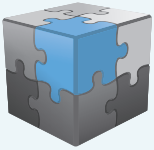
Jplus consulting
multivariate analytical technologies

Software tools for the global analysis of multiwavelength spectroscopic data

ReactLab™



adding new dimensions to chemical process analysis

ReactLab™ EQUILIBRIA

For the modeling and analysis of chemical equilibria

ReactLab™ KINETICS

For the modeling and analysis of kinetic processes

ReactLab software tools have been designed specifically to enable researchers and chemical engineers to gain the maximum reaction information from their multivariate chemical process measurements.

These tools will allow you to:

- Analyse spectroscopic data gathered during chemical process investigations such as equilibrium titrations or kinetic experiments
- Quantitatively characterise the chemical processes involved by globally fitting the fundamental parameters of the underlying reaction mechanism to the data
- Identify the reaction mechanism, the participating species, their spectra and concentration profiles and all rate and equilibrium constants
- Model and simulate key reactions to investigate and predict their behavior
- Optimise chemical processes

The Data

- Multiwavelength spectroscopic data including:
  - *Equilibrium spectra measured during automatic or manual titration experiments.*
  - *Time resolved spectra collected during kinetic experiments.*
- ReactLab™ is ideal for the analysis of measurements made using multichannel detectors such as photodiode arrays (PDA's).

ReactLab™ software tools bring significant advantages if your research involves:

- The quantitative analysis of chemical reaction processes.
- The elucidation of chemical reaction mechanisms and the determination of kinetic and equilibrium constants.
- Reaction modeling and simulation.
- Drug or ligand binding studies.
- Enzyme kinetics.
- Chemical process monitoring and optimization.

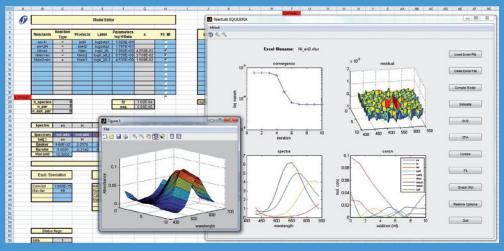
Global Analysis Advantage

- All available data are used for the analysis – there is no need for the selection of 'optimal' wavelengths.
- The model must account for features in the measurement throughout the wavelength range.
- Global analysis is essential for the robust determination of real chemical mechanisms providing:
  - *Superior definition of the parameters - rate and equilibrium constants*
  - *Superior definition of the correct chemical reaction model*
  - *Resulting spectra for all the interacting species.*
- Global error surface plots highlight discrepancies between all the measured data and the fitted reaction model.

Teaching and Education

ReactLab™ provides an ideal platform for teaching students the fundamentals of chemical equilibria and reaction kinetics allowing them to investigate theoretical mechanisms and generate simulated data for visualization and experimental analysis.

Compatible measurements include UV-Vis Absorbance, NIR, IR, Raman, ESR, CD, Fluorescence



Software Architecture

ReactLab™ applications are based on an innovative compiled Matlab-Excel architecture.

- All data, models and results are stored in portable Excel workbooks (derived from pre-formatted templates).
- The Re actLab™ analysis kernel and control GUI communicates with the Excel workbook via a robust Microsoft™ COM interface.
- Interactive 2D and 3D graphics provide flexible and interactive data and results visualization.
- Standard Excel functionality allows customised post-processing and additional charting of all experimental data and results.

Technical specifications:

Algorithms

- Least squares fitting of non-linear parameters (rate and equilibrium constants) using a modified Marquardt-Levenberg algorithm.
- Linear parameters (molar absorptivities or equivalent) are computed internally using explicit algorithms, no initial estimates are required.
- Advanced Newton-Raphson algorithm for equilibrium speciation calculations.
- 4th order Runge-Kutta numerical integration routines for computation of kinetic concentration profiles.
- Alternative variable order stiff solver may be selected if required.
- Unique combined speciation and numerical integration computations allow reaction rates and fast equilibria to be fitted together in kinetic models.
- pH changes arising from protonation equilibria are computed automatically allowing analysis of kinetics in buffered or un-buffered solutions.
- Alternative linear regression algorithms allow the option of bipolar or only non-negative spectra.
- Singular value decomposition (SVD) for the model free analysis of the data to identify the number of linearly independent components present.
- Evolving factor analysis (EFA) to visualise the appearance and disappearance of species and compute approximate concentration profiles and spectra.

ReactLab™ Deployment

ReactLab™ applications are compiled for deployment. They do not require Matlab to be installed on the host computer. They do require the freely available Matlab compiler runtime (MCR) library which is supplied. Excel 1997 or later must be installed on the host computer. See the Jplus Consulting website for more detailed system requirements.

ReactLab™ applications may be downloaded for a free fully functional 30 day trial period from our website. Thereafter a permanent computer locked license must be purchased to continue using the programs.

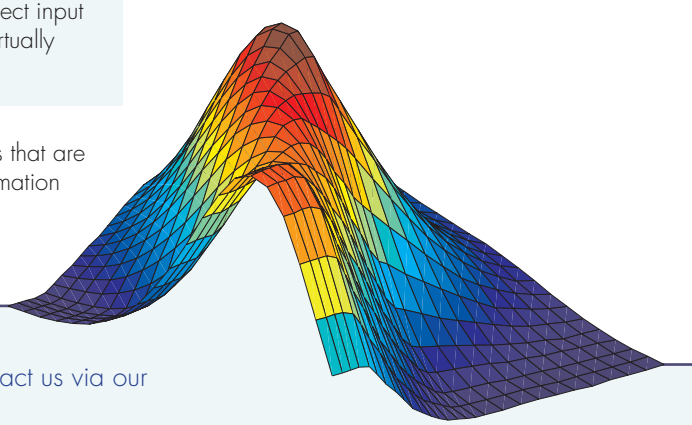
Features

ReactLab™ allows real reaction mechanisms to be fitted directly to the data. There is no requirement for data transforms or the fitting of empirical or arbitrary functions such as sums of exponentials.

- Pre-formatted Excel workbooks contain all data and results as well as the model entry interface. These provide a familiar environment into which data can easily be transferred from other sources.
- Output of all results to the Excel workbook allows easy post-analysis manipulation of the data using any of Excel's charting or spreadsheet functionality.
- Excel workbooks encapsulate the entire analysis session and are completely portable and self contained records. They can be subsequently shared and reviewed without a ReactLab™ installation.

A symbolic model editor allows direct input of chemical reaction schemes of virtually unlimited complexity.

- The standard non-linear parameters that are fitted are equilibrium constants, formation constants and rate constants.
- The spectra of all species are explicitly calculated during the analysis.
- Equilbrium models can be optionally defined in terms of equilibrium or formation constants.
- Kinetic models can include reversible reactions with kinetically observable rates to be fitted as well as rapid (instantaneous) equilibria.
- The fitted parameters are the corresponding forward/reverse rate constants and equilibrium/formation constants.
- When protonation equilibria are incorporated in a reaction model the autoprotolysis equilibrium of water is calculated automatically to correctly model accompanying pH changes.
- A unique auxiliary parameter feature allows the fitting of special parameters or the definition of a numerical relationship between standard parameters.
- Support is included for known (fixed) spectra.
- Reaction simulation enables artificial data sets to be created and analysed. This is an invaluable tool for exploring and predicting the behaviour of chemical mechanisms.



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