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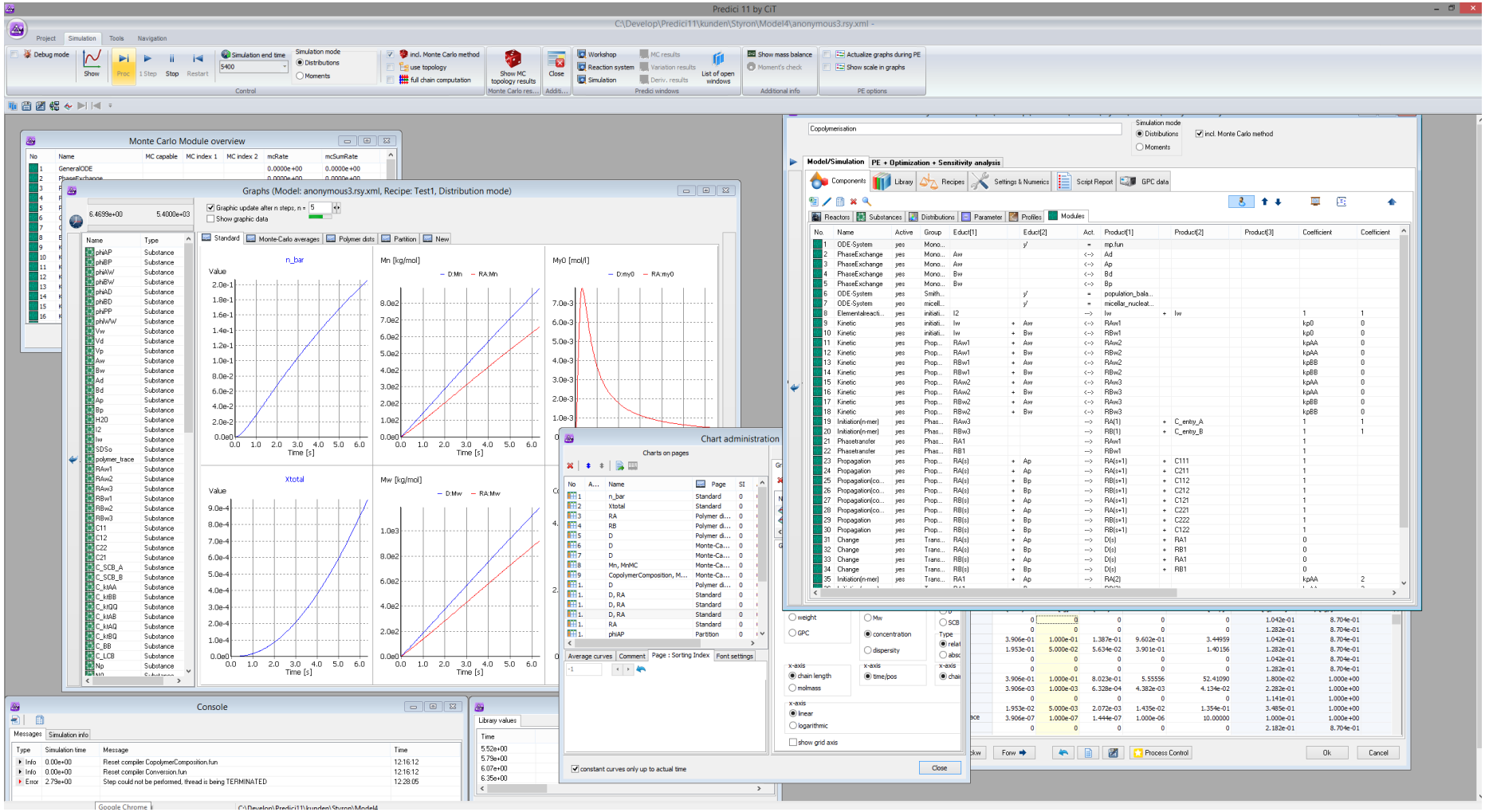
# Predici 11 – Quick Overview

PREDICI is the leading simulation package for kinetic, process and property modeling with a major emphasis on macromolecular systems. It has been successfully utilized to model radical copolymerization, living polymerizations (RAFT, NMP, ATRP), emulsion and suspension polymerizations and various Ziegler-Natta catalyzed systems.

