} + \gamma_{2p}x_{15} + 2k_{7p}x_{16}\left(\frac{\gamma_3}{k_{7m}}\right)\left(\frac{x_{14}}{\gamma_0+x_{14}}\right)^2 \\
Aa - tRNA & \quad \dot{x}_{15} = k_ax_{14} - 2k_{7p}x_{16}\left(\frac{\gamma_3}{k_{7m}}\right)\left(\frac{x_{14}}{\gamma_0+x_{14}}\right)^2 - \gamma_2x_{15} \\
T7RNAP_{mRNA} & \quad \dot{x}_{16} = k_{7m}\left(1 - \frac{\left(\frac{x_{12}}{K1}\right)^2}{\left(1+\frac{x_{12}}{K1}\right)^2}\right) - \gamma_3x_{16} \\
T7RNAP & \quad \dot{x}_{17} = k_{7p}x_{16}\left(\frac{\gamma_3}{k_{7m}}\right)\left(\frac{x_{14}}{\gamma_0+x_{14}}\right)^2 - \gamma_4x_{17} \\
lacZ_{mRNA} & \quad \dot{x}_{18} = \alpha_M\left(1 - \frac{\left(\frac{x_5}{K5}\right)^2}{\left(1+\frac{x_5}{K5}\right)^2}\right) - \gamma_Mx_{18} \\
\beta - Galactosidase & \quad \dot{x}_{19} = \alpha_Bx_{18} - \gamma_Bx_{19} \\
dye & \quad \dot{x}_{20} = \alpha_Ax_{19}
\end{aligned}
$$

2. Parameters

Parameter	Value	Unit	Name	Source
k_{ap}	0.1	$\frac{1}{s}$	EnvZ autophosphorelation rate	[3]
k_{ad}	0.001	$\frac{1}{s}$	EnvZ dephospholeration rate	[3]

Parameter	Value	Unit	Name	Source
k_{b1}	0.5	$\frac{1}{s}$	binding rate EnvZ-P & OmpR	[3]
k_{d1}	0.5	$\frac{1}{s}$	unbinding rate EnvZ-P.OmpR	[3]
k_{b2}	0.05	$\frac{1}{s}$	binding rate EnvZ & OmpR-P	[3]
k_{d2}	0.5	$\frac{1}{s}$	unbinding rate EnvZ.OmpR-P	[3]
k_{b3}	0.5	$\frac{1}{s}$	binding rate EnvZ & OmpR	[3]
k_{d3}	5	$\frac{1}{s}$	unbinding rate EnvZ.OmpR	[3]
k_{ph}	0.05	$\frac{1}{s}$	dephosphorelation rate EnvZ.OmpR-P	[3]
k_{pt}	1.5	$\frac{1}{s}$	phosphotransfer rate	[3]
k_1	1.54e-3	$\frac{1}{s}$	max transcription rate YcgF	[1]
k_2	0.848e-3	$\frac{1}{s}$	max transcription rate YcgE	[1]
k_3	0.167	$\frac{1}{s}$	max translation rate YcgF	[1]
k_4	0.167	$\frac{1}{s}$	max translation rate YcgE	[1]
k_{dim}	0.008	$\frac{1}{s}$	dimerization rate YcgF	[1]
k_{dis}	0.0058	$\frac{1}{s}$	dissociation rate YcgF dimer	[1]
k_{bind}	100	$\frac{1}{s}$	binding rate YcgF dimer to YcgE	[1]
k_{ubind}	1	$\frac{1}{s}$	unbinding rate YcgF.YcgE	[1]
γ_{mRNA}	2.3105e-3	$\frac{1}{s}$	degradation mRNA YcgE/YcgF	[1]
$\gamma_{Protein}$	1.9254e-5	$\frac{1}{s}$	degradation rate Protein YcgE/YcgF	[1]
k_t	$\frac{46.67}{60}$	$\frac{nM}{s}$	max transcription rate tRNA	[2]
k_a	$\frac{0.08}{60}$	$\frac{1}{s}$	synthesis rate Aa-tRNA	[2]
k_{7p}	$\frac{1.5625}{60}$	$\frac{nM}{s}$	max transcription rate T7RNAP	[2]
k_{7m}	$\frac{268*0.05}{60}$	$\frac{1}{s}$	max translation rate T7RNAP	[2]
k_S	0.3	$\frac{1}{nM}$	AND Gate rate	[2]
γ_0	1	-	threshold Aa-tRNA	guessed
γ_1	$\frac{1}{60*60}$	$\frac{1}{s}$	degradation of tRNA	[2]
γ_2	$\frac{1}{40*60}$	$\frac{1}{s}$	degradation of Aa-tRNA	[2]

