Evaluation of In Situ Bioremediation of 1,4-Dioxane by Metabolic and Cometabolic Bacteria Using a Contaminant Transport Model

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1,4-DIOXANE REMEDIATION CHALLENGES

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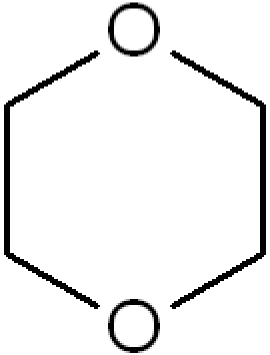
- Miscible in water, strong ether bonds
- *Ex Situ* advanced oxidation, UV, sonication (high cost)
- Phytoremediation (shallow aquifers/soils)
- *In Situ* bioremediation
  - Aerobic: metabolic or cometabolic
  - Anaerobic: insufficient evidence



1,4-Dioxane

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AEROBIC BIODEGRADATION of 1,4-DIOXANE

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METABOLISM		COMETABOLISM
No additional substrate		Higher affinity
Low risk of clogging		Potentially better at dilute plumes
Low oxygen demand	V.S.	THF, **propane**, methane
Pseudonocardia dioxanivorans **CB1190**		*Rhodococcus ruber* **ENV425** and mixed culture **ENV487**
Complete mineralization		Growth sustained

Which approach is best under what conditions? Need to know **kinetics**!

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METABOLIC or COMETABOLIC?

- Lack of information on kinetics for 1,4-dioxane co-metabolism for propane-oxidizing bacteria: ENV425 and ENV487
- Systematic approach to compare performance under *in situ* conditions?
- Effect of low dissolved oxygen concentrations on biodegradation kinetics?
- Incorporate species transport

***Rhodococcus ruber* ENV425**

OBJECTIVE

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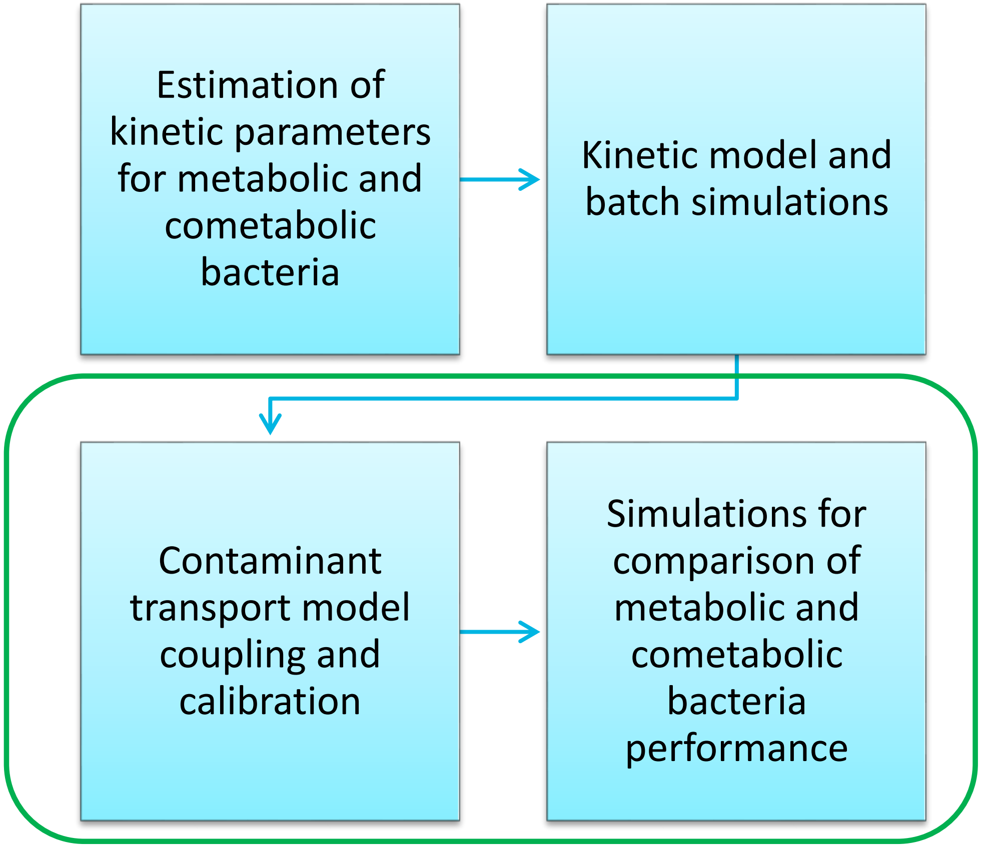
To provide a framework for a systematic approach that compares bioremediation alternatives involving aerobic metabolism and cometabolism of 1,4-dioxane under different in situ scenarios



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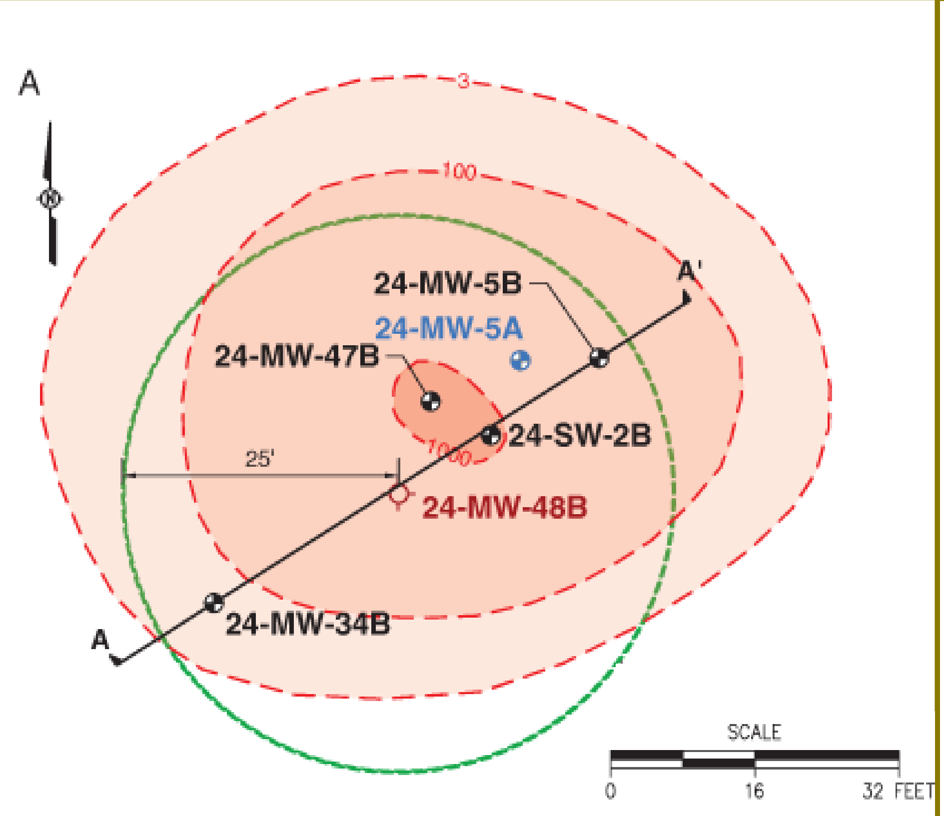
PROCEDURE

