
# Presto-Kinetics 11 – Overview

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# CiT...

CiT Dr. M. Wulkow Computing in Technology

- Founded in 1992, M. Wulkow is a mathematician
- Software for modeling and simulation in chemistry, mainly
  - PREDICI® (polymer kinetics)
  - PARSIVAL® (crystallization, particle systems)
  - PRESTO-KINETICS® (chemical and bio kinetics, spatial distributions)
- Clients
  - Many companies and universities world-wide

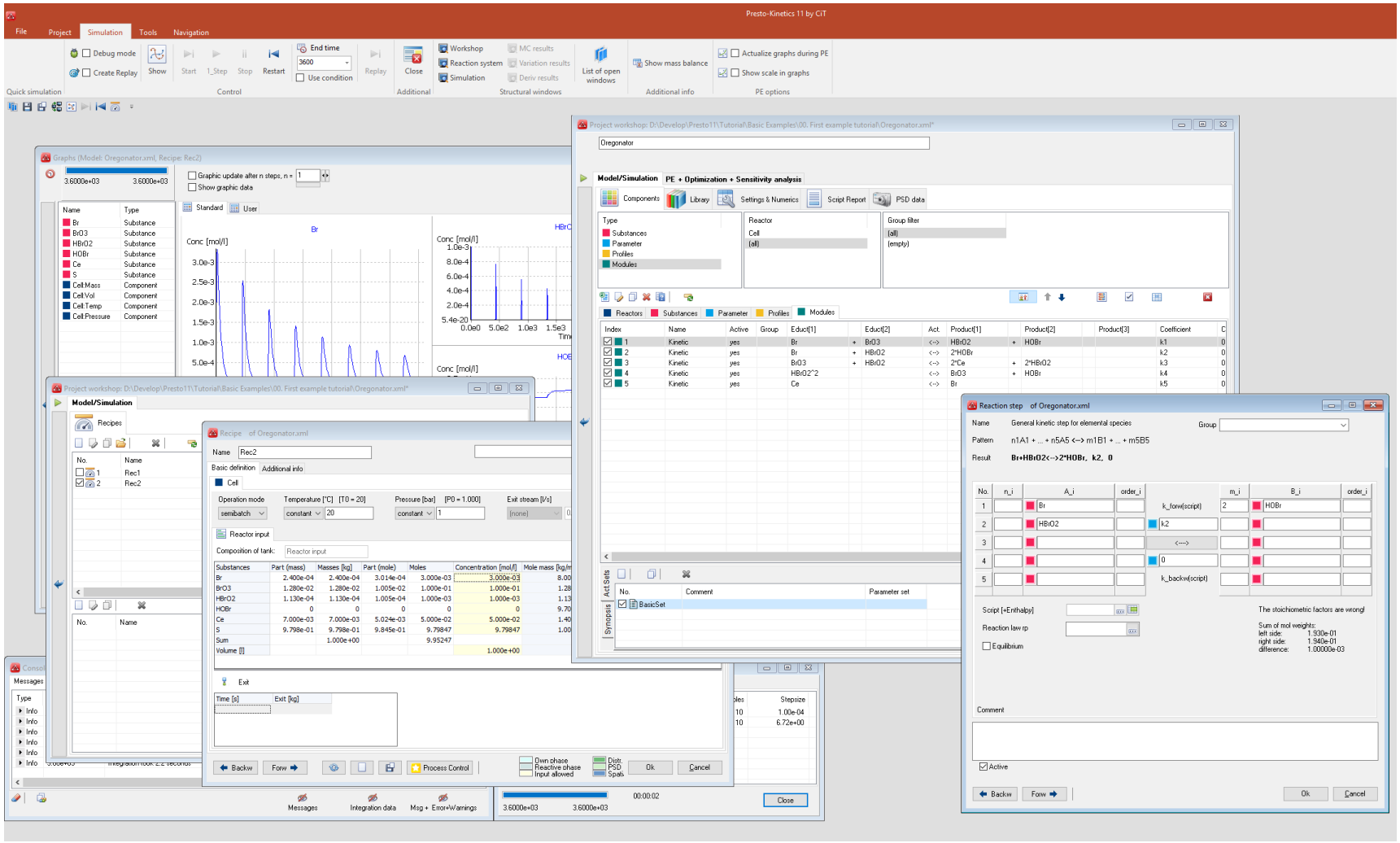
# Presto-Kinetics: Open and modular system

