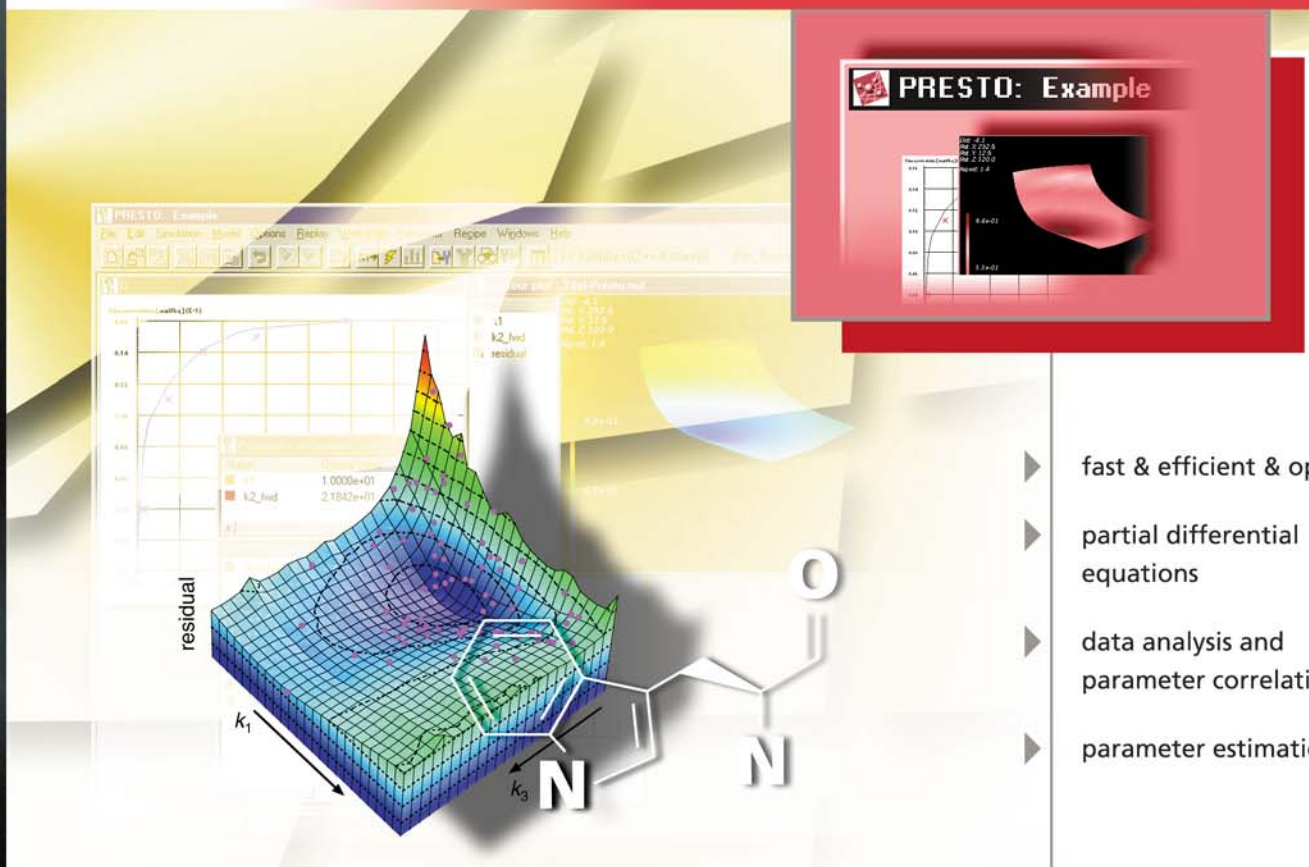
Computing in Technology

PRESTO-KINETICS

Advanced Kinetic and Process Modeling

simulation program



- fast & efficient & open
- partial differential equations
- data analysis and parameter correlations
- parameter estimation

solutions for chemical engineering

Dr. M. Wulkow Computing in Technology GmbH

PRESTO-KINETICS

simulation program

Simulation

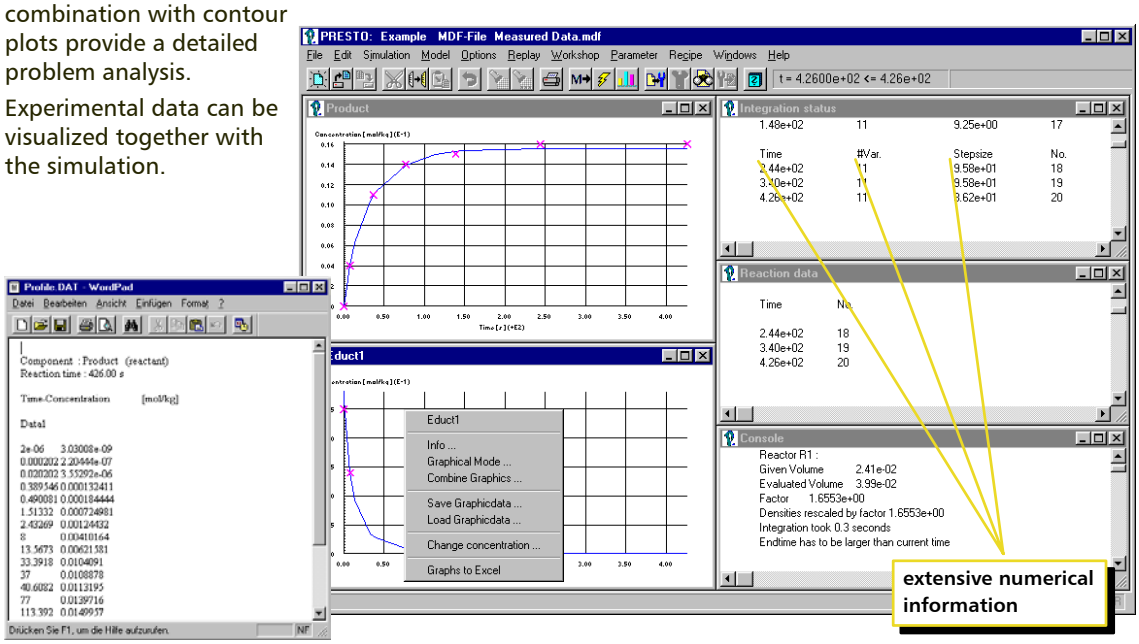
- unique numerical algorithms
- on-line information
- direct interaction
- open data formats
- off-line capabilities
- PDE's for spatial profiles
- 3D-visualization of time dependent spatial problems

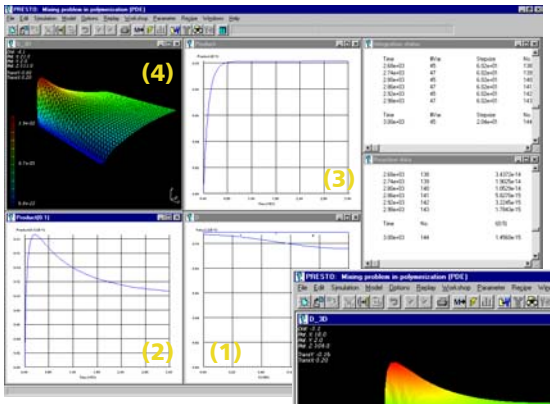
PRESTO is a sophisticated tool for the modeling of any kind of kinetic reactions. High-end mathematical techniques are combined with a state-of-the-art user-interface. Within this framework the definition of reactors, coefficients or species is completely open to the user. All data may be plotted to graphical output windows during simulation. The output can be updated after each individual integration time-step. Furthermore, during the simulation information about the actual chemical and numerical problem status is provided. The full simulation or selected parts can of it be recorded for later examination.