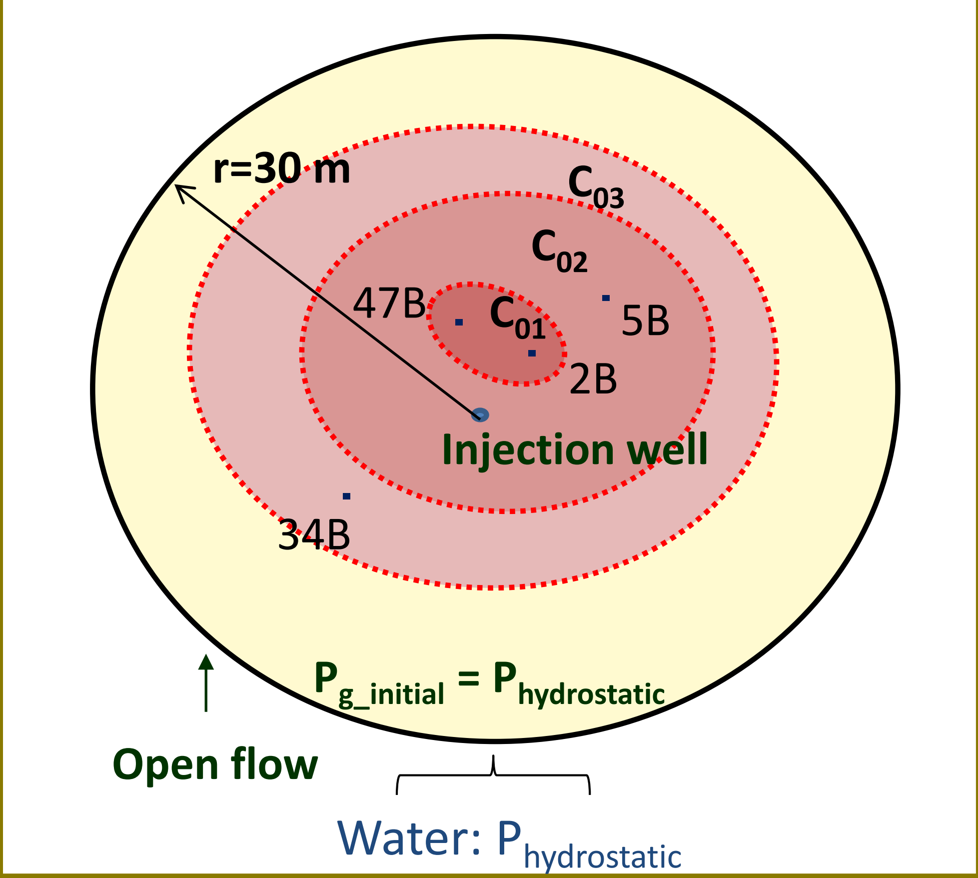
– Contaminant transport model in Comsol Multiphysics®
  - *In situ* air sparging
  - Biodegradation: Monod kinetics for CB1190 (Metabolism) and ENV425 (Cometabolism)
  - Calibrated with field data from a demonstration study (Lippincott et al., 2015) where 1,4-dioxane was successfully removed

Conceptual Model → Governing Equations → Model Calibration and Sensitivity Analysis → Model Simulations

