HelmholtzZentrum münchen
German Research Center for Environmental Health

ReKinSim: A numerical platform for parameter estimation of kinetically complex environmental systems

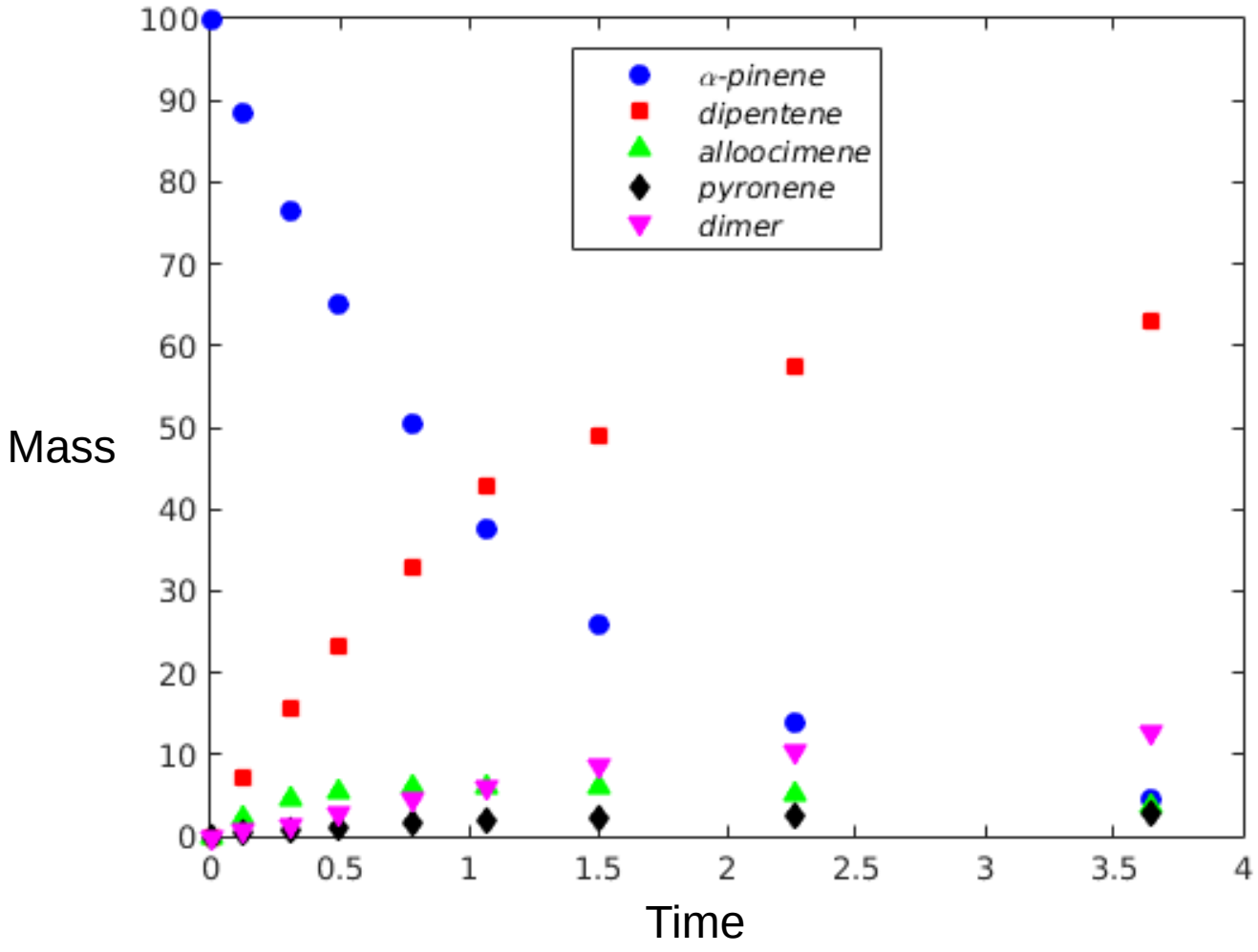
Mehdi Gharasoo, Martin Thullner, Martin Elsner

