SIMULATION AND DESIGN OF PHOTOREACTORS

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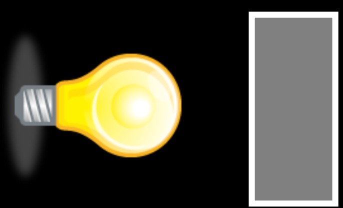
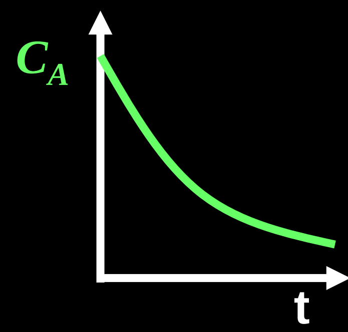
Outline

- 1.- Introduction — The Scaling-Up Problem
- 2.- Methodology — Proposed Scaling-Up Procedure
- 3.- Lab Scale
  - Photoreactor
  - Mass Balance
  - Kinetic Model
  - Radiation Model
  - Kinetic Parameters Estimation
- 4.- Bench Scale
  - Photoreactor
  - Radiation Model
  - Kinetic Model
  - Mass Balance
  - Scaling-Up Validation
- 5.- Conclusions

The Scaling-Up Problem

Laboratory Experiments





$$r = \frac{dC_A}{dt} = kC_A$$

$$r = \frac{dC_A}{dt} = k\frac{KC_A}{1 + KC_A}$$

The Scaling-Up Problem

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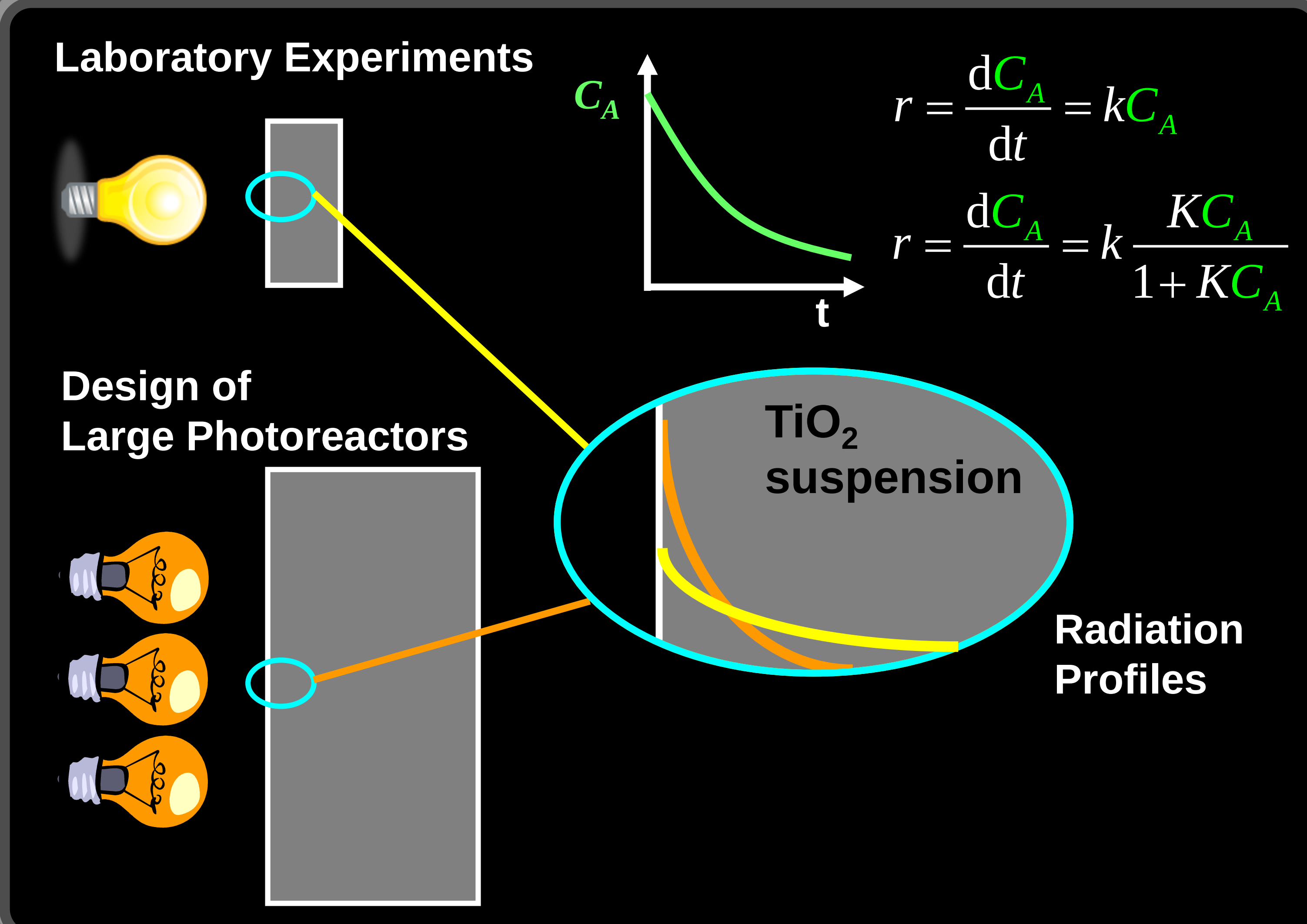
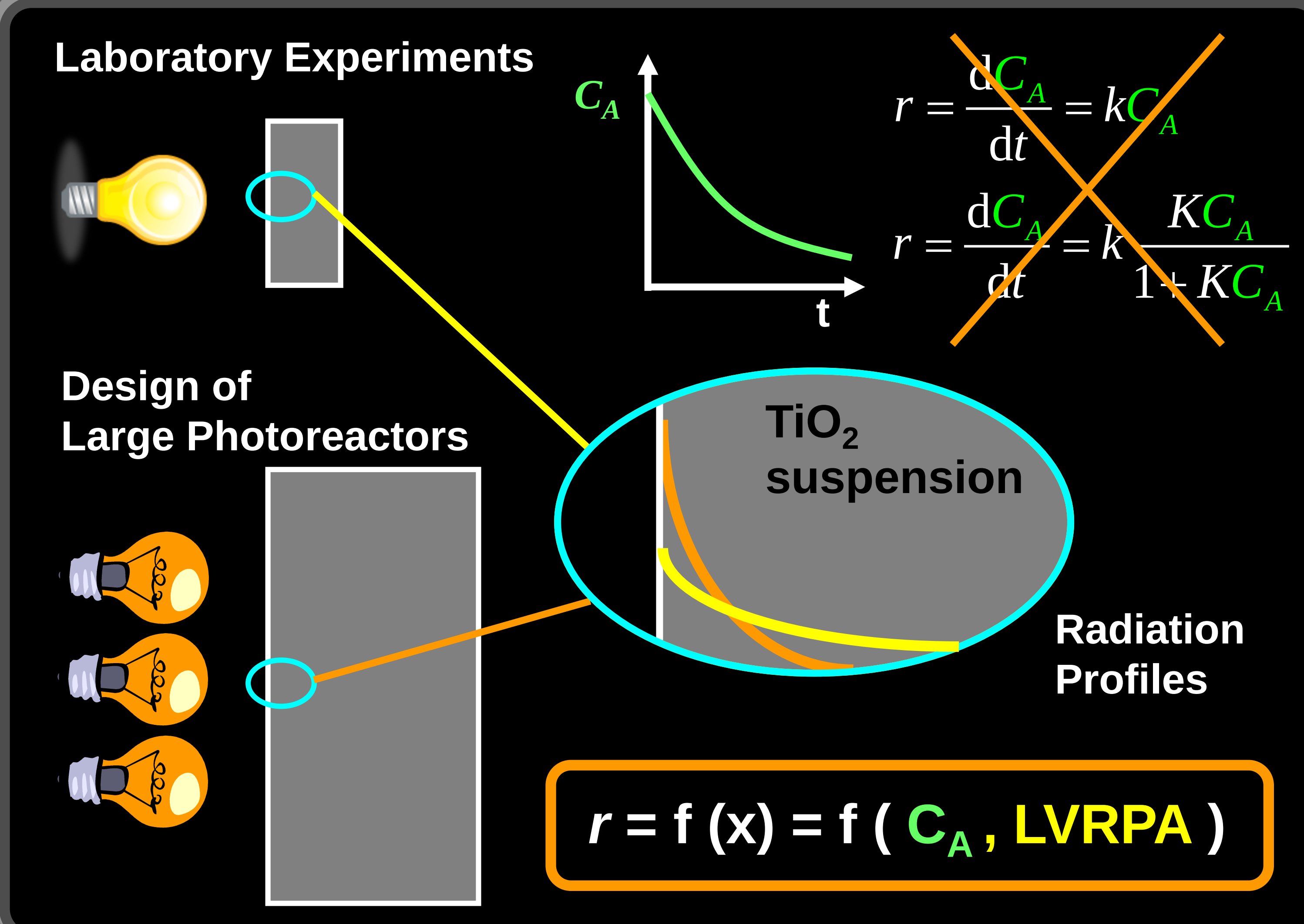
Conclusions.

