



CIT

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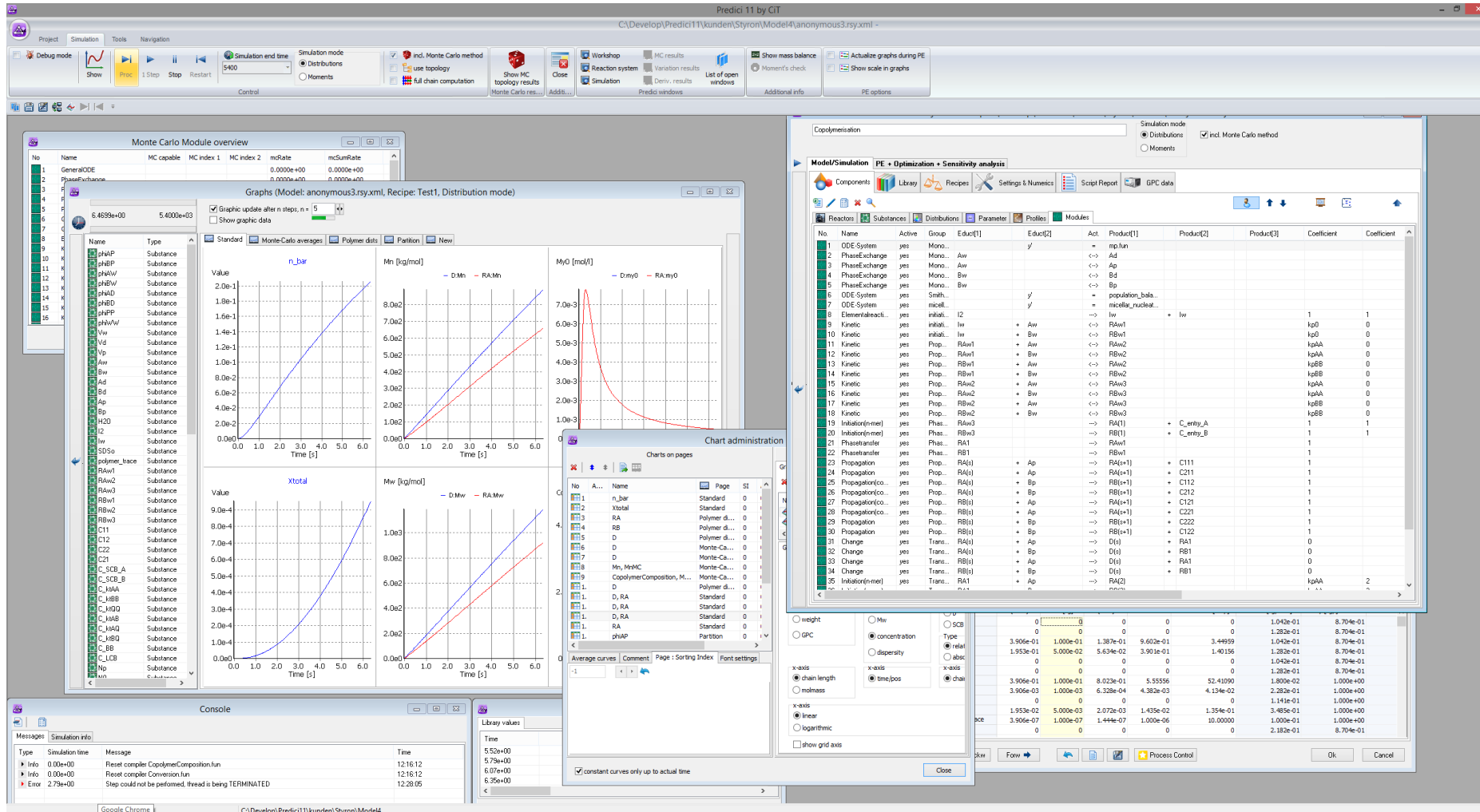
Predici 11 – Quick Overview