The ASCII format for in- and output files facilitates editing of any information by software of your convenience.

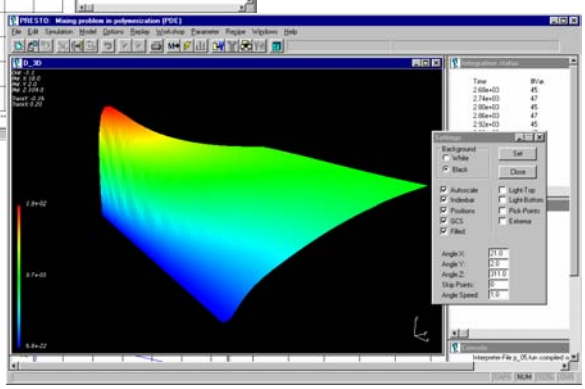
A sophisticated parameter estimator helps deriving the rate coefficients from experimental data. Standard algorithms, stochastic algorithms, and box search procedures in combination with contour plots provide a detailed problem analysis.

Experimental data can be visualized together with the simulation.





Spatial problems can be formulated using partial differential equations (PDE) considering diffusion, convection and spatial differentiated reaction rates. The highly efficient solver cares for automatic, self-adaptive and non-equidistant discretization with respect to the spatial coordinate and integration time axis. Thus the computational efforts are reduced to a minimum.

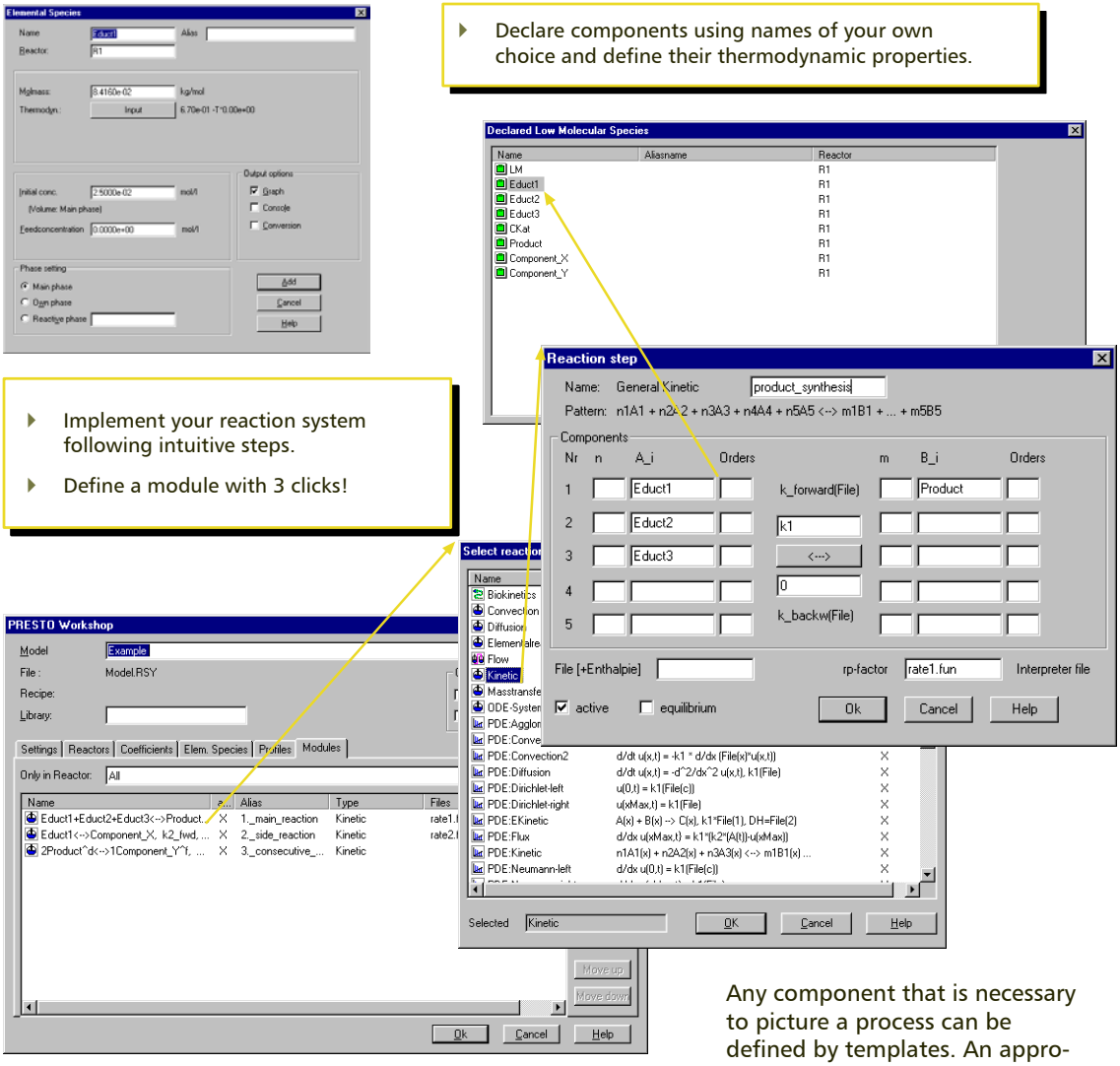


Example:

Polymer production and spatial equilibration after point-wise initiator feed.

Results are shown either as the full profiles at each time step[1], as time slices at a certain spatial coordinate[2], time dependent integrated value of each profile[3], or as time dependent evolution graphs of spatial species profiles[4].

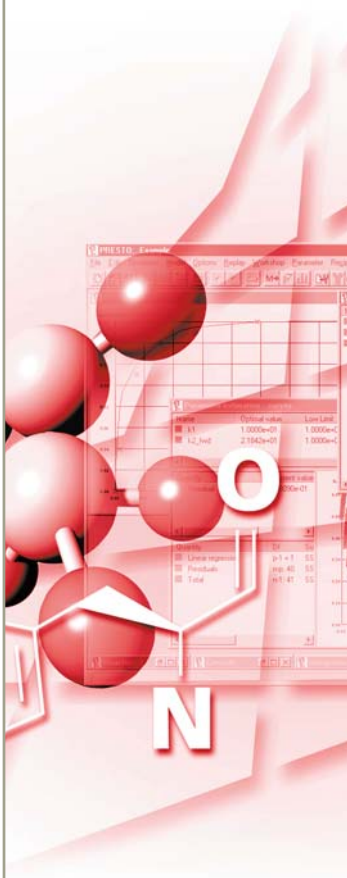
The creation of a model is supported by the comfortable Workshop. This Workshop is shared by all CiT tools to unify model implementation and to switch easily in-between the CiT tools without extended phases of individual training.



Any component that is necessary to picture a process can be defined by templates. An appropriate set of resources from the Windows GUI (graphical user interface) expects the user's input. It is demonstrated here for the definition of a general reaction step.

Interface

- easy-to-use GUI
- flat dialog structure
- intuitive
- efficient



Reactors: An arbitrary number of reactors can be defined, each having individual characteristics such as: temperature(-profiles), pressure, volume, heat-balance, operation mode (batch, feed-batch, continuous flow, CSTR or tubular). A powerful phase concept enables the treatment of multiple phases for heterogeneous reactions.

Coefficients: Rate coefficients and constants within a model may be defined as being temperature and pressure dependent following an Arrhenius term.

Reactants: Species and species profiles are defined by considering their thermodynamic properties, initial values of concentration and spatial profiles or feed-strategies.