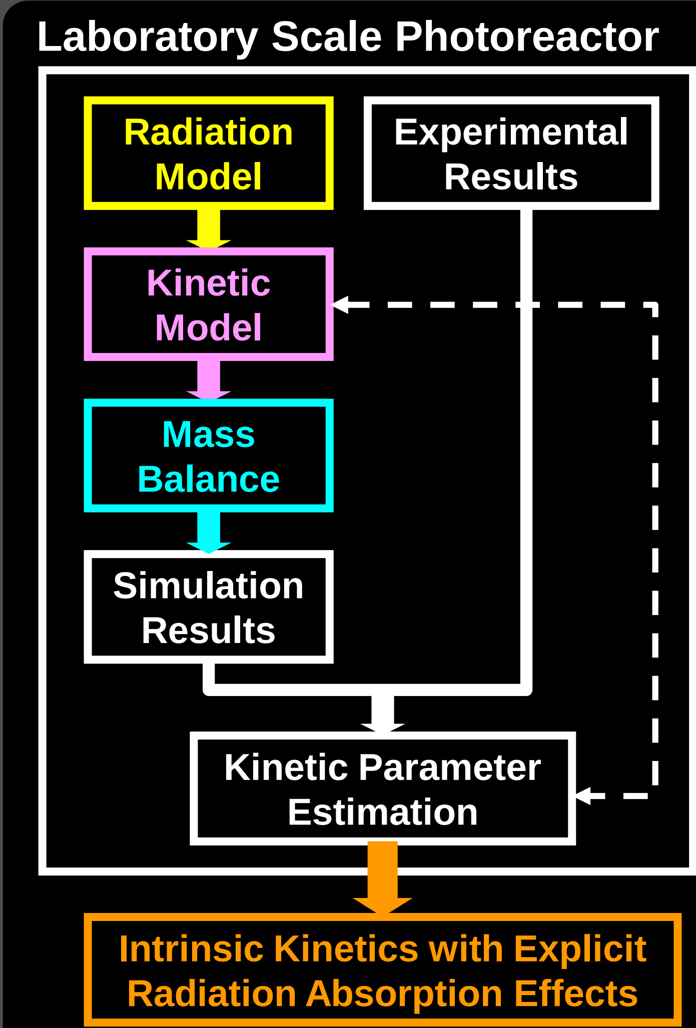


The Scaling-Up Problem



Proposed Scaling-Up Procedure

OUTLINE



Proposed Scaling-Up Procedure

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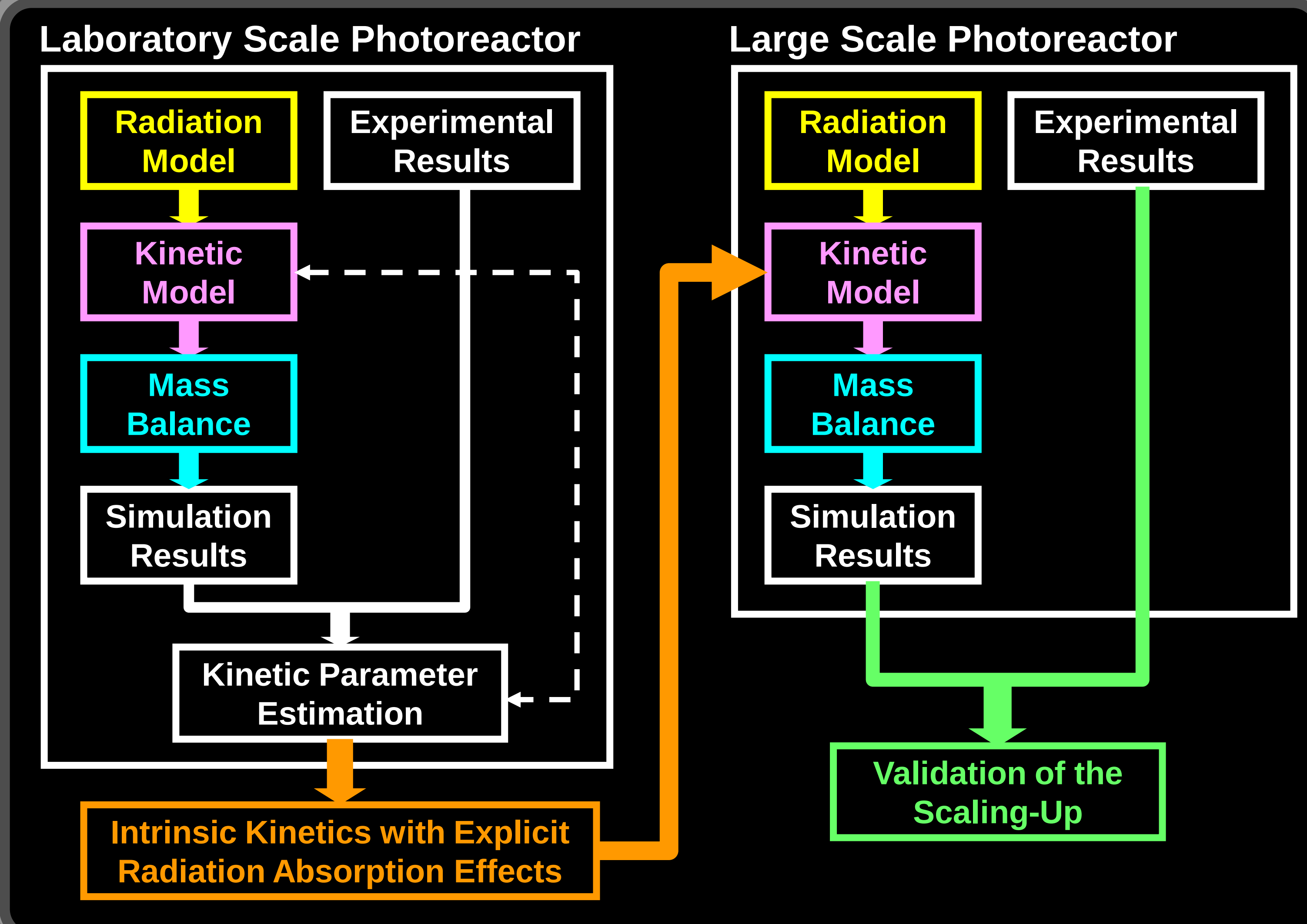
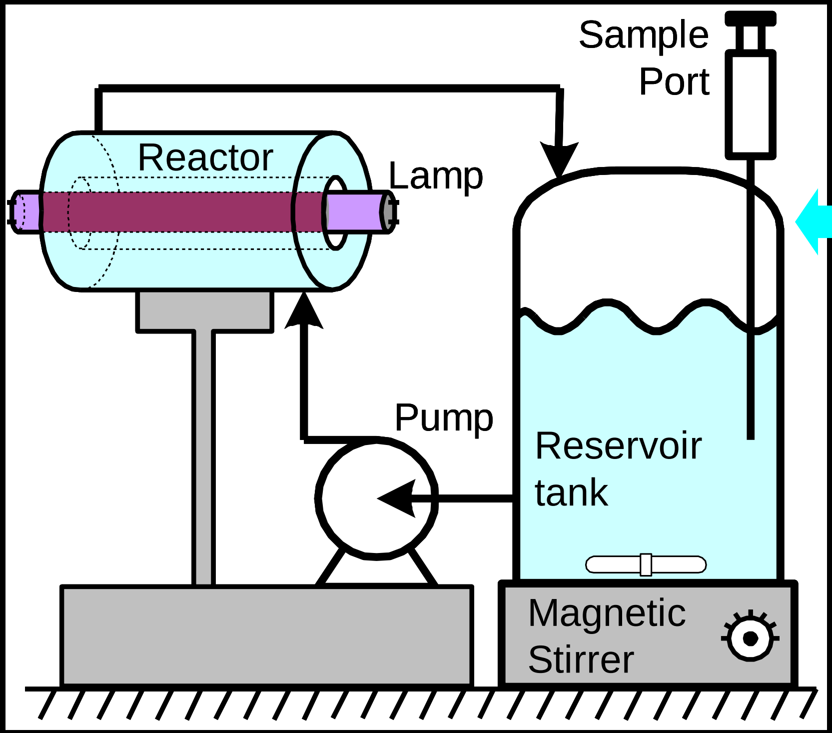


Lab Scale: Photoreactor & Experimental

OUTLINE



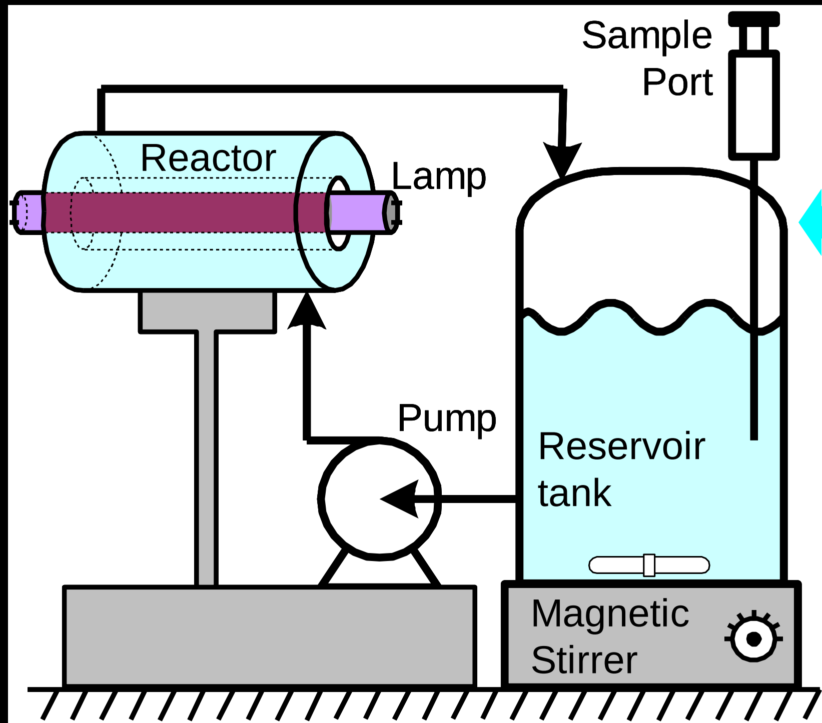
Laboratory scale reactor:

V_R = 188.5 cm^3, V_{Tot} = 1 L

Lamp: Philips TL 6W

L = 21 cm, Φ = 1.6 cm

Lab Scale: Photoreactor & Experimental



Laboratory scale reactor:

V_R = 188.5 cm^3, V_{Tot} = 1 L

Lamp: Philips TL 6W

L = 21 cm, Φ = 1.6 cm

Lamp + Neutral Filters

Actinometry

~ 40 W / m^2

Serial Dilutions + Plating

Catalyst: 0.02 – 0.2 g/L TiO_2 Degussa P25

Radiation: 0.8 – 2.7 × 10^{-6} Einstein / s

Microorg.: 10^3 – 10^6 CFU/mL *E.coli*

Lab Scale: Photoreactor: Mass Balance

ASSUMPTIONS:

1. The system is perfectly mixed.
2. No mass transport limitations.
3. Differential conversion per pass.
4. No parallel dark reactions.

$$\left.\frac{\mathrm{d}[\mathrm{B}](t)}{\mathrm{d}t}\right|_{Tank} = \frac{V_{React}}{V_{Tot}} \left\langle R_B(\underline{x},t) \right\rangle_{V_{React}}$$

$[\mathrm{B}]$	:	Bacterial concentration
t	:	Time
V_{React} / V_{Tot}	:	Reactor volume / Total volume
$\left\langle R_B(\underline{x},t) \right\rangle_{V_{React}}$	:	Bacterial reaction rate averaged over the reactor volume

Kinetic Model: Lab Scale Experimental Data

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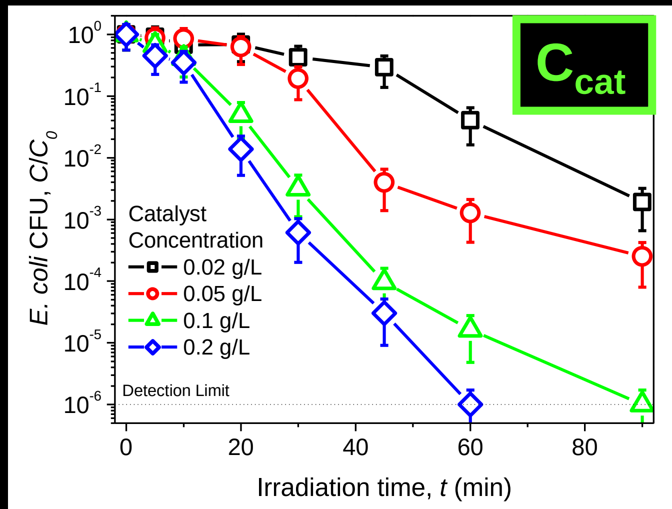
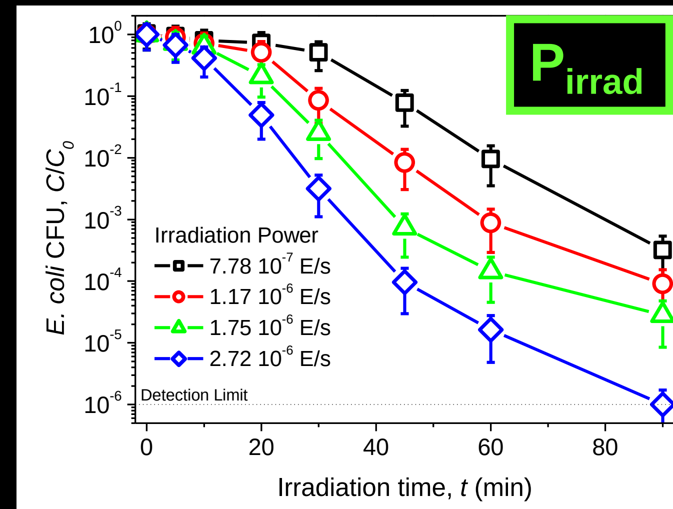
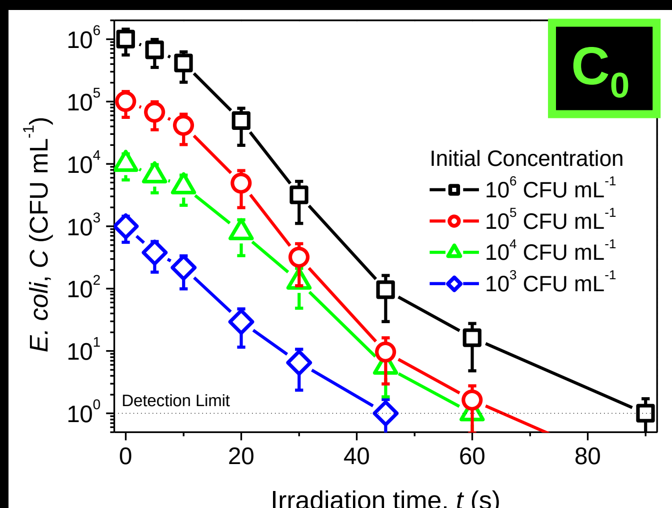
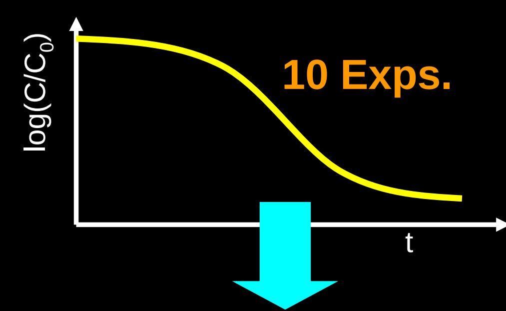