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



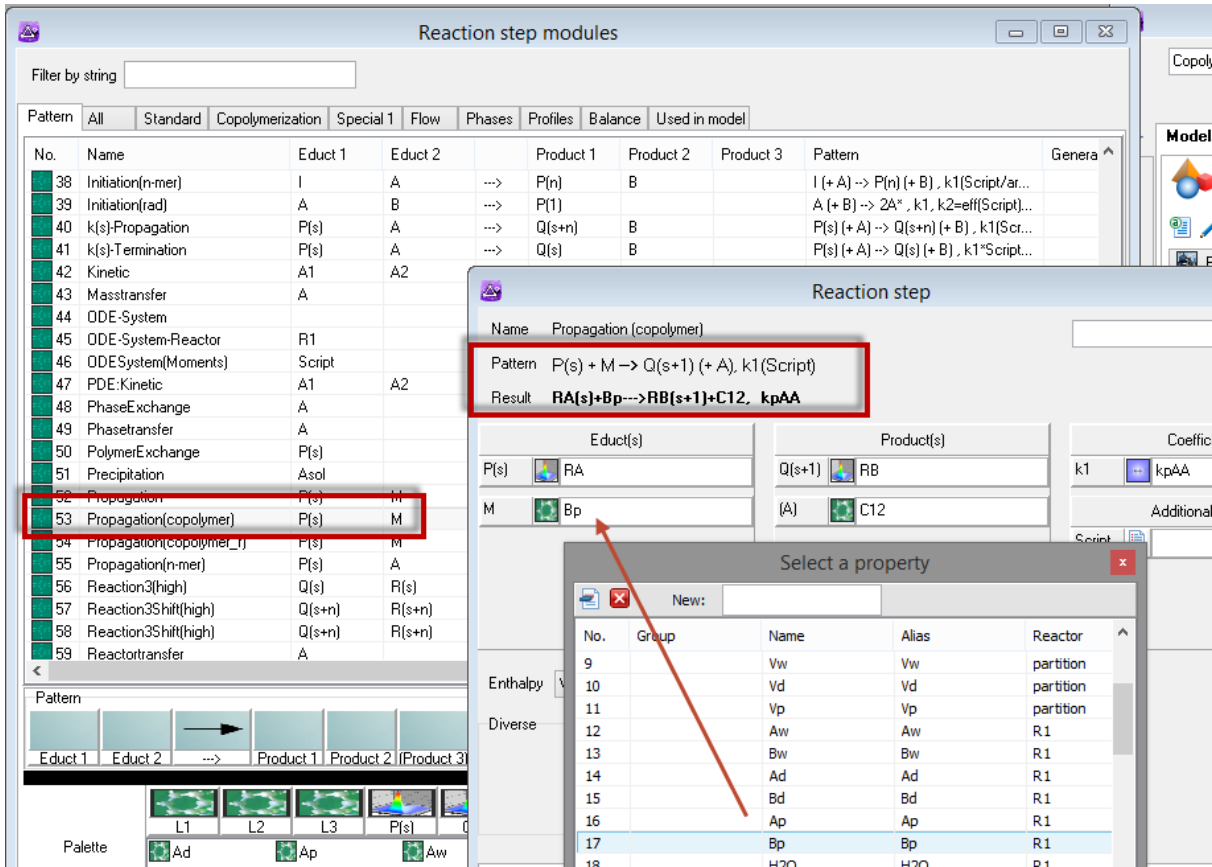
The screenshot displays the Predici 11 software interface, which is used for simulation and optimization. The main window is titled "Predici 11 by CIT" and shows a simulation setup for a copolymerization process. The interface is divided into several panels:

- Top Panel:** Contains simulation controls such as "Simulation end time" (set to 5400), "Simulation mode" (Distributions), and "Include Monte Carlo method".
- Left Panel:** A "Monte Carlo Module overview" table listing various substances and their properties. The table includes columns for Name, Type, MC capable, MC index, mRate, and mSumRate.
- Center Panel:** Displays "Graphs (Model: anonymous3.rxy.xml, Recipe: Test1, Distribution mode)". It features four sub-graphs:
 - n_bar:** A linear plot of n_bar vs Time [s].
 - Mn [g/mol]:** A linear plot of Mn vs Time [s].
 - Mw [g/mol]:** A linear plot of Mw vs Time [s].
 - MyO [mol/l]:** A plot showing MyO vs Time [s] with two curves (Dmyo and RAmyo).
- Right Panel:** A "Copolymerization" table showing reaction details. The table has columns for No., Name, Active, Group, Educt[1], Educt[2], Act., Product[1], Product[2], Product[3], Coefficient, and Coefficient. It lists various reactions like ODE-System, PhaseExchange, Kinetic, and Propagation.
- Bottom Panel:** A "Console" window showing simulation messages, including "Reset compiler: CopolymerComposition fun" and "Step could not be performed. Thread is being TERMINATED".
- Bottom-Right Panel:** A "Chart administration" dialog box with a table of charts and a "Charts on pages" section.