- Basic chemical kinetics
- Bio kinetics and systems biology
- Reactor models → batch, semi-batch, continuous, plug-flow, cascades
- Modules for
  - kinetics
  - phase changes
  - mass transfers
  - particle growth
  - reactor flows
  - spatial profiles
- Solver for partial differential equations
- Framework for multiple-phase systems
- Sophisticated parameter estimation based on unique algorithm

# Further important modules

- **PDE solver** for treatment of spatial profiles in catalysts or tube reactors
- **Sensitivity analysis** for parameters
- Recipe **variation**
- **Optimal control** module for stream and temperature control
- **Cape-Open** interface for access of thermodynamic property packages
- User **database** for handling of substance and kinetic data

# Full screen …


Presto-Kinetics 11 by CiT
File
Project
Simulation
Tools
Navigation
Graphs (Model: Oregonator.xml, Recipe: Rec2)
Project workshop: D:\Develop\Presto11\Tutorial\Basic Examples\00. First example tutorial\Oregonator.xml*
Oregonator
Model/Simulation
PE + Optimization + Sensitivity analysis
Components
Library
Settings & Numerics
Script Report
PSD data
Recipe of Oregonator.xml
Reaction step of Oregonator.xml
Messages
Integration data
Msg + Error+Warnings
Close

# Modular system for kinetics



- Typical scheme

$$A + 2B \xrightarrow{k_1} C \quad , \quad r_1 = k_1 A B^2$$

$$2C \xrightarrow{k_2} D + E \quad , \quad r_2 = k_2 C^2$$

$$A + E \xrightarrow{k_3} F + B \quad , \quad r_3 = k_3 A E$$

- Differential equations (ODEs)

$$A' = -r_1 - r_3 = -k_1 A B^2 - k_3 A E$$

$$B' = -2r_1 + r_3 = -2k_1 A B^2 + k_3 A E$$

$$C' = r_1 - 2r_2 = k_1 A B^2 - 2k_2 C^2$$

$$D' = r_2 = k_2 C^2$$

$$E' = r_2 - r_3 = k_2 C^2 - k_3 A E$$

$$F' = r_3 = k_3 A E$$

# Modular system for kinetics



- Often formally written in terms of matrix-vector product

$$\begin{bmatrix} A' \\ B' \\ C' \\ D' \\ E' \\ F' \end{bmatrix} = \begin{bmatrix} -1 & 0 & -1 \\ -2 & 0 & 1 \\ 1 & -2 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} k_1 AB^2 \\ k_2 C^2 \\ k_3 AE \end{bmatrix} = S \cdot r$$

- Implementation in plain code requires proper numbering
- In large systems single reactions are difficult to see

# Alternative: Presto-Kinetics approach



- Single reactions derive their “own” ODEs internally
- All terms are superposed, even kinetic steps and abstract ODEs
- All further terms are added automatically
- Once a kinetic step pattern is implemented and validated, it can be used again and again.
- Reaction rates can be arbitrarily complex
- Equilibrium reactions supported (requires extension of S and r otherwise)