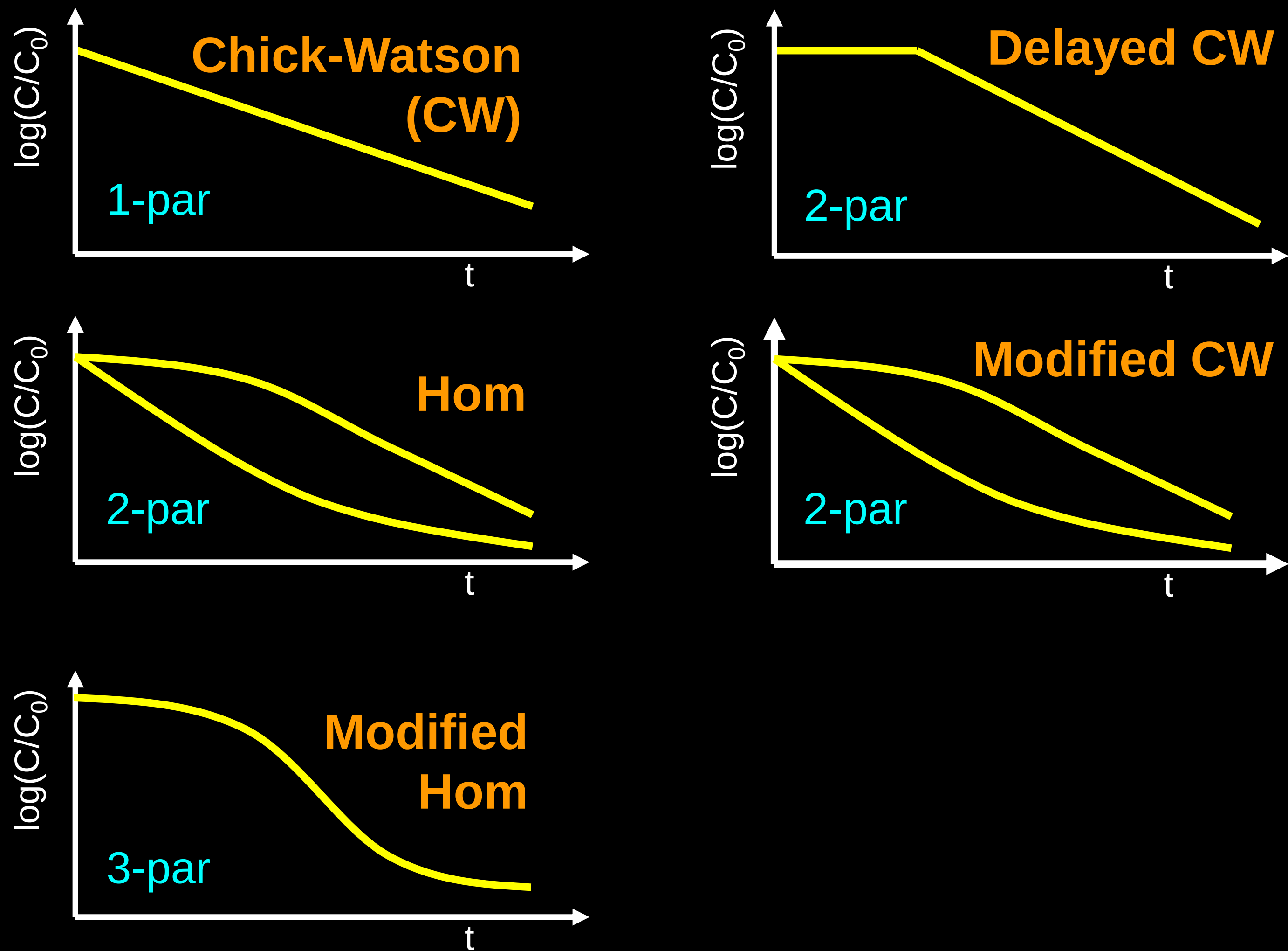




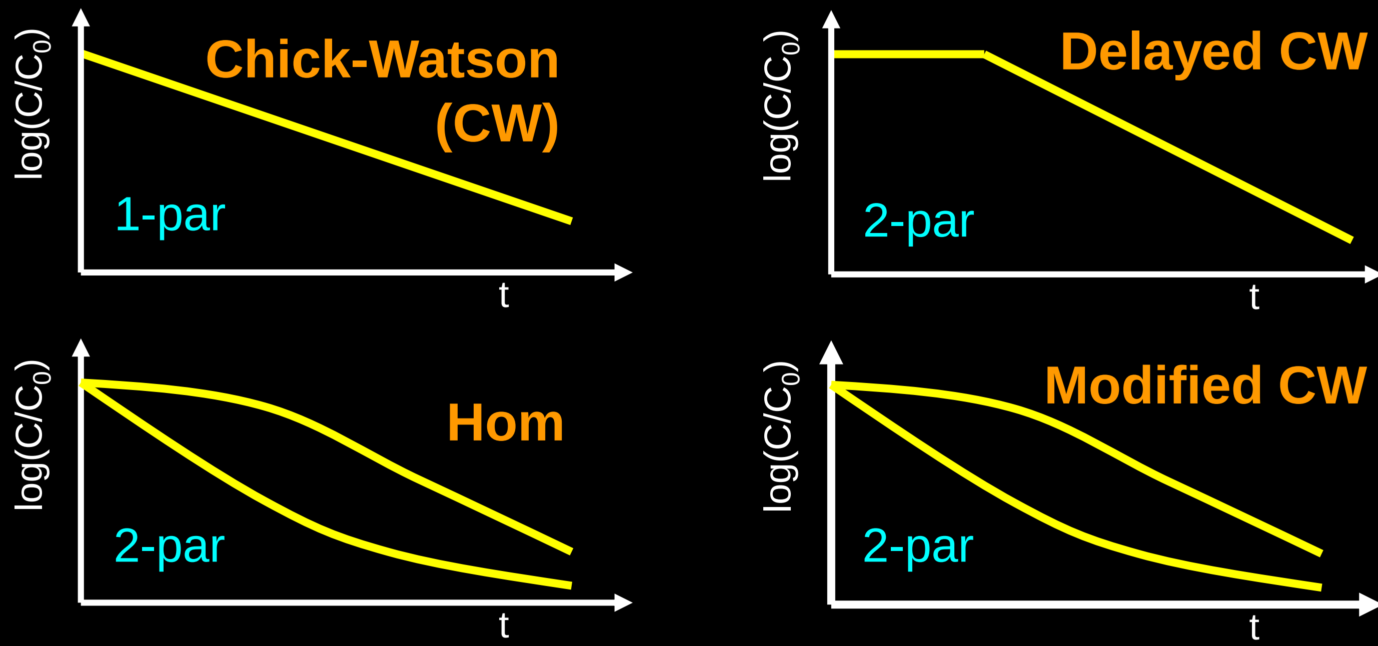


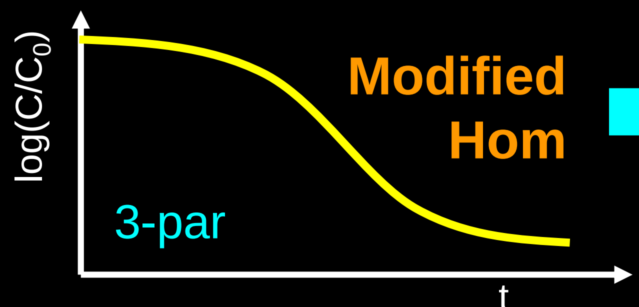
Kinetics Parameters for Reactor Design & Scaling-Up

Kinetic Model: Empiric Equations



Kinetic Model: Empiric Equations



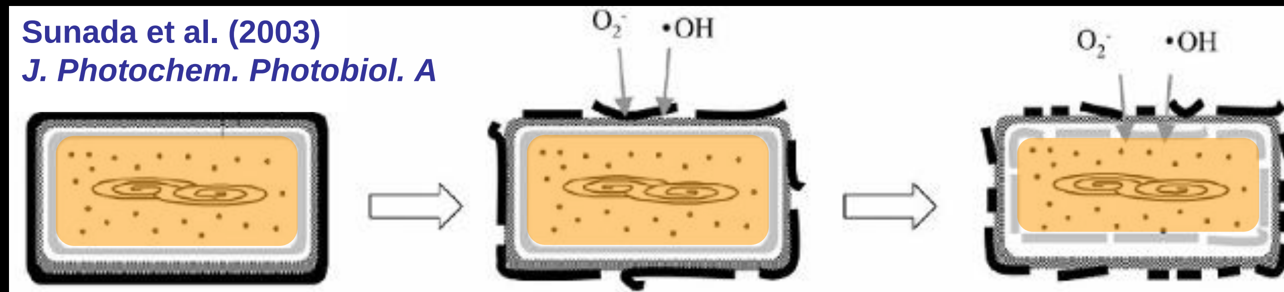


$$\log\left(\frac{C}{C_0}\right) = -k_1\left(1-\exp(-k_2 t)\right)^{k_3}$$

30 kinetic parameters !!!
(10 Exps).

Kinetic Model: Series Event Mechanism

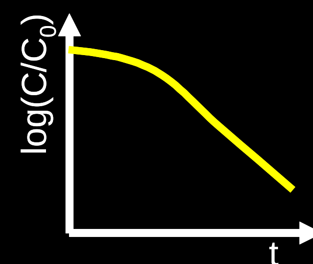
Sunada et al. (2003)
J. Photochem. Photobiol. A



Severin et al. (1983)
Water Res.

$$C_0 \rightarrow C_1 \rightarrow \ldots C_i \rightarrow \ldots C_{n-1} \rightarrow C_n$$

$$Log\frac{C}{C_0} = -kt + \ln\left(1 + \sum_{i=1}^{n}\frac{(kt)^i}{i!}\right)$$



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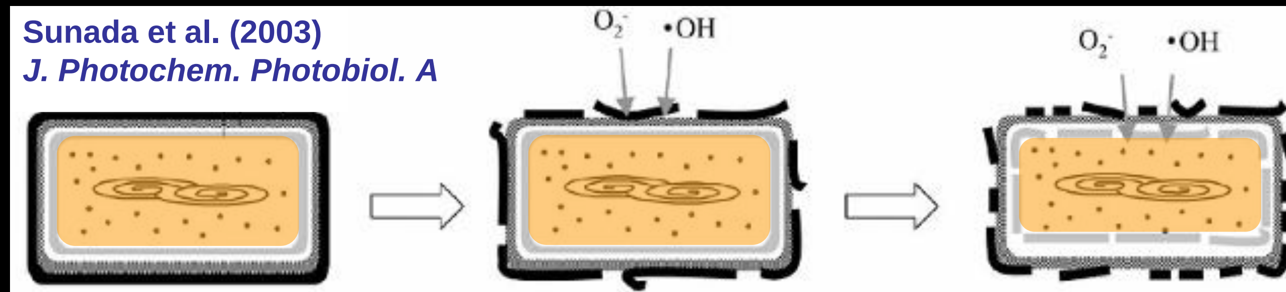

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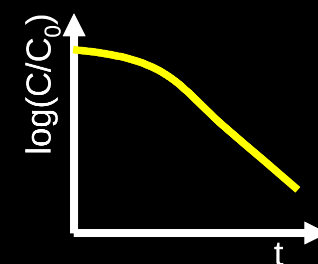

Photonic efficiency: ~ 10^{-11} bacteria / photon

10^9 ·OH / bacteria !!!

Marugán et al. (2008)
Appl. Catal. B: Environ

Kinetic Model: Pseudo-Mechanistic

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Conclusions.

Marugán et al. (2008)
Appl. Catal. B: Environ

$$C_{undam} \xrightarrow{k} C_{dam} \xrightarrow{k} C_{inact} \longrightarrow \dots$$

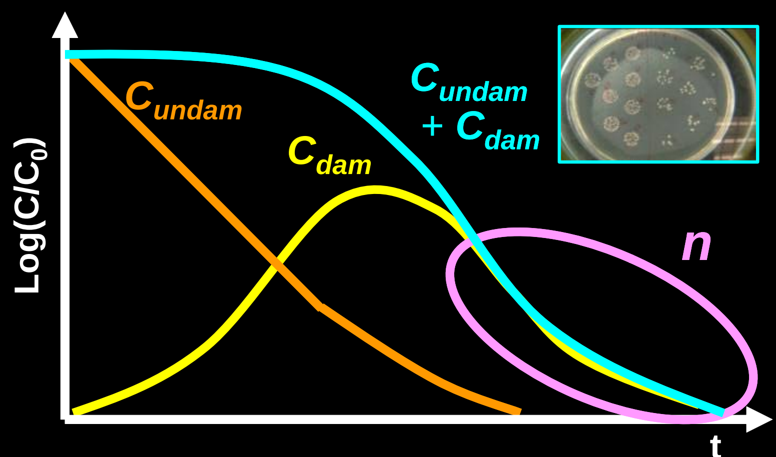
$$\frac{dC_{undam}}{dt} = -k \frac{K\ C_{undam}{}^{n}}{1 + K\ C_{undam}{}^{n} + K\ C_{dam}{}^{n}}$$

$$\frac{dC_{dam}}{dt} = k \frac{K\ C_{undam}{}^{n} - K\ C_{dam}{}^{n}}{1 + K\ C_{undam}{}^{n} + K\ C_{dam}{}^{n}}$$

k **:** **Kinetic constant**

K **:** **Pseudo-adsorption constant**

n **:** **Inhibition coeffient**



Kinetic Model: Pseudo-Mechanistic

Marugán et al. (2008)
Appl. Catal. B: Environ

$$C_{undam} \xrightarrow{k} C_{dam} \xrightarrow{k} C_{inact} \longrightarrow \dots$$

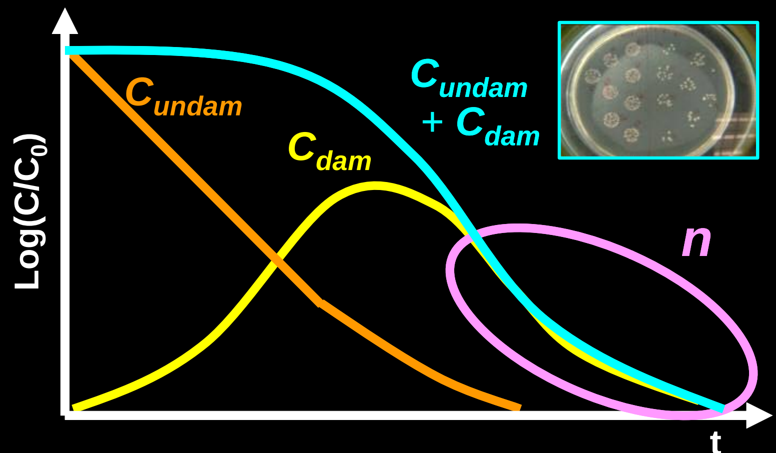
$$\frac{dC_{undam}}{dt} = -k \frac{K\, C_{undam}{}^{n}}{1 + K\, C_{undam}{}^{n} + K\, C_{dam}{}^{n}}$$

$$\frac{dC_{dam}}{dt} = k \frac{K\, C_{undam}{}^{n} - K\, C_{dam}{}^{n}}{1 + K\, C_{undam}{}^{n} + K\, C_{dam}{}^{n}}$$

k : Kinetic constant

K : Pseudo-adsorption constant

n : Inhibition coeffient



K, n : Constant

$k = f\,(C_{cat}, P_{irrad})$

Radiation Absorption

9 kinetic parameters
(10 Exps).