Institute of Groundwater Ecology, Helmholtz Zentrum München

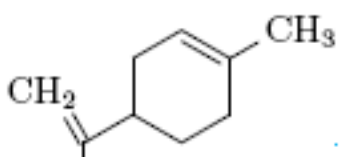
MICRODEGRADE

HELMHOLTZ ASSOCIATION

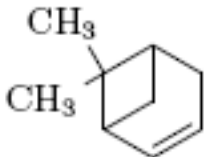
Experimental data

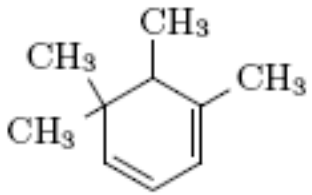


Speculate, design and describe the kinetic model



k1





Pyronene

k3

$$\frac{\partial[Pin]}{\partial t} = -k_1[Pin] - k_2[Pin]$$

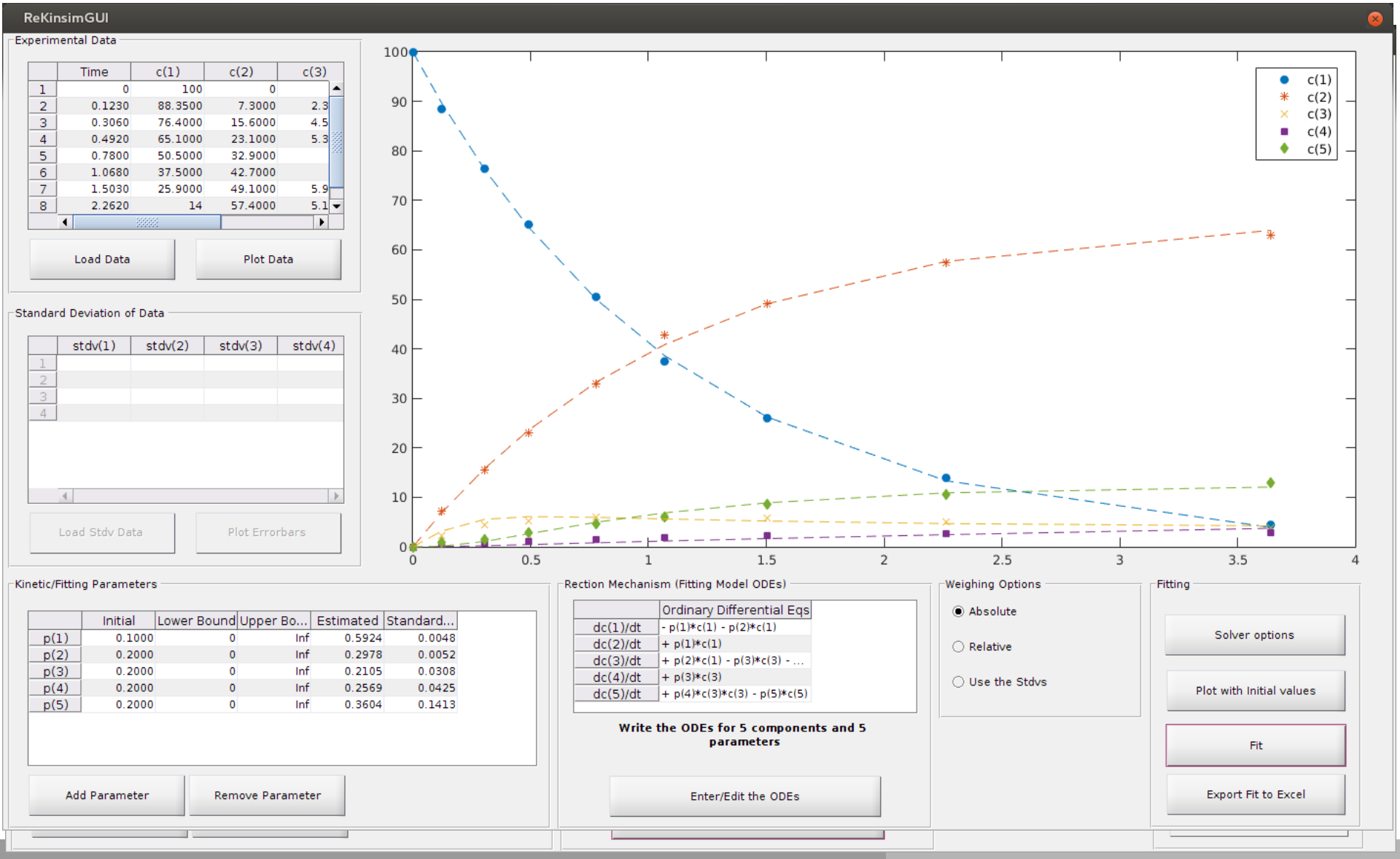
$$\frac{\partial[Dip]}{\partial t} = +k_1[Pin]$$

$$\frac{\partial[Allo]}{\partial t} = +k_2[Pin] - k_3[Allo] - 2k_4[Allo]^2 + 2k_5[Dim]$$

