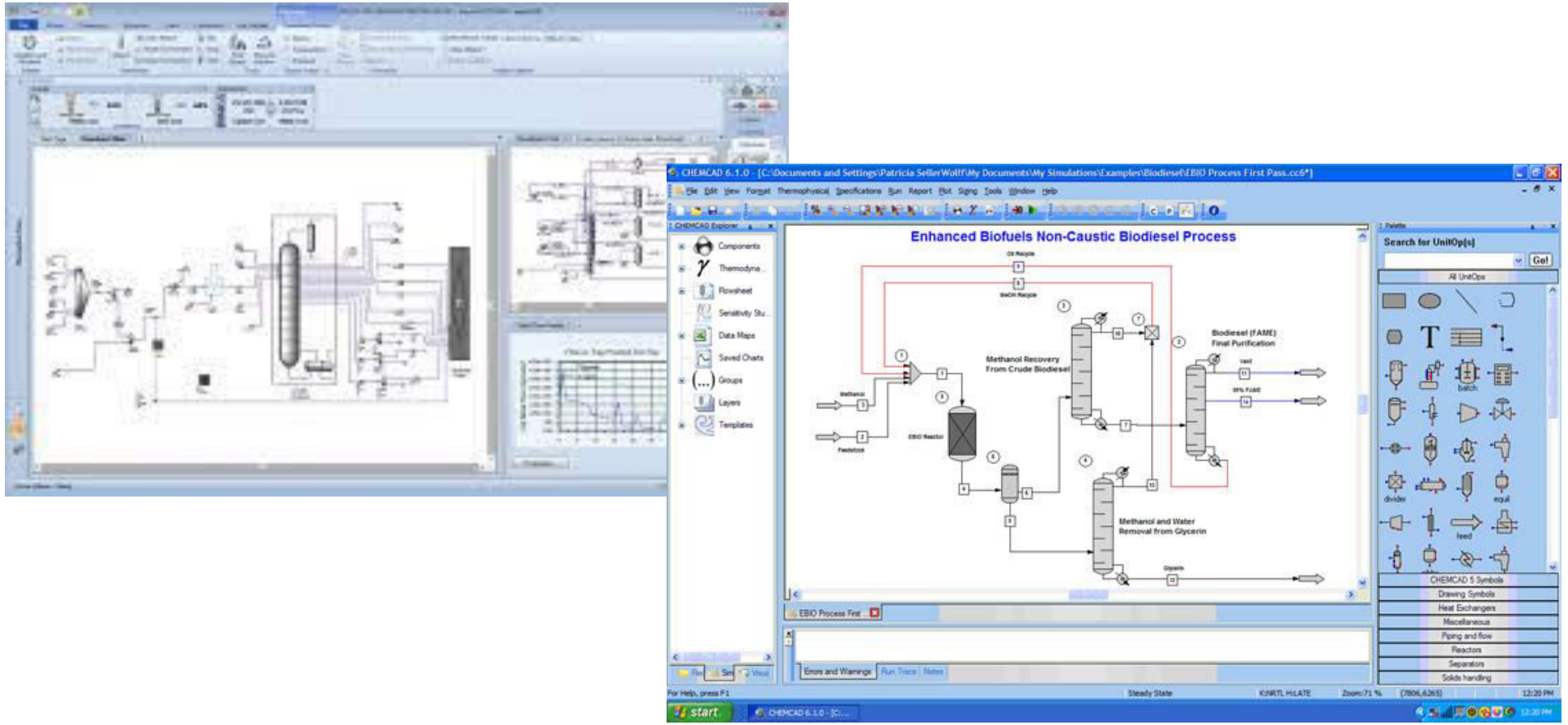
Introduction to a process simulation software



Process simulation

Process simulation is a model-based representation of chemical, physical, biological, processes and unit operations in software. Basic prerequisites are a thorough knowledge of chemical and physical properties of pure components and mixtures, of reactions, and of mathematical models which, in combination, allow the calculation of a process in computers.