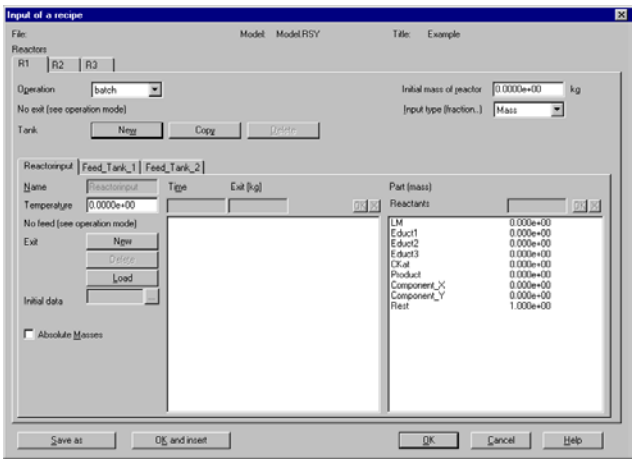
Reaction steps: Most of the reaction systems may be built up using the general kinetic step shown above. It provides any order of reaction with respect to the reactants or the direct implementation of the reaction rate. The stoichiometry may be defined totally free as well as the overall rate. Furthermore, there exists a large variety of modules especially designed for certain application fields. These include bio-kinetics, diffusion, convection, mass-transfer and several types of partial differential equations.

PRESTO-KINETICS

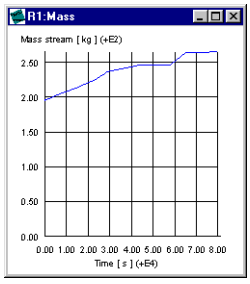
simulation program

Control

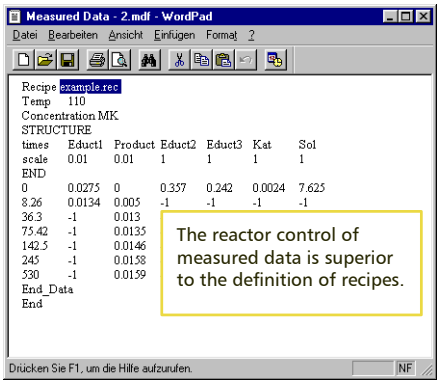
- recipe concept
- batch, feed-batch, CSTR, tubular, complex operation modes
- tracing experimental data



The definition of recipes allows an efficient control of the reactor operation strategy. The concept of tank recipes corresponds to strategies of batch and feed-batch operation as well as of continuous flow. Within each tank even species mixtures can be defined. For these feeds it is possible to import mass versus time profiles directly as ASCII data from your balance. When modeling processes that require multiple reactors, for each reactor an individual recipe can be defined.



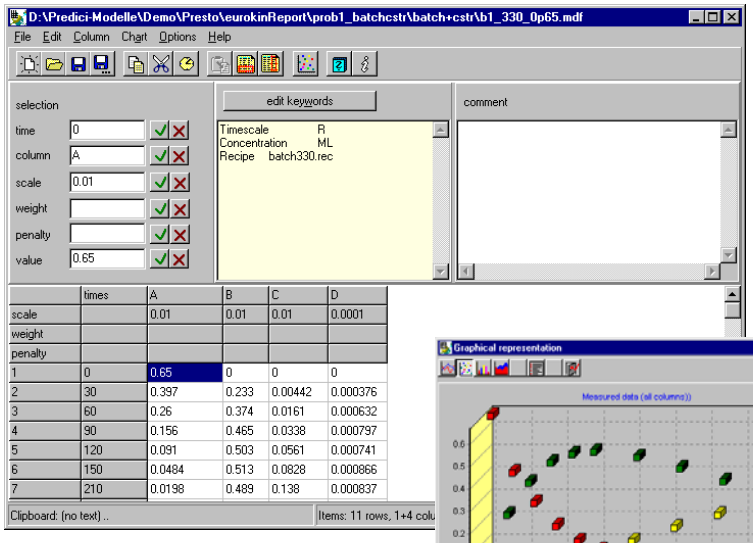
The reactor module accounts for continuous and discontinuous discharges from the reactor. Complete sampling programs can be simulated using this module. The volume control can be set manually or automatically; full mass balances are calculated in any case.



Special file formats for files containing experimental data allow recipe control by measured data sets.

Other special features are:

- By combining measured data files with recipes complex reactor operation programs are simulated that account for temperature and feed programs.
- Using this feature in combination with the parameter estimation tools, multiple rate coefficients can be estimated from whole sets of experimental data referring to dynamic reactor operation strategies simultaneously.
- Individual scaling or weight factors as well as penalty functions can be defined to account for differing precision of experimental data.



As an extra feature, a customized editor for the handling of measured data files is available. It simplifies editing data and key words considering all features of the parameter estimation tool. This tool is also capable of merging experimental data resulting from measurements on different time bases.

A graphical display is included for quick data inspection. This is useful for testing estimation procedures by in- or excluding groups of measured data.

Data Editing

- fast manipulation
- merging of different data sets
- quick display

Advanced Features

- bio-kinetics
- heat transfer
- thermodynamics
- multiple phase concept
- internal script language
- library

A flexible reactor concept provides stand-alone reactors or cascades. For each reactor the heat-balance and multiple phases can be defined. Special modules allow the species exchange in-between the phases.

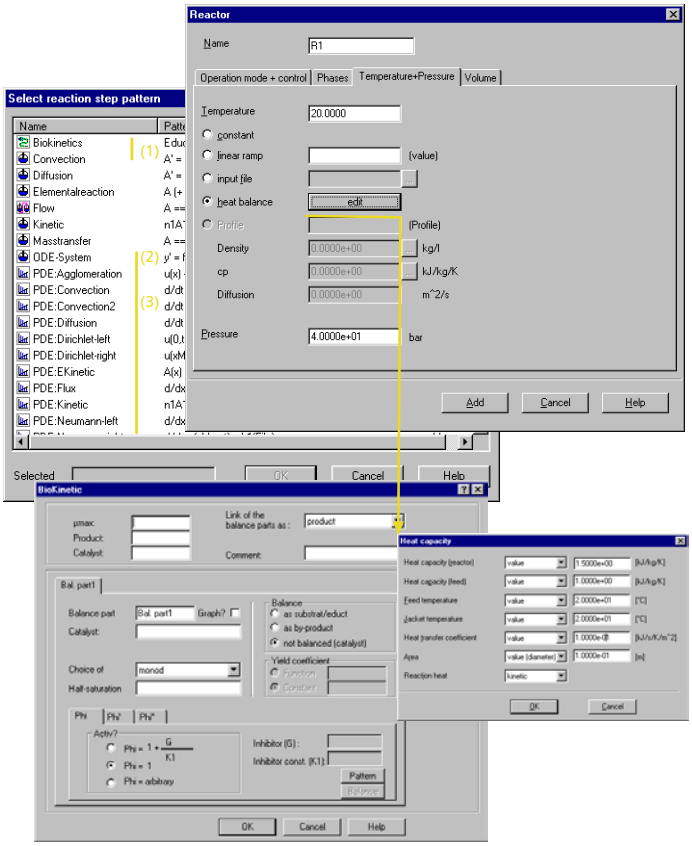
A bio-kinetic[1] pattern assists in modeling this significant class of processes.

Partial differential equations[3] (PDE-modules) facilitate the implementation of spatial profiles, particle distributions or reactions in heterogeneous reaction mixtures.