# Predici 11: Comparison to previous versions

| Features | Predici 11 | Predici 7 |
|---|---|---|
| Comprehensive list of reaction steps | X | X |
| Galerkin h-p- method for MWD simulation | X | X |
| Hybrid deterministic-stochastic solver | new | - |
| Recipe modules | advanced | basic |
| Parameter estimation tool | advanced, new handling | basic |
| Sensitivity analysis (Monte-Carlo) | new | - |
| Sensitivity analysis (sigma points) | new | - |
| Dynamic graphic and chart administration | new | - |
| PDE-solver and capabilities for particle size distributions | extended | X |
| Project search tool | new | - |
| Script interpreter | new editor | X |
| Export of underlying moment equations | including subroutines | X |
| Model comparison, exchange of objects between projects | new | X |
| All-in-one XML project files | new | - |
| Compatible import of PREDICI7 models | X | X |
| Petri chart for model analysis | new (using WinGraphviz) | - |
| Assignment of structure graphics to substances and reaction steps | new | - |
| Pattern finder for beginners | new | - |
| Cape-Open interface | integrated | separate DLL |
| Optimization module | integrated and improved | separate tool |
| OLE/COM interface | X | X |

# Predici 11: The completely new user interface



# Predici: An open and modular system

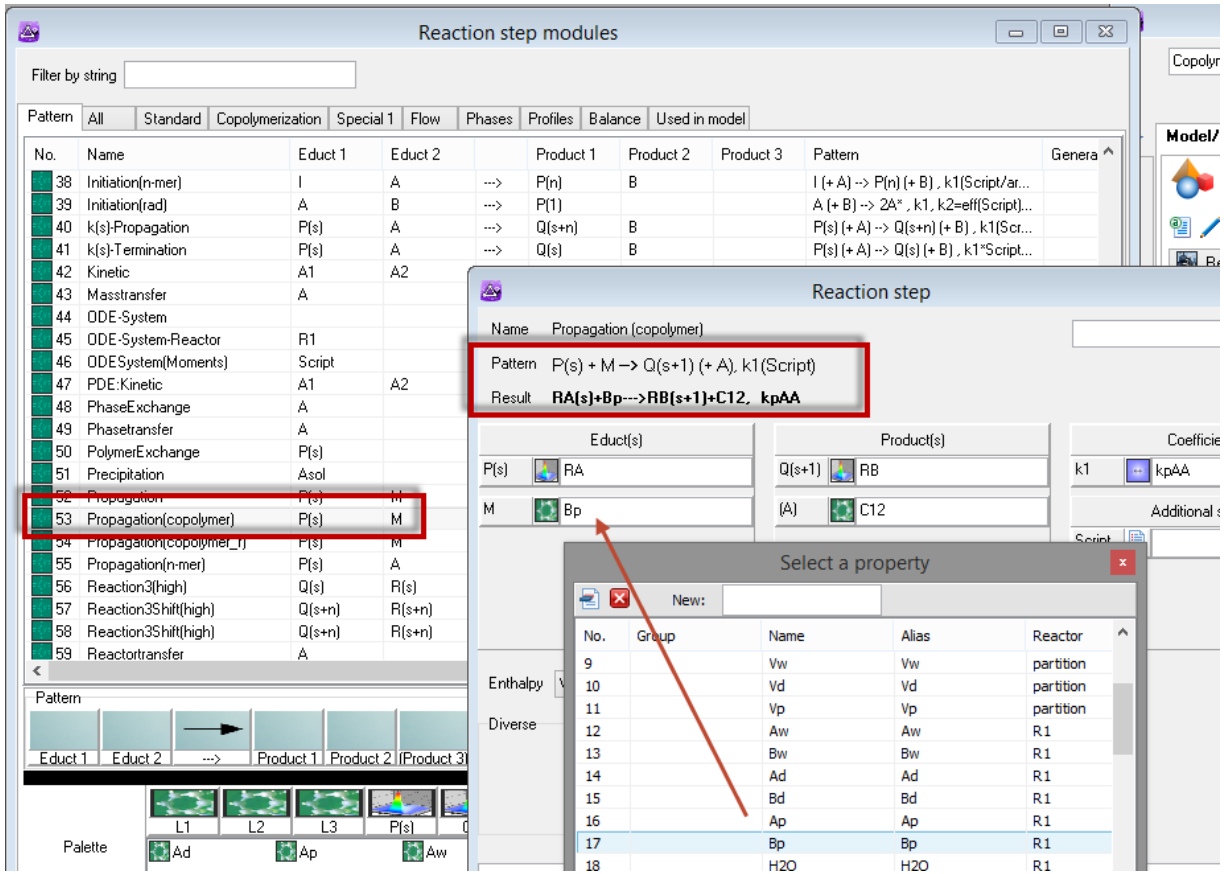
- Polymerization, e.g.
  - radical copolymerization
  - living polymerizations (RAFT, NMP, ATRP)
  - emulsion and suspension polymerizations
  - various Ziegler-Natta catalyzed systems
- Basic chemical kinetics
- Bio kinetics and systems biology
- Reactor models → batch, semi-batch, continuous, plug-flow, cascades
- Over 100 modules for
  - kinetics
  - phase changes
  - mass transfers
  - particle growth
  - reactor flows