Process simulation software describes processes in flow diagrams where unit operations are positioned and connected by streams. The software has to solve the mass and energy balance to find a stable operating point. The goal of a process simulation is to find optimal conditions for an examined process. This is essentially an optimization problem which has to be solved in an iterative process.

Process simulation

The development of models for a better representation of real processes is the core of the further development of the simulation software.

A model is a mathematical description of a chemical or physical phenomenon in which numerical parameters (for example a kinetic constant) and different variables (temperature, pressure, composition) are present.

Two main different types of models can be distinguished:

- Rather simple equations and correlations where parameters are fitted to experimental data.
- Predictive methods where properties are estimated.

The equations and correlations are normally preferred because they describe the property (almost) exactly. To obtain reliable parameters it is necessary to have experimental data which are usually obtained from factual data banks or, if no data are publicly available, from measurements.

Using predictive methods is much cheaper than experimental work and also than data from data banks. Despite this big advantage predicted properties are normally only used in early steps of the process development to find first approximate solutions and to exclude wrong pathways because these estimation methods normally introduce higher errors than correlations obtained from real data.

Steady state and dynamic process simulation

Initially process simulation was used to simulate steady state processes. **Steady-state models perform a mass and energy balance of a stationary process (a process in an equilibrium state) it does not depend on time.**

Dynamic simulation is an extension of steady-state process simulation whereby time-dependence is built into the models via derivative terms i.e. accumulation of mass and energy. The advent of dynamic simulation means that the time-dependent description, prediction and control of real processes in real time has become possible. This includes the description of starting up and shutting down a plant, changes of conditions during a reaction, holdups, thermal changes and more.

Dynamic simulations require increased calculation time and are mathematically more complex than a steady state simulation. It can be seen as a multiply repeated steady state simulation (based on a fixed time step) with constantly changing parameters.

A lot of efforts are made to develop new and improved models for the calculation of properties. This includes for example the description of

- thermophysical properties like vapor pressures, viscosities, caloric data, etc. of pure components and mixtures
- properties of different apparatuses like reactors, distillation columns, pumps, etc.
- chemical reactions and kinetics
- environmental and safety-related data

In this modern age of powerful computers, it often makes no sense to put pencil to paper like in the old days.
Now, new software can perform repetitive chemical engineering calculations in a fraction of the time it takes to execute them by hand.

Imagine you have been tasked to design a distillation column to produce a 90% benzene overhead product and a 95% toluene bottoms product. You look up the VLE data for benzene-toluene, carefully construct your x-y diagram, draw the feed line, and step off your McCabe-Thiele trays. Estimate tray efficiencies. Then you calculate your mass and energy balance, product and bottoms dew points and bubble points, and estimate your overhead condenser and column reboiler duties. Wrestle with those tedious hydraulics equations to determine the column diameter. Then dust off the old heat transfer equations and some time later you have your condenser and reboiler sized. Finally - the system is designed.

And then they decide they want 95% benzene, and by the way, the feed rate is 2,500 pounds per hour, not 1,500....

In this example, getting the initial solution using process simulation software would take....about the same amount of time.

BUT, when the design conditions are changed the speed and accuracy of process simulation begins to save tremendous time and money. And not only for design changes. In the example above, you had to select your reflux rate based on some old rule of thumb about the optimum reflux being some multiple of the minimum reflux. Wouldn't it be better to be able to plot reflux rate versus energy usage? Versus number of trays? And automatically, with one software command?