- 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

- 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

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



The screenshot displays the 'Reaction step modules' window with a list of reaction steps. Row 53, 'Propagation(copolymer)', is highlighted with a red box. Below it, the 'Reaction step' configuration window is open, showing the pattern $P(s) + M \rightarrow Q(s+1) (+ A), k1(\text{Script})$ and the result $RA(s)+Bp \rightarrow RB(s+1)+C12, kpAA$. A red box highlights the pattern and result. The 'Educt(s)' field contains 'P(s)' and 'M', and the 'Product(s)' field contains 'Q(s+1)', 'RB', and 'C12'. A 'Select a property' dialog is also open, showing a list of properties with 'Bp' selected.

No.	Name	Educt 1	Educt 2	Product 1	Product 2	Product 3	Pattern	Genera
38	Initiation(n-mer)	I	A	→	P(n)	B	$I (+ A) \rightarrow P(n) (+ B), k1(\text{Script}/ar...$	
39	Initiation(rad)	A	B	→	P(1)		$A (+ B) \rightarrow 2A^*, k1, k2=eff(\text{Script})...$	
40	k(s)-Propagation	P(s)	A	→	Q(s+n)	B	$P(s) (+ A) \rightarrow Q(s+n) (+ B), k1(\text{Scr}...$	
41	k(s)-Termination	P(s)	A	→	Q(s)	B	$P(s) (+ A) \rightarrow Q(s) (+ B), k1^*(\text{Scr}...$	
42	Kinetic	A1	A2					
43	Masstransfer	A						
44	ODE-System							
45	ODE-System-Reactor	R1						
46	ODESystem(Moments)	Script						
47	PDE:Kinetic	A1	A2					
48	PhaseExchange	A						
49	Phasetransfer	A						
50	PolymerExchange	P(s)						
51	Precipitation	Asol						
52	Propogation	P(s)	M					
53	Propagation(copolymer)	P(s)	M					
54	Propagation(copolymer_1)	P(s)	M					
55	Propagation(n-mer)	P(s)	A					
56	Reaction3(high)	Q(s)	R(s)					
57	Reaction3Shift(high)	Q(s+n)	R(s+n)					
58	Reaction3Shift(high)	Q(s+n)	R(s+n)					
59	Reactortransfer	A						

No.	Group	Name	Alias	Reactor
9		Vw	Vw	partition
10		Vd	Vd	partition
11		Vp	Vp	partition
12		Aw	Aw	R1
13		Bw	Bw	R1
14		Ad	Ad	R1
15		Bd	Bd	R1
16		Ap	Ap	R1
17		Bp	Bp	R1
18		H2O	H2O	R1