# Predici: Models and results

- Inputs
  - arbitrary kinetic schemes
  - parameters and rate expressions
  - additional differential equations
  - reactor operation (recipes)
  - experimental data
- Outputs
  - molecular weight distributions
  - concentrations of species and reactor variables
  - any other output based on state variables of the model
  - deterministic and statistical results
  - parameters
  - optimal controls

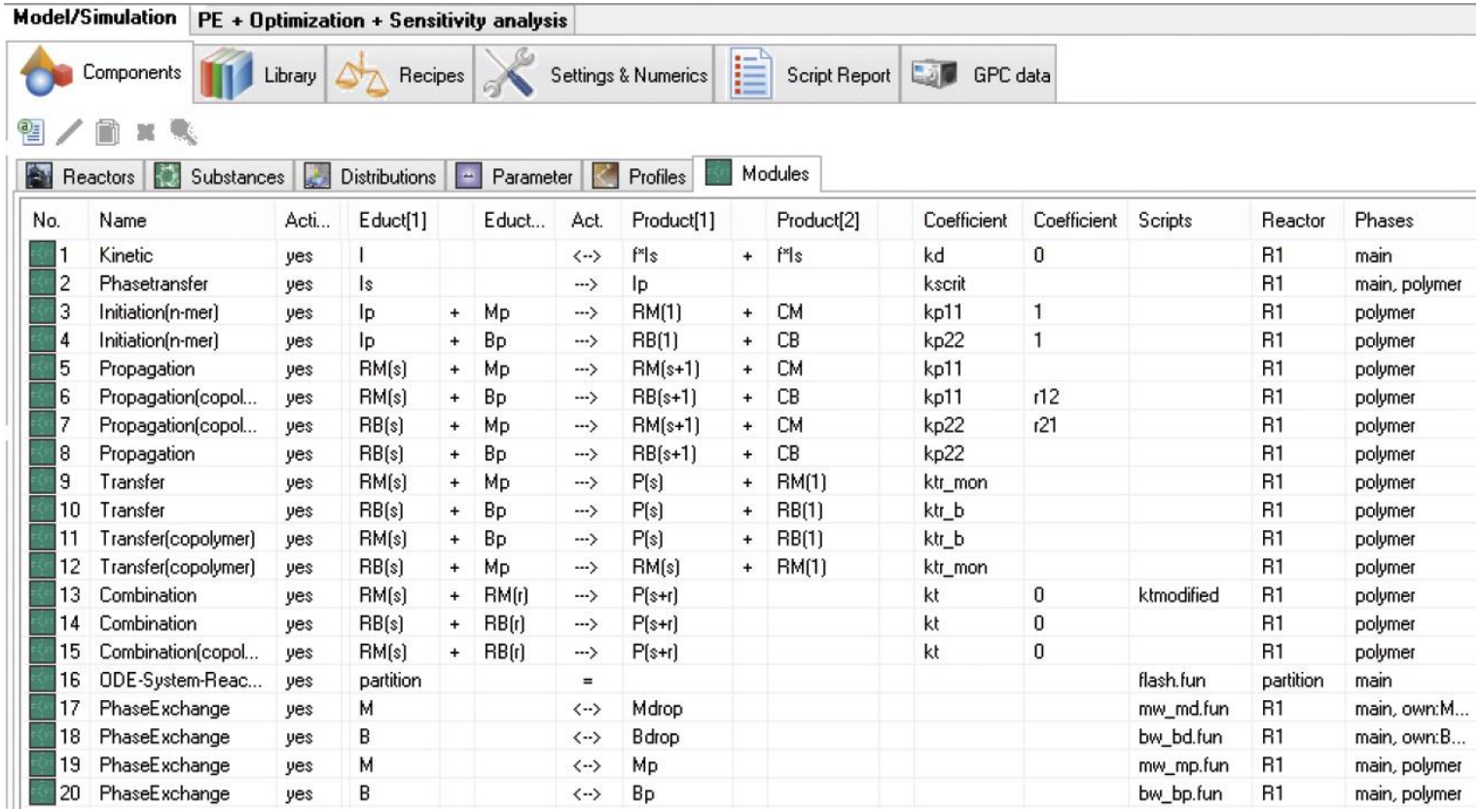
# Predici: Modular kinetics

- Select reaction step from comprehensive list using filters and “pattern finder”
- Assign species w.r.t modeling context