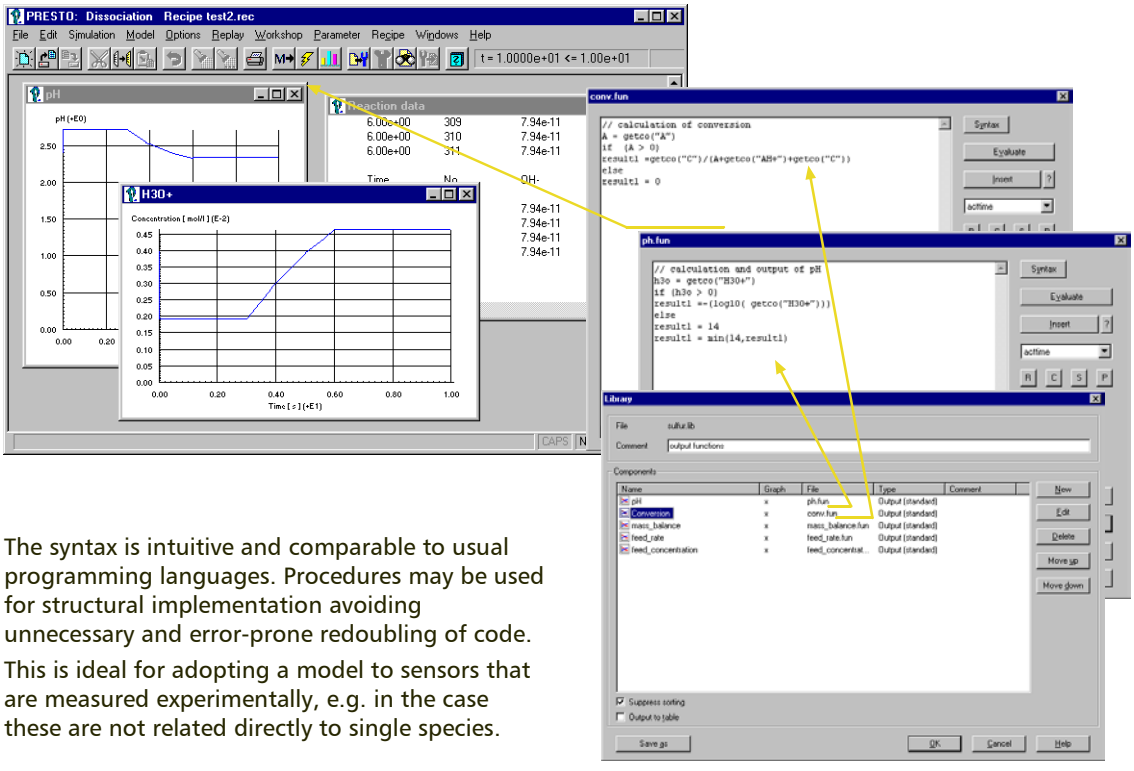
Using the integrated function interpreter (no external compilation) arbitrary functionalities may be implemented for heat-balance[4], phase-exchange, particle-formation, -agglomeration or -degradation.

For special demands ordinary differential equations (ODE) -modules[2] provide direct access and control e.g. to species, species distributions or balance variables.

There are several options to control feed and exit streams: directly, using the recipe module or by ODEs.



The library in combination with the function interpreter enables the calculation of self-defined quantities or implementation of control concepts, generating individual on-line output.



The syntax is intuitive and comparable to usual programming languages. Procedures may be used for structural implementation avoiding unnecessary and error-prone redoubling of code.

This is ideal for adopting a model to sensors that are measured experimentally, e.g. in the case these are not related directly to single species.

PRESTO-KINETICS

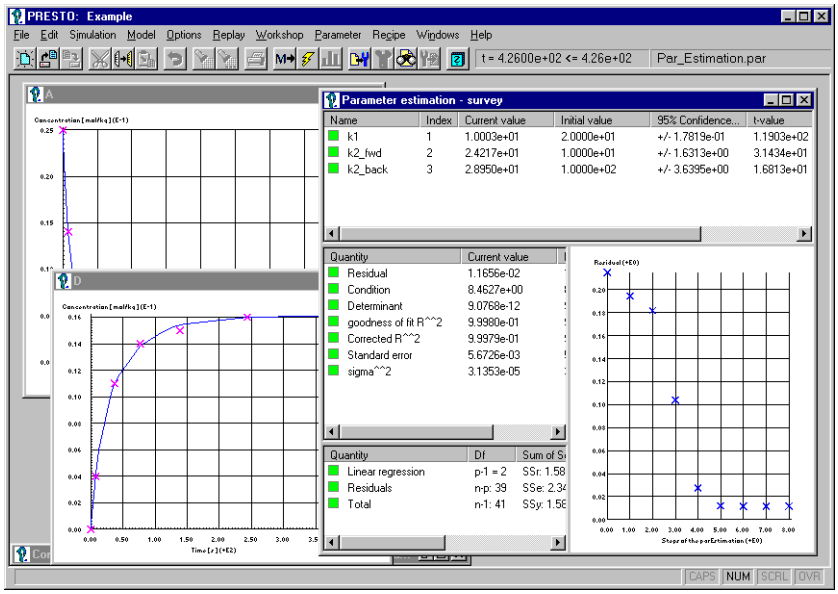
simulation program

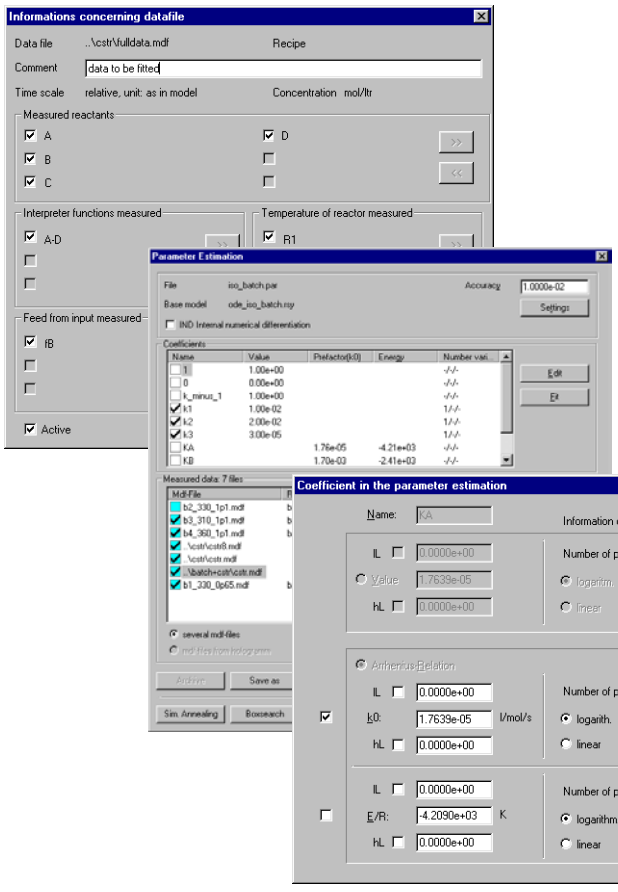
Parameter Estimation

- rate parameter
- Arrhenius estimation
- model parameter
- statistical information
- no sheet or data limitations
- value scaling
- value weighting
- free penalty functions

Rate coefficients and any other model parameters can be fitted by the parameter estimation tool. As sensors any species and system variable may act. Also quantities that are defined by the user via the function interpreter can be used.

An unlimited number of data sheets can be processed, each corresponding to an individual experiment having its own recipe, operation mode, temperature and feed profile.





Sophisticated statistical information is displayed on-line during the fitting procedure. Results providing criteria for the goodness of fit, correlation of parameters and individual sensitivity are available.