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

Model/Simulation PE + Optimization + Sensitivity analysis

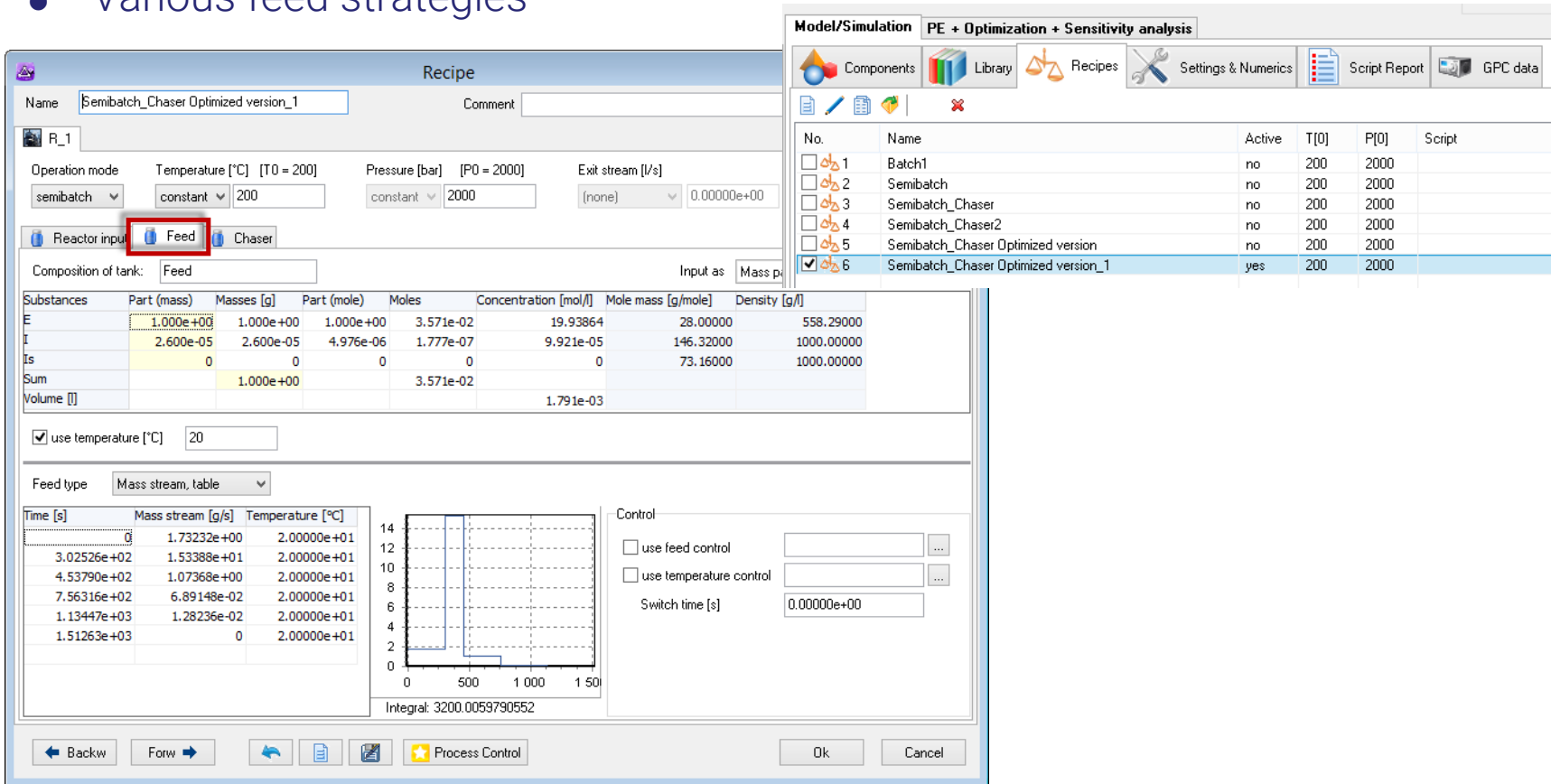
Components Library Recipes Settings & Numerics Script Report GPC data

Reactors Substances Distributions Parameter Profiles Modules

No.	Name	Acti..	Educt[1]	Educt...	Act.	Product[1]	Product[2]	Coefficient	Coefficient	Scripts	Reactor	Phases
1	Kinetic	yes	I		<->	I*s	+ I*s	kd	0		R1	main
2	Phasetransfer	yes	I		->	Ip		kscrip			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



The screenshot displays the software interface for configuring reactor recipes. The main window is titled "Recipe" and shows the configuration for "R_1". The "Operation mode" is set to "semibatch", with a "Temperature [°C]" of 200 and "Pressure [bar]" of 2000. The "Exit stream [l/s]" is set to 0.00000e+00. The "Feed" button is highlighted with a red box. Below the configuration, a table shows the composition of the tank, including substances, masses, moles, concentrations, and densities. The "Feed type" is set to "Mass stream, table", and a table shows the feed data over time. A graph plots the feed data, and a "Control" section allows for setting feed and temperature control parameters.