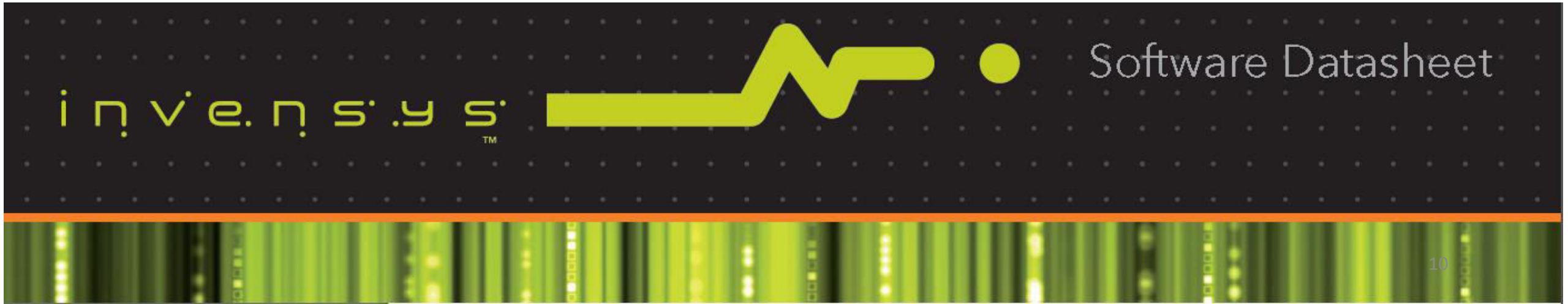
Multiple runs - quickly. Process design optimization - quickly. Such is the power of process simulation. The example given above is for a distillation tower, but the same holds true for any number of chemical engineering unit operations - heat exchangers, reactors, heaters, absorbers, extractors, crystallizers, evaporators; even pumps, compressors, and piping systems. In fact, even an entire plant - in one model.

Several simulation software are available!!!

These lists are taken from wikipedia

Software	Developer	Applications	Operative system	License
Ariane	ProSim	Utilities management and power plant optimization		
APMonitor		Data reconciliation, real-time optimization, dynamic simulation and nonlinear predictive control		
Aspen Plus	Aspen Technology	Process simulation and optimization		
Aspen HYSYS	Aspen Technology	Process simulation and optimization		
ASSETT	Kongsberg Oil & Gas Technologies AS	Dynamic process simulation		
BatchColumn	ProSim	Simulation and Optimization of batch distillation columns		
BatchReactor	ProSim	Simulation of chemical reactors in batch mode		
D-SPICE	Kongsberg Oil & Gas Technologies AS			
K-Spice	Kongsberg Oil & Gas Technologies AS	Dynamic process simulation and multiphase pipeline simulation		
CADSIM Plus	Aurel Systems Inc.	Steady-state and dynamic process simulation		
ChromWorks	ChromWorks, Inc.	Continuous/Batch chromatography process simulator		
CHEMCAD	Chemstations	Software suite for process simulation		
Cycle-Tempo	Asimptote	Thermodynamic analysis and optimization of systems for the production of electricity, heat and refrigeration		
COCO simulator	AmsterCHEM	Steady state simulation		free of charge
Design II for Windows	WinSim Inc.	Process simulation		
Distillation expert trainer	ATR	Operator training simulator for distillation process		
PIPE-FLO Professional	Engineered Software Inc.			
PEL Software Suite				
Petro-SIM	KBC Advanced Technologies			
PETROX	Petrobras	General Purpose, Static, Sequential-Modular Process Simulator	Windows	internal users only
Prode Properties	Prode Software			
Prode simulator	Prode Software			
ProSim DAC	ProSim	Dynamic Adsorption Column Simulation		
ProSimPlus	ProSim	Process simulation and optimization		
ProSimulator	Sim Infosystems			
Pro-Steam	KBC Advanced Technologies			
ProMax	Bryan Research and Engineering			
TSWEET	Bryan Research and Engineering			
PROSIM				
PRO/II	SimSci			
DYNSIM	SimSci			
ROMeo (process optimizer)	SimSci			
RecoVR	VRTech			
Simulis Thermodynamics	ProSim	Mixture properties and fluid phase equilibria calculations		
SimCreate	TSC Simulation			
SPEEDUP	Roger W.H. Sargent and students			
SolidSim	SolidSim Engineering GmbH	Flowsheet simulation of solids processes		
SuperPro Designer	Intelligen			
SysCAD				

Introduction to a process simulation software: PRO II by Invensys, Simulation Science®



Why we will use PRO II?

We will use PRO II as an example of excellent commercial software. There are no particular reasons for this choice, respect others commercial software.

We use this software with satisfactory results in several research applications.

Very important: we have a regular license of this software!

Another very used simulation software in academic and industrial field is Aspen Hysys

Optimize Hydrocarbon Processes with Aspen HYSYS®.