CONCEPTUAL MODEL

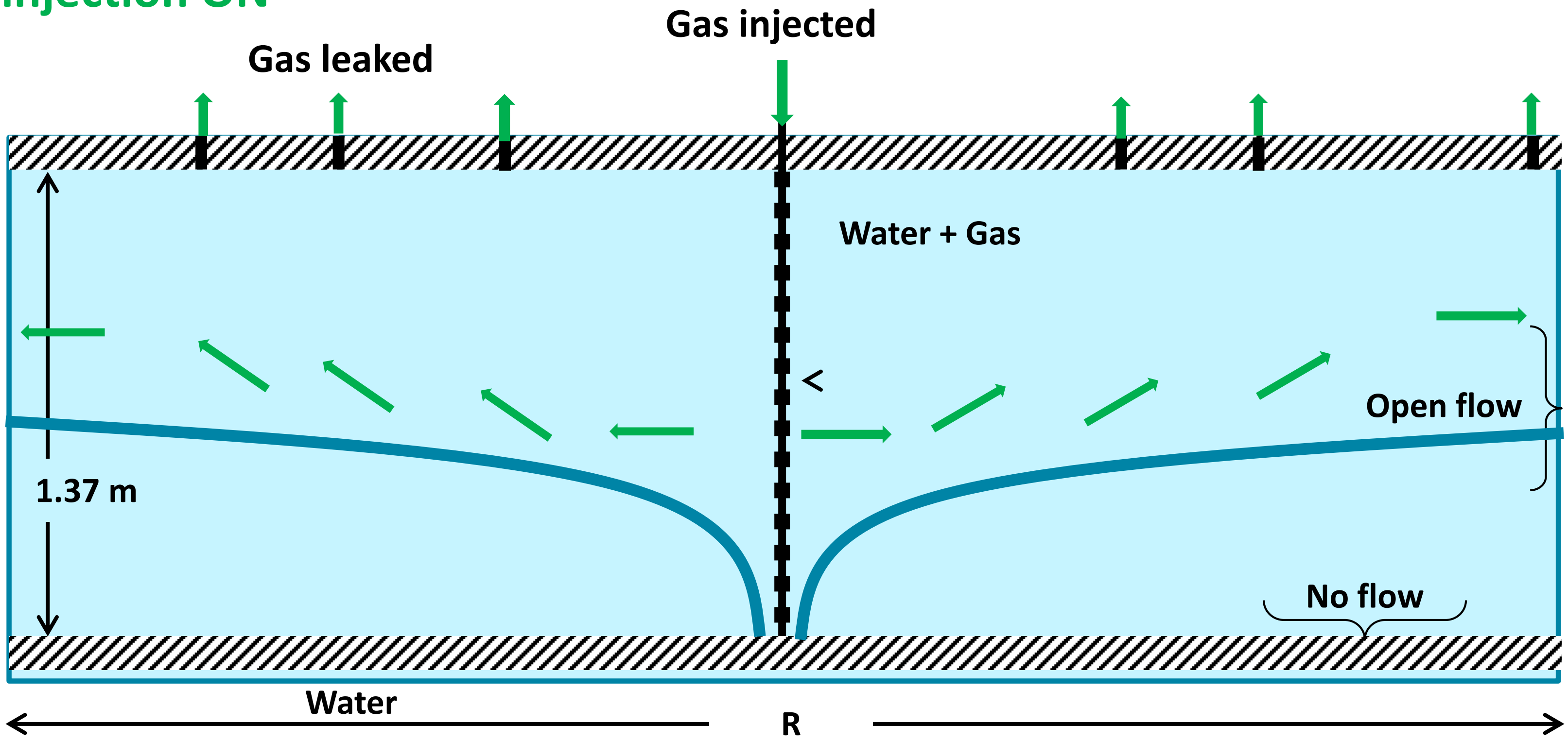


Lippincott et al. (2015)