Recipe Configuration:

- Name: Semibatch_Chaser Optimized version_1
- Operation mode: semibatch
- Temperature [°C]: constant 200
- Pressure [bar]: constant 2000
- Exit stream [l/s]: (none) 0.00000e+00
- Reactor input: Feed
- Composition of tank: Feed
- Input as: Mass p

Substances Table:

Substances	Part (mass)	Masses [g]	Part (mole)	Moles	Concentration [mol/l]	Mole mass [g/mole]	Density [g/l]
E	1.000e+00	1.000e+00	1.000e+00	3.571e-02	19.93864	28.00000	558.29000
I	2.600e-05	2.600e-05	4.976e-06	1.777e-07	9.921e-05	146.32000	1000.00000
Is	0	0	0	0	0	73.16000	1000.00000
Sum		1.000e+00		3.571e-02			
Volume [l]					1.791e-03		

Feed Data Table:

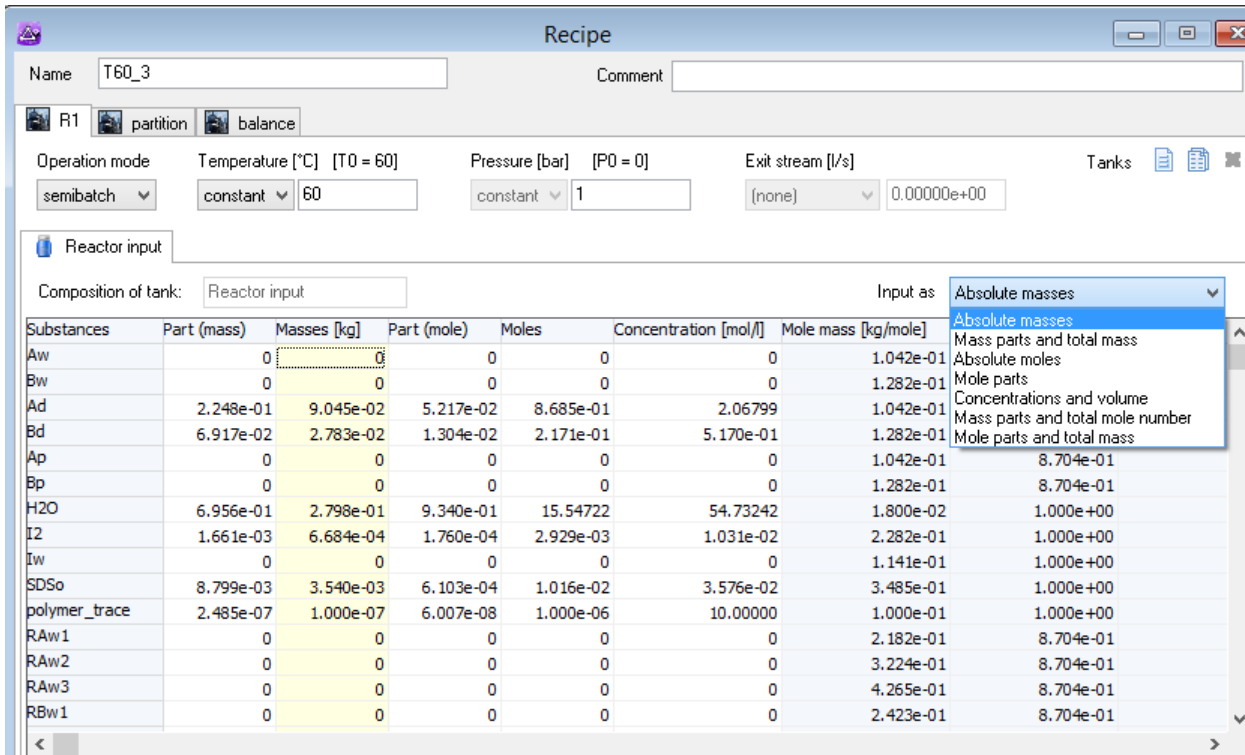
Time [s]	Mass stream [g/s]	Temperature [°C]
0	1.73232e+00	2.00000e+01
3.02526e+02	1.53388e+01	2.00000e+01
4.53790e+02	1.07368e+00	2.00000e+01
7.56316e+02	6.89148e-02	2.00000e+01
1.13447e+03	1.28236e-02	2.00000e+01
1.51263e+03	0	2.00000e+01

Recipe List Table:

No.	Name	Active	T[0]	P[0]	Script
<input type="checkbox"/>	1 Batch1	no	200	2000	
<input type="checkbox"/>	2 Semibatch	no	200	2000	
<input type="checkbox"/>	3 Semibatch_Chaser	no	200	2000	
<input type="checkbox"/>	4 Semibatch_Chaser2	no	200	2000	
<input type="checkbox"/>	5 Semibatch_Chaser Optimized version	no	200	2000	
<input checked="" type="checkbox"/>	6 Semibatch_Chaser Optimized version_1	yes	200	2000	

Recipes: Many new input options

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



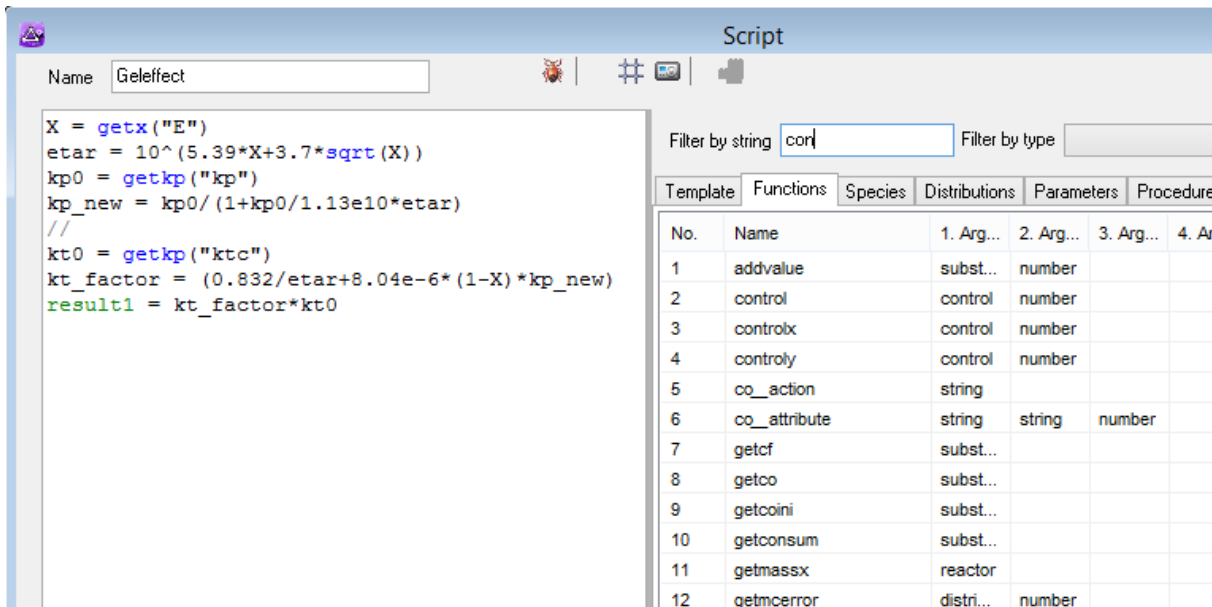
The screenshot shows the 'Recipe' window with the following settings:

- Name: T60_3
- Comment: (empty)
- Operation mode: semibatch
- Temperature [°C]: constant, 60
- Pressure [bar]: constant, 1
- Exit stream [l/s]: (none), 0.00000e+00
- Reactor input: Reactor input

The 'Composition of tank' table is as follows:

Substances	Part (mass)	Masses [kg]	Part (mole)	Moles	Concentration [mol/l]	Mole mass [kg/mole]	Input as
Aw	0	0	0	0	0	1.042e-01	Absolute masses
Bw	0	0	0	0	0	1.282e-01	Absolute masses
Ad	2.248e-01	9.045e-02	5.217e-02	8.685e-01	2.06799	1.042e-01	Mass parts and total mass
Bd	6.917e-02	2.783e-02	1.304e-02	2.171e-01	5.170e-01	1.282e-01	Absolute moles
Ap	0	0	0	0	0	1.042e-01	Mole parts
Bp	0	0	0	0	0	1.282e-01	Concentrations and volume
H2O	6.956e-01	2.798e-01	9.340e-01	15.54722	54.73242	1.800e-02	Mass parts and total mole number
I2	1.661e-03	6.684e-04	1.760e-04	2.929e-03	1.031e-02	2.282e-01	Mole parts and total mass
Iw	0	0	0	0	0	1.141e-01	8.704e-01
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