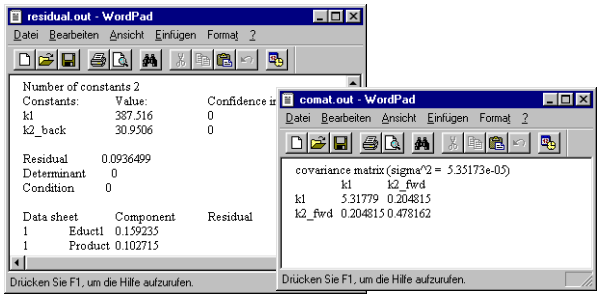
There are no principle limitations with respect to the number of data sheets or parameters to be estimated.

Concerning rate coefficients, either their absolute values may be fitted and evaluated as Arrhenius term further on, or the Arrhenius parameters may be estimated directly. During estimation limiting bounds may be set.

Quick sensitivity tests can be performed without changing the general setup of the estimation arrangement via activating or deactivating individual constants or data sheets.

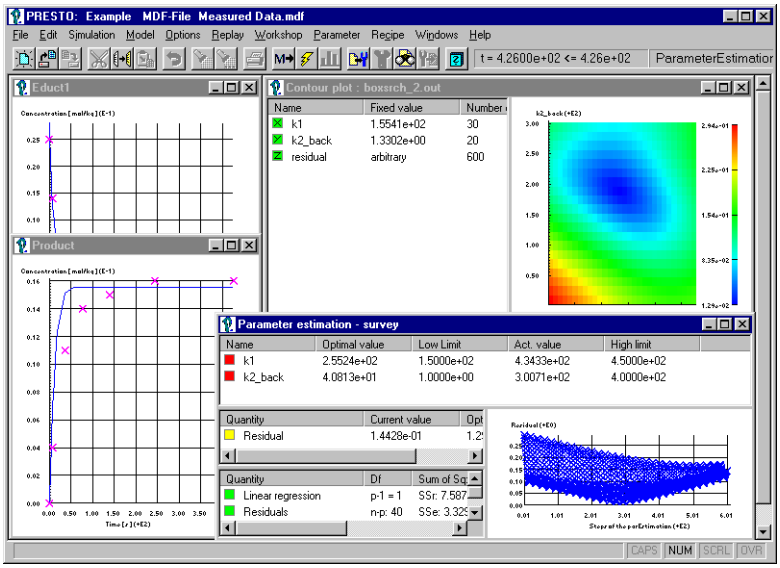
The configuration summarizeses the data collection, model and rate coefficients as well as scaling and weighting preferences together with penalty functions.

ASCII log-files provide a history of the fitting procedure for later inspection of the efficiency of the estimation process. All statistical information together with the course of parameter estimates are collected. Even detailed information about individual contributions of single compounds to the residual within each experiment is available.



Parameter Estimation

- box-search
- simulated annealing
- 3D-visualization

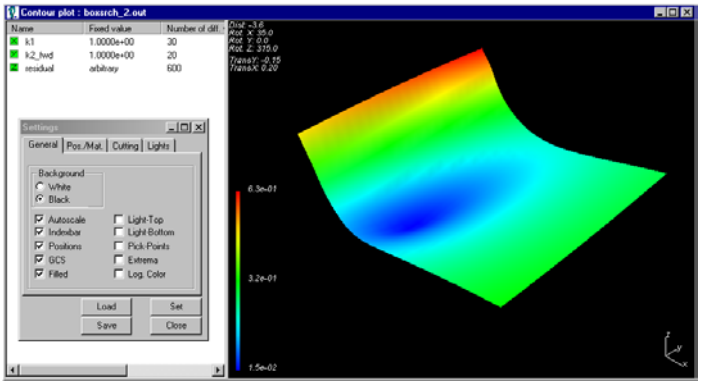


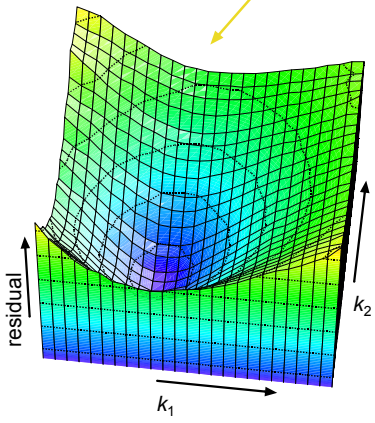
The box-search is the ideal tool for taking a first glance at a fitting problem and getting an idea about parameter sensitivities or correlations, leading to efficient initial values.

For the fitting of more than two parameters, the sensitivity of any of their combinations may be inspected using the internal contour plot function.

ASCII output files enable the processing and the visualization of data using other programs.

The integrated 3D OpenGL visualization helps to inspect sensitivity matrices and correlations of estimated parameters efficiently. The surface may be zoomed, shifted and rotated by any axis. It may be displayed as colored or shaded surface as well as transparent grid.

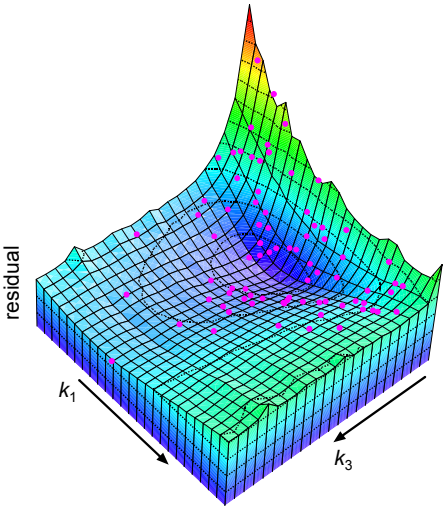




This feature is also available as stand-alone tool for the visualization of matrices.

In order to avoid laborious screening, a simulated annealing algorithm is implemented for a statistical search. The combination of gradient and random walk techniques assures finding identical solutions from varying initial conditions while concentrating computational efforts on the sensitivity area of interest.

The data are logged into ASCII files for later inspection and graphical representation by other sophisticated programs.