Intrinsic Kinetic Model: Proposed Mechanism

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STEP	REACTION	RATE
Activation	$TiO_2 \xrightarrow{h\nu} TiO_2 + e^- + h^+$	r_g
Recombination	$e^- + h^+ \rightarrow heat$	$\nu_i\, k_2 [e^-][h^+]$
Electron trapping	$e^- + O_2 \rightarrow \bullet O_2^-$	$\nu_i\, k_3 [e^-][O_2]$
Hole trapping	$h^+ + H_2O \rightarrow \bullet OH + H^+$	$\nu_i\, k_4 [h^+][H_2O]$
Hydroxyl attack	$B_u + \ell \bullet OH \rightarrow B_d$	$\nu_i\, k_5 [\bullet OH]^\ell [B_u]$
	$B_d + \ell \bullet OH \rightarrow B_i$	$\nu_i\, k_6 [\bullet OH]^\ell [B_d]$
	$B_i + \ell \bullet OH \rightarrow B_{p1} + B_{p2} + \ldots B_{pi} \ldots + B_{pn}$	$\nu_i\, k_7 [\bullet OH]^\ell [B_i]$
	$B_{p1} + \ell \bullet OH \rightarrow Products$	$\nu_i\, k_{81} [\bullet OH]^\ell [B_{p1}]$
	$B_{p2} + \ell \bullet OH \rightarrow Products$	$\nu_i\, k_{82} [\bullet OH]^\ell [B_{p2}]$
	…	…
	$B_{pi} + \ell \bullet OH \rightarrow Products$	$\nu_i\, k_{8i} [\bullet OH]^\ell [B_{pi}]$
	…	…
	$B_{pn} + \ell \bullet OH \rightarrow Products$	$\nu_i\, k_{8n} [\bullet OH]^\ell [B_{pn}]$
Adsorption	$cell\,site + TiO_{2,bulk} \leftrightarrow TiO_{2,ads}$	K_{ads}

Intrinsic Kinetic Model: General Equation

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$$B_u \xrightarrow{k_5} B_d \xrightarrow{k_6} B_i \xrightarrow{k_7} \left\{ \begin{array}{l} B_{p1} \xrightarrow{k_{81}} \\ B_{p2} \xrightarrow{k_{82}} \\ \quad \cdots \\ B_{pn} \xrightarrow{k_{8n}} \end{array} \right\} \text{Products}$$

$$R_u\left(\frac{\mathrm{CFU}}{\mathrm{s\,cm^3}}\right) = -\alpha_1 \left(\frac{K_{ads} C_{cat}}{1+K_{ads} C_{cat}}\right) \frac{[B_u]^2}{[B_u]+\alpha_4[B_d]+\alpha_3\left([B]_0-[B_u]-[B_d]\right)} \left[-1+\sqrt{1+\frac{\alpha_2 e^a}{S_g C_{cat}}}\right]$$

$$R_d\left(\frac{\mathrm{CFU}}{\mathrm{s\,cm^3}}\right) = \alpha_1 \left(\frac{K_{ads} C_{cat}}{1+K_{ads} C_{cat}}\right) \frac{[B_u]^2-\alpha_4[B_d]^2}{[B_u]+\alpha_4[B_d]+\alpha_3\left([B]_0-[B_u]-[B_d]\right)} \left[-1+\sqrt{1+\frac{\alpha_2 e^a}{S_g C_{cat}}}\right]$$

5 kinetic parameters
≠ f (Nº Exps).

α_1 , α_2 , α_3 , α_4 , K_{ads}

R = f (C_{cat} , e^a , $[B]_0$)

e^a = f (C_{cat} , P_{irrad}, geometry)

Intrinsic Kinetic Model: Limiting Cases

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$$R_u\left(\frac{\mathrm{CFU}}{\mathrm{s\,cm^3}}\right)=-\alpha_1\left(\frac{K_{ads}C_{cat}}{1+K_{ads}C_{cat}}\right)\frac{[\mathrm{B_u}]^2}{[\mathrm{B_u}]+\alpha_4[\mathrm{B_d}]+\alpha_3\left([\mathrm{B}]_0-[\mathrm{B_u}]-[\mathrm{B_d}]\right)}\left[-1+\sqrt{1+\frac{\alpha_2 e^a}{S_g C_{cat}}}\right]$$

$$R_d\left(\frac{\mathrm{CFU}}{\mathrm{s\,cm^3}}\right)=\alpha_1\left(\frac{K_{ads}C_{cat}}{1+K_{ads}C_{cat}}\right)\frac{[\mathrm{B_u}]^2-\alpha_4[\mathrm{B_d}]^2}{[\mathrm{B_u}]+\alpha_4[\mathrm{B_d}]+\alpha_3\left([\mathrm{B}]_0-[\mathrm{B_u}]-[\mathrm{B_d}]\right)}\left[-1+\sqrt{1+\frac{\alpha_2 e^a}{S_g C_{cat}}}\right]$$

$K_{ads}C_{cat} >> 1$

~~K_{ads}~~

4 kinetic parameters

α_1, α_2, α_3, α_4

Meaningless simulation results for C_{cat} effect

$K_{ads}C_{cat} \rightarrow 0$

$\alpha = \alpha_1 K_{ads}$

4 kinetic parameters

α, α_2, α_3, α_4

Intrinsic Kinetic Model: Limiting Cases

$$\ldots \sim \left[-1+\sqrt{1+\frac{\alpha_2 e^a}{S_g C_{cat}}}\right]$$

$$\frac{\alpha_2 e^a}{S_g C_{cat}} >> 1 \qquad\qquad \frac{\alpha_2 e^a}{S_g C_{cat}} << 1$$

$$\alpha = \alpha_1 \sqrt{\alpha_2}\, K_{ads} \qquad\qquad \alpha = \frac{\alpha_1\, \alpha_2\, K_{ads}}{2}$$

$$\ldots \sim \sqrt{e^a} \qquad\qquad \ldots \sim e^a$$

Square-root dependence

3 kinetic parameters

α , α_3 , α_4

Linear dependence

3 kinetic parameters

α , α_3 , α_4

Lab Scale Photoreactor: Radiation Model

$$\frac{\mathrm{d}I_{\lambda,\underline{\Omega}}}{\mathrm{d}s} = -\underbrace{\kappa_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{ABSORPTION}} - \underbrace{\sigma_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{OUT-SCATTERING}} + \underbrace{\frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} p \cdot I_{\lambda,\underline{\Omega}'}\mathrm{d}\Omega'}_{\text{IN-SCATTERING}}$$

Lab Scale Photoreactor: Radiation Model

$$\frac{dI_{\lambda,\underline{\Omega}}}{ds} = -\underbrace{\kappa_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{ABSORPTION}} - \underbrace{\sigma_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{OUT-SCATTERING}} + \underbrace{\frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} p \cdot I_{\lambda,\underline{\Omega}'}\, d\Omega'}_{\text{IN-SCATTERING}}$$

RTE Solution → $I_{\lambda,\underline{\Omega}}$

INTENSITY OF RADIATION
Monochromatic, Directional

Lab Scale Photoreactor: Radiation Model

OUTLINE

$$\frac{dI_{\lambda,\underline{\Omega}}}{ds} = -\underbrace{\kappa_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{ABSORPTION}} - \underbrace{\sigma_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{OUT-SCATTERING}} + \underbrace{\frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} p \cdot I_{\lambda,\underline{\Omega}'} d\Omega'}_{\text{IN-SCATTERING}}$$

RTE Solution → $I_{\lambda,\underline{\Omega}}$

INTENSITY OF RADIATION
Monochromatic, Directional

Integration on the spherical space of directions

$$G_\lambda = \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} d\Omega$$

INCIDENT RADIATION

Lab Scale Photoreactor: Radiation Model

$$\frac{dI_{\lambda,\underline{\Omega}}}{ds} = \underbrace{-\kappa_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{ABSORPTION}} \underbrace{- \sigma_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{OUT-SCATTERING}} + \underbrace{\frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} p \cdot I_{\lambda,\underline{\Omega}'} d\Omega'}_{\text{IN-SCATTERING}}$$

RTE Solution

$$I_{\lambda,\underline{\Omega}}$$

INTENSITY OF RADIATION
Monochromatic, Directional

Integration on the spherical space of directions

$$G_\lambda = \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} d\Omega$$

INCIDENT RADIATION

$$e_\lambda^a = \kappa_\lambda \cdot G_\lambda$$

MONOCHROMATIC RADIATION ABSORPTION

Lab Scale Photoreactor: Radiation Model

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$$\frac{dI_{\lambda,\underline{\Omega}}}{ds} = -\underbrace{\kappa_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{ABSORPTION}} - \underbrace{\sigma_\lambda \cdot I_{\lambda,\underline{\Omega}}}_{\text{OUT-SCATTERING}} + \underbrace{\frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} p \cdot I_{\lambda,\underline{\Omega}'} d\Omega'}_{\text{IN-SCATTERING}}$$

RTE Solution

$$I_{\lambda,\underline{\Omega}}$$

INTENSITY OF RADIATION
Monochromatic, Directional

Integration on the spherical space of directions

$$G_\lambda = \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} d\Omega$$

INCIDENT RADIATION

$$e^a_\lambda = \kappa_\lambda \cdot G_\lambda$$

MONOCHROMATIC RADIATION ABSORPTION

Integration on wavelength

$$\text{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} e^a_\lambda d\lambda$$

LOCAL VOLUMETRIC RATE OF PHOTON ABSORPTION

RTE Resolution

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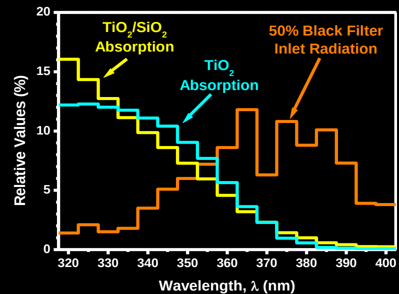
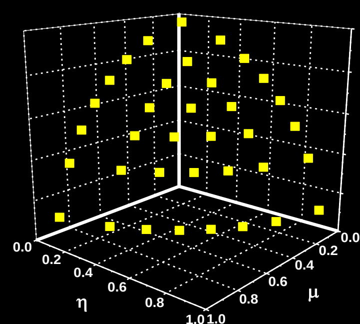
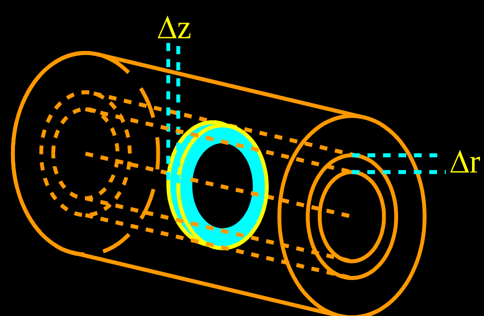
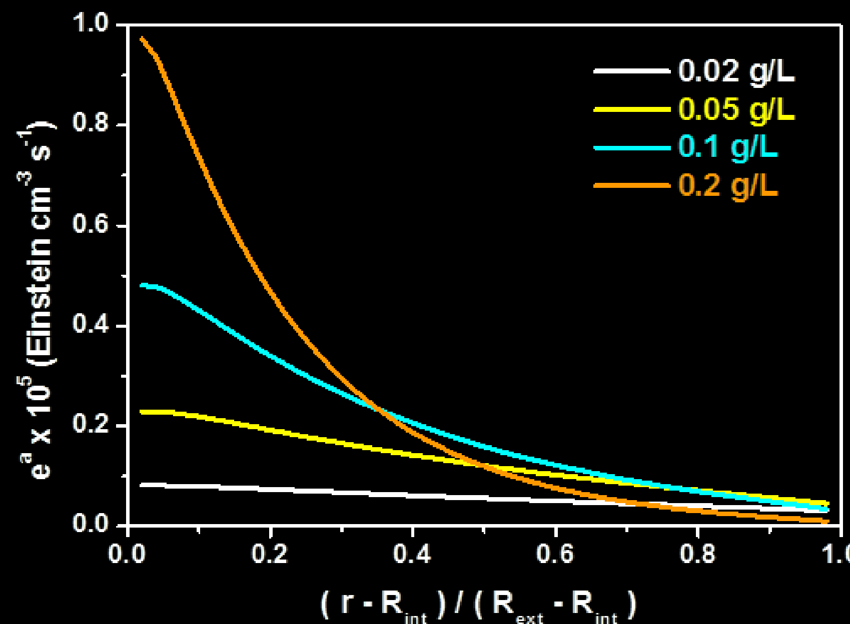


$$\frac{dI_{\lambda,\underline{\Omega}}}{ds} = -\kappa_\lambda \cdot I_{\lambda,\underline{\Omega}} - \sigma_\lambda \cdot I_{\lambda,\underline{\Omega}} + \frac{\sigma_\lambda}{4\pi}\int_{\underline{\Omega}'=4\pi} p \cdot I_{\lambda,\underline{\Omega}'} d\underline{\Omega}'$$