$$A + 2B \xrightarrow{k_1} C \quad , \quad r_1 = k_1 A B^2$$

$$A' = -k_1 r A B^2$$

$$B' = -2k_1 A B^2$$

$$C' = k_1 A B^2$$

$$2C \xrightarrow{k_2} D + E \quad , \quad r_2 = k_2 C^2$$

$$C' = -2k_2 C^2$$

$$D' = k_2 C^2$$

$$E' = k_2 C^2$$

$$A + E \xrightarrow{k_3} F + B \quad , \quad r_3 = k_3 A E$$

$$A' = -k_3 A E$$

$$E' = -k_3 A E$$

$$B' = k_3 A E$$

$$F' = k_3 A E$$

# Presto-Kinetics framework

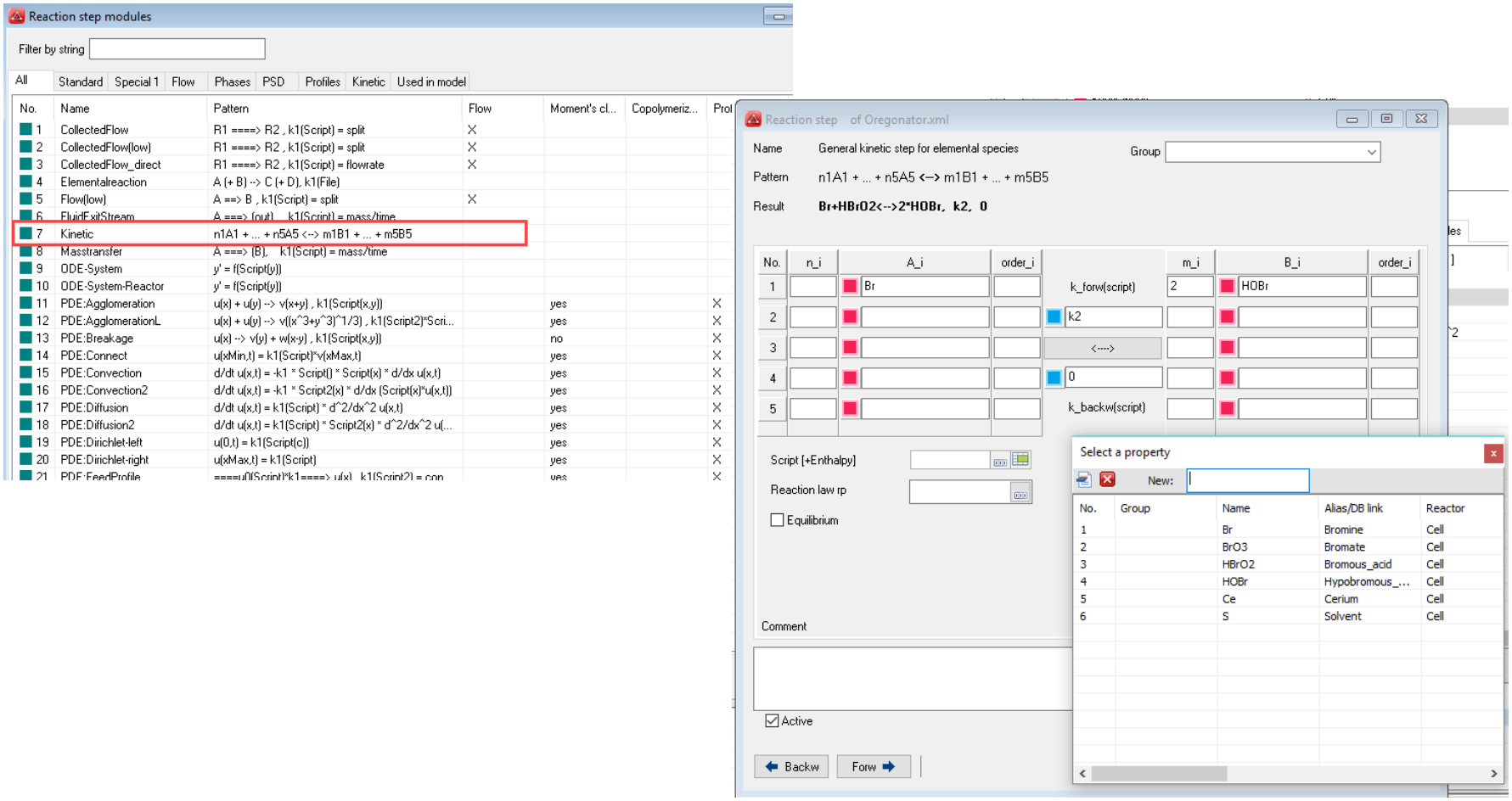


- Internal treatment of species based on mol/volume
- Volume treatment important in many applications
- Recipe input allows all kind of inputs that is transformed to basic units
- Reaction rates have to be returned in terms of mol/volume/time
- Volume influenced by streams and density changes