V8

The energy industry's leading process simulation software.

Aspen HYSYS is a comprehensive process modeling system used by the world's leading oil & gas producers, refineries, and engineering companies to optimize process design and operations.

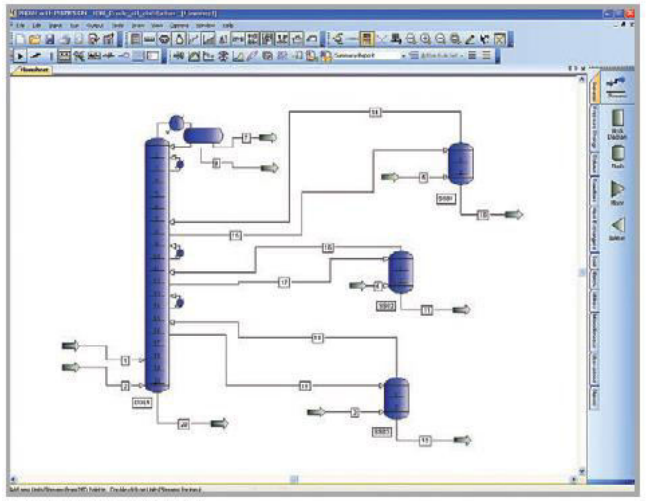
aspentech

PRO/II is a professional simulation tool that offers a comprehensive simulation solution for process design, revamp, and operational analysis. PRO/II performs rigorous mass and energy balances for processes ranging from oil and gas separation to reactive distillation.

PRO/II has the power and flexibility to simulate a wide range of processes at steadystate, from refining to chemicals. PRO/II provides robust and accurate results based on industry-standard thermodynamic methods and physical property data. PRO/II is a valuable tool allowing engineers and management to enhance the bottom line of their process or plant.

SIMULATION USES

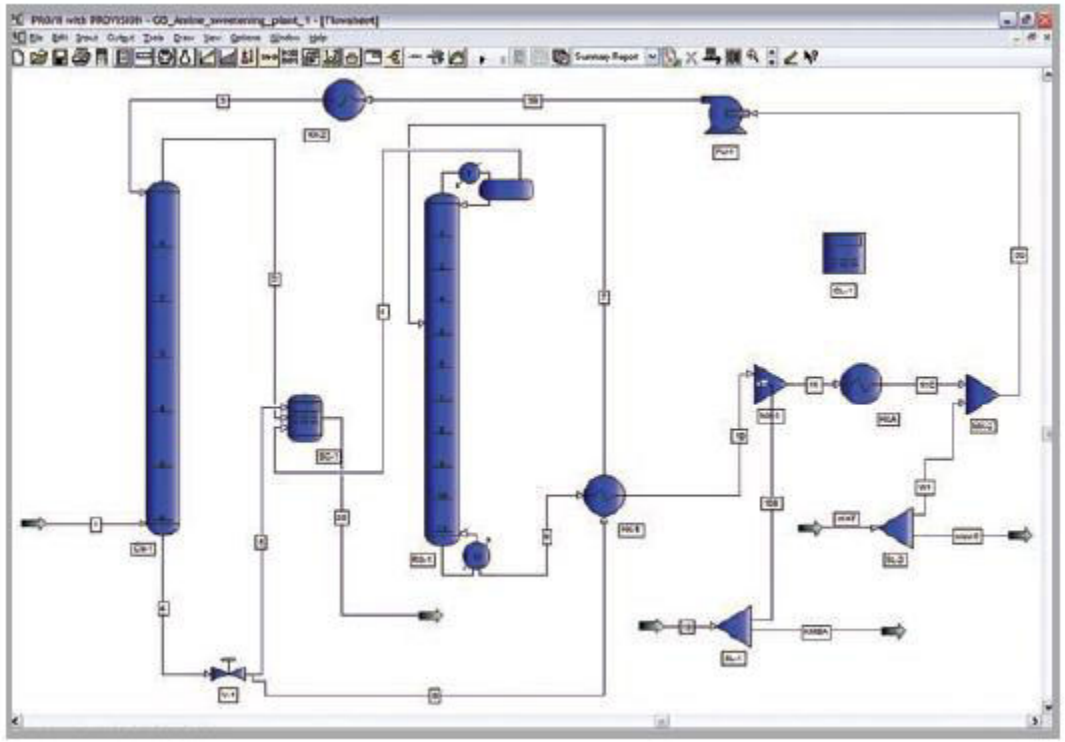
- Design new processes
- Evaluate alternate plant configurations
- Modernize or revamp existing plants
- Assess and document compliance within environmental regulations
- Troubleshoot and debottleneck plant processes
- Monitor, optimize, and improve plant yields and profitability