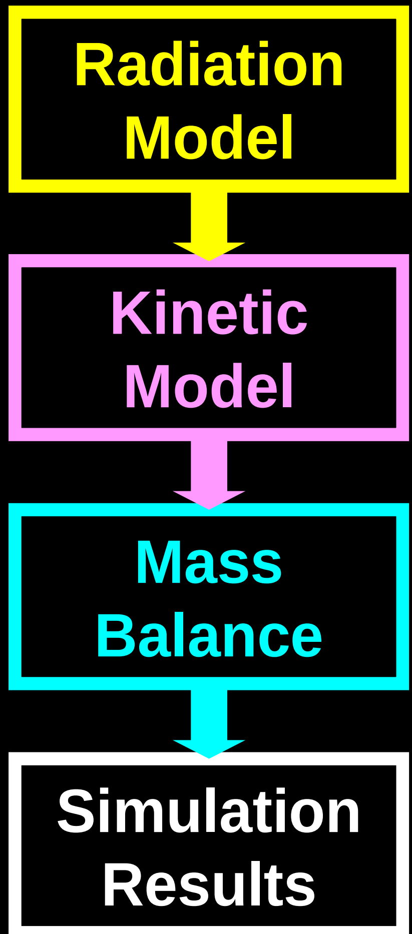
$I_\lambda(r, z, \Omega)$ → $e^a\ (C_{cat}, P_{irrad})$







Kinetic Parameters Estimation



RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\text{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, \mathrm{d}\Omega \, \mathrm{d}\lambda$$

Kinetic Parameters Estimation

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Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\text{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, \mathrm{d}\Omega \mathrm{d}\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^a, [\mathrm{B}]_0\right)$$

Kinetic Parameters Estimation

Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\mathrm{LVRPA} = e^{a} = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, \mathrm{d}\Omega \mathrm{d}\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^{a}, [\mathrm{B}]_0\right)$$

$$\left.\frac{\mathrm{d}[\mathrm{B_u}](t)}{\mathrm{d}t}\right| = \frac{V_{React}}{V_{Tot}} \langle R_u(\underline{x},t) \rangle_{V_{React}} \qquad \left.\frac{\mathrm{d}[\mathrm{B_d}](t)}{\mathrm{d}t}\right| = \frac{V_{React}}{V_{Tot}} \langle R_d(\underline{x},t) \rangle_{V_{React}}$$

Kinetic Parameters Estimation

Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\text{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, \mathrm{d}\Omega \, \mathrm{d}\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^a, [\mathrm{B}]_0\right)$$

$$\left.\frac{\mathrm{d}[\mathrm{B_u}](t)}{\mathrm{d}t}\right| = \frac{V_{React}}{V_{Tot}} \left\langle R_u(\underline{x}, t)\right\rangle_{V_{React}} \qquad \left.\frac{\mathrm{d}[\mathrm{B_d}](t)}{\mathrm{d}t}\right| = \frac{V_{React}}{V_{Tot}} \left\langle R_d(\underline{x}, t)\right\rangle_{V_{React}}$$

$$[\mathrm{B_u} + \mathrm{B_d}](t)$$

Kinetic Parameters Estimation

Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\mathrm{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, d\Omega \, d\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^a, [\mathrm{B}]_0\right)$$

$$\left.\frac{d[\mathrm{B_u}](t)}{dt}\right| = \frac{V_{React}}{V_{Tot}} \left\langle R_u(\underline{x},t)\right\rangle_{V_{React}}$$

$$\left.\frac{d[\mathrm{B_d}](t)}{dt}\right| = \frac{V_{React}}{V_{Tot}} \left\langle R_d(\underline{x},t)\right\rangle_{V_{React}}$$

$[\mathrm{B_u} + \mathrm{B_d}](t)$ ***vs* Experimental**

Simulation Results: 5-Par Model

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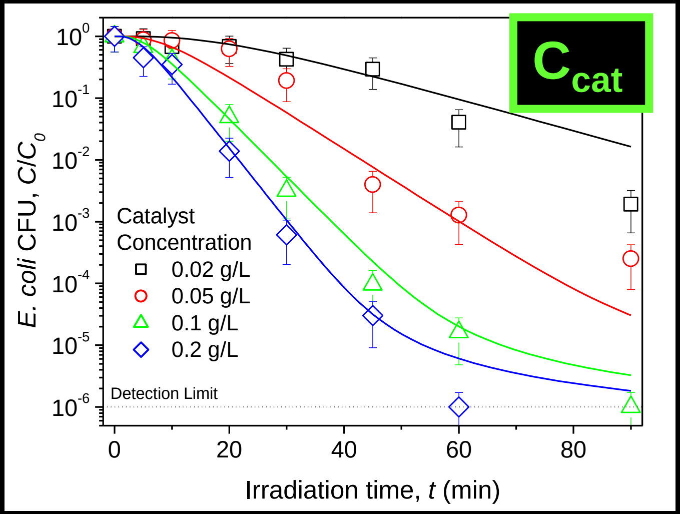
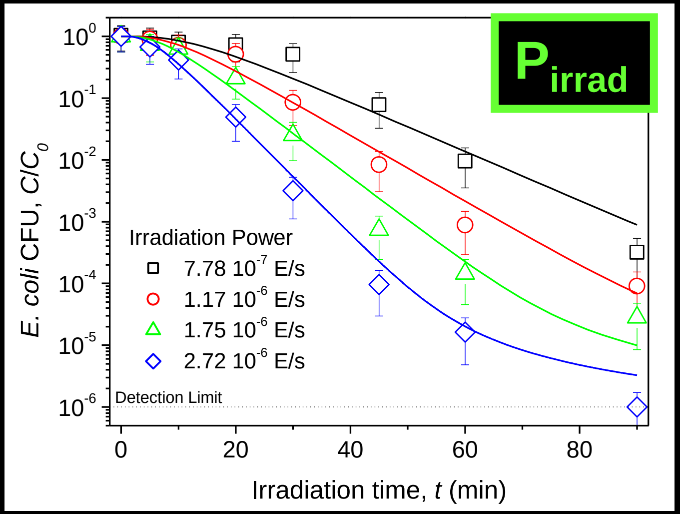
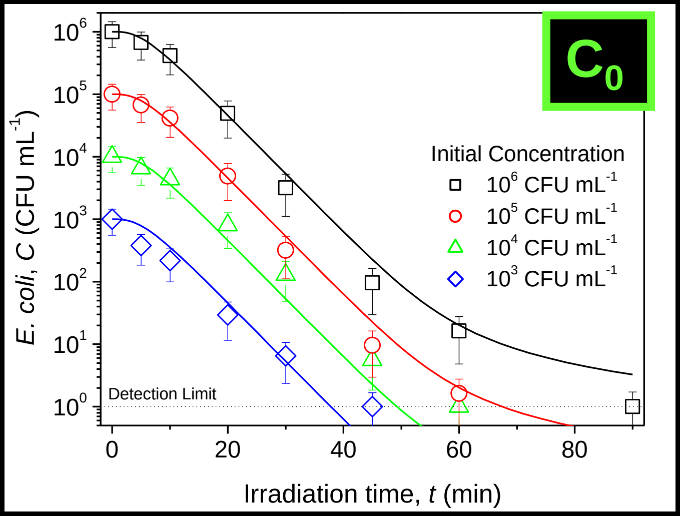
Conclusions.







$\alpha_1 = 1.64 \times 10^2\ s^{-1}$

$\alpha_2 = 1.13 \times 10^{11}\ cm^2 \cdot s \cdot E^{-1}$

$\alpha_3 = 3.11 \times 10^{-6}$

$\alpha_4 = 1.00 \times 10^{-1}$

$K_{ads} = 1.00\ cm^3 \cdot g^{-1}$

SSLE = 6.64

Simulation Results: 4-Par Model

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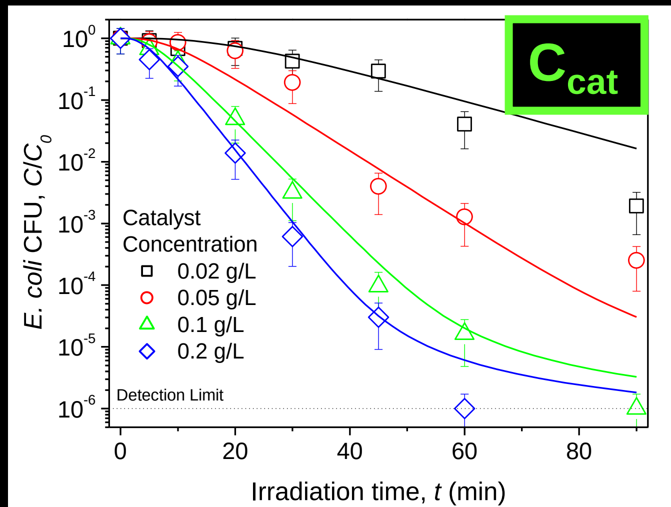

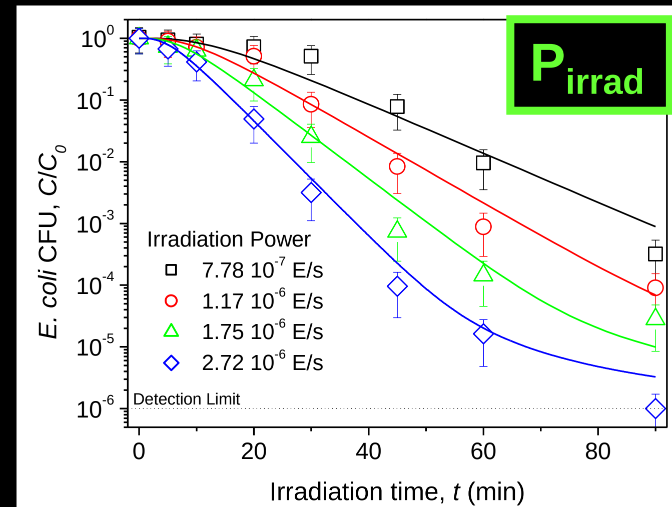

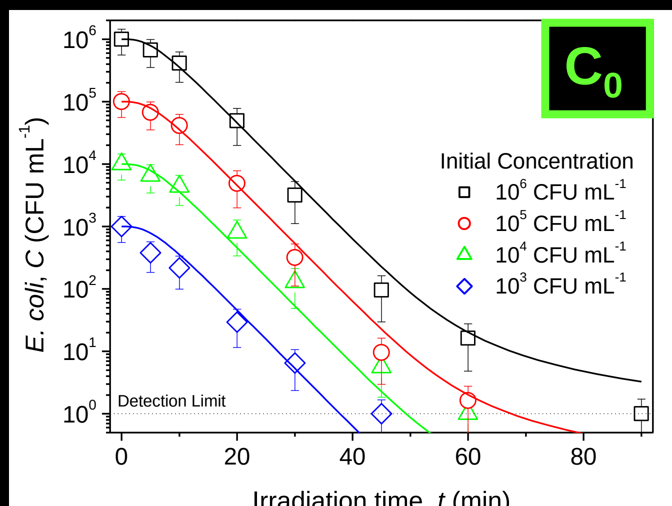

$$K_{ads} C_{cat} \to 0 \qquad \alpha = \alpha_1 K_{ads}$$

α = 1.64 x 10^{2} cm^{3}·s^{-1}·g^{-1}

α_2 = 1.13 x 10^{11} cm^{2}·s·E^{-1}

α_3 = 3.37 x 10^{-6}

α_4 = 1.07 x 10^{-1}

SSLE = 6.64

Simulation Results: 3-Par Model ~ $e^{a\,0.5}$

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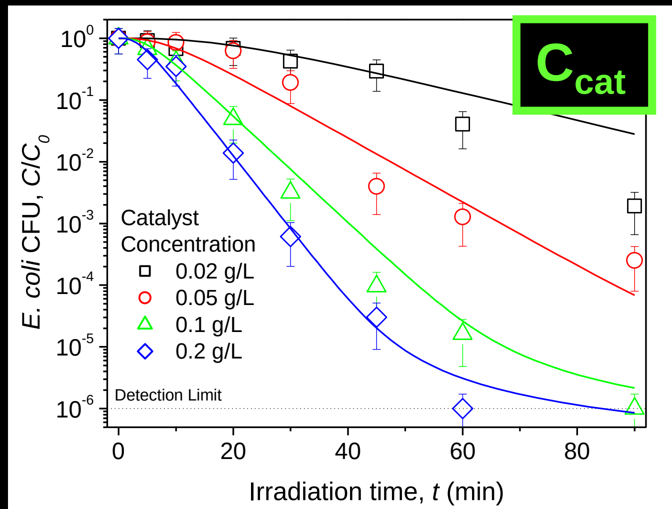