$$\frac{dA}{dt} = r_A^{total} - \frac{V_R'}{V} A - \frac{V_\rho'}{V} A$$

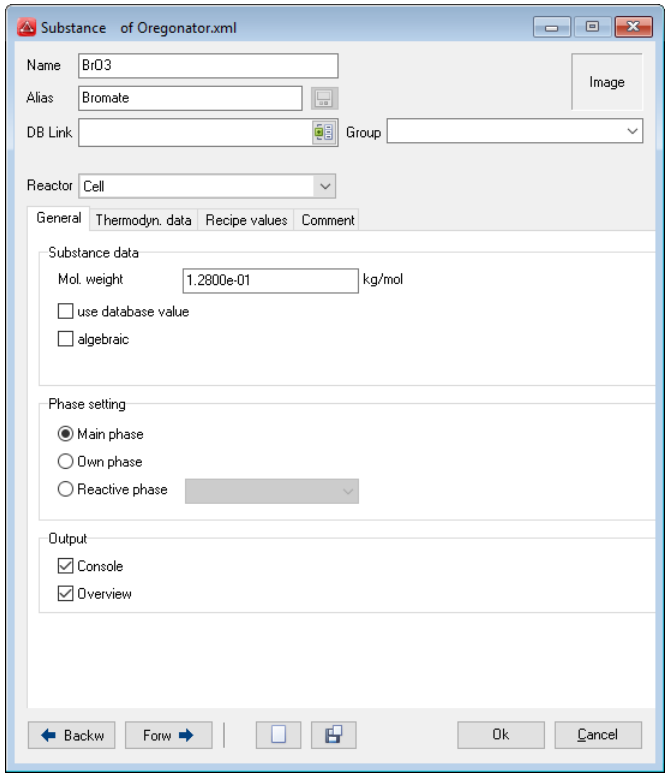
# Modular kinetics

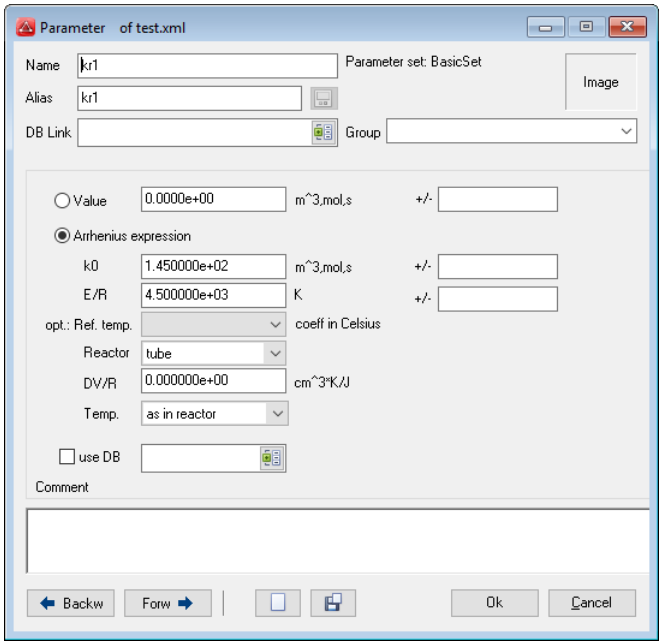
- Select reaction step pattern from list using, e.g. “General kinetic”
- Assign species w.r.t modeling context



# Model administration – components

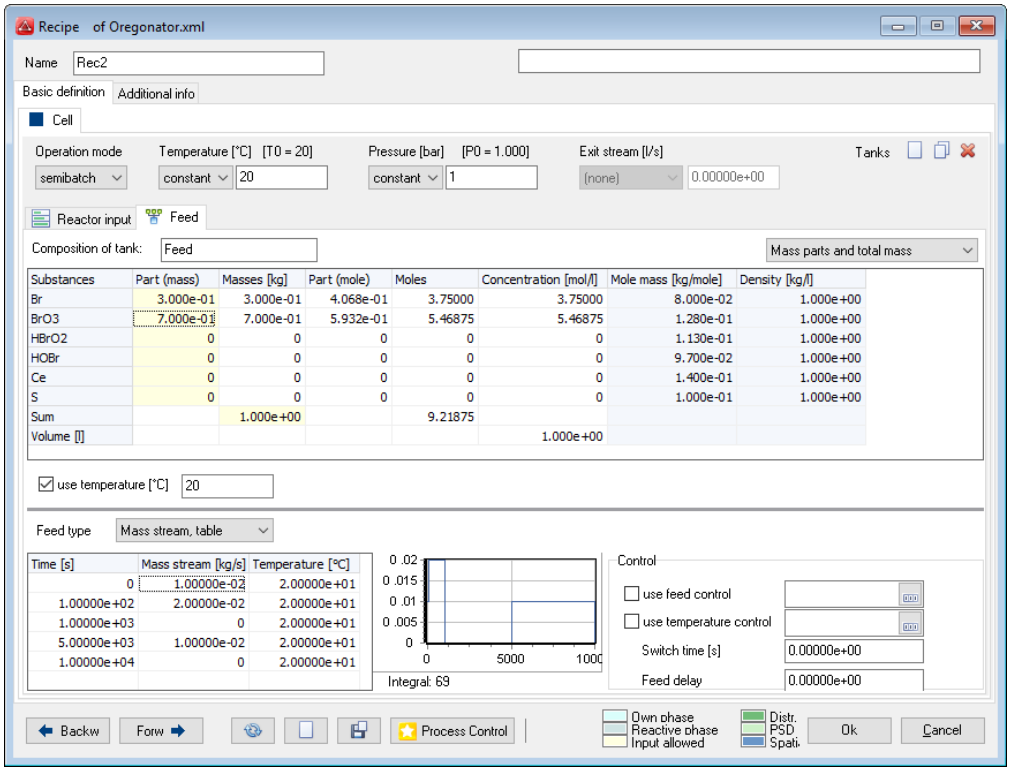
- Various properties and settings
- Comfortable editing
- Access to user-database
- Extension by user-scripts possible