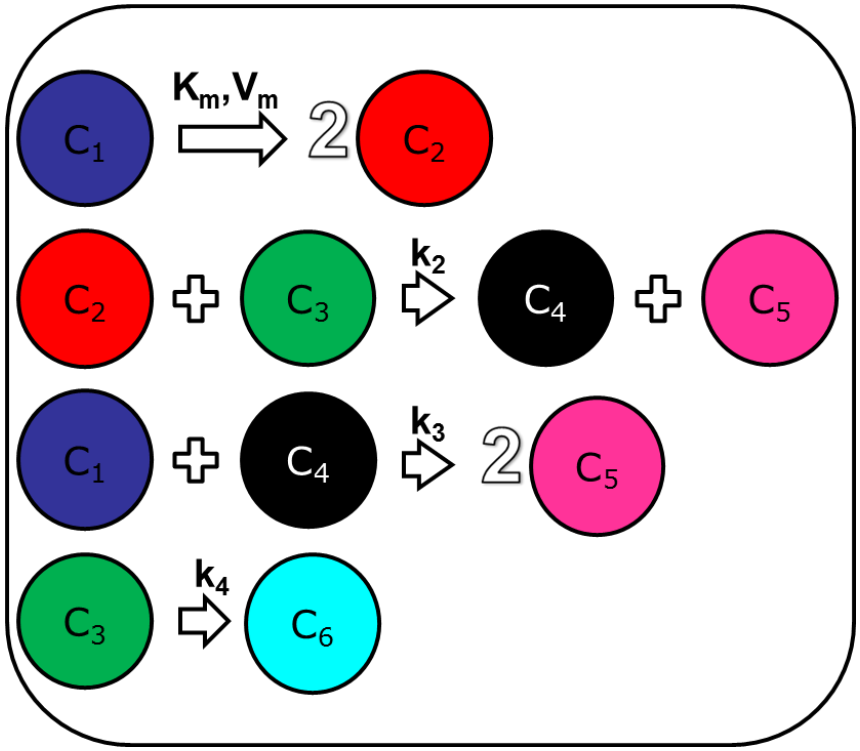
$$\frac{\partial[Pyr]}{\partial t} = +k_3[Allo]$$

$$\frac{\partial[Dim]}{\partial t} = +k_4[Allo]^2 - k_5[Dim]$$

ReKinSim (GUI mode)



Hypothetical test case



- Michealis-Menten reaction (K_m and V_m)
- A second order reaction (k_2)
- Another second order reaction (k_3)
- A first order reaction (k_4)