# Predici: Modular kinetics

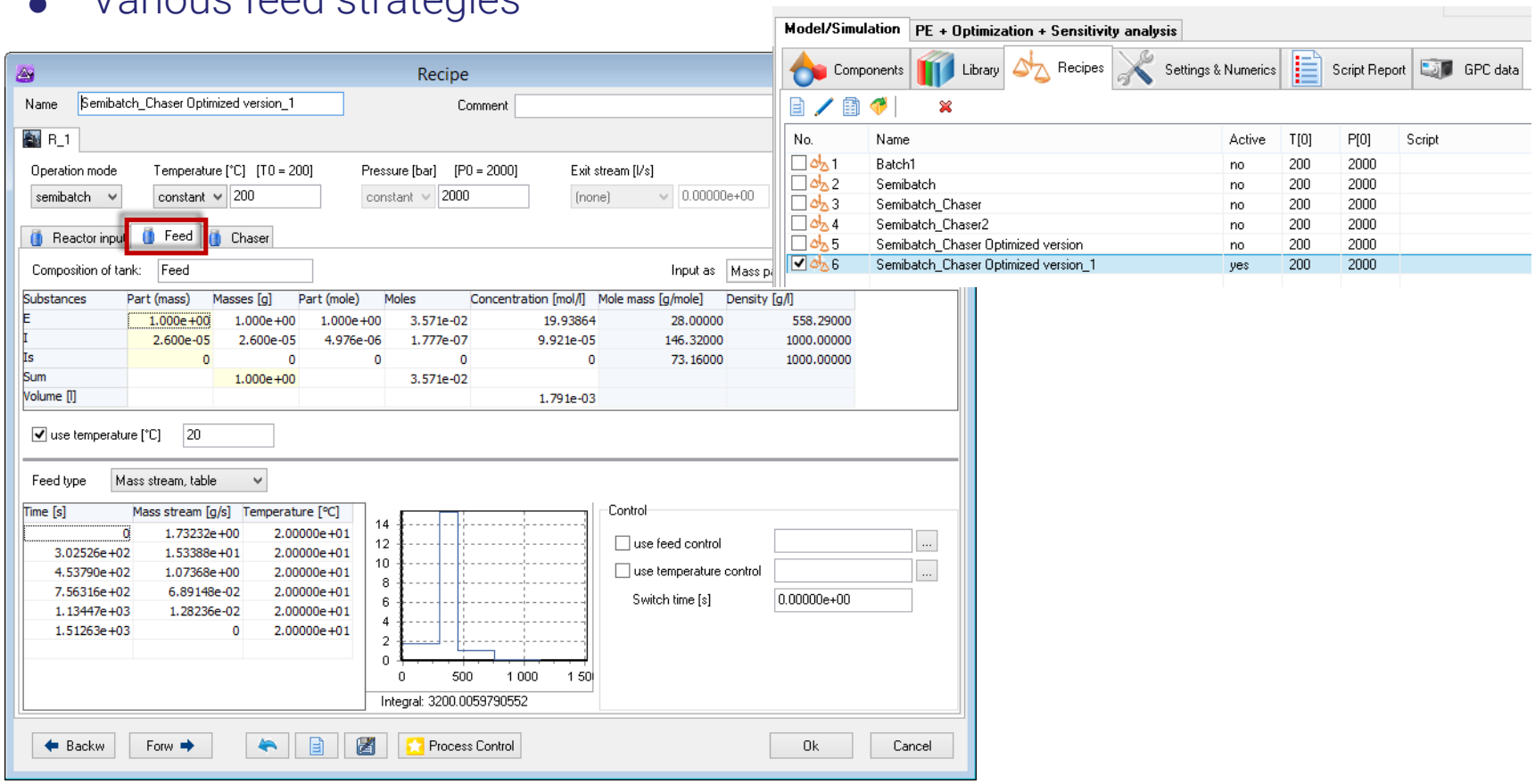
- Create any kind of kinetic system
- Link parameters and user-defined rate expressions (optional)