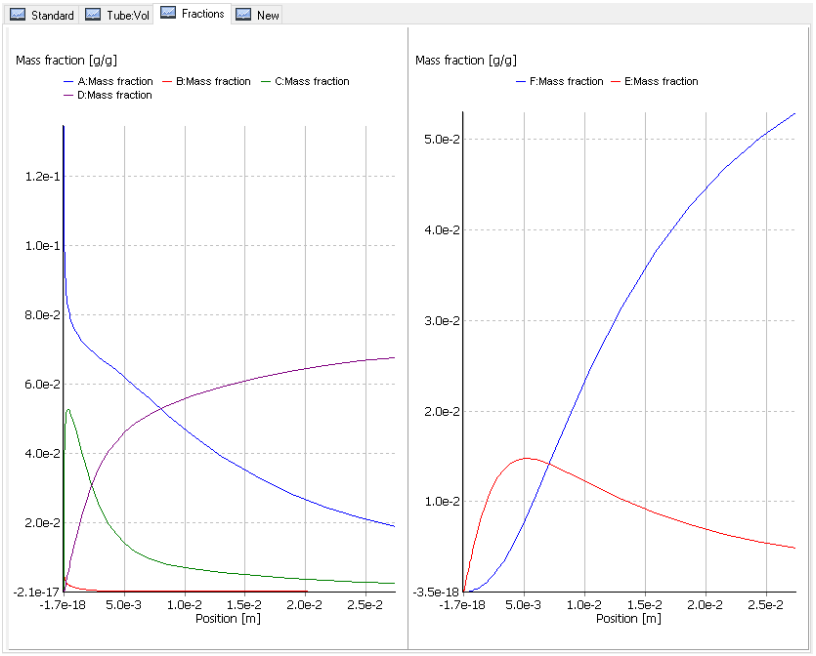
# Recipes

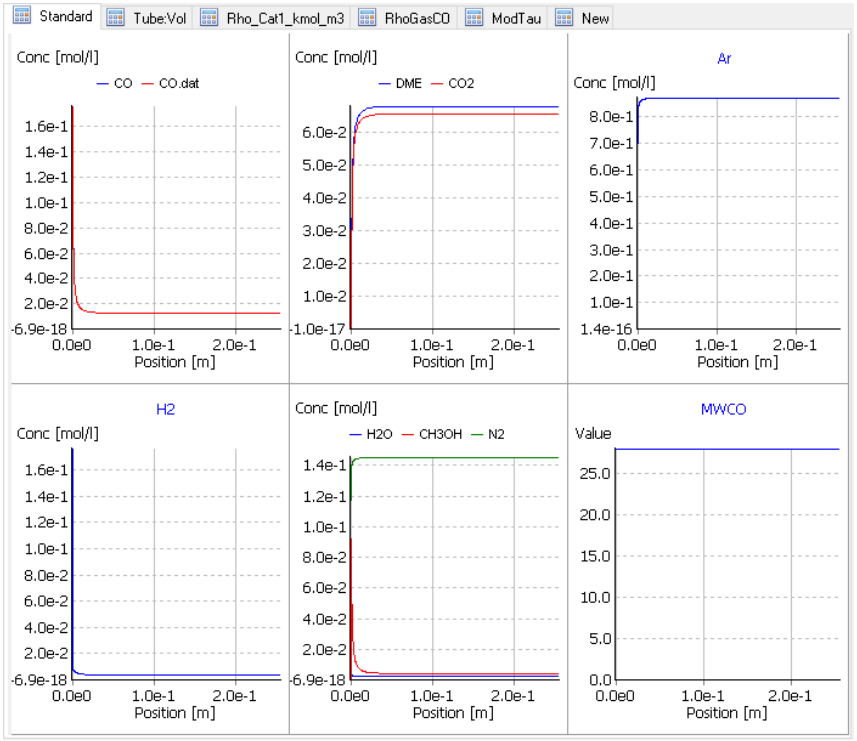
- All input of all species entered in terms of recipes
- Various input types
- Multi-reactor treatment
- Temperature and pressure control
- Project contains list of recipes, one active
- Various feed and control strategies



