

# REX™ Suite

Reaction Analysis and Optimization Software



www.optience.com

Strategic Solutions through  
Optimization Science

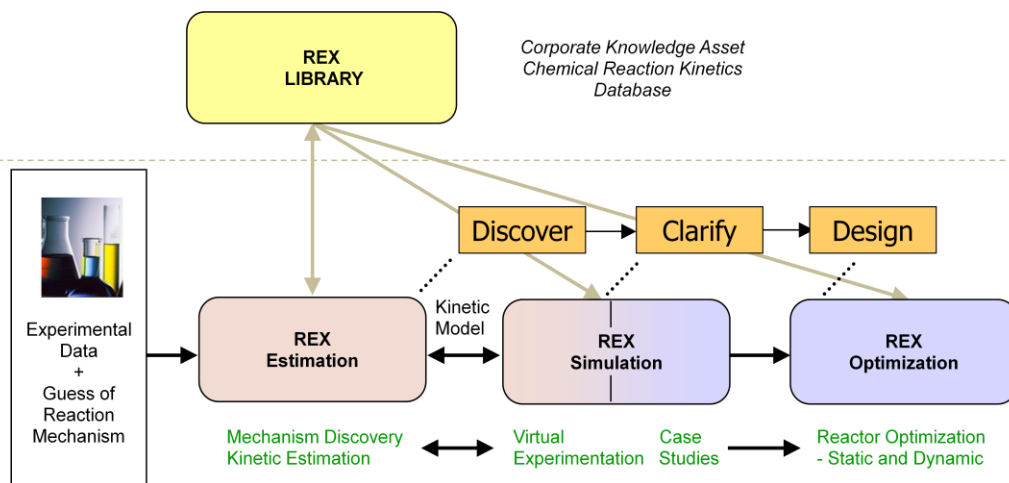
Optience REX™ is a comprehensive software suite that aids chemists and chemical engineers to analyze chemical reaction systems and thereby develop strategies to maximize their yield performance.

## REX™ Blends with your Workflow

Your Thinking Partner

The software components in REX™ aid in decision making at every step of your workflow:

You may start your journey with REX™ from reaction route evaluation, continuing on to reasoning of experimental data through kinetic modeling, evaluation of alternate strategies for the reaction system, and finally optimization of the reaction system to meet performance objectives. REX™ allows you to reason through the bottlenecks in your reaction system, identify the causes for yield loss and by-product formation, and devise strategies to maximize the performance of the reaction system.



## REX™ Architecture

The REX™ Suite has two products:  
REX™ Projects and REX™ Library

- **REX™ Projects**  
Allows the user to perform tasks ranging from Kinetic Estimation, Reactor Simulation, Virtual Experimentation and Reactor Dynamic Optimization.
- **REX™ Library**  
Serves as the knowledge management of the REX Suite, and allows you to explore reaction kinetics databases.

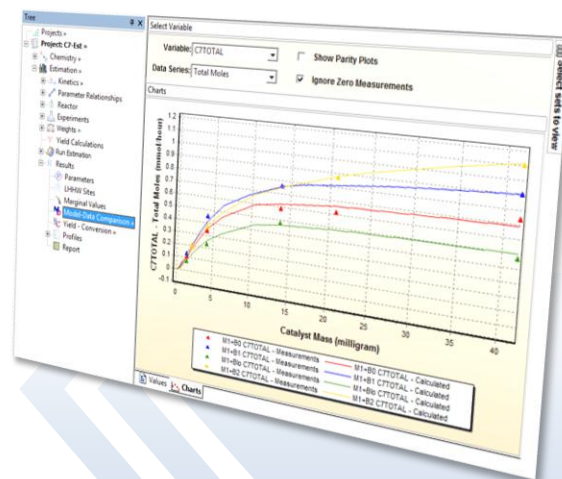
## Proven Applications

REX has enabled our customers to maximize reaction performance across a spectrum of chemical reactions ranging from:

- Petrochemicals
- Polymer Systems
- Pharmaceuticals and Fine Chemicals

## Wide Range of Applicability

REX™ has facilitated the analysis of reaction systems for a wide range of applications from petrochemicals to pharmaceuticals synthesis. REX™ allows the user to select reaction mechanisms with kinetics ranging from power law to complex Langmuir-Hinshelwood-Hougen-Watson kinetics. Reactor types can range from batch, semi-batch, continuous stirred tank, fixed bed and flow reactors. The differential algebraic models that represent the kinetic estimation and reactor optimization models are solved with sophisticated algorithms, ensuring flexibility and robustness.



