

1. EQUATIONS

$$\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}{(\frac{1}{2}+BL)^2} + 2k_{dis}x_{10} - \gamma_{Protein}x_9 \\
YcgF_{dimer} \quad \dot{x}_{10} &= 2k_{dim}x_9^2 \frac{BL^2}{(\frac{1}{2}+BL)^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{(\frac{x_5}{K_1})^2}{(1+\frac{x_5}{K_1})^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{(\frac{x_{12}}{K_1})^2}{(1+\frac{x_{12}}{K_1})^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{(\frac{x_5}{K_5})^2}{(1+\frac{x_5}{K_5})^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	Sal
k_{ad}	0.001	$\frac{1}{s}$	EnvZ dephospholeration rate	Sal

Parameter	Value	Unit	Name	Source
k_{b1}	0.5	$\frac{1}{s}$	binding rate EnvZ-P & OmpR	Sal
k_{d1}	0.5	$\frac{1}{s}$	unbinding rate EnvZ-P.OmpR	Sal
k_{b2}	0.05	$\frac{1}{s}$	binding rate EnvZ & OmpR-P	Sal
k_{d2}	0.5	$\frac{1}{s}$	unbinding rate EnvZ.OmpR-P	Sal
k_{b3}	0.5	$\frac{1}{s}$	binding rate EnvZ & OmpR	Sal
k_{d3}	5	$\frac{1}{s}$	unbinding rate EnvZ.OmpR	Sal
k_{ph}	0.05	$\frac{1}{s}$	dephosphorelation rate EnvZ.OmpR-P	Sal
k_{pt}	1.5	$\frac{1}{s}$	phosphotransfer rate	Sal
k_1	1.54e-3	$\frac{1}{s}$	max transcription rate tRNA	KU Leuven 2009
k_2	0.848e-3	$\frac{1}{s}$	max transcription rate tRNA	KU Leuven 2009
k_3	0.167	$\frac{1}{s}$	max translation rate T7RNAP	KU Leuven 2009
k_4	0.167	$\frac{1}{s}$	max translation rate T7RNAP	KU Leuven 2009
k_{dim}	0.008	$\frac{1}{s}$	dimerization rate YcgF	KU Leuven 2009
k_{dis}	0.0058	$\frac{1}{s}$	dissociation rate YcgF dimer	KU Leuven 2009
k_{bind}	100	$\frac{1}{s}$	binding rate YcgF dimer to YcgE	KU Leuven 2009
k_{ubind}	1	$\frac{1}{s}$	unbinding rate YcgF.YcgE	KU Leuven 2009
γ_{mRNA}	2.3105e-3	$\frac{1}{s}$	degradation mRNA YcgE/YcgF	KU Leuven 2009
$\gamma_{Protein}$	1.9254e-5	$\frac{1}{s}$	degradation rate Protein YcgE/YcgF	KU Leuven 2009
k_t	$\frac{46.67}{60}$	$\frac{nM}{s}$	max transcription rate tRNA	PKU Beijing 2009
k_a	$\frac{0.08}{60}$	$\frac{1}{s}$	synthesis rate Aa-tRNA	PKU Beijing 2009
$k_{\tau p}$	$\frac{1.5625}{60}$	$\frac{nM}{s}$	max transcription rate T7RNAP	PKU Beijing 2009
$k_{\tau m}$	$\frac{268*0.05}{60}$	$\frac{1}{s}$	max translation rate T7RNAP	PKU Beijing 2009
k_S	0.3	$\frac{1}{nM}$	AND Gate rate	PKU Beijing 2009
γ_0	1	-	threshold Aa-tRNA	guessed
γ_1	$\frac{1}{60*60}$	$\frac{1}{s}$	degradation of tRNA	PKU Beijing 2009
γ_2	$\frac{1}{40*60}$	$\frac{1}{s}$	degradation of Aa-tRNA	PKU Beijing 2009

Parameter	Value	Unit	Name	Source
γ_3	$\frac{1}{4.4*60}$	$\frac{1}{s}$	degradation of T7RNAP mRNA	PKU Beijing 2009
γ_4	$\frac{46.67}{40*60}$	$\frac{1}{s}$	degradation of T7RNAP	PKU Beijing 2009
$K1$	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	Chaos Lac
α_B	$\frac{1.661e-5}{60}$	$\frac{1}{s}$	max translation rate lacZ	Chaos Lac
α_A	$\frac{20}{60}$	$\frac{1}{s}$	enzymatic reaction rate	Chaos Lac
γ_M	$\frac{0.411}{60}$	$\frac{1}{s}$	degradation lacZ mRNA	Chaos Lac
γ_B	$\frac{8.331e-4}{60}$	$\frac{1}{s}$	degradation β -Galactosidase	Chaos Lac

3. INITIAL DATA

Name	Variable	Initial Value	Comment
$EnvZ$	x_1	$\frac{3500}{0.60221}$	3500 molecules per cell
$EnvZ - P$	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
$EnvZ.OmpR$	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
<i>tRNA</i>	x_{14}	0	
<i>Aa - tRNA</i>	x_{15}	0	
<i>T7RNAP_{mRNA}</i>	x_{16}	0	
<i>T7RNAP</i>	x_{17}	0	
<i>lacZ_{mRNA}</i>	x_{18}	0	
<i>β - Galactosidase</i>	x_{19}	0	
<i>dye</i>	x_{20}	0	

4. ANALYSIS

TBD

5. REFERENCE

The red light sensor was modeled according to the paper “Hysteretic and graded responses in bacterial two-component signal transduction”

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.

The Expression of lacZ is an adaption of the model given by “Dynamics and bistability in a reduced model of the lac operon”