# Powerful online chart administration

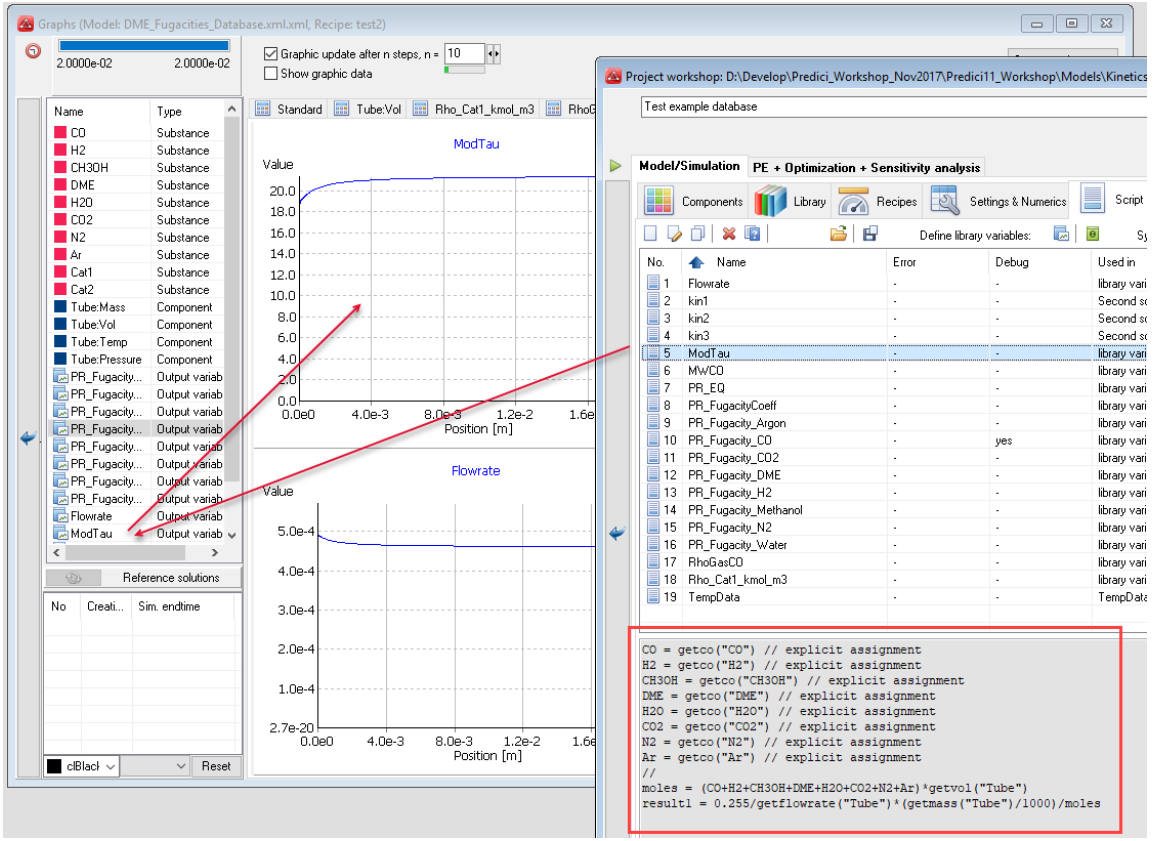
- Create own graphic tabs, even during a simulation
- Drag & drop curves to graphic tab
- Combine graphics in one chart
- Loaded reference data are stored within the project