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



The screenshot shows a software interface with a script editor on the left and a function list on the right. The script editor is titled "Script" and has a name field containing "Geleffect". The script code is as follows:

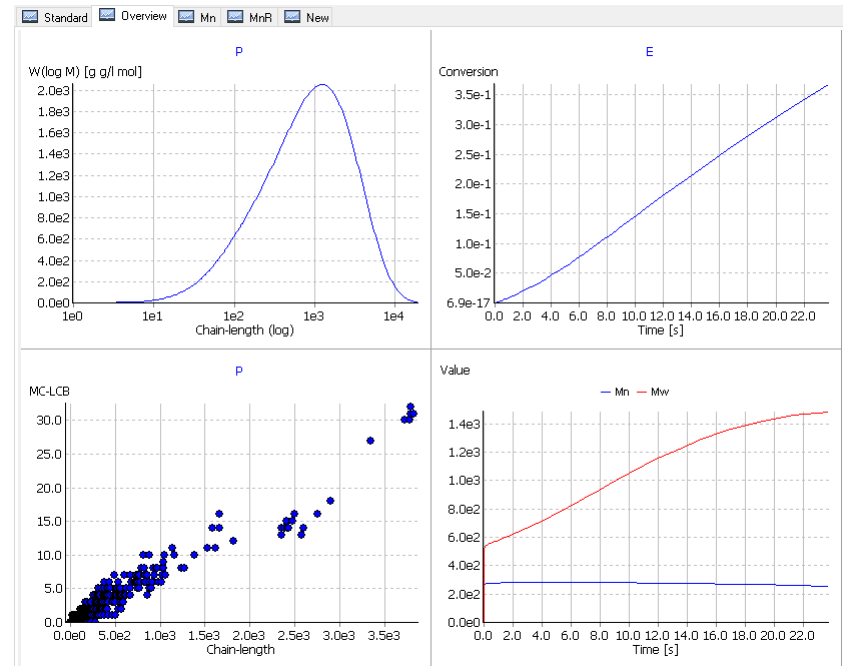
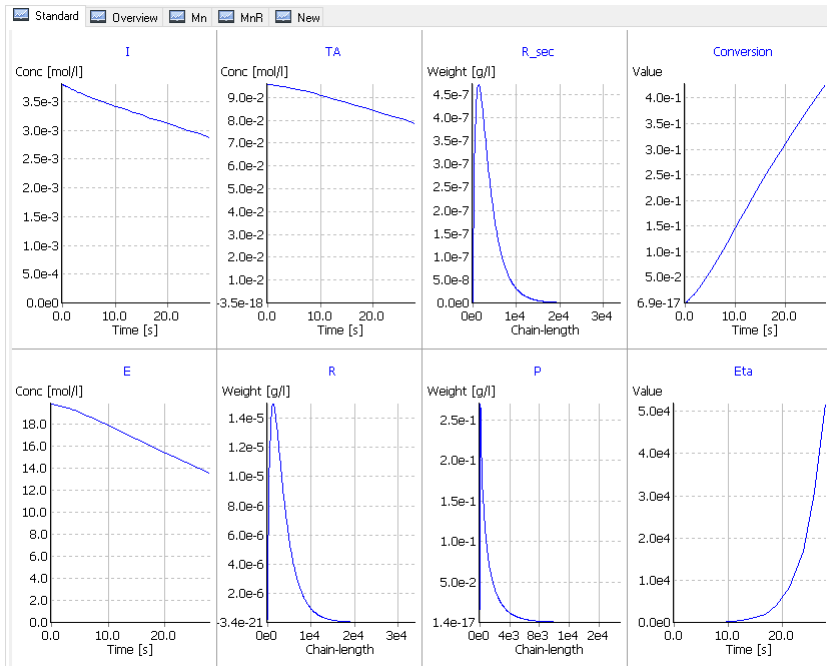
```
X = getx("E")
etar = 10^(5.39*X+3.7*sqrt(X))
kp0 = getkp("kp")
kp_new = kp0/(1+kp0/1.13e10*etar)
//
kt0 = getkp("kct")
kt_factor = (0.832/etar+8.04e-6*(1-X))*kp_new
result1 = kt_factor*kt0
```