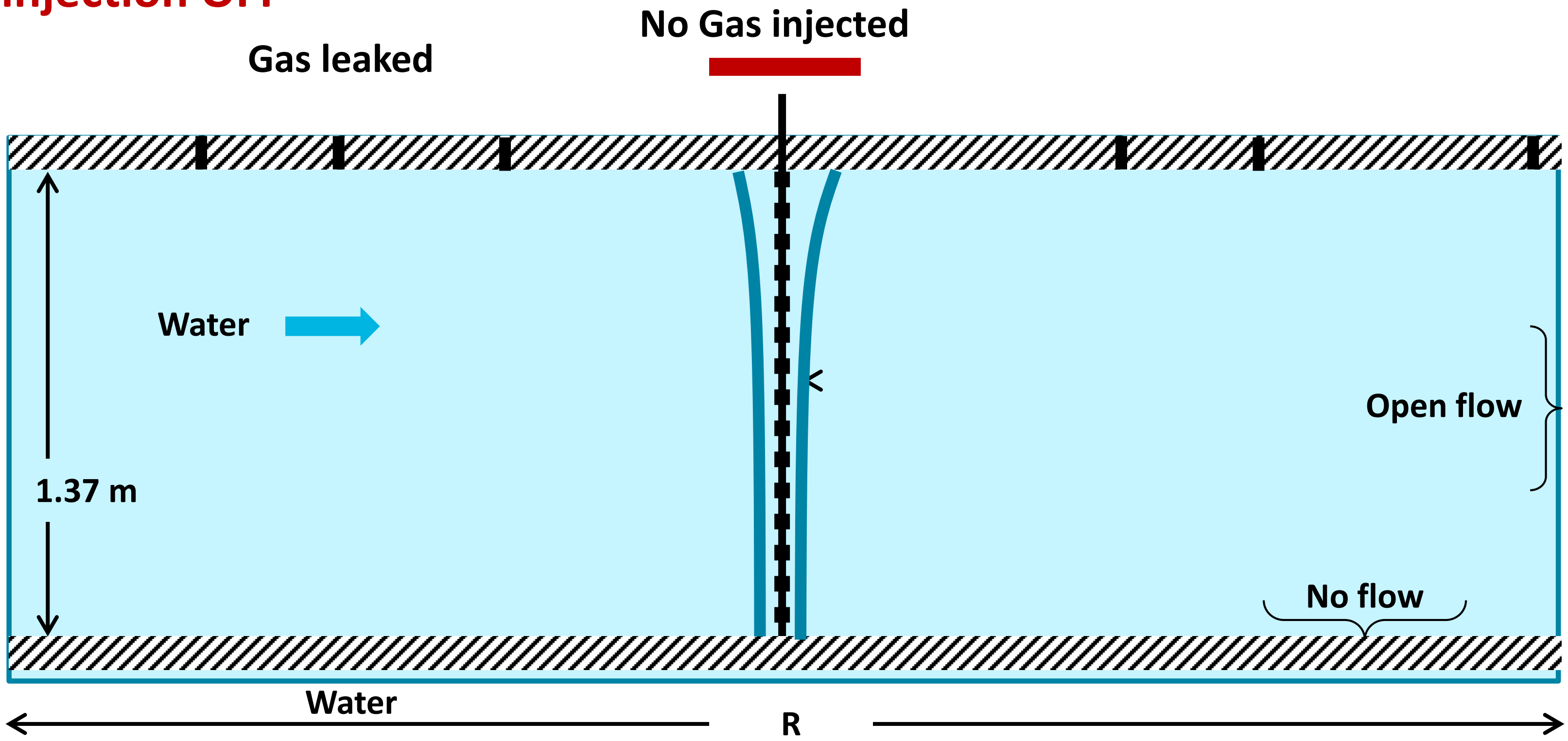
CONCEPTUAL MODEL: TRANSIENT FLOW

Gas injection ON



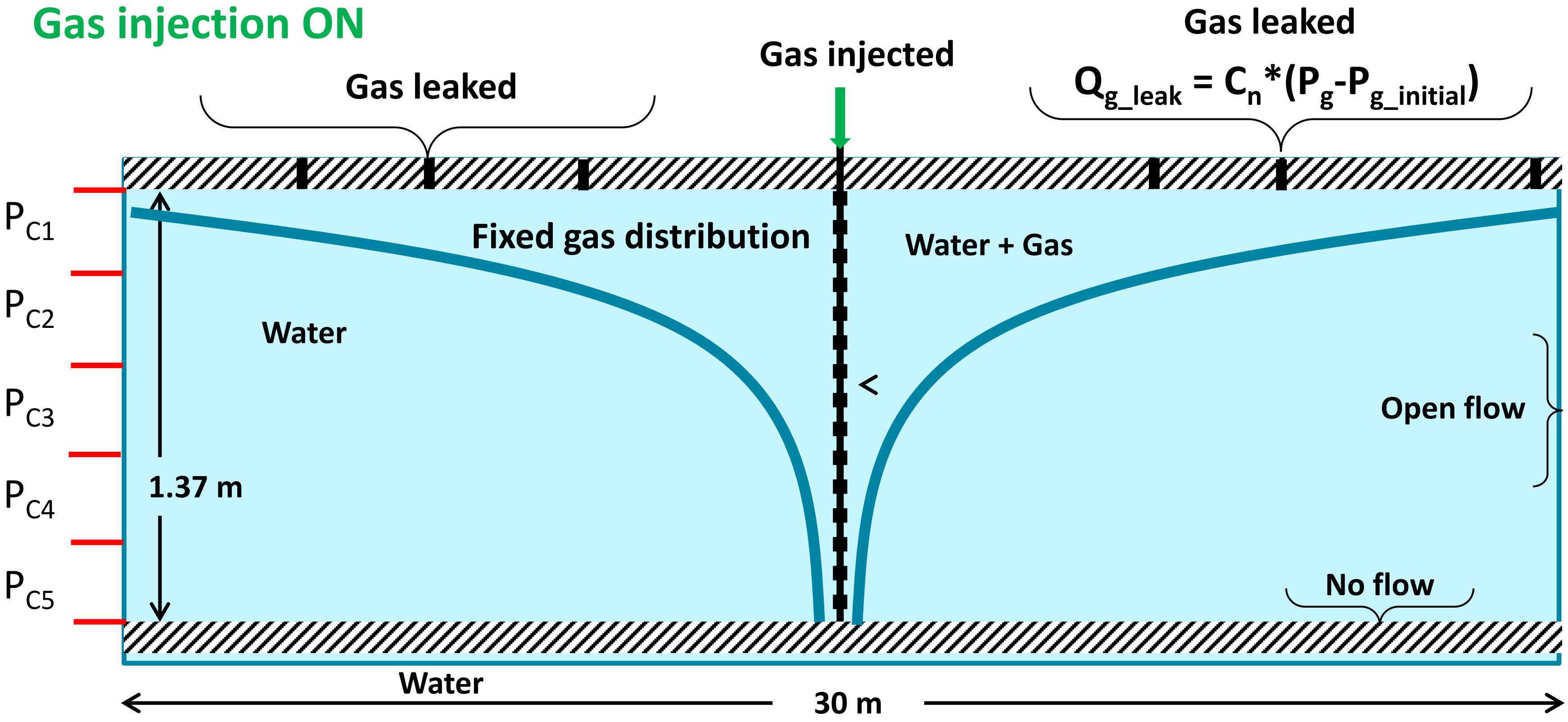
CONCEPTUAL MODEL: TRANSIENT FLOW

Gas injection OFF



CONCEPTUAL MODEL: STEADY STATE FLOW

Gas injection ON



CONCEPTUAL MODEL: ASSUMPTIONS

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– Aquifer thickness
  - Small and divided into 5 segments; capillary pressures from each segment (P_C) are averaged
– Steady state flow
  - Constant injection rate
  - No water movement
– Dispersion in water
  - Adjusted to field data
  - Not dependent on velocity

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GOVERNING EQUATIONS: GAS and WATER FLOW

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Conservation of mass

Darcy flow

$$\nabla \cdot (\rho_g \vec{u}_g) = \varepsilon \dot{S}_g$$

Gas Phase

$$\vec{u}_g = -\frac{k_{rg} k}{\mu_g} (\nabla P_g)$$

$$\nabla \cdot (\rho_w \vec{u}_w) = \varepsilon \dot{S}_w$$

Water Phase

$$\vec{u}_w = -\frac{k_{rw} k}{\mu_w} (\nabla P_w)$$

Flow · **Source/Sink**

Relative permeability · **Intrinsic permeability** · **Velocity** · **Viscosity** · **Pressure gradient**

GOVERNING EQUATIONS: AQUEOUS TRANSPORT

1,4-dioxane, propane, O_2, biomass

$$\frac{dC}{dt} = -\nabla \cdot (\vec{u_w} C) + \nabla \cdot \left(\left(\varepsilon_w \cdot (D_{e,w,C} + D_{h,w,C}) \right) \nabla C \right) - q_C \cdot X$$

$$\frac{dS}{dt} = -\nabla \cdot (\vec{u_w} S) + \nabla \cdot \left(\left(\varepsilon_w \cdot (D_{e,w,S} + D_{h,w,S}) \right) \nabla S \right) - q_S \cdot X + \dot{S}_S$$

$$\frac{dO}{dt} = -\nabla \cdot (\vec{u_w} O) + \nabla \cdot \left(\varepsilon_w \cdot (D_{e,w,O} + D_{h,w,O}) \nabla O \right) - q_O \cdot X + \dot{S}_O$$

$$\frac{dX}{dt} = -\nabla \cdot (\vec{u_w} X) + \nabla \cdot \left(\left(\varepsilon_w \cdot (D_{e,w,X} + D_{h,w,X}) \right) \nabla X \right) - q_X \cdot X$$

Change in time = Advection + Dispersion + Biodegradation + Mass transfer

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GOVERNING EQUATIONS: GAS TRANSPORT

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Propane, O_2

$$\frac{dS_{gas}}{dt} = -\nabla \cdot \left(\vec{u_g} S_{gas}\right) + \nabla \cdot \left(\left(\varepsilon_g \cdot (D_{e,g,Sgas} + \alpha_g^S v_g)\right)\nabla S_{gas}\right) - \dot{S}_{S_{gas}}$$

$$\frac{dO_{gas}}{dt} = -\nabla \cdot \left(\vec{u_g} O_{gas}\right) + \nabla \cdot \left(\left(\varepsilon_g \cdot (D_{e,g,Ogas} + \alpha_g^O v_g)\right)\nabla O_{gas}\right) - \dot{S}_{O_{gas}}$$