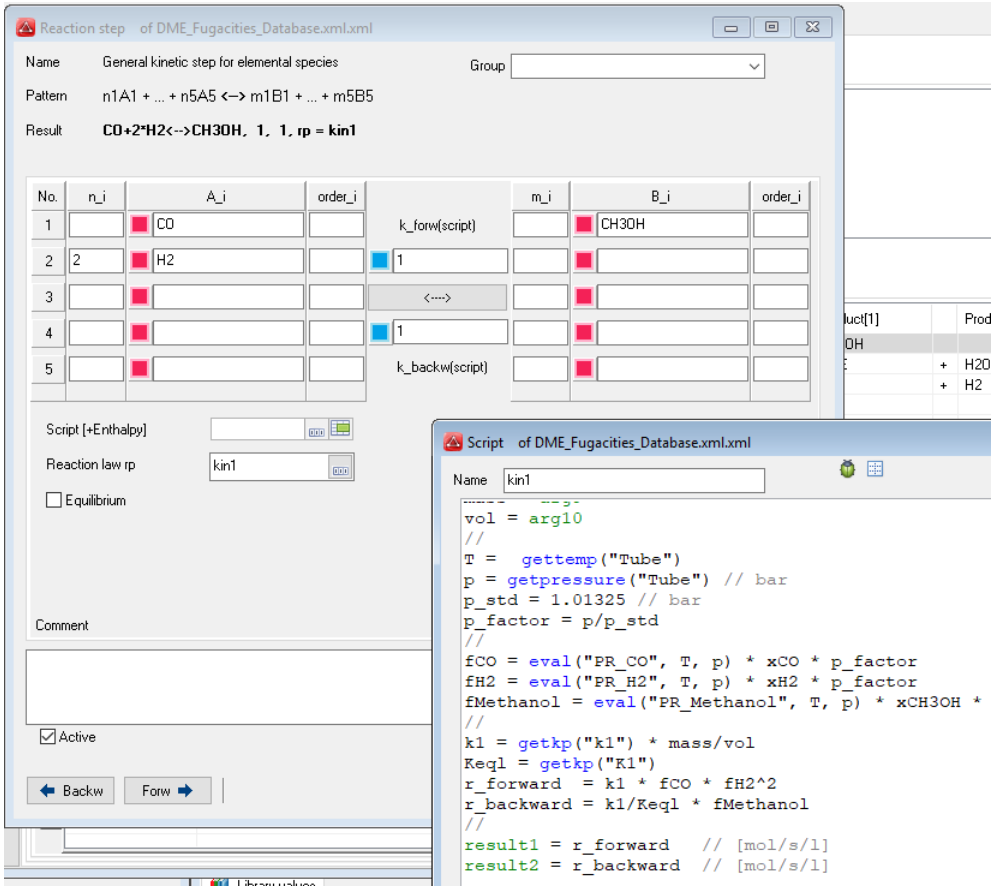
# Scripts

- Direct output of user-defined expressions of any kind
- User-defined equations and rates
- Access to all system variables
- Export of results



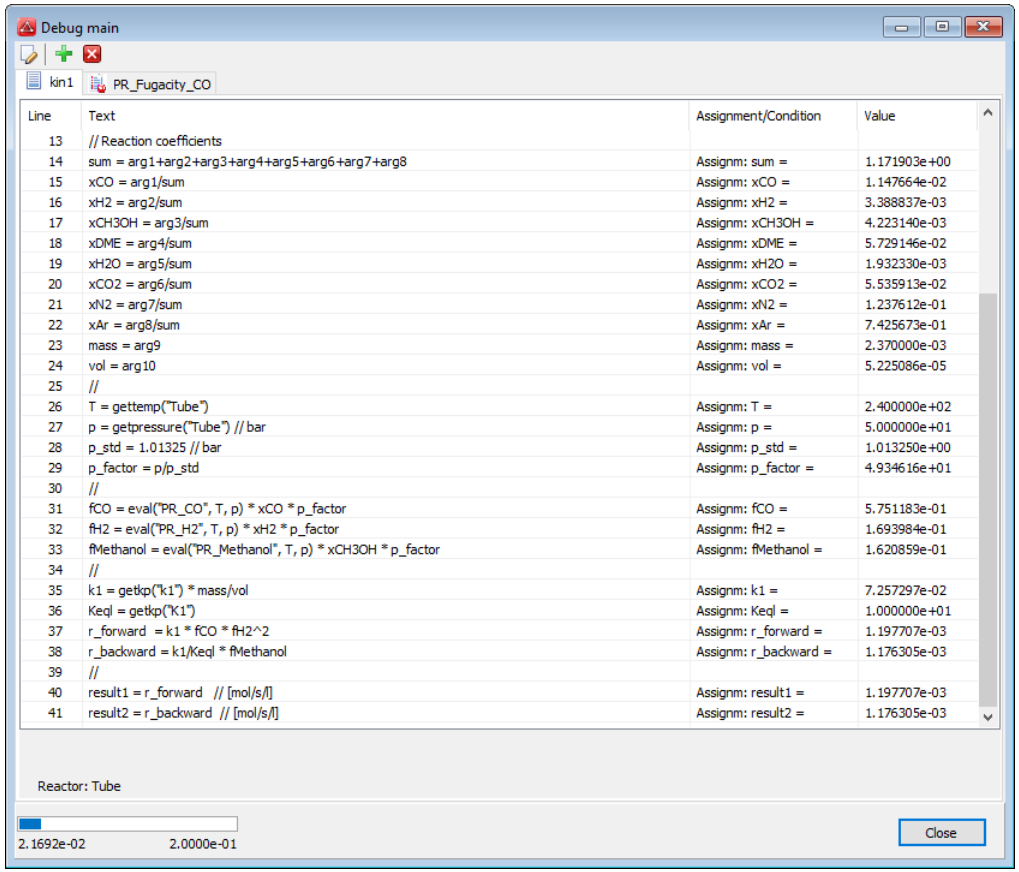
# Scripts

- Reaction rates
  - Presto-Kinetics combines stoichiometry, rate parameters and reaction law
  - Scripts may re-define any part of a kinetics step