| No. | Name | Acti... | Educt[1] | | Educt... | Act. | Product[1] | | Product[2] | | Coefficient | Coefficient | Scripts | Reactor | Phases |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Kinetic | yes | I | | | <--> | f*Is | + | f*Is | | kd | 0 | | R1 | main |
| 2 | Phasetransfer | yes | Is | | | ---> | Ip | | | | kscrit | | | R1 | main, polymer |
| 3 | Initiation(n-mer) | yes | Ip | + | Mp | ---> | RM(1) | + | CM | | kp11 | 1 | | R1 | polymer |
| 4 | Initiation(n-mer) | yes | Ip | + | Bp | ---> | RB(1) | + | CB | | kp22 | 1 | | R1 | polymer |
| 5 | Propagation | yes | RM(s) | + | Mp | ---> | RM(s+1) | + | CM | | kp11 | | | R1 | polymer |
| 6 | Propagation(copol... | yes | RM(s) | + | Bp | ---> | RB(s+1) | + | CB | | kp11 | r12 | | R1 | polymer |
| 7 | Propagation(copol... | yes | RB(s) | + | Mp | ---> | RM(s+1) | + | CM | | kp22 | r21 | | R1 | polymer |
| 8 | Propagation | yes | RB(s) | + | Bp | ---> | RB(s+1) | + | CB | | kp22 | | | R1 | polymer |
| 9 | Transfer | yes | RM(s) | + | Mp | ---> | P(s) | + | RM(1) | | ktr_mon | | | R1 | polymer |
| 10 | Transfer | yes | RB(s) | + | Bp | ---> | P(s) | + | RB(1) | | ktr_b | | | R1 | polymer |
| 11 | Transfer(copolymer) | yes | RM(s) | + | Bp | ---> | P(s) | + | RB(1) | | ktr_b | | | R1 | polymer |
| 12 | Transfer(copolymer) | yes | RB(s) | + | Mp | ---> | RM(s) | + | RM(1) | | ktr_mon | | | R1 | polymer |
| 13 | Combination | yes | RM(s) | + | RM(r) | ---> | P(s+r) | | | | kt | 0 | ktmodified | R1 | polymer |
| 14 | Combination | yes | RB(s) | + | RB(r) | ---> | P(s+r) | | | | kt | 0 | | R1 | polymer |
| 15 | Combination(copol... | yes | RM(s) | + | RB(r) | ---> | P(s+r) | | | | kt | 0 | | R1 | polymer |
| 16 | ODE-System-Reac... | yes | partition | | | = | | | | | | | flash.fun | partition | main |
| 17 | PhaseExchange | yes | M | | | <--> | Mdrop | | | | | | mw_md.fun | R1 | main, own:M... |
| 18 | PhaseExchange | yes | B | | | <--> | Bdrop | | | | | | bw_bd.fun | R1 | main, own:B... |
| 19 | PhaseExchange | yes | M | | | <--> | Mp | | | | | | mw_mp.fun | R1 | main, polymer |
| 20 | PhaseExchange | yes | B | | | <--> | Bp | | | | | | bw_bp.fun | R1 | main, polymer |

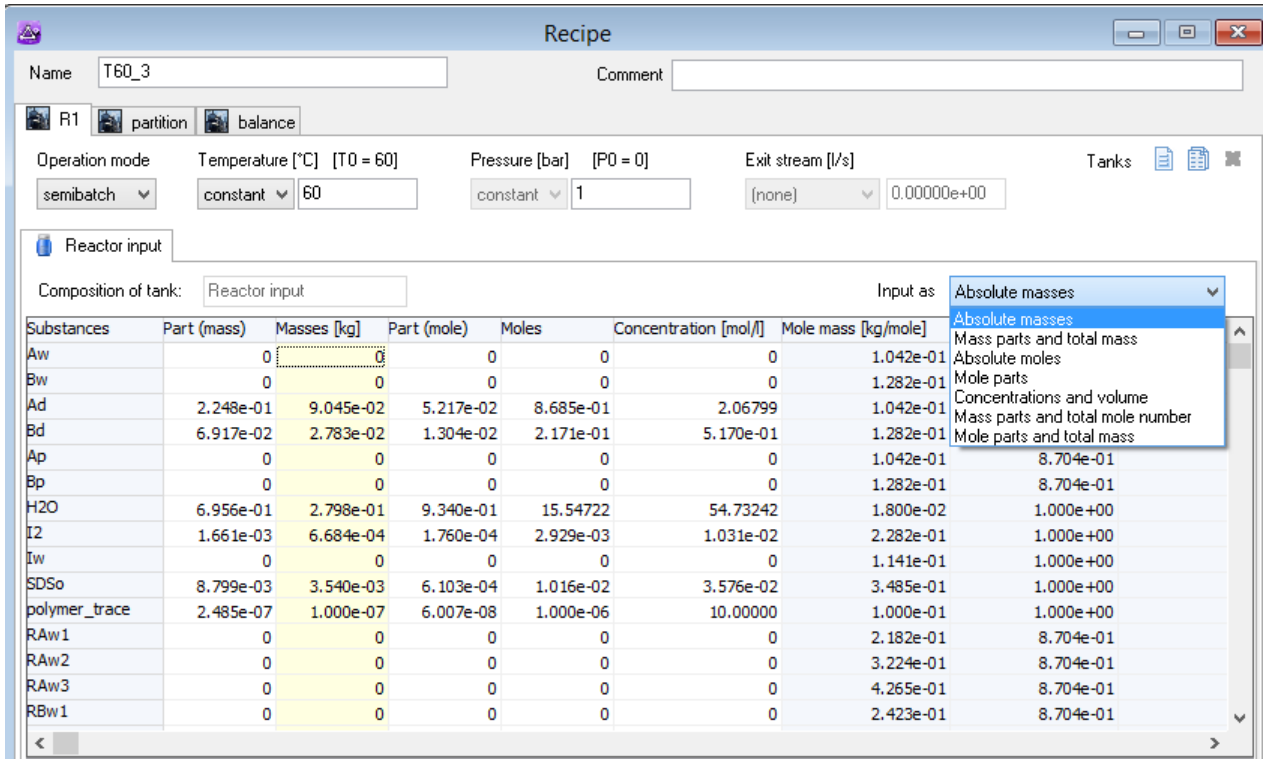
# Recipes: Input of all kinds of reactor operation modes