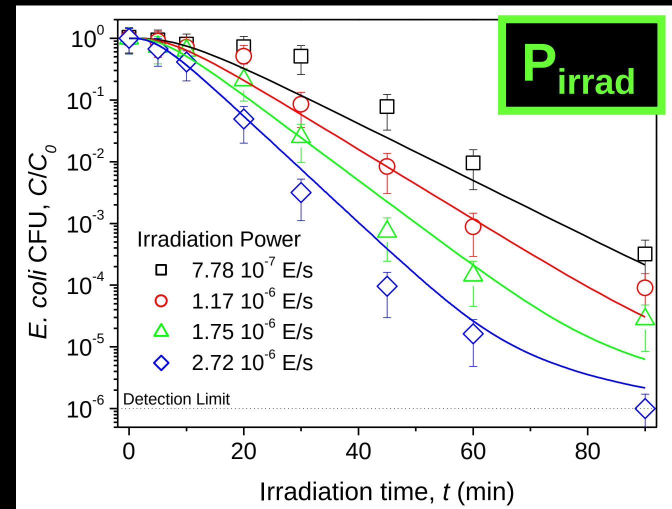

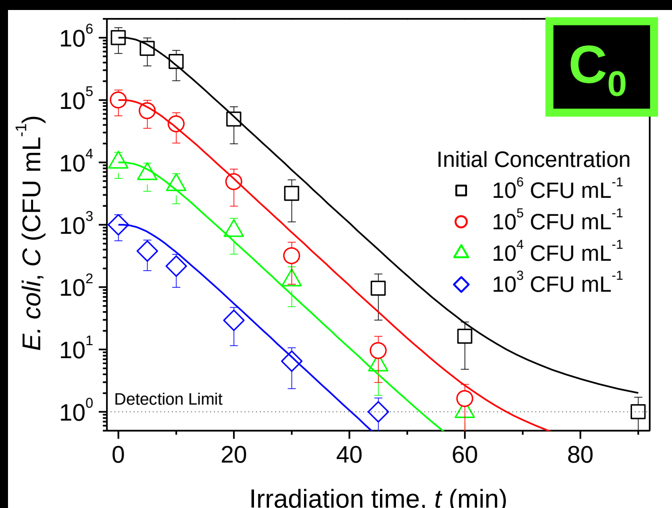

$$\ldots \sim \sqrt{e^{a}} \qquad \alpha = \alpha_1 \sqrt{\alpha_2}\, K_{ads}$$

α = 3.86 x10^{7} cm^{4}·g^{-1}·s$^{-0.5}$·E$^{-0.5}$

α_3 = 2.06 x10^{-6}

α_4 = 1.67 x10^{-1}

SSLE = 7.12

Simulation Results: 3-Par Model ~ e^a

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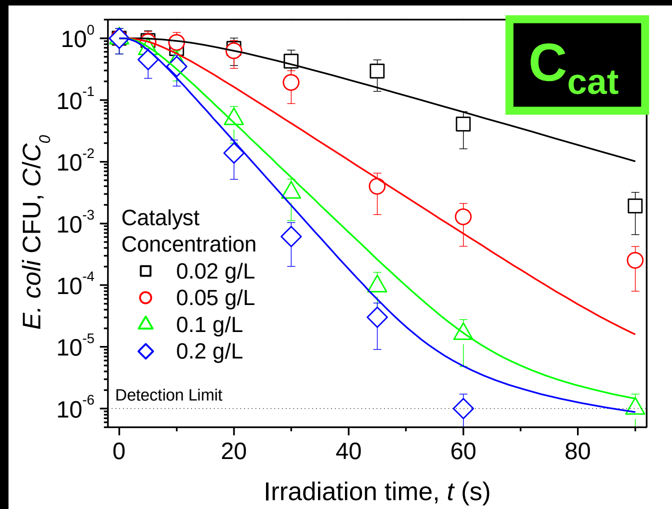
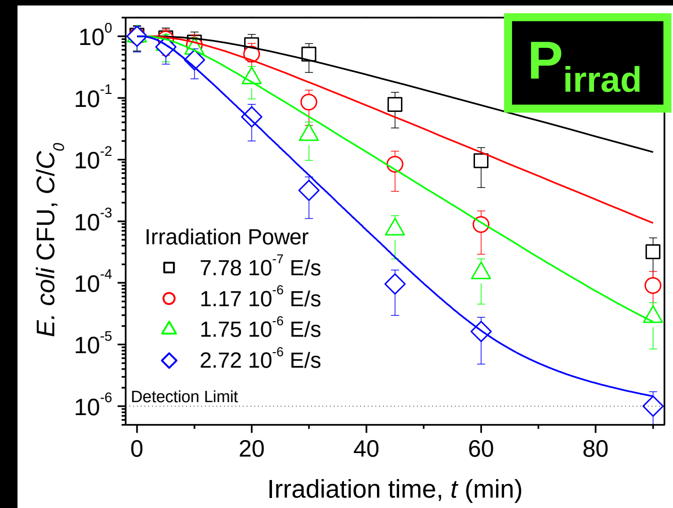
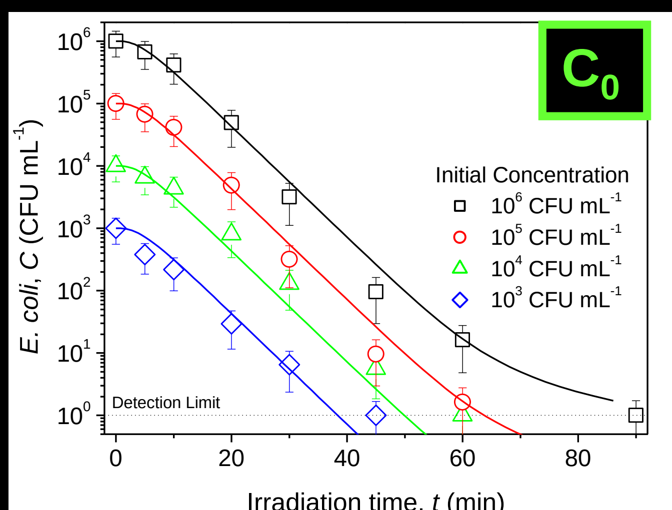
Conclusions.







$$\ldots \sim e^{a} \qquad \alpha = \frac{\alpha_1 \alpha_2 K_{ads}}{2}$$

α = 3.66 x 10^{12} $cm^5 \cdot g^{-1} \cdot E^{-1}$

α_3 = 2.00 x 10^{-6}

α_4 = 2.18 x 10^{-1}

SSLE = 14.28

Bench Scale Photoreactor

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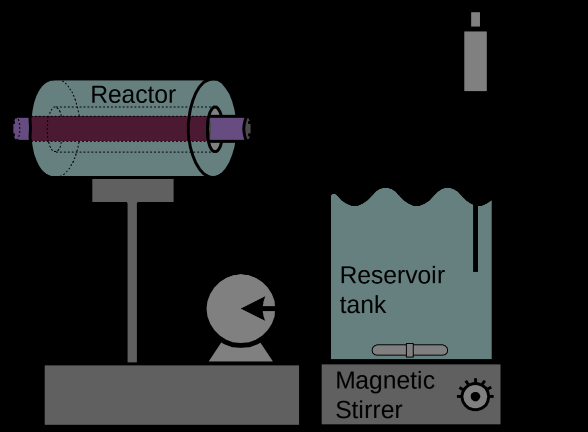


Laboratory scale reactor:

V_R = 188.5 cm^3 , V_{Tot} = 1 L

Lamp: Philips TL 6W

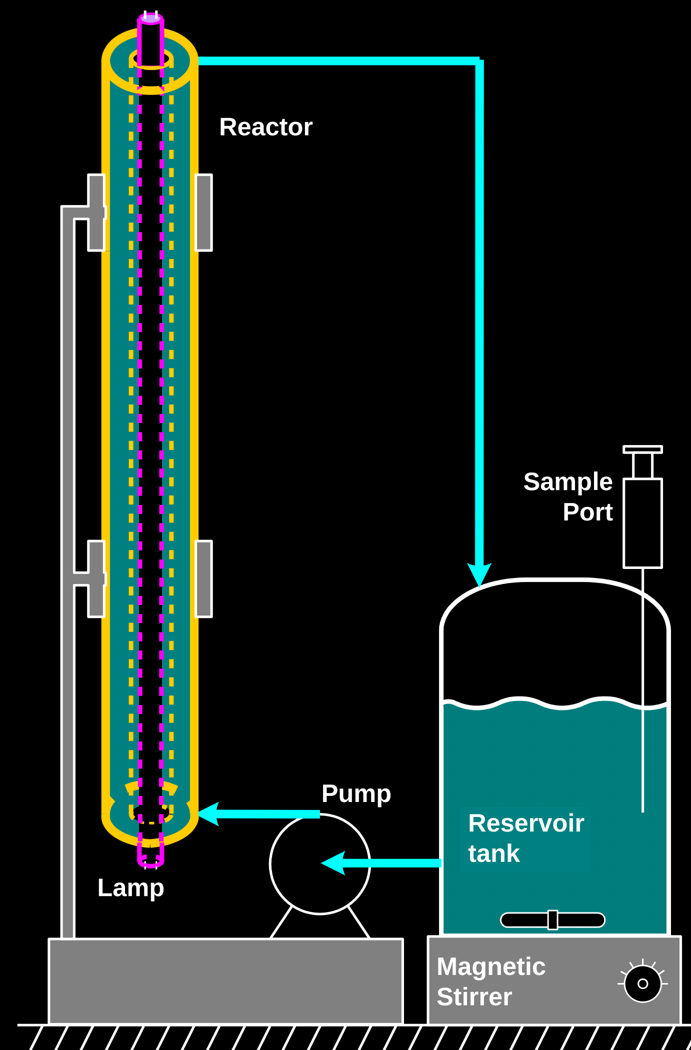
L = 21 cm, Φ = 1.6 cm

Bench scale reactor:

V_R = 1250 cm^3 , V_{Tot} = 5 L

Lamp: Osram L 36W

L = 120 cm, Φ = 2.6 cm



Bench Scale Photoreactor

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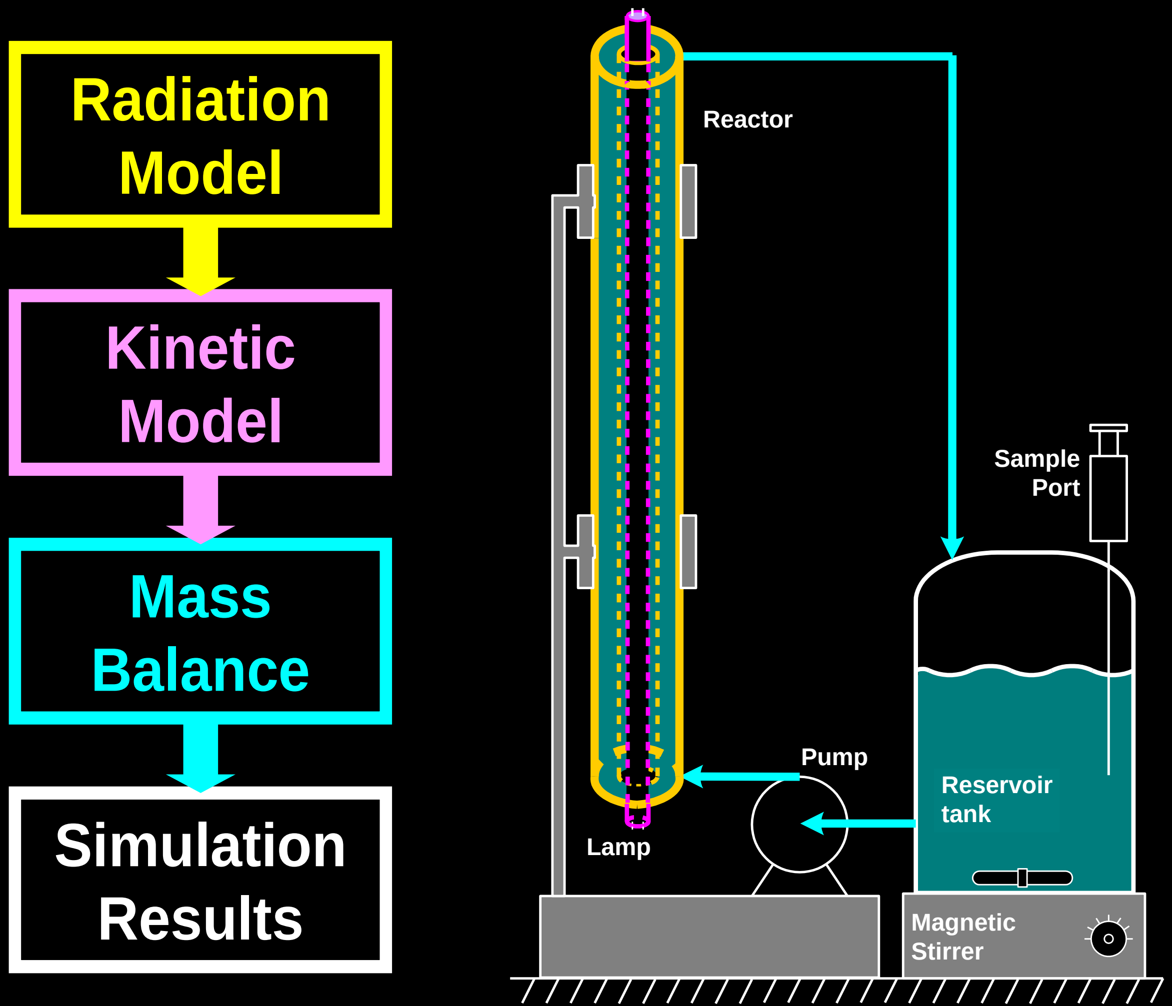
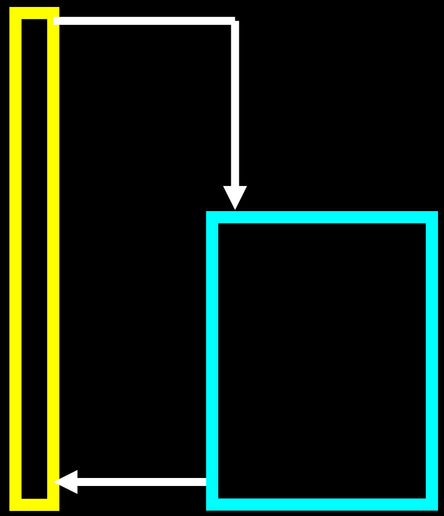


