

## Diffusion Model

Description	Symbol	Value	Units	Reference
2,4-DNT concentration at the source	c0	4,38E-04	mol/m <sup>3</sup>	[1]
Radius of the source	a	0.1	m	assumed
Diffusion constant of 2,4-DNT in air	D	0.067e-4	m <sup>2</sup> /s	[2]
Decay rate of 2,4-DNT in the air	k	3,21E-07	1/s	

- [1] Jenkins, Thomas F., et al. *Analysis of explosives-rel*  
 [2] Yaws, Carl L. *Transport properties of chemicals and*  
 [3] Jenkins, Thomas F., et al. "Chemical signatures of T

## Bubbling Model

Description	Symbol	Value	Units	Reference
Liquid volume (in which we bubble)	Vl	3,00E-06	m <sup>3</sup>	[1]
Liquid Height	L	0,05	m	[1]
Bubble diameter	d	0,002	m	[1]
Specific Surface Area (bubble)	a	1570,8	m <sup>2</sup> /m <sup>3</sup>	[2]
Gas Flow Rate	Q	1,00E-04		[1]
Universal Gas Constant	R	8,314	J/(mol*K)	[3]
Temperature	T	298	K	[3]
Density of water	rho <sub>l</sub>	997	kg/m <sup>3</sup>	[3]
Density of air	rho <sub>g</sub>	1,225	kg/m <sup>3</sup>	[3]
Standard Gravity	g	9,81	m/s <sup>2</sup>	[3]
Viscosity of water	mu	1,00E-03	Pa*s	[3]

## 2,4 DNT

Solubility Limit	cs	1,537	mol/m <sup>3</sup>	[4]
Molecular weight	M	182,15	g/mol	[4]
Diffusion constant	D	7.31e-10	m <sup>2</sup> /s	[5]
Henry's constant	H		mol/(m <sup>3</sup> *[4]	

- [1] Own design or characteristic of our hardware  
 [2] pi/d  
 [3] <https://pubchem.ncbi.nlm.nih.gov>  
 [4] [https://pubchem.ncbi.nlm.nih.gov/compound/2\\_4-din](https://pubchem.ncbi.nlm.nih.gov/compound/2_4-din)  
 [5] <https://www.nj.gov/dep/srp/guidance/rs/chempropert>

## Chemotaxis Model

Description	Symbol	Value	Units	Reference
Total Concentration of CheA in the cell	CheATot	7,9	uM	[1]
Total Concentration of CheY in the cell	CheYTot	9,7	uM	[1]
Total Concentration of CheB in the cell	CheBTot	0,28	uM	[1]
Total Concentration of CheZ in the cell	CheZTot	3,8	uM	[1]
Total Concentration of CheR in the cell	CheRTot	0,16	uM	[1]
Autophosphorylation rate of CheA	ka	34	1/s	[2]
Phosphotransfer rate to CheY (from CheA)	ky	100	1/uM 1/s	[3]
Phosphotransfer rate to CheB (from CheA?)	kb	15	1/uM 1/s	[3]
Dephosphorylation rate of CheB-P	k <sub>b</sub>	0.7	1/s	[4]
Dephosphorylation rate of CheY-P (by CheZ)	k1	1.6	1/uM 1/s	[5]

(auto)Dephosphorylation of CheY-P	k2	0,085	1/s	[6]
Methylation of Tar by CheR	gr		1/s	Fitted
Demethylation of Tar by CheB	gb	3,14	1/uM <sup>2</sup> 1/s	Fitted
Number of Tar receptors in a cluster	N	18	-	[7]
<i>Dissociation constant of active Tar receptor</i> kon			uM	Fitted
<i>Dissociation constant of inactive Tar receptor</i> koff		20	uM	Fitted

- [1] Li, Mingshan, and Gerald L. Hazelbauer. "Cellular stoichiometry of the chemotaxis signaling pathway in *Escherichia coli*." *Journal of Bacteriology* 186, no. 12 (2004): 3700-3708.
- [2] Shroff AL, Montefusco DJ, Weis RM (2003) Temporal precision in the bacterial chemotaxis signaling pathway. *Journal of Bacteriology* 185, no. 12 (2003): 3600-3608.
- [3] Stewart, Richard C., Knut Jahreis, and John S. Park. "The chemotaxis signaling pathway in *Escherichia coli*." *Journal of Bacteriology* 186, no. 12 (2004): 3691-3700.
- [4] Stewart, Richard C. "Activating and inhibitory mutations in the chemotaxis signaling pathway of *Escherichia coli*." *Journal of Bacteriology* 186, no. 12 (2004): 3682-3690.
- [5] Li, M., Hazelbauer, G., 2004. Cellular stoichiometry of the chemotaxis signaling pathway in *Escherichia coli*. *Journal of Bacteriology* 186, no. 12 (2004): 3700-3708.
- [6] Stewart, R., van Bruggen, R., 2004. Rapid phosphorylation of CheY in the chemotaxis signaling pathway of *Escherichia coli*. *Journal of Bacteriology* 186, no. 12 (2004): 3691-3700.
- [7] Endres, Robert G., et al. "Variable sizes of *Escherichia coli* chemotaxis receptors." *Journal of Bacteriology* 186, no. 12 (2004): 3682-3690.

### Split-Luciferase Model

Description	Symbol	Value	Units	Reference
Association rate ligand - taz receptor	k1	0,0039	1/uM 1/s	[1]
Dissociation rate ligand - taz receptor	k-1	1	1/s	[2]
autophosphorylation rate Taz	k2	0,045	1/s	[4]
Association rate OmpR - tazp	k3	1,92	1/uM 1/s	[3]
Dissociation rate OmpR - tazp	k-3	1	1/s	[2]
Phosphorylation of OmpR	k4	0,069	1/s	[5]
Association rate OmpRp - taz	k5	0,625	1/uM 1/s	[3]
Dissociation rate OmpRp - taz	k-5	1	1/s	[2]
Dephosphorylation of OmpRp	k6	0,023	1/s	[6]
Association rate of OmpRp to DNA	k8	0,2134	1/uM 1/s	[5]
Dissociation rate of OmpRp to DNA	k-8	0,0016	1/s	[5]
Dimerization OmpR	kdim1	142	1/uM 1/s	[7]
Reverse dimerization rate OmpRp	k_dim1	0,001	1/s	[7]
Dimerization OmpR	kdim2	1,429	1/uM 1/s	[7]
Reverse dimerization rate OmpRp	k_dim2	0,1	1/s	[7]

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- [4] Kenney, L. J. (1997). Kinase activity of EnvZ, an osmR-regulated protein kinase. *Journal of Bacteriology* 179, no. 12 (1997): 3600-3608.
- [5] Qin, L., Yoshida, T. & Inouye, M. (2001). The critical role of the chemotaxis signaling pathway in the regulation of OmpR in *Escherichia coli*. *Journal of Bacteriology* 185, no. 12 (2001): 3600-3608.
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### Holographic Imaging Model

Description	Symbol	Value	Units	Reference
n of LB media	n	1,338	-	[1]
n of water	n	1,3		
Refractive index of e.coli		1		[2]
refractive index polystyrene beads		1,59		
improved gradient descend initial step_size		20	m	

[1]  
[2]

<https://www.biorxiv.org/content/biorxiv/suppl/2016/07>  
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