# Scripts

- Script debugger
  - line-by-line check of code
  - check at any time during simulation possible (step mode)



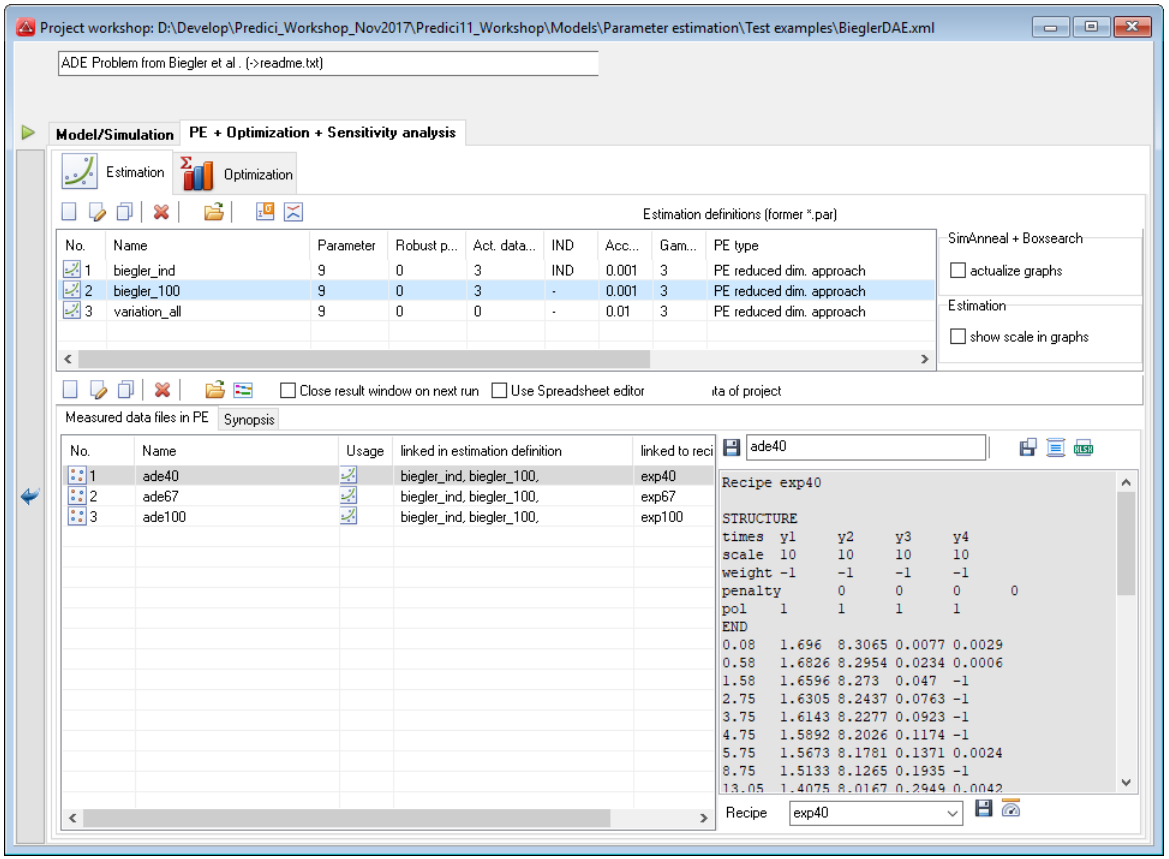
# Parameter estimation



- Task: fit any set of model parameters vs. set of experimental data of all kind
  - concentrations
  - temperature
  - user-defined script expressions
- Important aspects
  - sensitivities
  - scaling
  - dependencies
- Algorithms
  - box search
  - simulated annealing
  - sophisticated Gauss-Newton algorithm with damping strategy
  - extension: algorithm to detect dependencies among parameters
  - New: Bayesian analysis and uncertainty quantification

# Parameter estimation

- Definition includes all necessary information
  - parameter definitions
  - experimental data files and recipes
  - various settings



# Parameter estimation

- Values of fitted parameters including statistic values
- Estimation of essential degrees of freedom
- Detailed presentation of residuals and parameters