CRC 1253 CATCHMENTS AS REACTORS

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From Chemostat/Retentostat to Soil: Modeling bioavailability limitations on atrazine degradation

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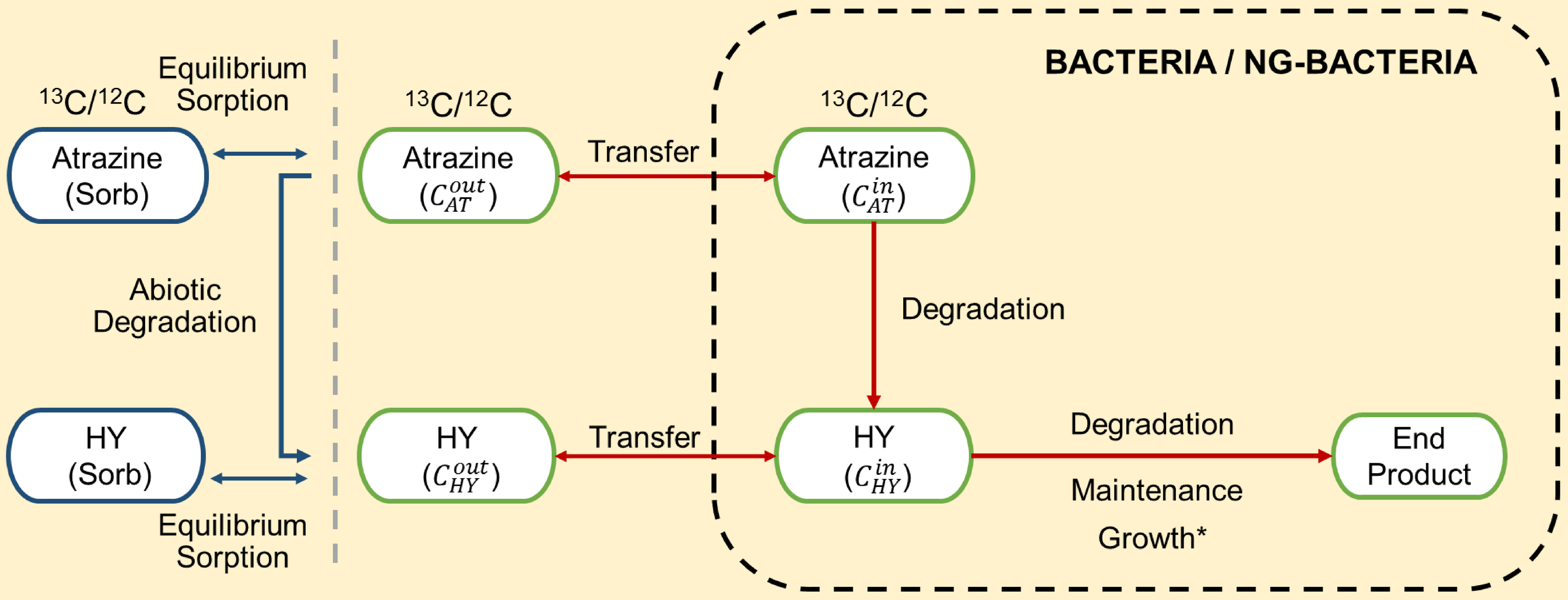
I. Motivation

- Atrazine presents an environmental threat due to its persistence and ecotoxicity.
- Although soil bacteria have evolved effective biodegradation pathways, atrazine persists in soils at low concentrations - converting soils to potential continuous sources of groundwater pollution.
- Limited mass transfer across the cell membrane might control atrazine degradation at low concentrations.

II. Objectives

- Parameterize a mathematical model of atrazine degradation in engineered systems - chemostat/retentostat - using laboratory data.
- Integrate this modeling approach into a soil model to determine the role of mass transfer across bacterial cell membranes against other rate limiting processes in complex environmental systems.

III. Modeling approach for simplified systems (Chemostat/Retentostat)



Model extension for soil simulations.