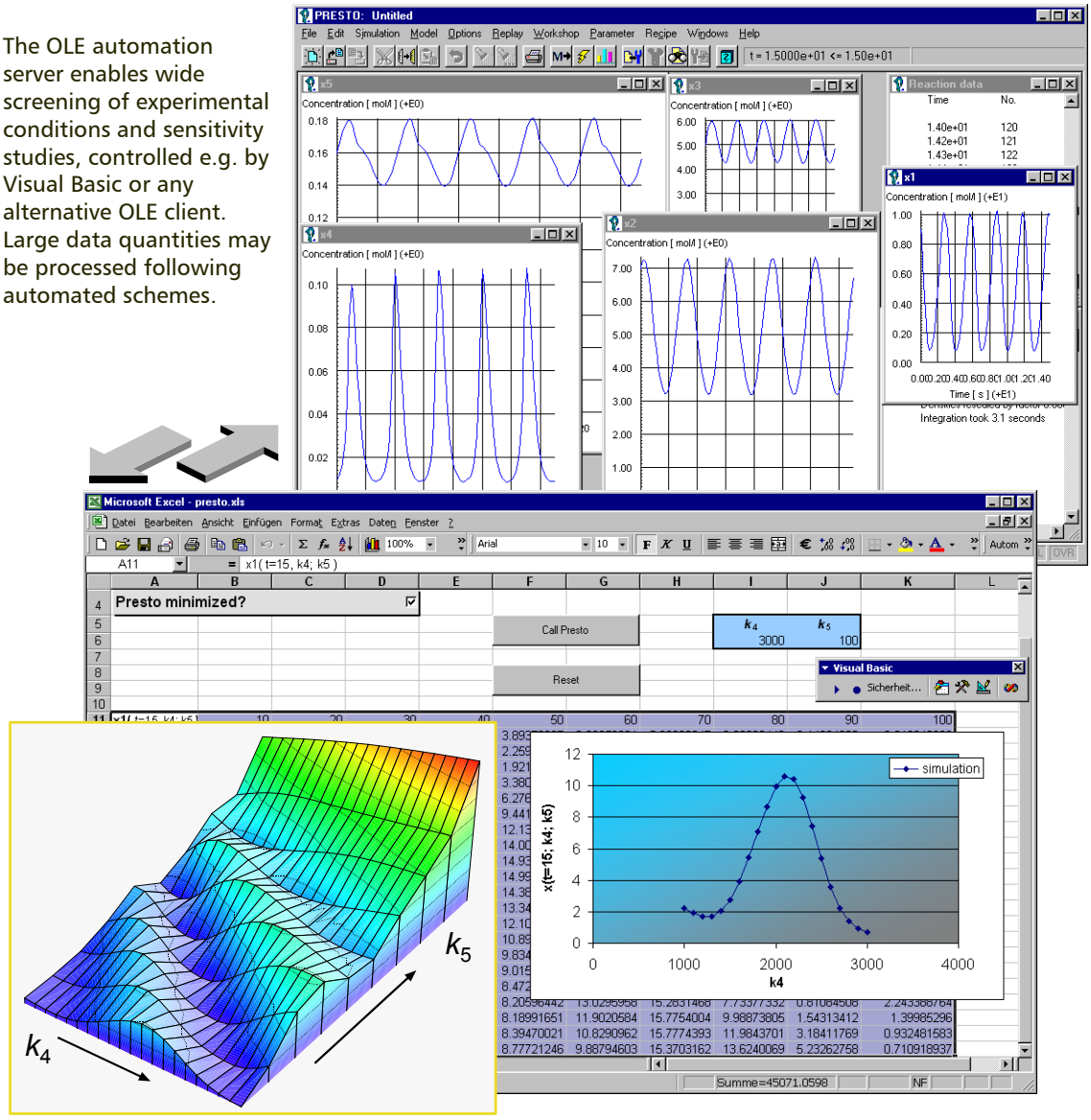
PRESTO-KINETICS

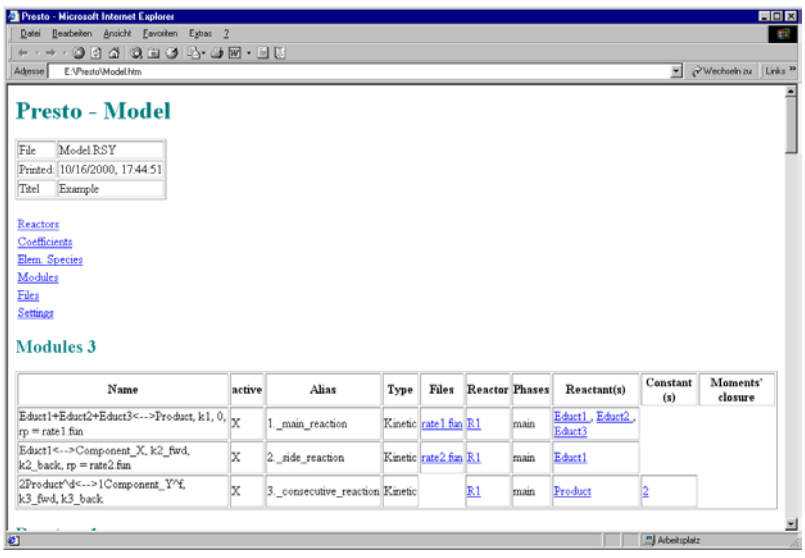
simulation program

Connectibility

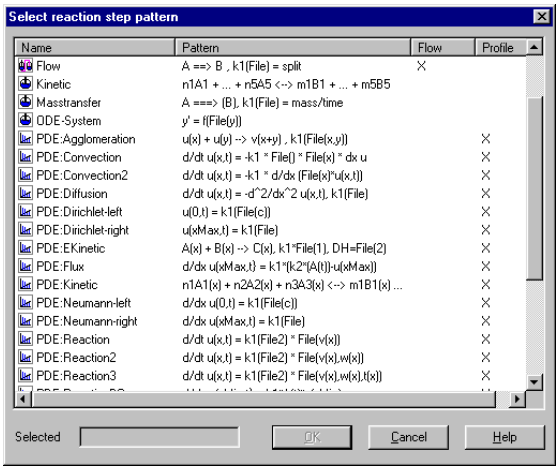
- open data formats for import / export
- batch automation
- OLE capability
- Web-functionality

The OLE automation server enables wide screening of experimental conditions and sensitivity studies, controlled e.g. by Visual Basic or any alternative OLE client. Large data quantities may be processed following automated schemes.





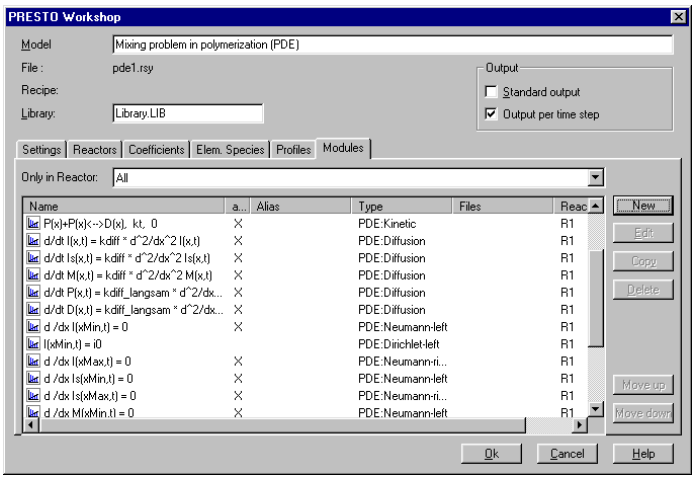
HTML functionalities simplify documentation. The ouput files in HTML-format include the model description, an archive that may be run directly with PRESTO and simulation results. These files can be used as a stand-alone documentation or as input files for other text processors. Furthermore, they can be published on the inter- or intranet.

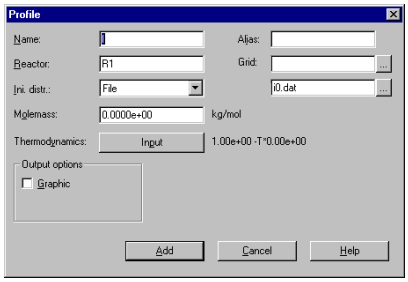


PRESTO is not only a very efficient tool for kinetic systems described by ordinary and algebraic differential equations, but includes a leading solver for systems of partial-differential equations.

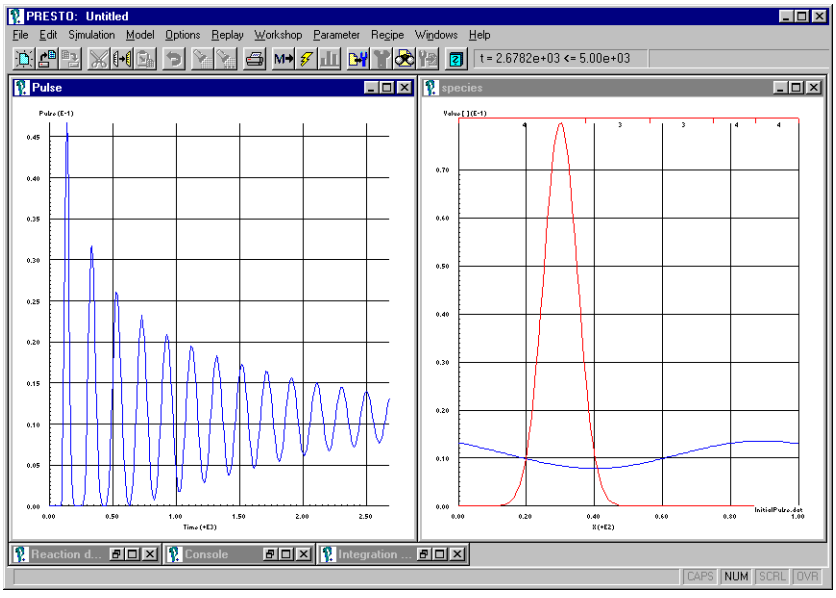
Numerous modules for a general description of convection, transport, diffusion, dispersion, boundary conditions, agglomeration and arbitrary kinetic reactions allow an easy transfer of kinetic schemes to distributed variables (e.g. axial or radial co-ordinates in a non-stationary tubular reactor, mixing problems, general PDE's). Parameter and coefficients of these processes can be formulated as spatial dependent.

