



webZyme – A Web-Based Enzyme Simulation System for Education and Research

Bruce A. Palfey, Brian Haber, and Rebecca L. Fagan

Department of Biological Chemistry, University of Michigan Medical School, Ann Arbor, MI

Check it out! http://brupalf.googlepages.com/example_enzymes

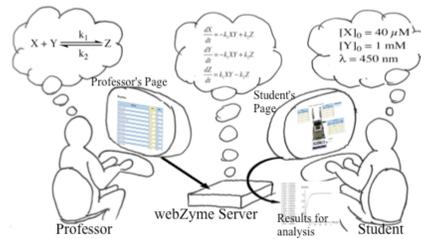
Use it in your class - brupalf@umich.edu

The Problem:

- Kinetics is essential to understand enzymes.
- Students are intimidated by the math.
- Students do not easily connect abstract analyses to real experiments.
- Building kinetic models is not easily learned as a spectator.

Our Solution: webZyme

- Instructors create “virtual enzymes” on a web-server.
- Students perform virtual experiments using their browser.
- Data are downloaded and analyzed independently of webZyme.
- Mechanism is a “black-box” to the student.
- Quality of the results depends on a student’s experimental design; fosters the development of good judgement.
- Reactions defined with an intuitive syntax.
- Many types of experiments are possible.
- Allows model-building & hypothesis-testing.



Current Capabilities

- Absorbance Stopped-Flow
- Steady-State Velocities

Coming Very Soon

- Quenching
- Fluorescence Stopped-Flow

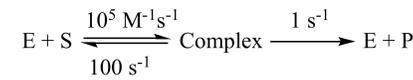
Unique Capabilities

- Calculates reactions between the contents of syringes in the virtual stopped-flow prior to a shot.
- All data have experimental noise at a level controlled by the instructor.
- Nothing to install.
- Independent of platform & location.
- Works on my iPhone.
- Possible to create unique enzymes for each student.

webZyme is not (yet)...

- ...a data-analysis/curve-fitting program.
- ...a substitute for standard simulation programs (e.g., KINSIM, Berkeley Madonna, Gepasi).
- ...expensive. Use webZyme on our server for free – just send Bruce an e-mail (brupalf@umich.edu).
- ...finished. Features are still being added, and bugs are still being found (and fixed).

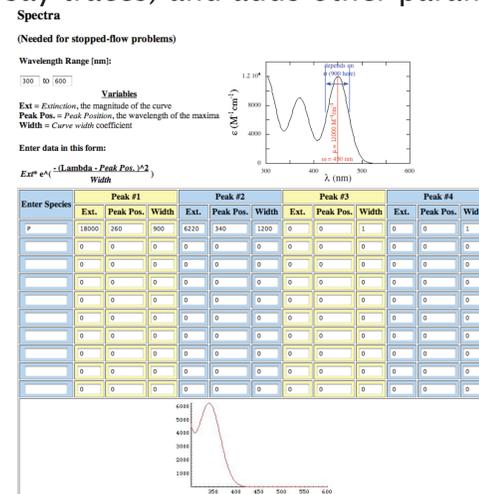
Example: Simple Michaelis-Menten



Instructor enters reactions & rate constants.

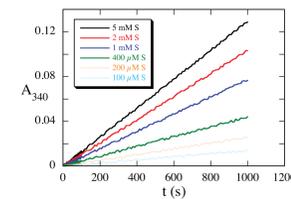
Reaction	kfwd	krev
E+S<>Complex	1e5	100
Complex>E+P	1	1e6
Enter rxn here	Fwd	Bkwd
Enter rxn here	Est	Bkwd

Instructor creates absorbance spectra (for assay traces) and adds other parameters.



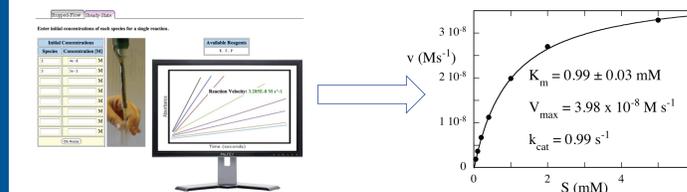
Students could collect assay traces...

<http://palfeybiochem.med.umich.edu:8080/webMathematica/webZyme/Students/MM/Prob1/StopFlow/>

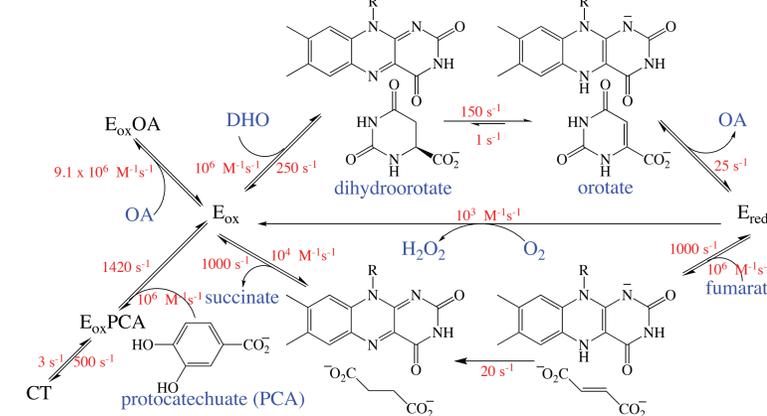


...or students could get velocities directly.