- All input of all species entered in terms of recipes
- Project contains list of recipes, one set to be active
- Various feed strategies



# Recipes: Many new input options

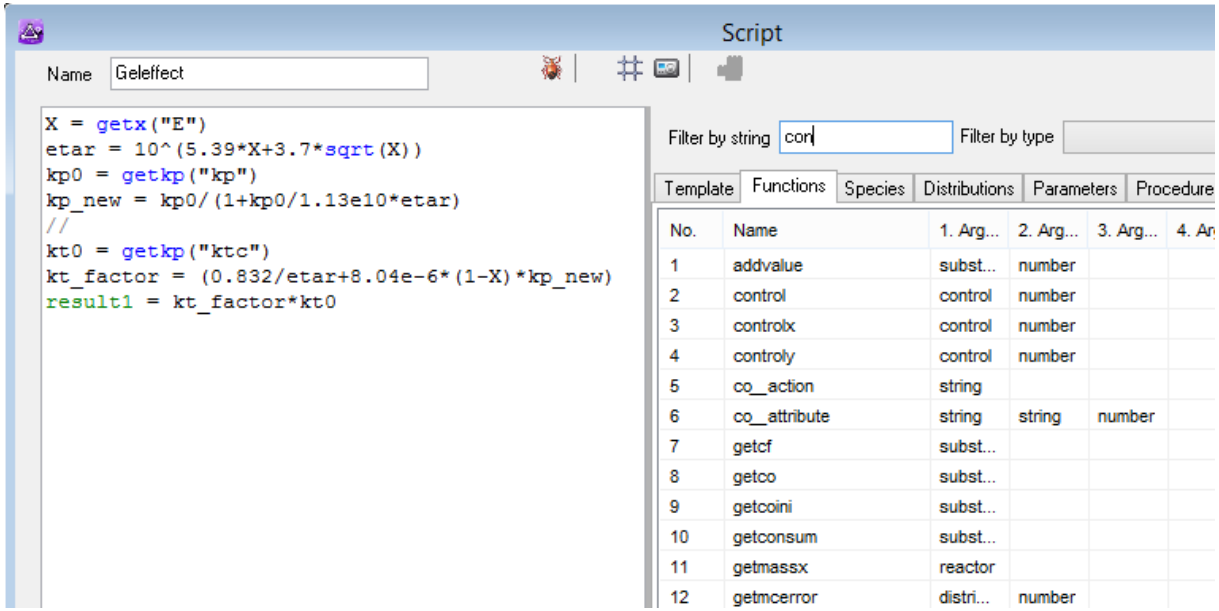
- Various input types
- Multi-reactor treatment
- Temperature and pressure control




| Substances | Part (mass) | Masses [kg] | Part (mole) | Moles | Concentration [mol/l] | Mole mass [kg/mole] | |
|---|---|---|---|---|---|---|---|
| Aw | 0 | 0 | 0 | 0 | 0 | 1.042e-01 | |
| Bw | 0 | 0 | 0 | 0 | 0 | 1.282e-01 | |
| Ad | 2.248e-01 | 9.045e-02 | 5.217e-02 | 8.685e-01 | 2.06799 | 1.042e-01 | |
| Bd | 6.917e-02 | 2.783e-02 | 1.304e-02 | 2.171e-01 | 5.170e-01 | 1.282e-01 | |
| Ap | 0 | 0 | 0 | 0 | 0 | 1.042e-01 | 8.704e-01 |
| Bp | 0 | 0 | 0 | 0 | 0 | 1.282e-01 | 8.704e-01 |
| H2O | 6.956e-01 | 2.798e-01 | 9.340e-01 | 15.54722 | 54.73242 | 1.800e-02 | 1.000e+00 |
| I2 | 1.661e-03 | 6.684e-04 | 1.760e-04 | 2.929e-03 | 1.031e-02 | 2.282e-01 | 1.000e+00 |
| Iw | 0 | 0 | 0 | 0 | 0 | 1.141e-01 | 1.000e+00 |
| SDSo | 8.799e-03 | 3.540e-03 | 6.103e-04 | 1.016e-02 | 3.576e-02 | 3.485e-01 | 1.000e+00 |
| polymer_trace | 2.485e-07 | 1.000e-07 | 6.007e-08 | 1.000e-06 | 10.00000 | 1.000e-01 | 1.000e+00 |
| RAw1 | 0 | 0 | 0 | 0 | 0 | 2.182e-01 | 8.704e-01 |
| RAw2 | 0 | 0 | 0 | 0 | 0 | 3.224e-01 | 8.704e-01 |
| RAw3 | 0 | 0 | 0 | 0 | 0 | 4.265e-01 | 8.704e-01 |
| RBw1 | 0 | 0 | 0 | 0 | 0 | 2.423e-01 | 8.704e-01 |