Parameter	Value	Unit	Name	Source
γ_3	$\frac{1}{4.4*60}$	$\frac{1}{s}$	degradation of T7RNAP mRNA	[2]
γ_4	$\frac{46.67}{40*60}$	$\frac{1}{s}$	degradation of T7RNAP	[2]
$K1$	5	nM	response param. OmpR-P,tRNA	guessed
$K3$	600	nM	response param. YcgE,T7RNAP	guessed
$K5$	$\frac{k7p}{4*\gamma_4}$	nM	response param T7RNAP,lacZ	guessed
α_M	$\frac{0.997}{60}$	$\frac{nM}{s}$	max transcription rate lacZ	[4]
α_B	$\frac{1.661e-5}{60}$	$\frac{1}{s}$	max translation rate lacZ	[4]
α_A	$\frac{20}{60}$	$\frac{1}{s}$	enzymatic reaction rate	[4]
γ_M	$\frac{0.411}{60}$	$\frac{1}{s}$	degradation lacZ mRNA	[4]
γ_B	$\frac{8.331e-4}{60}$	$\frac{1}{s}$	degradation β-Galactosidase	[4]

3. Initial Data

Name	Variable	Initial Value	Comment	Source
$EnvZ$	x_1	$\frac{3500}{0.60221}$	3500 molecules per cell	[3]
$EnvZ-P$	x_2	0		
$EnvZ-P.OmpR$	x_3	0		
$EnvZ.OmpR-P$	x_4	0		
$OmpR-P$	x_5	0		
$OmpR$	x_6	$\frac{100}{0.60221}$	100 molecules per cell	[3]
$EnvZ.OmpR$	x_7	0		
$YcgF_{mRNA}$	x_8	$\frac{k_1}{\gamma_{mRNA}}$	steady state	
$YcgF_{inactive}$	x_9	$\frac{k_3}{\gamma_{Protein}}\frac{k_1}{\gamma_{mRNA}}$	steady state	
$YcgF_{dimer}$	x_{10}	0		
$YcgE_{mRNA}$	x_{11}	$\frac{k_2}{\gamma_{mRNA}}$	steady state	
$YcgE$	x_{12}	$\frac{k_4}{\gamma_{Protein}}\frac{k_2}{\gamma_{mRNA}}$	steady state	
$YcgE.YcgF$	x_{13}	0		

Name	Variable	Initial Value	Comment	Source
$tRNA$	x_{14}	0		
$Aa - tRNA$	x_{15}	0		
$T7RNAP_{mRNA}$	x_{16}	0		
$T7RNAP$	x_{17}	0		
$lacZ_{mRNA}$	x_{18}	0		
$\beta - Galactosidase$	x_{19}	0		
dye	x_{20}	0		

4. Simulation

TBD

5. Attribution

The red light sensor was modeled according to the paper "Hysteretic and graded responses in bacterial two-component signal transduction"[3]

The blue light sensor was modeled with help of the model by the iGEM team KU Leuven 2009[1]

The model for our AND-Gate is based on the model of the iGEM team PKU Beijing 2009 for their AND-Gate1. We modified the equations such that the change in tRNA and Aa-tRNA does not include the degradation of the mRNA which caused negativity of some concentrations in our model.[2]

The Expression of lacZ is an adaption of the model given by "Dynamics and bistability in a reduced model of the lac operon"[4]

References

1. KU Leuven 2009, *Blue light receptor: Modeling*, 2009.
2. PKU Beijing 2009, *And gate 1*, 2009.
3. Oleg A Igoshin, Rui Alves, and Michael A Savageau, *Hysteretic and graded responses in bacterial two-component signal transduction*, Mol Microbiol **68** (2008), no. 5, 1196–215.
4. N Yildirim, M Santillan, D Horike, and MC Mackey, *Dynamics and bistability in a reduced model of the lac operon*, CHAOS **14** (2004), no. 2, 279–292 (English).