$$\frac{\partial C_1}{\partial t} = -\frac{V_m C_1}{C_1 + K_m} - k_3 C_1 C_4$$

$$\frac{\partial C_2}{\partial t} = +2\frac{V_m C_1}{C_1 + K_m} - k_2 C_2 C_3$$

$$\frac{\partial C_3}{\partial t} = -k_2 C_2 C_3 - k_4 C_3$$

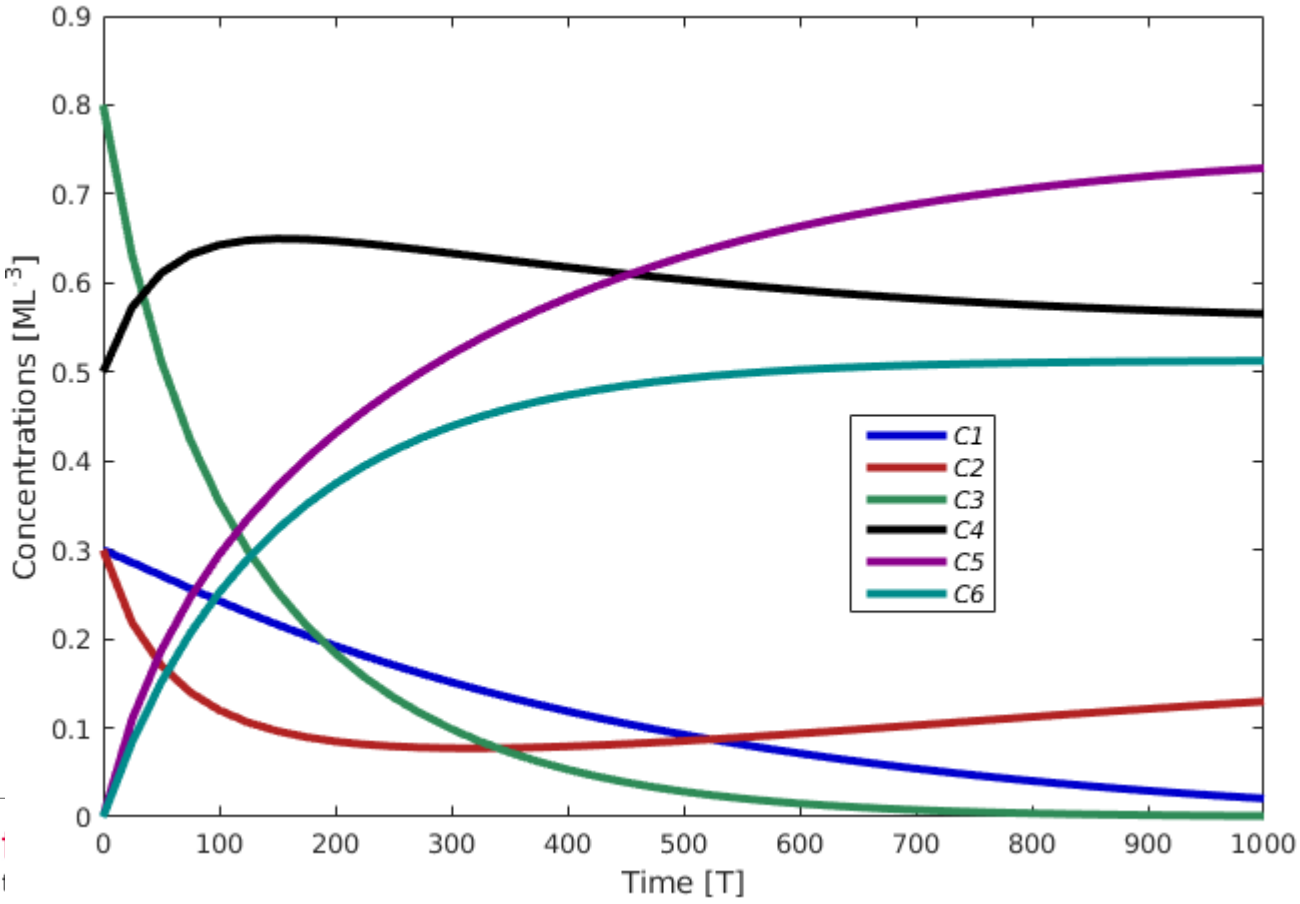
$$\frac{\partial C_4}{\partial t} = +k_4 C_3 - k_3 C_1 C_4$$