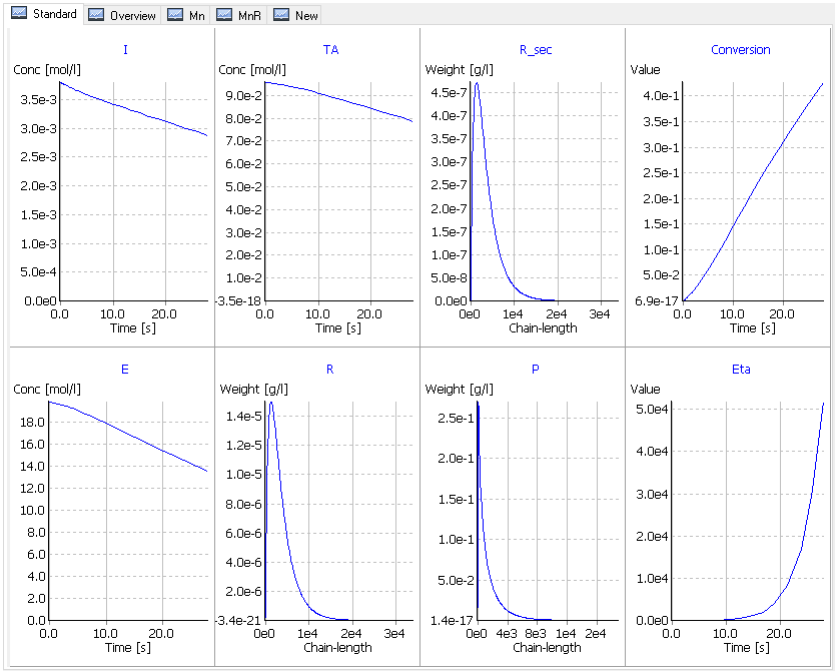
# Integrated scripting: User-defined extensions

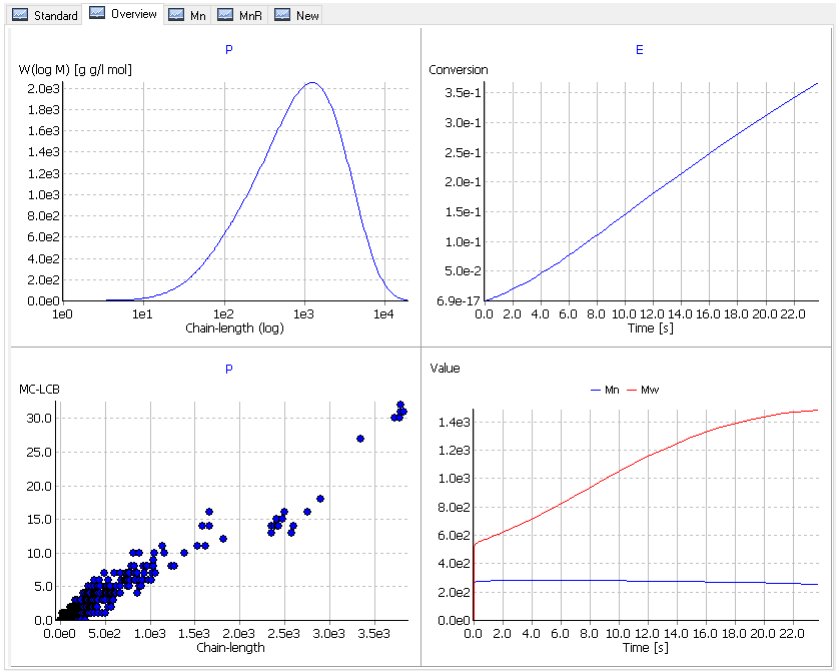
- Add own code for
  - additional output
  - rate expressions
  - additional equations
- Simple script language, access to all system variables by high-level script commands