The Galerkin h-p-algorithm works full self-adaptively, all discretizations are error-controlled. In connection with a parameter estimation procedure, the algorithm is even more efficient. The drawbacks of other solvers (poor error control, missing adaptivity, large number of approximating variables, restriction to local operators, method-of-lines approach), are avoided and overcome in PRESTO. A series of challenging problems could be solved with this tool in a unique way. Even free boundary problems (e.g. single particle models) can easily be solved in PRESTO using these powerful features. The handling of large PDE systems is as simple as for standard kinetics.





By this, in the same manner as for standard models complex simulation models may be defined by linking elementary basic objects. Recycle operators provide the facility to model loop reactors in an intuitive way. For results of the polymerization model shown here see page 2.

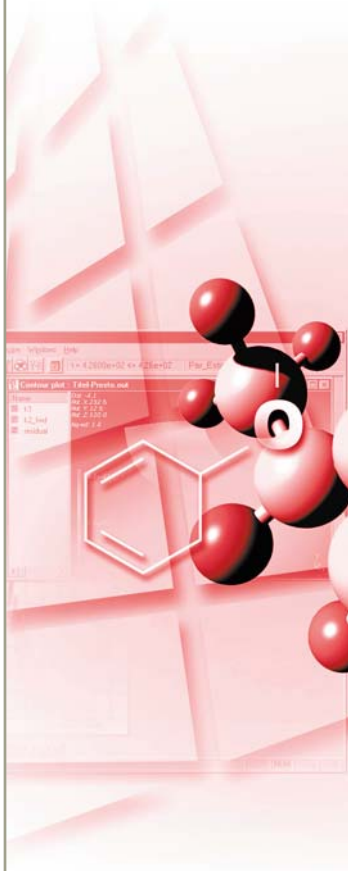


The profile species may be displayed as time dependent integral, time slices at a certain coordinate using the output functions of the library or as full time dependent 3D profiles using OpenGL techniques (see also page 2).

The example graphs show the behavior of a tracer pulse within a loop reactor where the backmixing characteristic is modeled by diffusion and convection operators.

Partial Differential Equations

- spatial gradients
- species profiles
- dynamic computation



PRESTO-KINETICS

simulation program

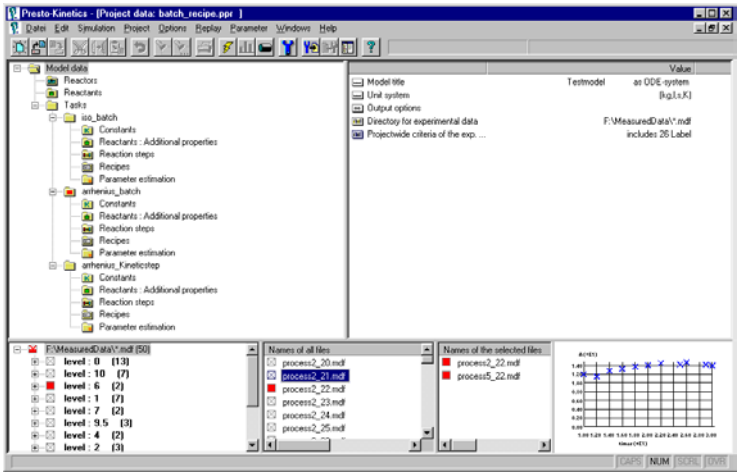
Extended Project Management

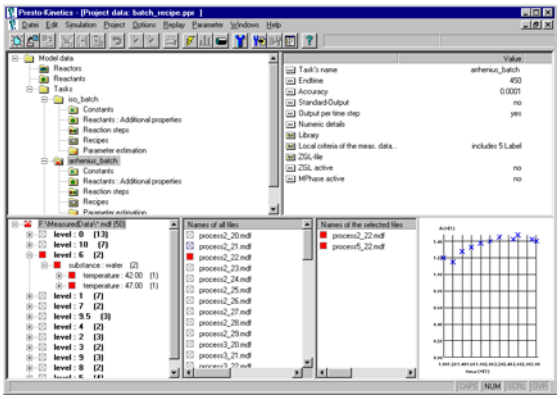
- multiple projects for a single model
- quick process change
- direct access to measured data

PRESTO is available in a second version (PRESTO-Kinetics II), that supports extended project management and shares the outstanding mathematical techniques.

It is developed to accompany multi-purpose plants. Plant specific data such as reactor configuration and specified substances are stored superior to individual project tasks.

The project tasks contain process specific items such as the kinetic model, rate coefficients, recipes and parameter estimation configuration.





Any of the project tasks has access to a common database of experimental data for comparison and parameter estimation.

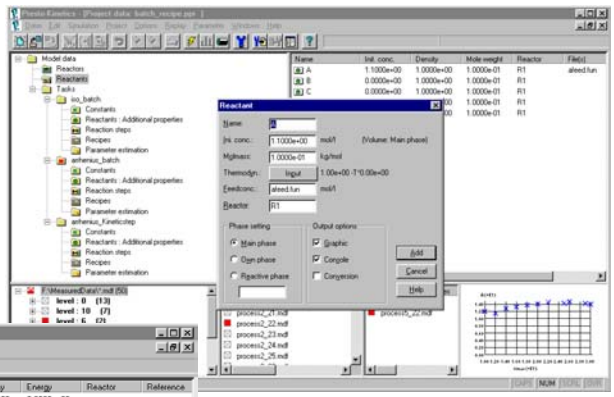
By changing tasks models may be tested very efficiently without changing the gobal project. Any development of model or process adaption is summarized within the same gobal project to keep things together.

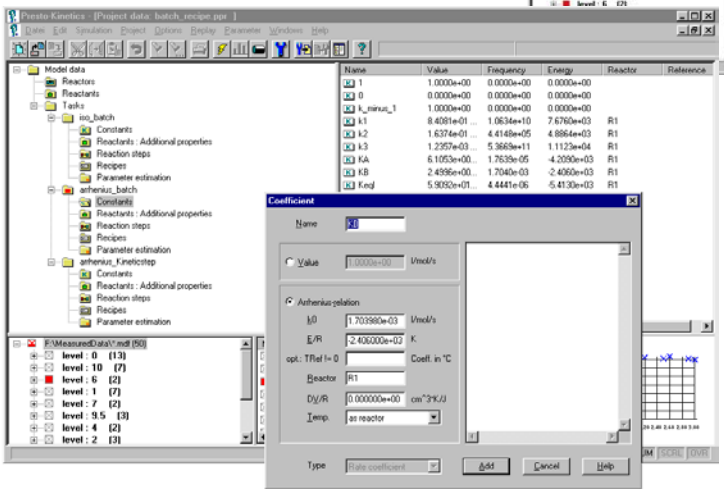
Moreover, an interface is available to link species to databases for calculation of thermodynamic properties such as activity coefficients.