$$\frac{\partial C_5}{\partial t} = +2k_3 C_1 C_4 + k_2 C_3 C_2$$

$$\frac{\partial C_6}{\partial t} = +k_4 C_3$$

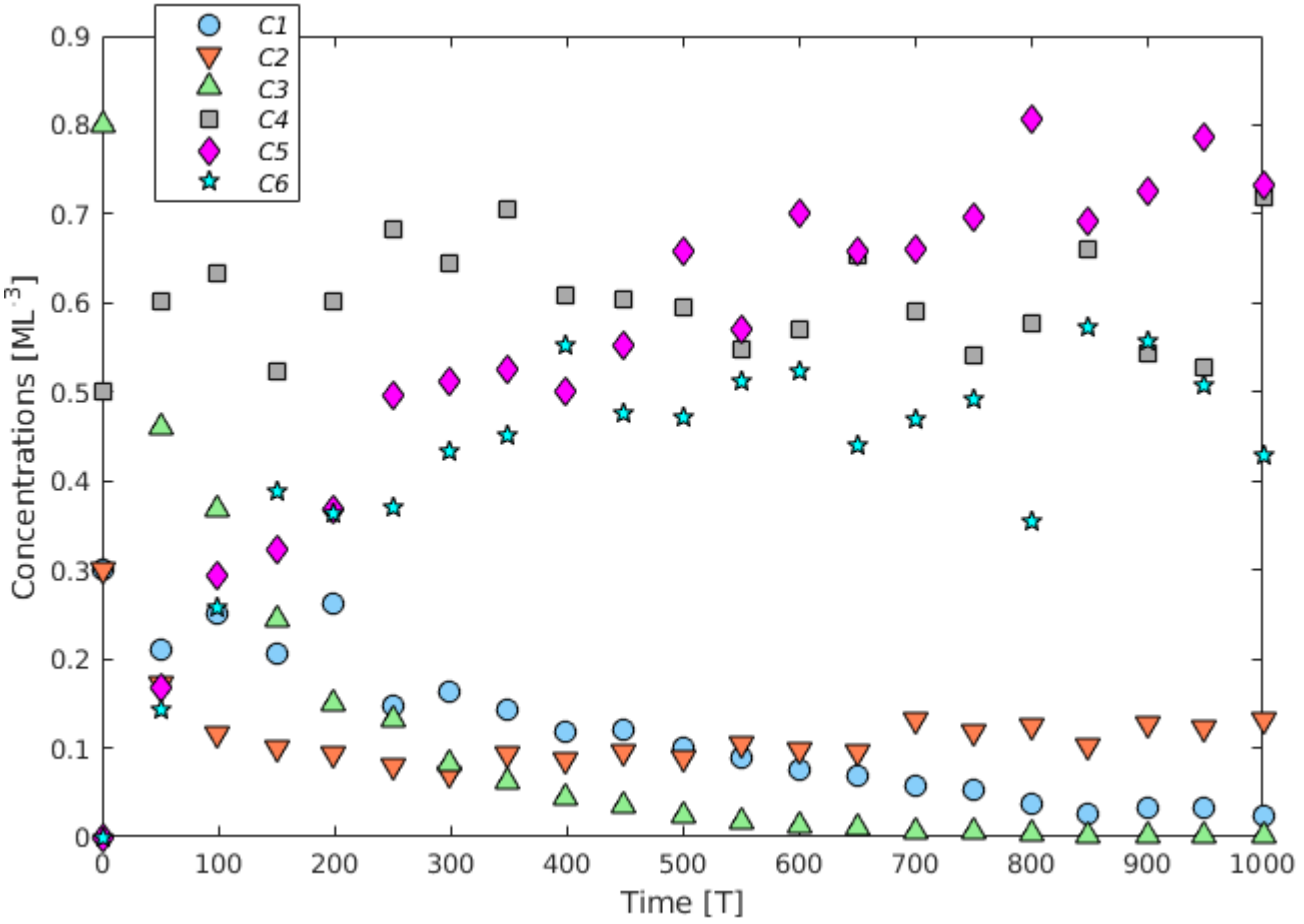
Hypothetical test case

- The actual values of parameters: $V_m = 1e\text{-}4[ML^{-3}T^{-1}]$, $K_m = .06[ML^{-3}]$, $k_2 = .02[M^{-1}L^3T^{-1}]$, $k_3 = .003[M^{-1}L^3T^{-1}]$, $k_4 = .005[T^{-1}]$.
- Initial concentrations: $C_1 = .3$, $C_2 = .3$, $C_3 = .8$, $C_4 = .5$, $C_5 = 0$ v, $C_6 = 0[ML^{-3}]$
- The solution over **1000 unit of time**:

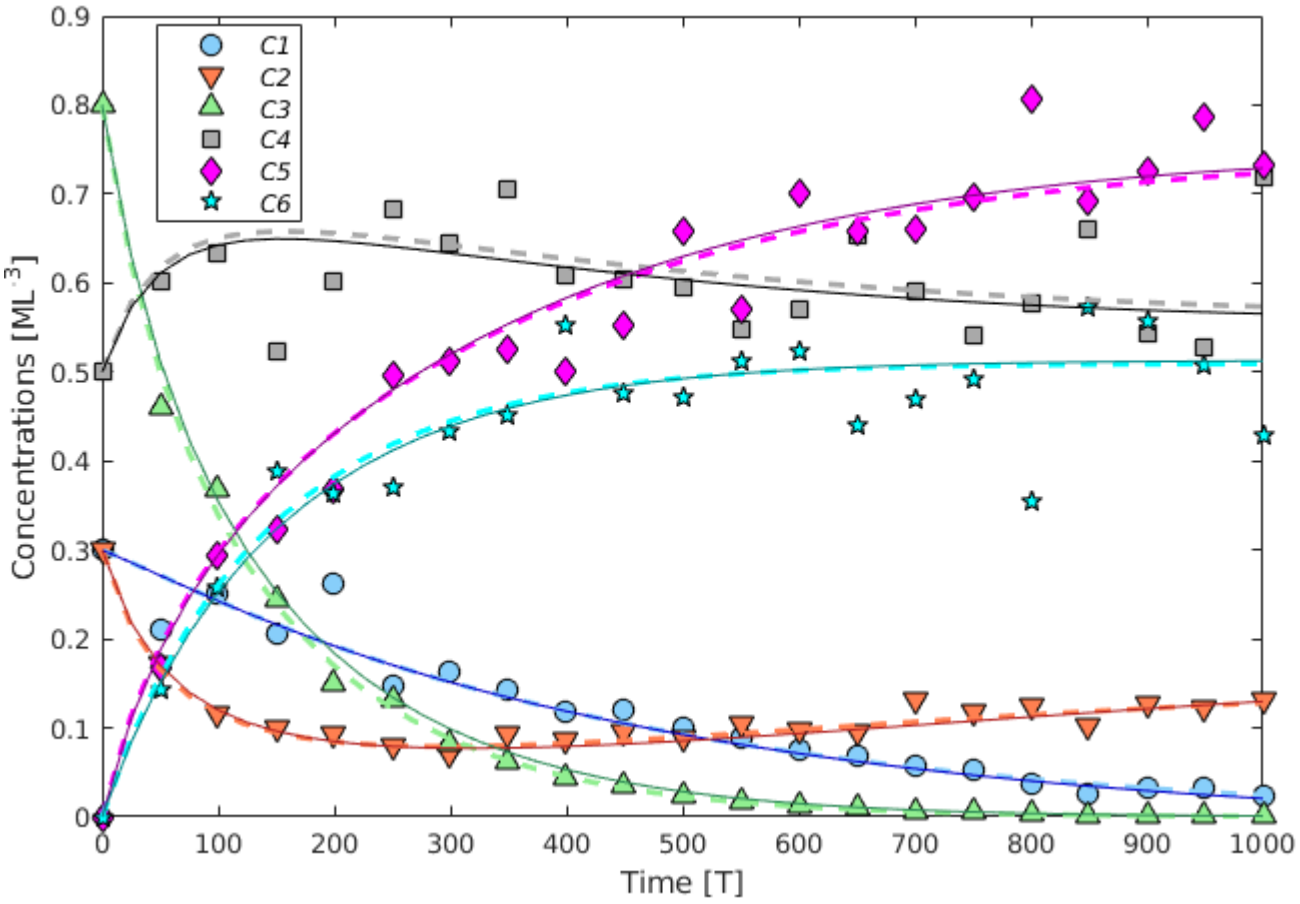


Hypothetical test case

- noisy observations are artificially created from the model solution by adding normally distributed pseudorandom errors.



Hypothetical test case



KinTek Explorer test case

Purchase PDF Export

Search ScienceDirect Advanced

ELSEVIER

Analytical Biochemistry

Volume 387, Issue 1, 1 April 2009, Pages 20-29

Global Kinetic Explorer: A new computer program for dynamic simulation and fitting of kinetic data

Kenneth A. Johnson[a, b], Zachary B. Simpson[b], Thomas Blom[a]

Show more

https://doi.org/10.1016/j.ab.2008.12.024

Get rights and content

Abstract

We describe a new dynamic kinetic simulation program that allows multiple data sets to be fit simultaneously to a single model based on numerical integration of the rate equations describing the reaction mechanism. Unlike other programs that allow fitting based on numerical integration of rate equations, in the dynamic simulation rate constants, output factors, and starting concentrations of reactants can be scrolled while observing the change in the shape of the simulated reaction curves. Fast dynamic simulation facilitates the exploration of initial parameters that serve as the starting point for nonlinear regression in fitting data and facilitates exploration of the relationships between individual constants and observable reactions. The exploration of parameter space by dynamic simulation provides a powerful tool for learning kinetics and for evaluating the extent to which parameters are constrained by the data. This feature is critical to avoid overly complex models that are not supported by the data.