# Output: Enhanced online charts

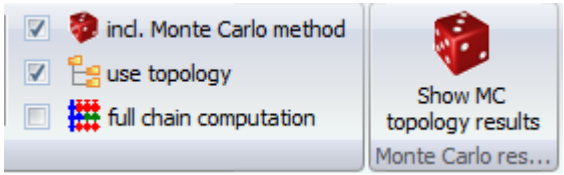
- Create own graphic tabs, even during a simulation
- Drag & drop curves to graphic tab
- Combine graphics in one chart
- Selective export of all graphic data possible

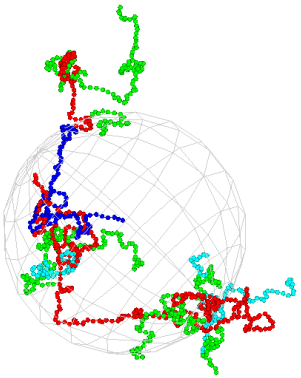


# New algorithm: Hybrid Monte-Carlo method

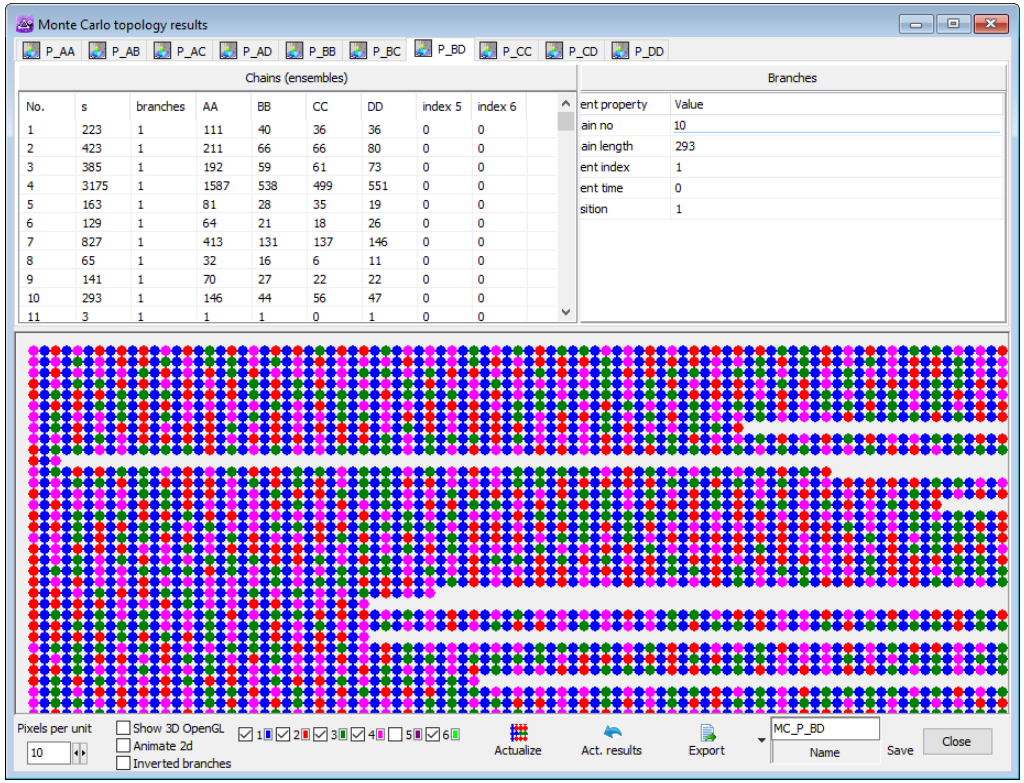
- Predici performs **deterministic** calculations based on Galerkin h-p-method.
- For all distributions after each time step an ensemble of chains is updated by Gillespie-type algorithm applying the deterministic results.
- A number of **property indexes** as well as **topology** information is tracked.
- The most important reaction steps are available for Monte-Carlo simulations
- Output
  - total and relative number of property indexes in chains
  - mean values of chain ensemble from MC (compare to h-p-method)
  - sequence distributions of indexes in chains
  - topology of polymer molecules based on random walk



# Hybrid Monte-Carlo method: Complete polymer chains

- All events along a chain can a stored, e.g. incorporation of different monomers
- Built-in sequence length analysis of copolymers
- Analysis of any single event along all chains possible



# Parameter estimation: New handling, improved algorithms

- Fit of any set of model parameters vs. any set of experimental data
  - concentrations
  - temperature
  - product properties: mean values, composition, full distributions
  - user-defined script expressions
- Important new functionalities in Predici
  - project administration of data and configurations
  - powerful sensitivity analysis
  - comprehensive administration, output and export of results
- Algorithms
  - Gauss-Newton with damping strategy (accurate local search)
  - special algorithm detecting dependencies among parameters
  - box search (deterministic scan of parameter range)
  - simulated annealing (stochastic global search)

# Parameter estimation: New options to analyze results

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