Change in time = Advection + Dispersion + Mass transfer

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GOVERNING EQUATIONS

Model calibration

- 1,4-dioxane and propane field data

Sensitivity analysis

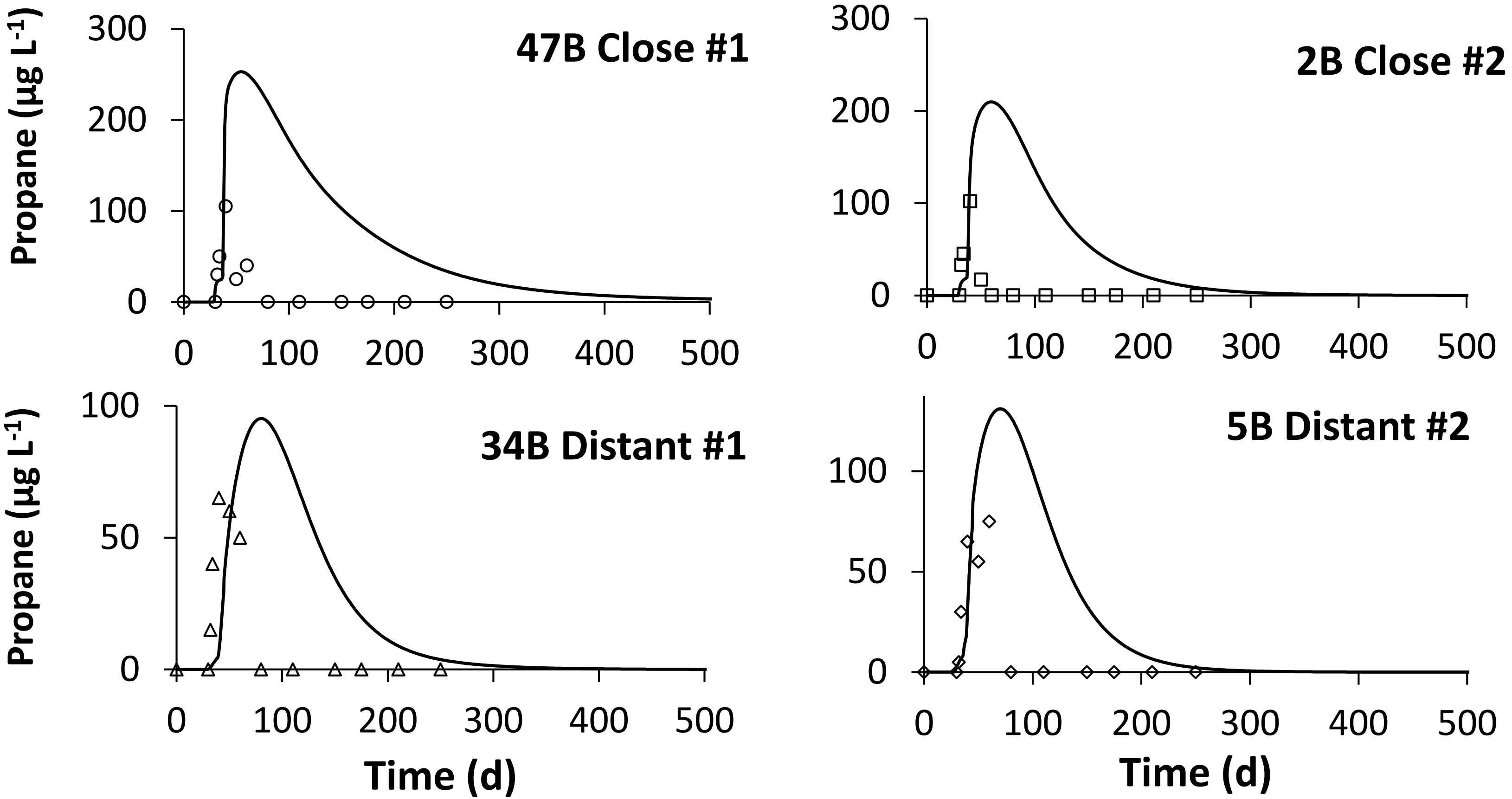
- *Biomass decay*
- *Dispersion Coefficients*
- *Maximum specific 1,4-dioxane biodegradation rate*

Comparison between metabolism (**CB1190**) and cometabolism (**ENV425**)

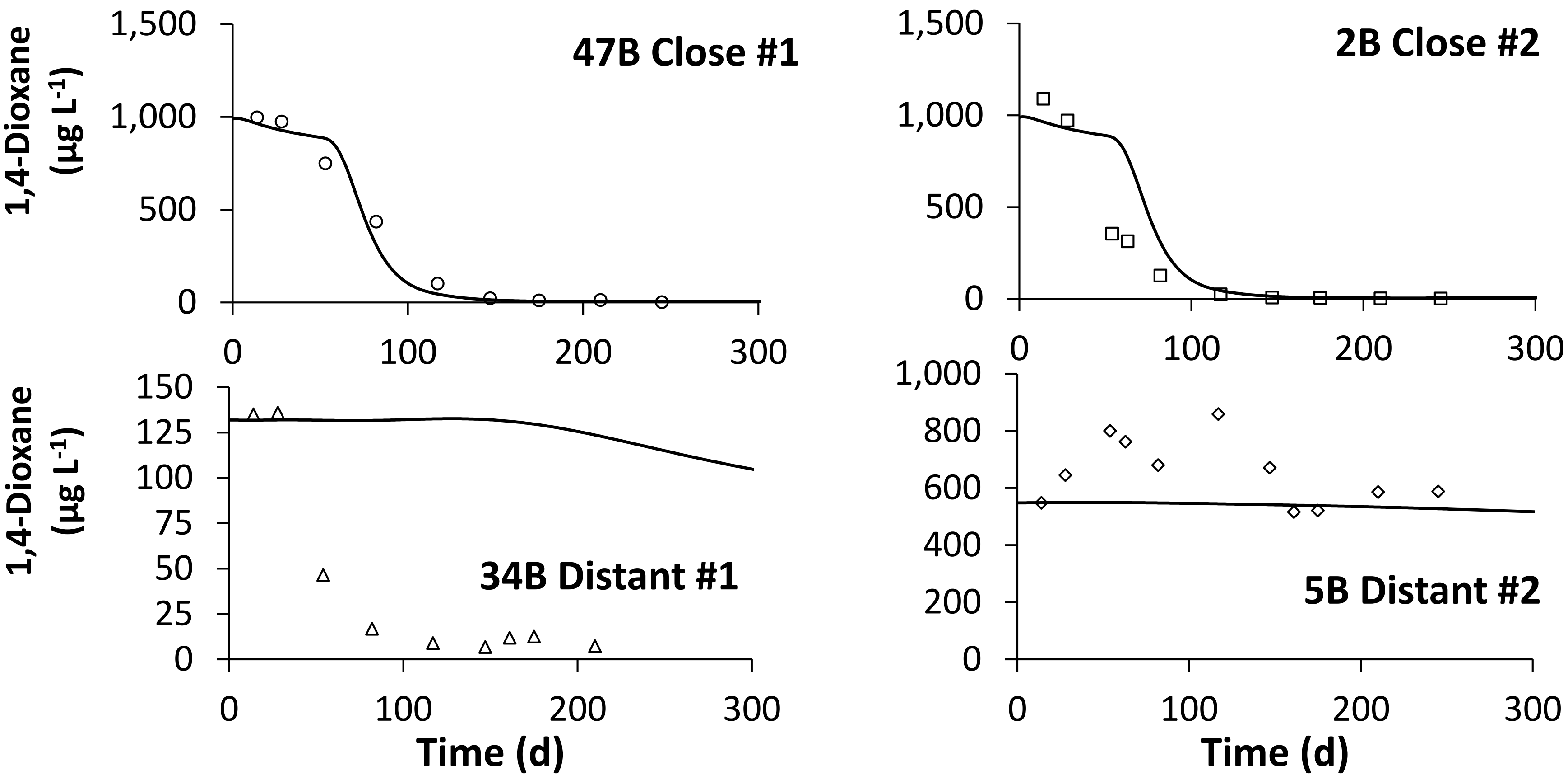
Simulations for different scenarios varying:

- *1,4-Dioxane*
- *Biomass*
- *Propane*
- *Oxygen*

RESULTS: MODEL CALIBRATION



RESULTS: MODEL CALIBRATION



SIMULATIONS RESULTS

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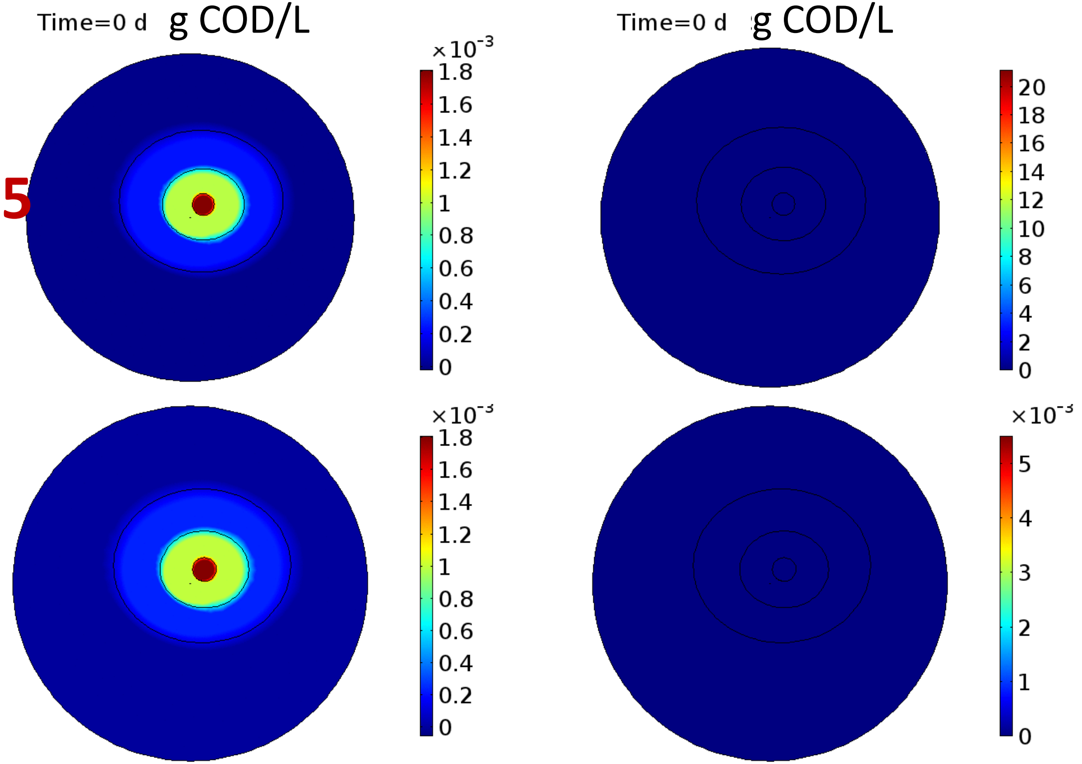
1,4-Dioxane | **Biomass**