Recommended articles

FitSpace Explorer: An algorithm to evaluate multid...
Analytical Biochemistry, 2009, pp. 30-41
Download PDF View details

Chapter 23 Fitting Enzyme Kinetic Data with KinTe...
Methods in Enzymology, 2009, pp. 601-626
Download PDF View details

Analysis of numerical methods for computer simul...
Analytical Biochemistry, 1983, pp. 134-145
Download PDF View details

View more articles

Citing articles (202)

Modulation effect of acidulated human serum albu...
2017, Journal of Inorganic Biochemistry
View details

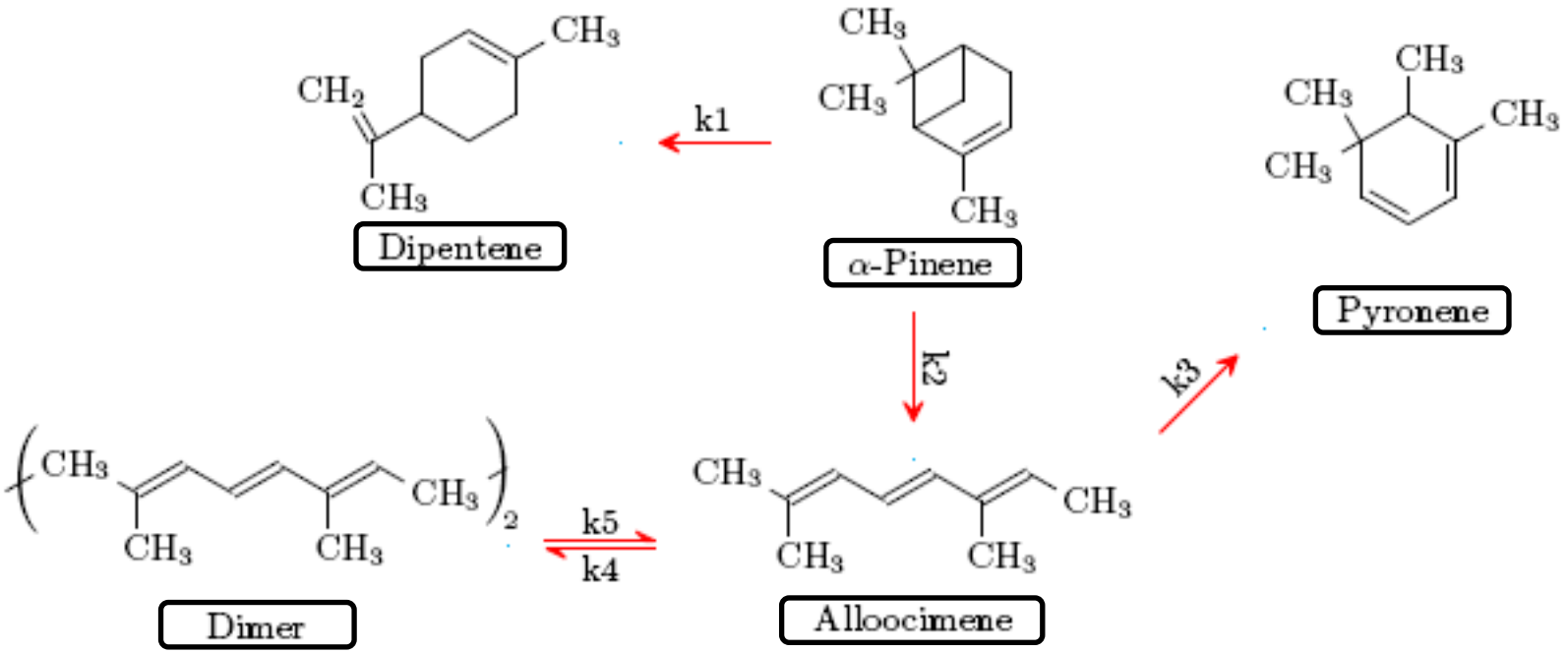
Modeling the Actin.myosin ATPase Cross-Bridge ...
2017, Biophysical Journal
View details