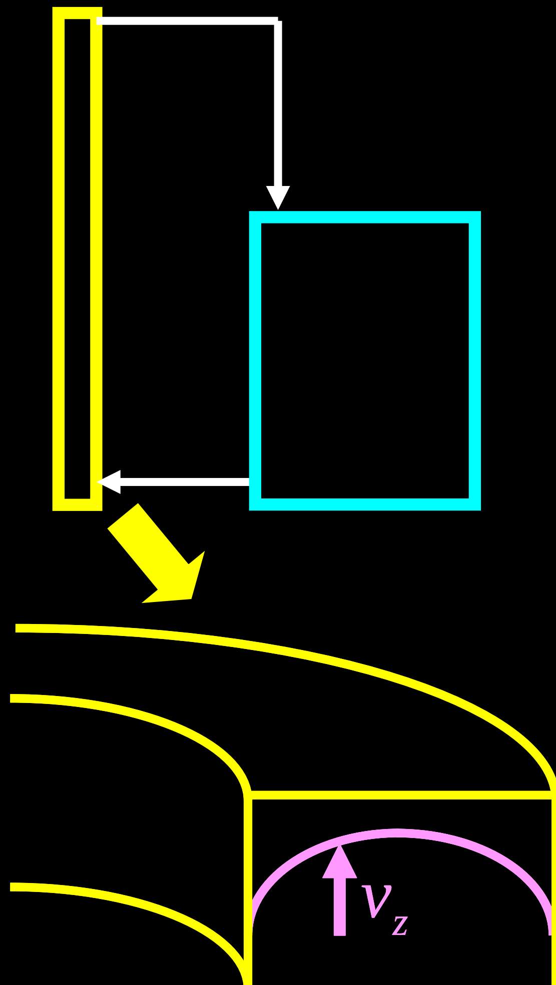
Bench Scale Photoreactor: Mass Balance



$$\left.\frac{d[\mathrm{B}](t)}{dt}\right|_{Tank} = \frac{1}{\tau_{Tank}}\left([\mathrm{B}]^{inlet}(t) - [\mathrm{B}](t)\right)$$

$$[\mathrm{B}](0) = [\mathrm{B}]^{0}$$

Bench Scale Photoreactor: Mass Balance



$$\left.\frac{\mathrm{d}[\mathrm{B}](t)}{\mathrm{d}t}\right|_{Tank} = \frac{1}{\tau_{Tank}}\left([\mathrm{B}]^{inlet}(t) - [\mathrm{B}](t)\right)$$

$$[\mathrm{B}](0) = [\mathrm{B}]^0$$

$$v_z \frac{\partial[\mathrm{B}]}{\partial z} = D^0_{B-Water}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial[\mathrm{B}]}{\partial r}\right)\right) + R_B$$

$$[\mathrm{B}](z)0,r) = [\mathrm{B}](t)$$

$$\frac{\partial[\mathrm{B}](z,r_{int})}{\partial r} = \frac{\partial[\mathrm{B}](z,r_{ext})}{\partial r} = 0$$

Bench Scale Photoreactor: Simulation

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Conclusions.

Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\mathrm{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, \mathrm{d}\Omega \, \mathrm{d}\lambda$$

Bench Scale Photoreactor: Simulation

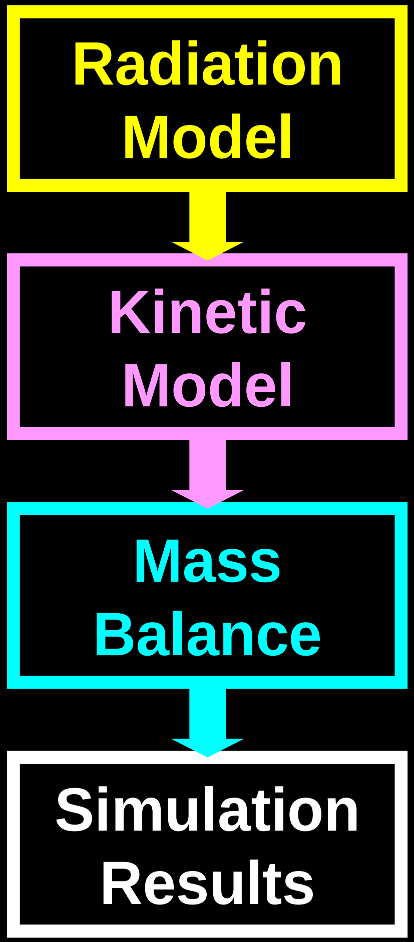
Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\underline{\Omega}} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\text{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\underline{\Omega}} \, \mathrm{d}\Omega \, \mathrm{d}\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^a, [\mathrm{B}]_0\right)$$

Bench Scale Photoreactor: Simulation



RTE → $I_{\lambda,\Omega} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\text{LVRPA} = e^{a} = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\Omega}\, \mathrm{d}\Omega\, \mathrm{d}\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^{a}, [\mathrm{B}]_0\right)$$

$$v_z \frac{\partial [\mathrm{B}]}{\partial z} = D^0_{B-Water}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial [\mathrm{B}]}{\partial r}\right)\right) + R_B$$

$$\left.\frac{\mathrm{d}[\mathrm{B}](t)}{\mathrm{d}t}\right|_{Tank} = \frac{1}{\tau_{Tank}}\left([\mathrm{B}]^{inlet}(t) - [\mathrm{B}](t)\right)$$

Bench Scale Photoreactor: Simulation

Radiation Model → **Kinetic Model** → **Mass Balance** → **Simulation Results**

RTE → $I_{\lambda,\Omega} = f\left(C_{cat}, P_{irrad}, geometry\right)$

$$\text{LVRPA} = e^a = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda \int_{\Omega=4\pi} I_{\lambda,\Omega} \, \mathrm{d}\Omega \, \mathrm{d}\lambda$$

$$R_u, R_d = f\left(\alpha_1, \alpha_2, \alpha_3, \alpha_4, K_{ads}, C_{cat}, e^a, [\mathrm{B}]_0\right)$$

$$v_z \frac{\partial [\mathrm{B}]}{\partial z} = D^0_{B-Water}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial [\mathrm{B}]}{\partial r}\right)\right) + R_B$$

$$\left.\frac{\mathrm{d}[\mathrm{B}](t)}{\mathrm{d}t}\right|_{Tank} = \frac{1}{\tau_{Tank}}\left([\mathrm{B}]^{inlet}(t) - [\mathrm{B}](t)\right)$$

$$[\mathrm{B}](t)$$

Simulated Results

Universidad Rey Juan Carlos

Bench Scale Photoreactor: Simulation

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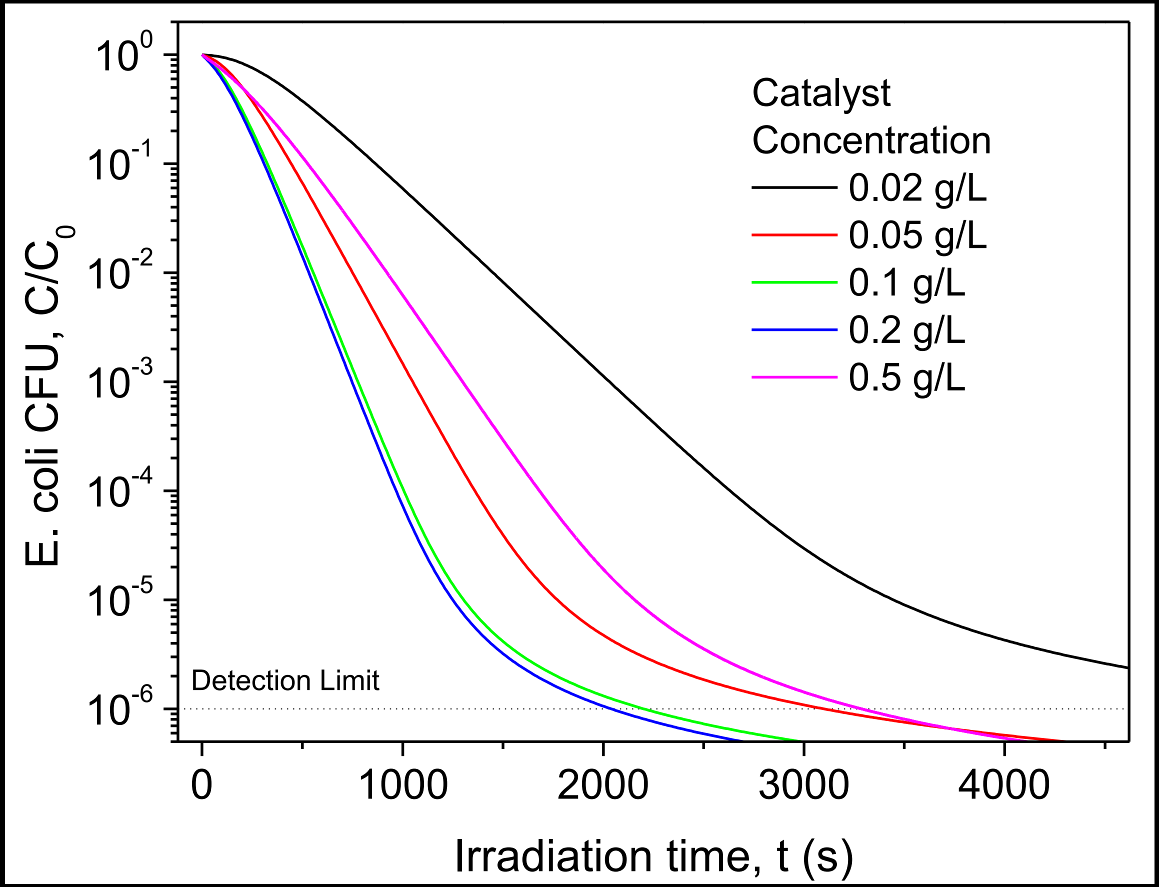

Maximum Activity 0.1-0.2 g/L TiO_2
Significant decrease in activity for 0.5 g/L TiO_2