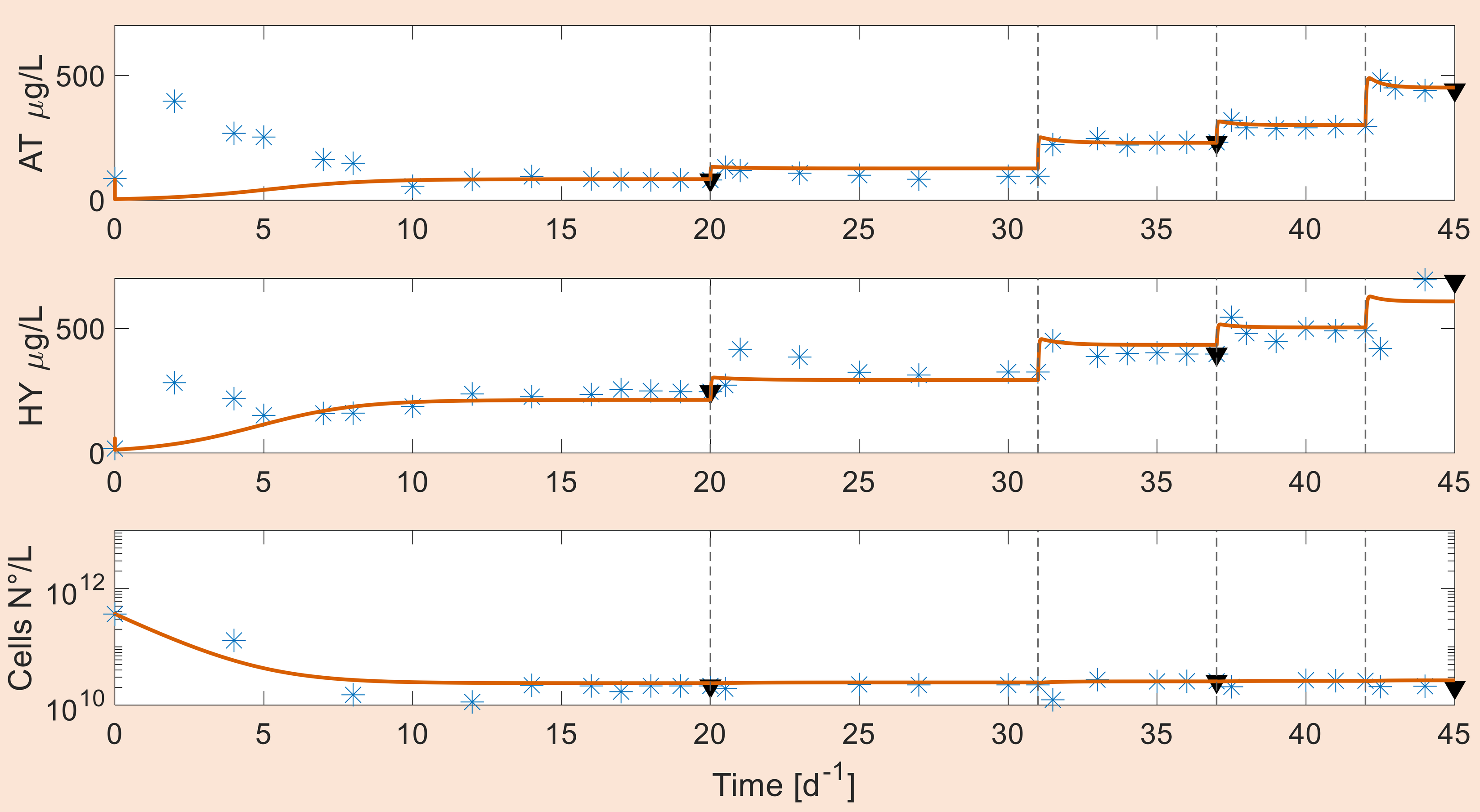
* Only for growing bacteria.