Cometabolic, ENV425

Metabolic, CB1190



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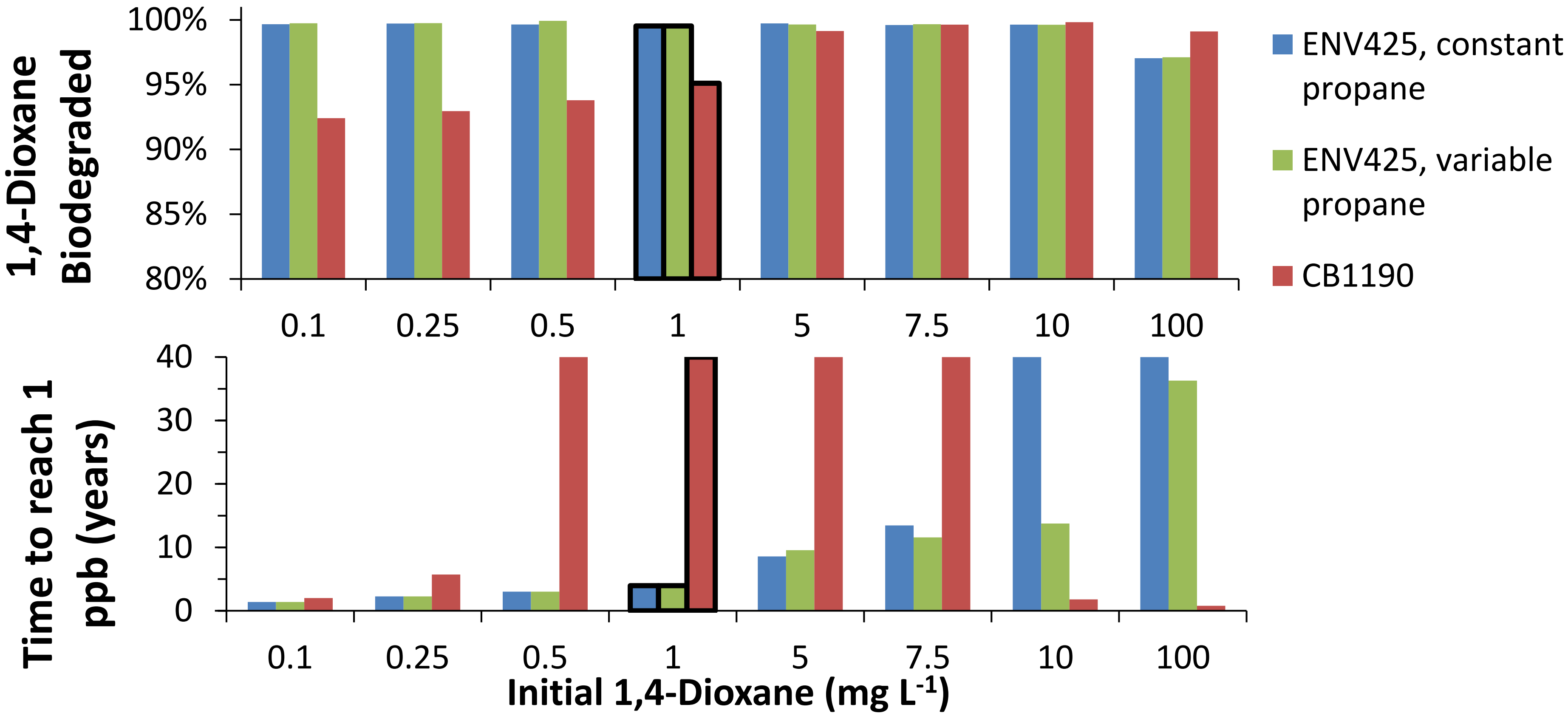
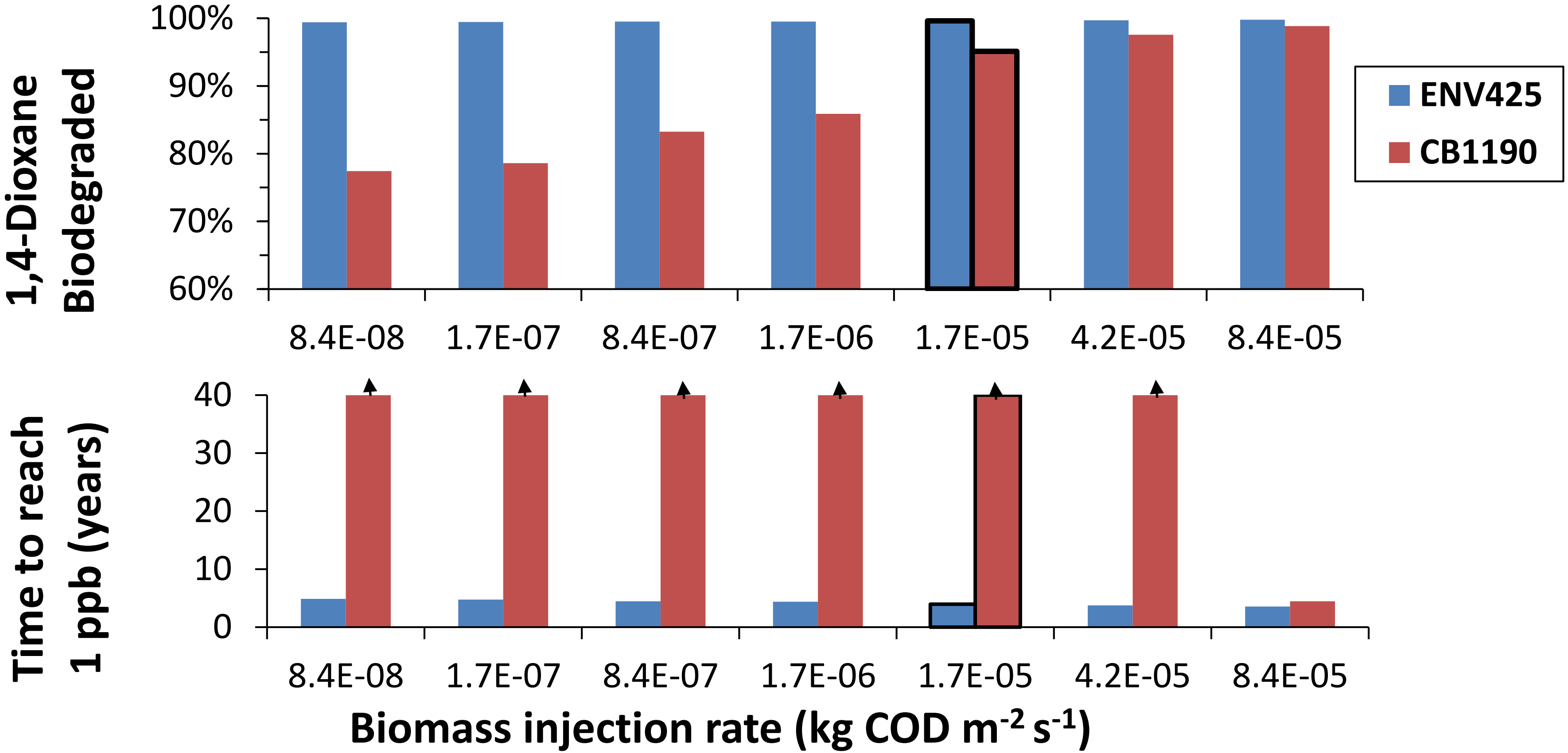
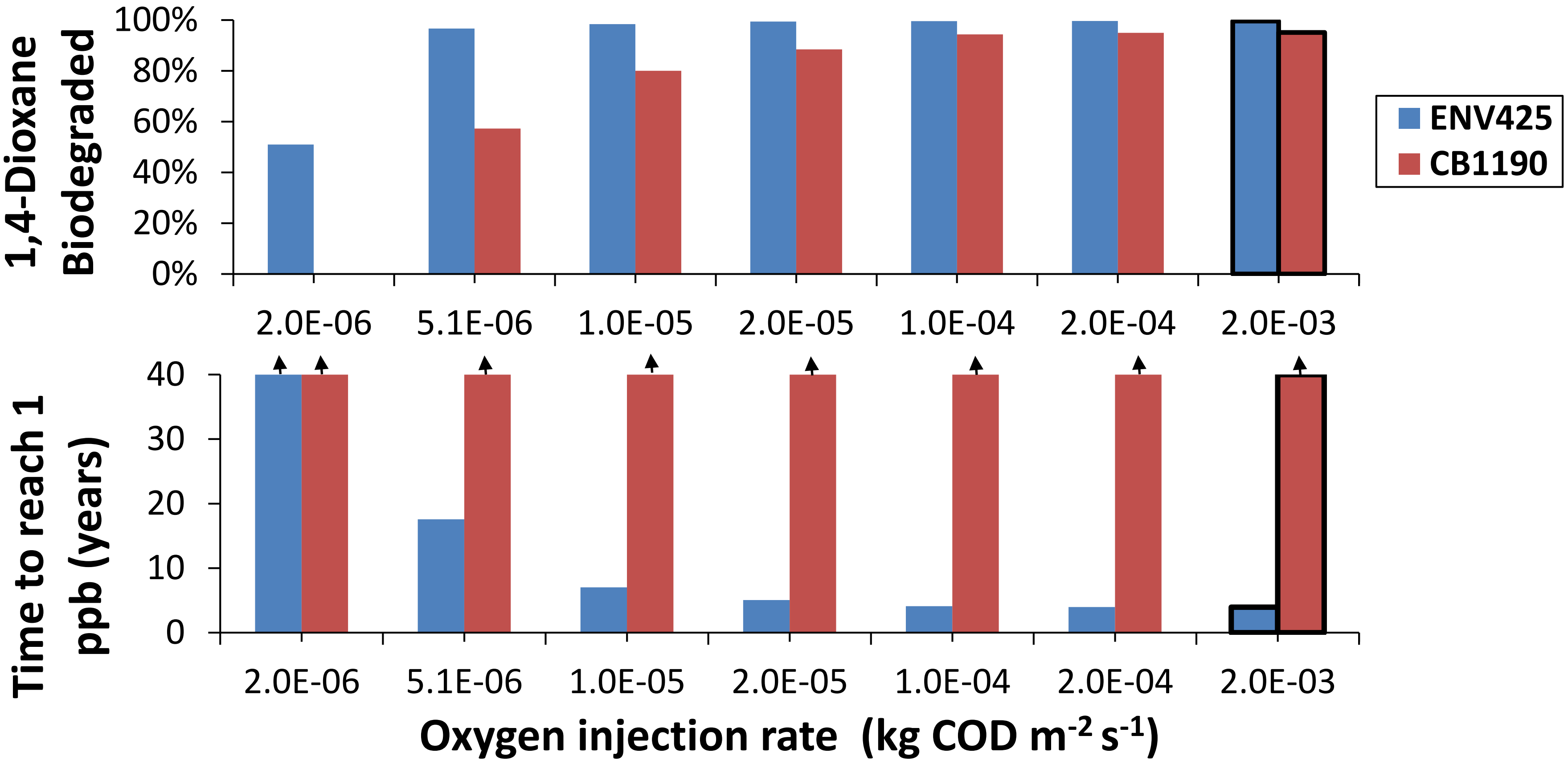
EFFECT of INITIAL 1,4-DIOXANE CONCENTRATION



