ORDINARY DIFFERENTIAL EQUATIONS USED TO SIMULATE THE MODEL

· **Production of *mRNA*$_{amo}$,** from its transcription

$$\frac{d[mRNA_{amo}]}{dt} = C_{AMO} \cdot DNA_{amo} - d_{mRNAamo} \cdot [mRNA_{amo}]$$

· **Formation of $COCl_2$** from *AMO protein* and *bacterium inlet chloroform*. An *AMO protein* and *bacterium inlet chloroform* complex is formed during the $COCl_2$ yield

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$$\frac{d[AMO]}{dt} = v_{amo} \cdot [mRNA_{amo}] + k_{COCl_2} \cdot [AMO:chlor] + k_{-1} \cdot [AMO:chlor] - k_1 \cdot [chlor][AMO] - d_{AMO} \cdot [AMO]$$

$$\frac{d[chlor]}{dt} = \frac{P \cdot A_{\text{int}}}{V_{cell}} \cdot ([Cb] - [chlor]) - k_1 \cdot [chlor] \cdot [AMO]$$

$$\frac{d[AMO:chlor]}{dt} = k_1 \cdot [chlor] \cdot [AMO] - k_{-1} \cdot [AMO:chlor] + k_{COCl_2} \cdot [AMO:chlor] - d_{AMO:chlor} \cdot [AMO:chlor]$$

$$\frac{d[COCl_2]}{dt} = k_{COCl_2} \cdot [AMO:chlor] + k_{-2} \cdot [factor:COCl_2] - k_2 \cdot [factor][COCl_2]$$

· **Production of *mRNA*$_{factor}$, from its transcription**

$$\frac{d[mRNA_{factor}]}{dt} = C_{factor} \cdot DNA_{factor} - d_{mRNA_{factor}} \cdot [mRNA_{factor}]$$

· **Formation of the *complex:promoter* that later is transcripted to *mRNA*$_{GFP}$,** that allows the formation of the fluorescence protein *GFP*. Note that one step reaction is pH dependent. Two complexes are produced before reaching the formation of the *complex:promoter*.

$$\frac{d[factor]}{dt} = v_{factor}\cdot[mRNA_{factor}] - k_2\cdot[factor]\cdot[COCl_2] + k_{-2}\cdot[factor:COCl_2]$$
$$- k_I\cdot[factor]\cdot(1+10^{a-pH}+10^{b\cdot pH-c}) + k_{-I}\cdot[factor:H^+] - d_{factor}\cdot[factor]$$

$$\frac{d[factor:H^+]}{dt} = k_I\cdot[factor]\cdot(1+10^{a-pH}+10^{b\cdot pH-c}) - k_{-I}\cdot[factor:H^+] - d_{fH}\cdot[factor:H^+]$$

$$\frac{d[factor:COCl_2]}{dt} = k_2\cdot[factor]\cdot[COCl_2] - k_{-2}\cdot[factor:COCl_2] - k_3\cdot[factor:COCl_2]\cdot[poly]$$
$$+ k_{-3}\cdot[complex:poly] - d_{factor:COCl_2}\cdot[factor:COCl_2]$$

$$\frac{d[complex:poly]}{dt} = k_3\cdot[factor:COCl_2]\cdot[poly] - k_{-3}\cdot[complex:poly] - k_4\cdot[complex:poly]\cdot[promoter]$$
$$+ k_{-4}\cdot[complex:promoter] - d_{complex:poly}\cdot[complex:poly]$$

$$\frac{d[complex:promoter]}{dt} = k_4\cdot[complex:poly]\cdot[promoter] + k_{-4}\cdot[complex:promoter] - d_{complex:promoter}\cdot[complex:promoter]$$

· **Production of *mRNA*$_{factor}$, from its transcription**

$$\frac{d[mRNA_{GFP}]}{dt} = C_{GFP}\cdot[complex:promoter] - d_{mGFP}\cdot[mRNA_{GFP}]$$

· **Formation of *GFP***

$$\frac{d[GFP_{im}]}{dt} = v_{GFP_{im}}\cdot[mRNA_{GFP}] - k_{mis}\cdot[GFP_{im}] - k_{fol}\cdot[GFP_{im}] - d_{GFP_{im}}\cdot[GFP_{im}]$$

$$\frac{d[GFP_{mis}]}{dt} = k_{mis}\cdot[GFP_{im}] + k_5\cdot[GFP] - k_{-5}\cdot[GFP_{mis}] - d_{mis}\cdot[GFP_{mis}]$$

$$\frac{d[GFP]}{dt} = k_{fol}\cdot[GFP_{im}] - k_5\cdot[GFP] + k_{-5}\cdot[GFP_{mis}] - d_{GFP}\cdot[GFP]$$

· **Diffusion through the bacterial membrane**

It is important to take into account that the chloroform added into the culture medium has to pass through the lipid bilayer of the bacterium. The equation used to model that fact is Fick's law and film theory, in general is written as follows:

$$j = -D\left(\frac{dC}{dx}\right) = k_L(c - c^*) \qquad \text{where} \qquad k_L = \frac{D}{\delta}$$

Solving this equation the mass flow is known but it is necessary to calculate the interfacial area where the phenomenon is going to be. Therefore, an approximate value of the bacterial radius is needed.

After that brief introduction the two remaining ordinary differential equation can be written (the first one describe the evolution in time of the chloroform on the solution and the second one on the gas phase).

$$\frac{d[C_b]}{dt} = -\frac{P \cdot A_{int}}{V_b} \cdot ([C_b] - m_{in} \cdot [chlor]) - \frac{k_{Dg}}{V_b} \cdot ([C_b] - m_g \cdot [C_g])$$

$$\frac{d[C_g]}{dt} = \frac{k_{Dg}}{V_g} \cdot ([C_b] - m_g \cdot [C_g])$$