## Easy to Model and Easy to Use

REX™ Projects comes with an easy to use graphical user interface that allows you to rapidly build the chemistry and provide experimental data for kinetic estimation projects. Different kinetic mechanisms can be evaluated against experimental data for easy analysis. Once the kinetic mechanism and rate parameters are obtained, Virtual Experimentation and Reactor Optimization studies can also be conducted by building several cases simultaneously. Comprehensive graphing options allow for easy trend analysis and comparison between cases.

REX™ relieves the user from the burden of building the differential equation models, thus allowing the user to focus on the chemistry and performance improvement of the reaction system. Models can be built consistently and fast, resulting in savings in engineering time alone in the order of days.

Include	Data Point	Time (sec)	Temperature (C)	Volume (lit)	HK2 (mmol)	HK (mmol)	AX (mmol)
<input type="checkbox"/>	1	0	0	1	0.1525	0	0.204125
<input type="checkbox"/>	2	10	0	1	0.1625	0	0.186875
<input type="checkbox"/>	3	20	0	1	0.1285	0	0.18475
<input type="checkbox"/>	4	30	0	1	0.12675	0	0.1645
<input type="checkbox"/>	5	40	0	1	0.110225	0	0.136125
<input type="checkbox"/>	6	50	0	1	0.0915625	0	0.1219
<input type="checkbox"/>	7	60	0	1	0.078075	0	0.107775
<input type="checkbox"/>	8	70	0	1	0.07095	0	0.0903875
<input type="checkbox"/>	9	80	0	1	0.0612875	0	0.08795
<input type="checkbox"/>	10	90	15	1	0.0483875	0	0.0869625
<input type="checkbox"/>	11	100	15	1	0.0384125	0	0.0573625
<input type="checkbox"/>	12	110	15	1	0.0271625	0	0.040075
<input type="checkbox"/>	13	120	30	1	0.02525	0	0.035375
<input type="checkbox"/>	14	130	30	1	0.018575	0	0.0250125
<input type="checkbox"/>	15	140	30	1	0.0148875	0	0.0182375
<input type="checkbox"/>	16	150	30	1	0.01163	0	0.0094575
<input type="checkbox"/>	17	160	30	1	0.008925	0	0.00115

## Unique in Design and Features

REX™ design is unique in its understanding of the research workflow and thus combining the tasks of estimation, simulation and optimization in one framework, with easy transfer of information between these steps. Kinetic Estimation can be done for a variety of reactors and reaction kinetics types. Furthermore, REX™ is unique in its ability to perform flexible dynamic optimization of temperature, pressure and compound addition or removal profiles for batch systems.

## Continuous Improvement and Customization

The software architecture of Optience products allows us to flexibly customize our interfaces and models. We listen to our customers, and Optience is committed to continuous improvement of our products to meet their needs.

## Contact Us

Optience believes that an engaged approach with the client can provide superior results. We also arrange short-courses on reaction analysis both on-site and at our office.

## Proven Technology and Superior Service

REX™ is built on the success and experience of improving yields for numerous projects in petrochemical, polymers and pharmaceutical synthesis. REX™ is also backed by an experienced consulting and training services team that can ensure effective utilization to generate superior results when it comes to your reaction yields.

## Seamless Transfer of Knowledge

As projects on reaction analysis are completed in REX™ Projects, the resulting chemistry and kinetics can be seamlessly transferred to your corporate database for archival. This allows company researchers to query the corporate database and use this information for new projects.

For more information on REX™ Suite, please visit:  
<http://www.optience.com/rex>  
or contact us at  
[information@optience.com](mailto:information@optience.com)