EFFECT of BIOMASS INJECTION RATE



EFFECT of OXYGEN INJECTION RATE



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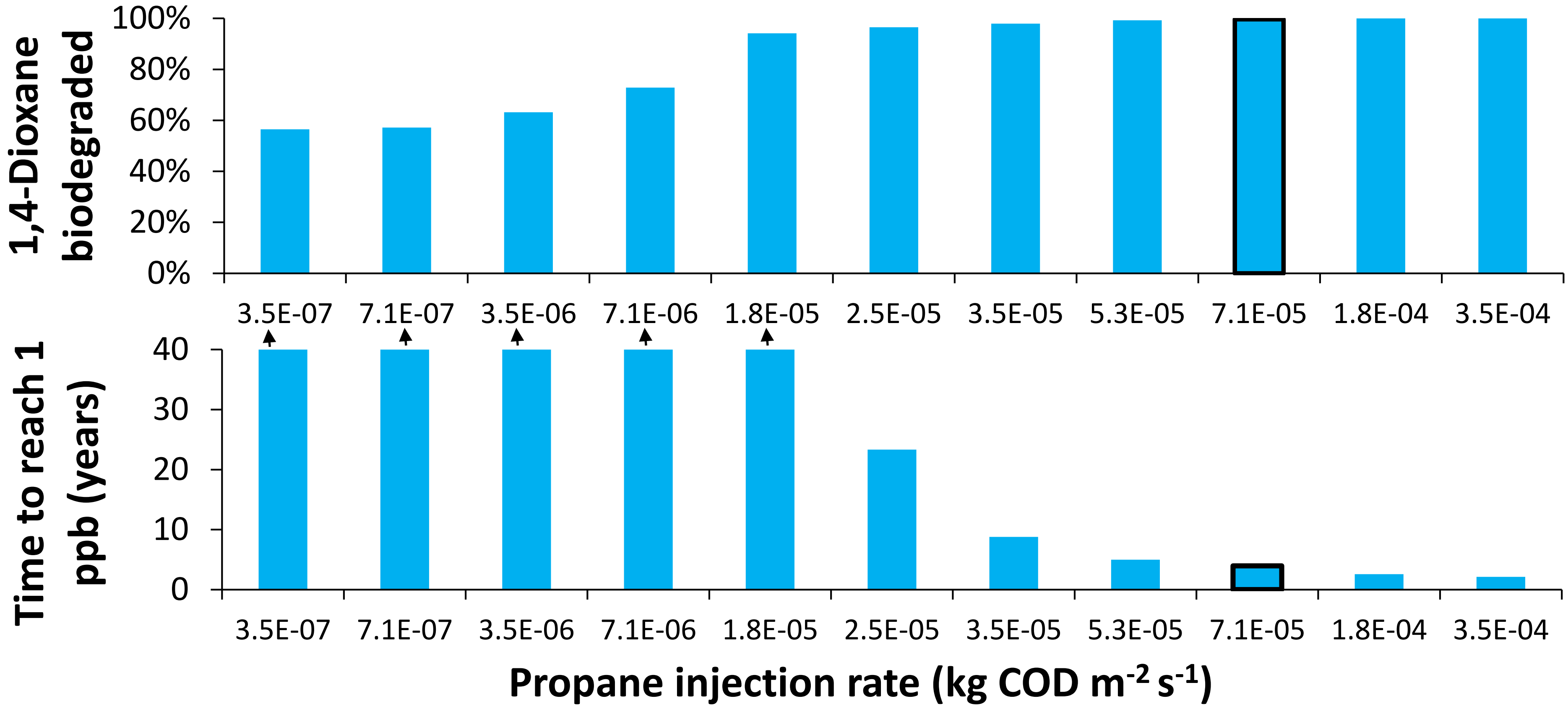
EFFECT of PROPANE INJECTION RATE



SUMMARY AND CONCLUSIONS

- Model calibrated
  - Model fit 1,4-dioxane field data: decrease in two closest wells
  - Model mismatch on one distant well due to heterogeneities and preferential flow in aquifer
- Sensitivity analysis on remediation times and biodegradation
  - Heavily impacted by **decay**, maximum specific 1,4-dioxane degradation rate, and biomass dispersion (data not shown)

SUMMARY AND CONCLUSIONS

- Metabolic and cometabolic comparison:
  - **Cometabolic** culture superior at **~0.1 to 10 mg L^{-1}** of 1,4-dioxane
  - Metabolism similar below ~0.1 mg L^{-1} due to decreased effect of decay
  - Metabolism more affected by **biomass** and **oxygen** injection rates
  - Lowest oxygen rates affected both cultures
  - Propane injection rate effect on remediation times reached a plateau; propane added in excess in the field study

- First step towards a framework for evaluating aerobic bioremediation strategies for 1,4-dioxane plumes that require treatment

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Thank You!

Francisco Barajas