Behind this advanced interface for multiple project management there exist the same user-friendly dialogues as in PRESTO-Kinetics.

Therefore there is no need for retraining when switching to PRESTO-Kinetics II and back.

Project tasks are fully compatible with models of PRESTO-Kinetics II and vice versa.

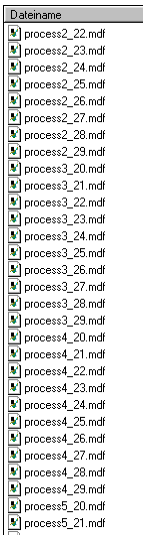




Dr. M. Wulkow Computing in Technology GmbH

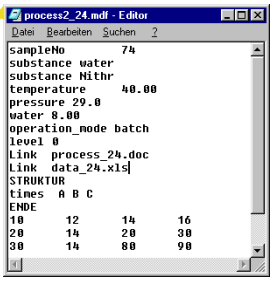
Data Hologram

- free label and group definition
- object oriented data classification
- application bounded links for files
- graphical representation of data



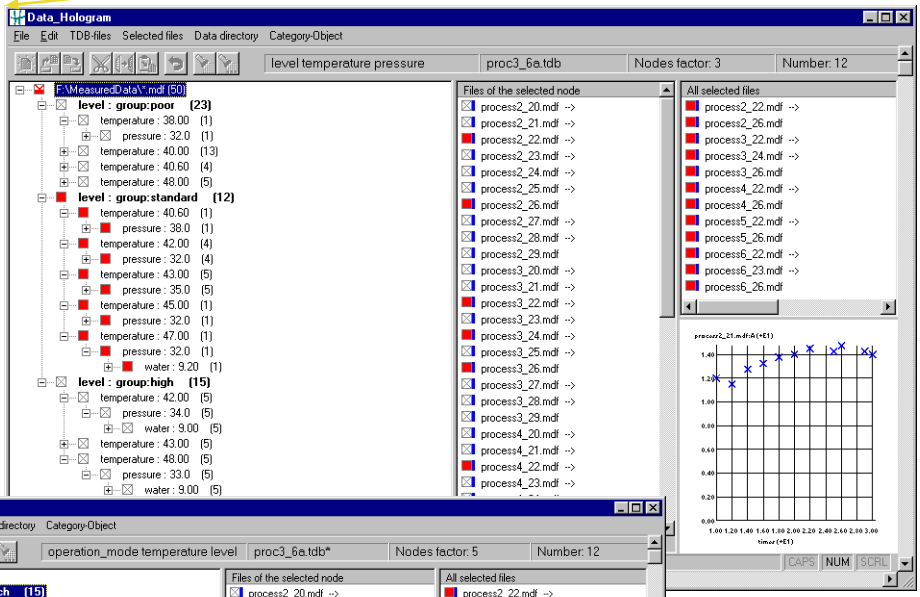
Initial situation:

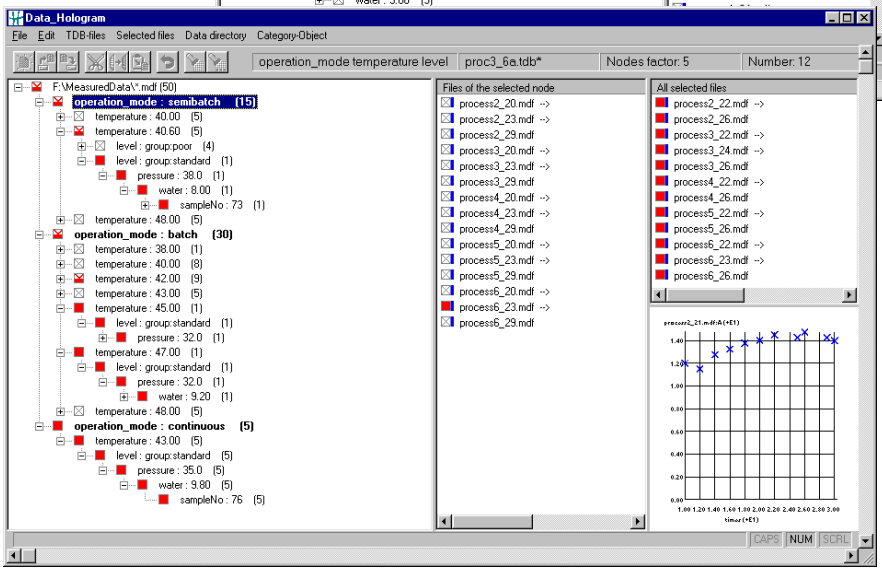
Unstructured collection consisting of individual data files with inhomogeneous content ...



Organization using the hologram:

User defined labels in arbitrary order describe the content of the data file and build the basic structure that has to be followed ...





... collect labels and data ranges to groups of your own choice and parse them hierarchically to find the data sets of your interest ...

- multi-dimensional overview of extended file collections for experimental data
- hierarchical structurization follows flexible differing aspects of interest
- labels for structurization are based on the individual files content
- user-defined labels that describe numerical data, abstract meanings, ranges of subjects
- user defined filters
- summarizing labels or numerical data in self-defined groups
- (easy) automatic scanning of labels

PRESTO-KINETICS

simulation program

Further Tools

Potential applications of PRESTO range from simulating general kinetic schemes up to treating 2-dimensional problems or bio-kinetics. And there are more products of CiT that share all the same outstanding numerical technology:

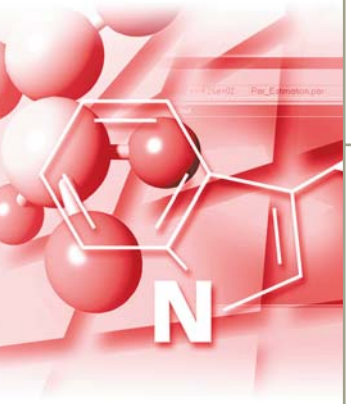
Predici:
- rigorous treatment of complete molecular weight distributions in arbitrary polymerization processes
- reaction step patterns for propagation, termination, transfer (monomer, agent, polymer), depolymerization and polymer degradation, description of oligomers, chain-length dependent reactions
- copolymerization with any number of monomer species
- treatment of composition and branching distributions
- particle size distributions in heterogeneous systems
- parameter estimation (multiple experiments)
- temperature- and pressure profiles as well as recipes for reactors or cascades of reactors
- manipulation of kinetic rate coefficients and reactants by use of an interpreter mechanism
- analysis of polymer properties
- input of measured concentrations as well as molecular weight distributions

Parsival:
- rigorous treatment of particle size distributions in heterogeneous process units (e.g. crystallization)
- reaction step patterns for particle growth, nucleation, agglomeration, breakage, fine's dissolution, convection, diffusion, boundary conditions, kinetic reactions
- flow sheets with classified flow and exit
- parameter estimation

Rioval:
- management tool for water quality modeling in streams
- interface for the description of rivers and input from treatment plants
- simulation based on a comprehensive and well-tested biofilm model

References

The products of CiT are used world-wide in academia and industry.
On your request it will be a pleasure for us providing a comprehensive list of reference customers and projects.



Dr. Michael Wulkow Computing in Technology GmbH
Oldenburger Straße 200
D - 26180 Rastede

Germany

Tel.: +49 (0) 44 02 / 84 2 48
Fax: +49 (0) 44 02 / 939 927
mwulkow-cit@t-online.de
http://www.wst.shuttle.de/cit/

Version 3.03.06