The function list on the right is titled "Script" and has a filter by string field containing "con". The list is organized into tabs: Template, Functions, Species, Distributions, Parameters, and Procedure. The Functions tab is selected, showing a table of functions:

No.	Name	1. Arg...	2. Arg...	3. Arg...	4. An
1	addvalue	subst...	number		
2	control	control	number		
3	controtx	control	number		
4	controly	control	number		
5	co_action	string			
6	co_attribute	string	string	number	
7	getcf	subst...			
8	getco	subst...			
9	getcoini	subst...			
10	getconsum	subst...			
11	getmassx	reactor			
12	getmccerror	distri...	number		

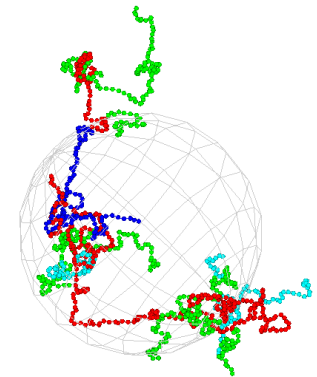
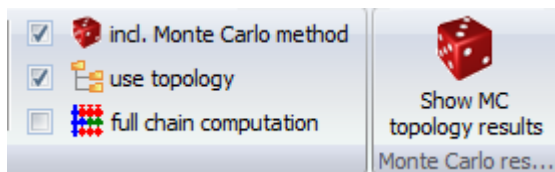
Output: Enhanced online charts

- 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



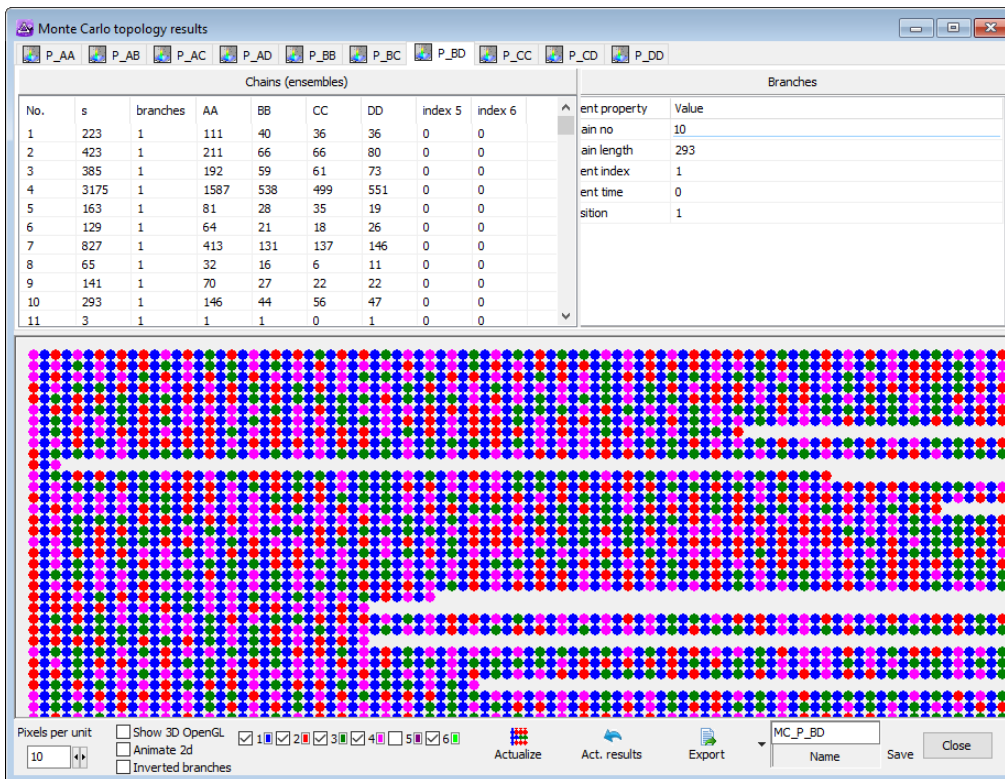
New algorithm: Hybrid Monte-Carlo method

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



- 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