Model Features:

- Growing and non-growing (NG) bacteria
- Degradation rates for both atrazine (AT) isotopologues
- Hydroxyatrazine (HY) degradation coupled with growth and maintenance
- Density-dependent growth
- Compromise maintenance model
- Correction factor for changeable bacterial volume

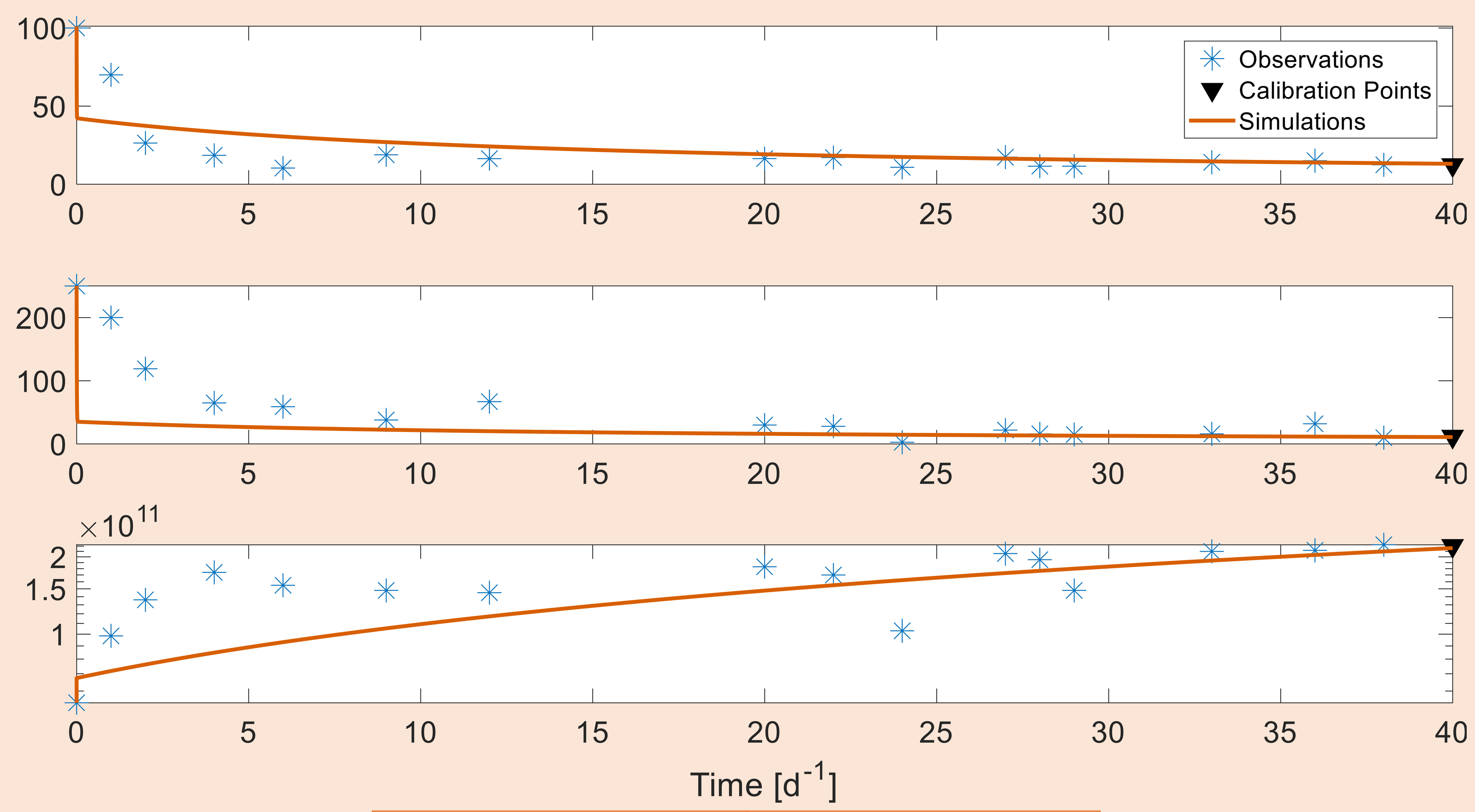
IV. Preliminary Results (Chemostat/Retentostat)

Chemostat – No mass-transfer limitation



$\epsilon^{13}_{measured}$	$\epsilon^{13}_{simulated}$
5.4 ‰	4.7 ‰

Retentostat – Mass-transfer limitation



$\epsilon^{13}_{measured}$	$\epsilon^{13}_{simulated}$
0.45 ‰	0.46 ‰

V. Conclusions and Outlook

- The current model simulates mass-transfer and not mass-transfer limiting systems independently.
- We will calibrate the model for both systems together if possible and extend it for soil systems.

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