<http://palfeybiochem.med.umich.edu:8080/webMathematica/webZyme/Students/MM/Prob1/SS/>



Example: Dihydroorotate Dehydrogenase



Instructor enters all reactions, rate constants, spectra, etc.

Reaction	kfwd	krev
Eox+DHO<>EoxDHO	1e6	250
EoxDHO<>EredDHO	157	0.6
EredDHO<>EredOA	25	1e5
Ered+O2<>EredH2O2	1e6	1000
EredH2O2<>EoxH2O2	20	1e6
EoxH2O2<>EoxOA	1000	1e5
Eox+OA<>EoxOA	9.1e6	40
Ered+O2<>EredH2O2	3000	1e6
Eox+PCA<>EoxPCA	1e6	1420
EoxPCA<>CT	500	3

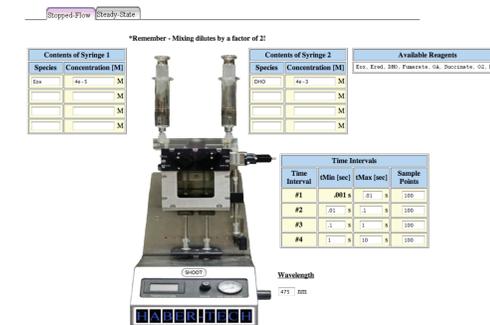
Enter Species	Est.	Peak Pos.	Width									
EoxDHO	5000	280	1100	920	380	1200	410	1200	3	0	0	1
CT	3000	290	1100	810	390	1200	460	1300	140	400	140	100
EredDHO	4000	280	1100	600	340	1400	400	1100	1400	140	100	100
EoxOA	4000	280	1100	700	350	1400	410	1100	1400	140	100	100
EoxDHO	5000	280	1100	810	390	1200	410	1200	470	1100	0	1

Based on data from:

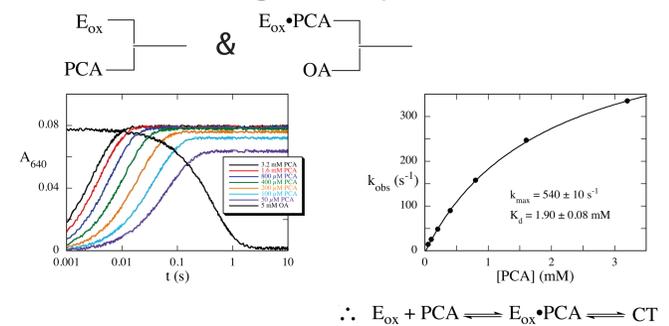
- Fagan, Jensen, Björnberg, & Palfey (2007) *Biochemistry*, 46, 4028–4036
- Wolfe, Thymark, Gattis, Fagan, Hu, Johansson, Arent, Larsen, & Palfey (2007) *Biochemistry*, 46, 5741–5753
- Unpublished results

Students explore transient kinetics...

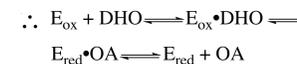
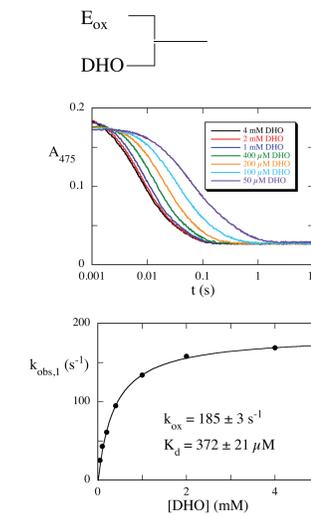
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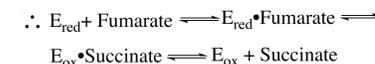
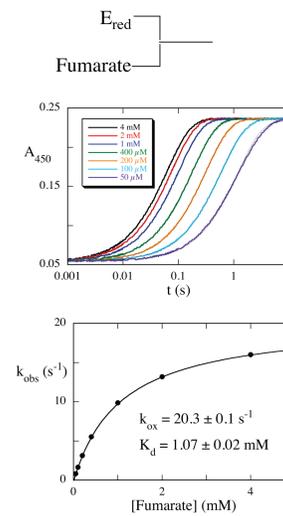
Inhibitor Binding & Competition



Reductive Half-Reaction



Oxidative Half-Reaction



Reaction with O₂