On the estimation errors of KM and V from time-c...
2016, Biophysical Chemistry
View details

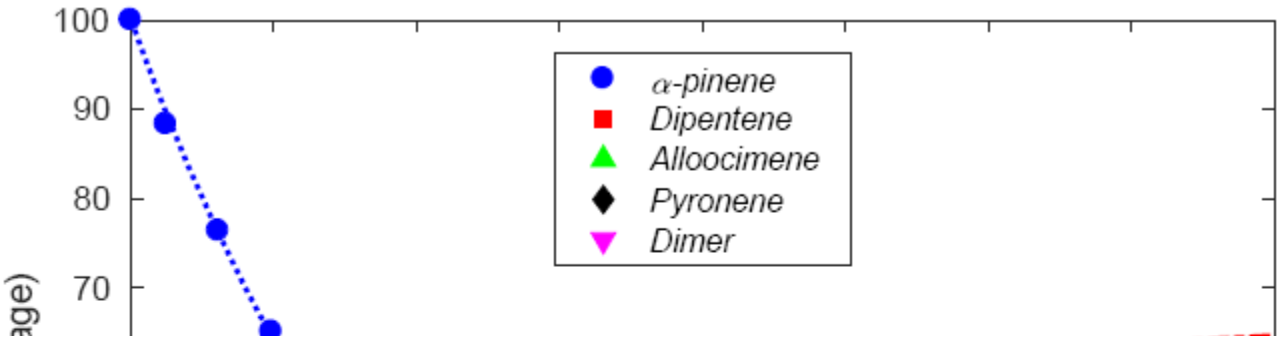
View more articles

Feedback

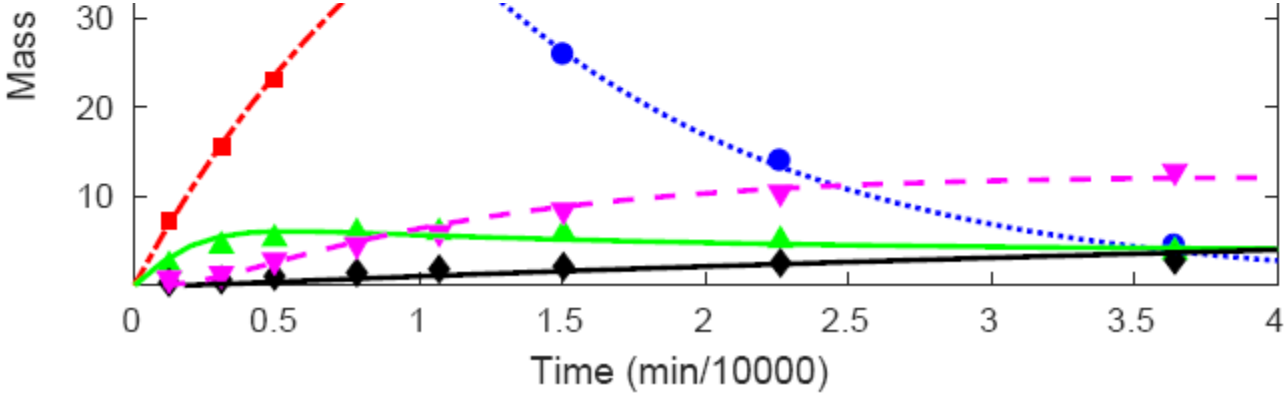
Thermal isomerization of α-pinene



Thermal isomerization of α-pinene



$\times 10^5$	$k_1[min^{-1}]$	$k_2[min^{-1}]$	$k_3[min^{-1}]$	$k_4[min^{-1}\%^{-1}_{Allo}]$	$k_5[min^{-1}]$
KinTek Explorer	6.0	3.0	1.6	2.5	5
ReKinSim	5.9 ± 0.005	3.0 ± 0.005	2.1 ± 0.029	2.6 ± 0.04	3.6 ± 0.134



Take away messages

- A parameter estimation platform for kinetically complex problems was introduced (ReKinSim)

- ReKinSim is shown by comparison in par or superior to other similarly oriented programs such as Aquasim and KinTek Explorer in terms of flexibility and adoptability.

- ReKinSim is offered in two different modes:
  - With a GUI
  - Code based