Bench Scale Photoreactor: VALIDATION

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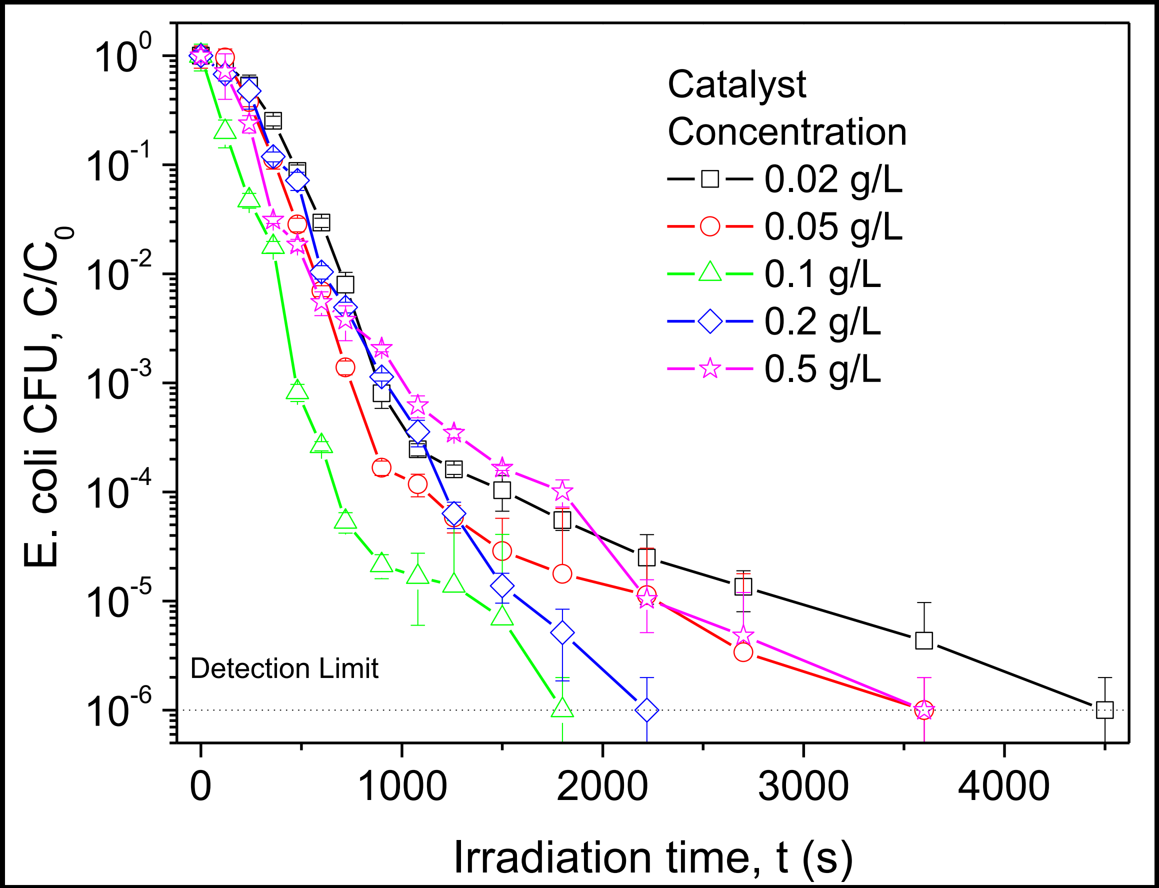
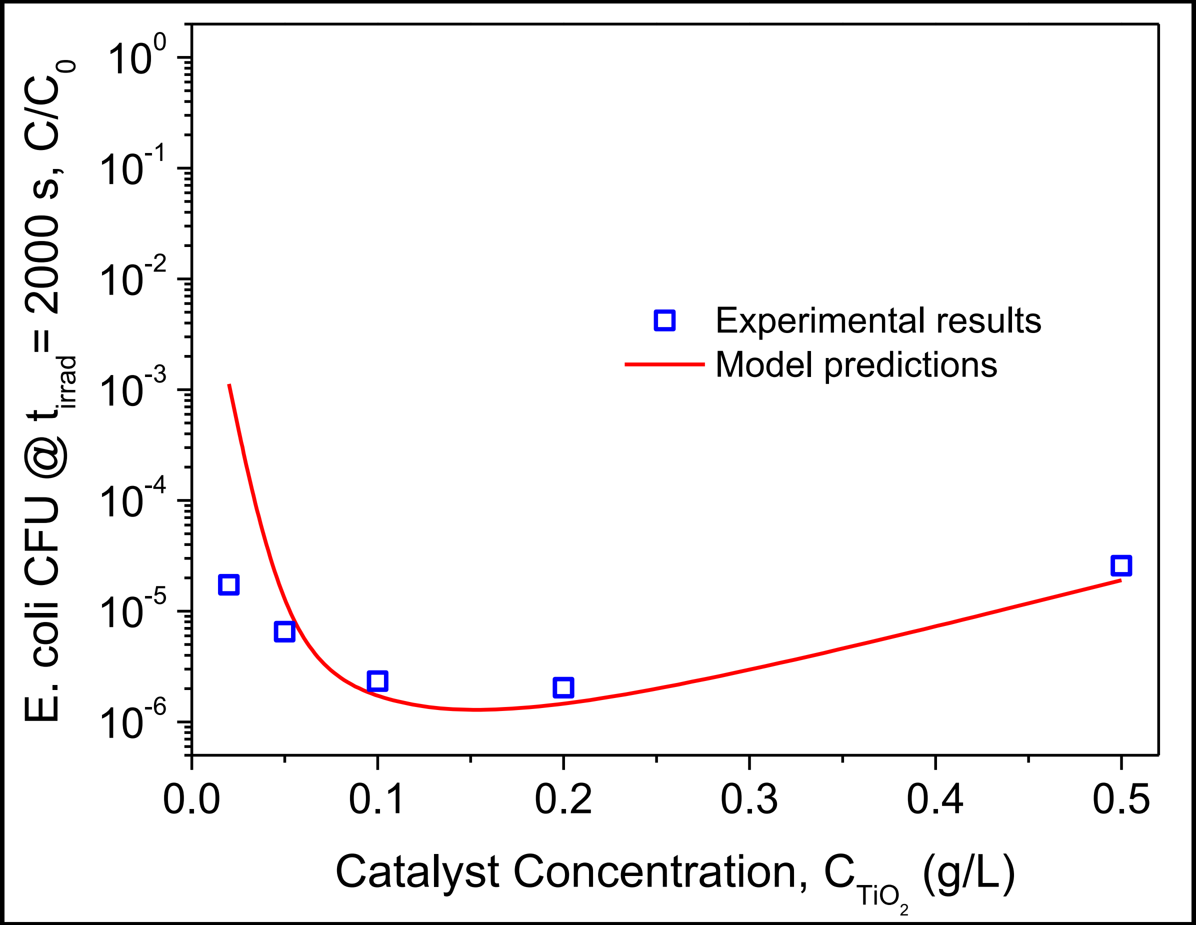
Conclusions.



Maximum Activity 0.1 g/L TiO_2
Significant decrease in activity for 0.5 g/L TiO_2

Bench Scale Photoreactor: VALIDATION



Perfil de Concentración (0.5 g/L)

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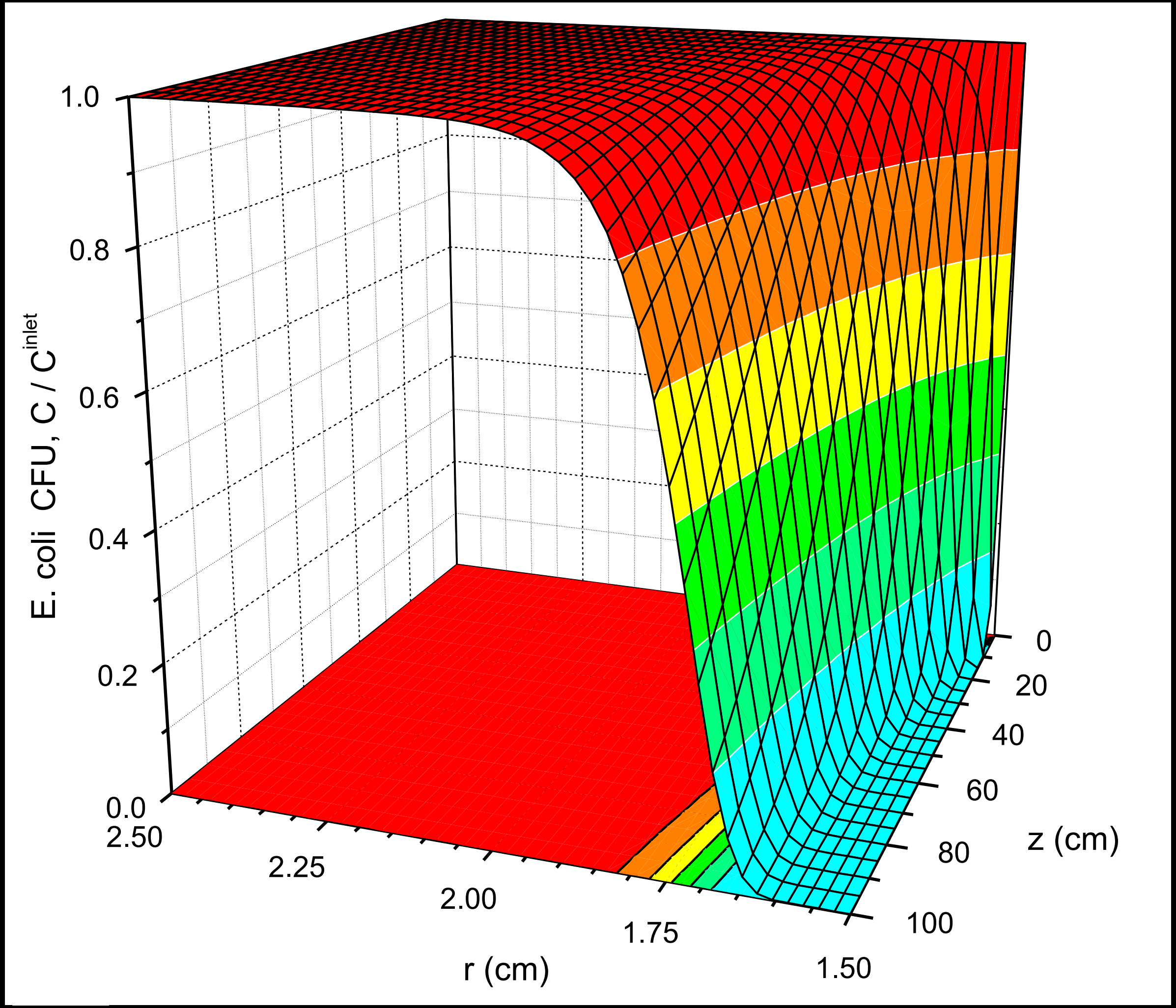


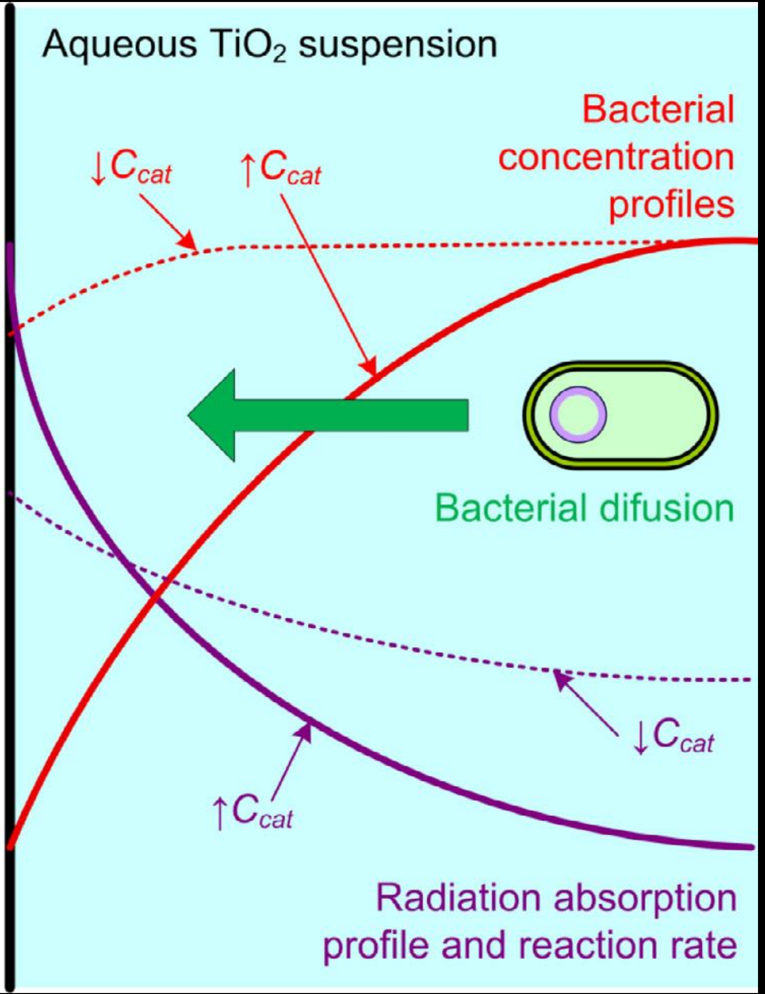
Optimum [TiO_2]: Bacteria vs Molecules

$$D^0_{CN^-} = 1.25 \times 10^{-5} cm^2 s^{-1}$$

Sun et al. (1996)
Metall. Mater. Trans.

$$D^0_{Ecoli} = 9.2 \times 10^{-7} cm^2 s^{-1}$$

Ford & Harvey. (2007)
Adv. Water Res.



Conclusions

- **The performance of large scale photocatalytic reactor has been simulated following an absolutely predictive procedure based on the intrinsic kinetics and the information about the geometry, irradiation source and operation conditions.**
- **The only experimental information required to be determined at laboratory scale is the intrinsic kinetics that describes the explicit dependence of the reaction rate with the LVRPA.**
- **The proposed method for the scaling-up of slurry reactors for the photocatalytic inactivation of *E. coli* with TiO_2 in suspension has been successfully validated in a ten times higher irradiated volume reactor, including the predicted optimum concentration of catalyst predicted by the model.**

Thanks for your attention!

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SIMULATION AND DESIGN OF PHOTOREACTORS

Javier Marugán

Universidad Rey Juan Carlos

AOPs PhD School

Summer School 2017

Porto, 11th July 2017