KEY FEATURES

- Comprehensive thermodynamics and physical property data
- Creation and management of custom component data
- Comprehensive rigorous unit operation modeling
- Application across multiple industries

- Green Engineering
- Refining
- Oil & Gas Processing
- Petrochemicals
- Chemicals
- Polymers
- Pharmaceuticals



Business Value

Decrease capital costs

- Decrease operating costs
- Increase efficiency
- Increase productivity
- Reduce learning curves
- Increase profitability

Component Databanks

- 1,700+ pure component library
- Solids properties
- 1900+ components/species electrolyte databank
- Integration with Spiral CrudeSuite provides access to libraries for crude assays
- Non-library components
- Pseudocomponents and assay characterization
- User libraries
- Property prediction from UNIFAC and PROPRED structures
- Multiple assay blends
- Thermodynamic Data Manager (TDM) the ability to create, regress and manage custom libraries

THERMODYNAMIC METHODS

Refining/Oil & Gas/Petrochemicals

- Soave-Redlich-Kwong (SRK)
- Peng-Robinson (PR)
- Huron-Vidal mixing rule (SRK & PR)
- Kabadi-Danner mixing rule (SRK & PR)
- Panagiotopoulos & Reid mixing rule (SRK & PR) original & modified
- SIMSCI mixing rule (SRK)
- Temperature-dependent Kijs
- Lee-Kesler
- Lee-Kesler-Plocker
- Chao-Seader
- Grayson-Streed
- Braun K10
- Ideal library methods
- BWRS
- Costald
- API density method
- Single and multi-fluid Rackett densities
- IF97 Steam Tables
- Free-water decant

Petrochemical/Chemicals/Polymers

- UNIFAC (VLE, LLE, & VLLE)
- UNIFAC-FV (free volume)
- UNIWAALS
- UNIQUAC
- NRTL-8 coefficient form
- Wilson
- Van Laar
- Regular solution model
- Acid dimerization
- Henry's law for non-condensibles
- Henry's law for dilute aqueous systems
- Three-phase equilibrium
- Heat of mixing
- Hayden-O'Connell
- Electrolyte models (OLI)
- Advanced Lattice Model (ALM) for polymers
- Flory-Huggins with Chi for polymers
- SAFT EOS for polymers
- PHSC EOS for polymers

UNIT OPERATIONS

General Flowsheet Models

- Flash, valve, compressor, expander, pump, pipe, AMSIM module, fuel cell, membrane separator
- Simple integration of custom units using the Excel unit operation

Heat Exchanger Models

- Shell and tube exchanger, simplified exchanger, LNG exchanger, fired heater, air cooled exchanger, heating/cooling curves
- HTRI integration, zone analysis

Flowsheet Control

- Feed-forward control, feedback controller, multivariable controller, optimizer
- Parameter cross-referencing, auto-sequencing

Polymer Modeling

- Continuous stirred tank reactor, plug flow reactor, wiped film evaporator
- Kinetics mechanism
  - Homogeneous Ziegler-Natta
  - Chain polymerization
  - Condensation polymerization

Distillation Models

- Multiple advanced solution algorithms
- Multiple initial estimate generators
- Two/Three phase distillation
- Electrolytic distillation
- Reactive and batch distillation
- Liquid-liquid extraction
- Column and tray sizing or rating
- Thermosiphon reboiler
- RATEFRAC & BATCHFRAC

Solids Modeling

- Crystallizer/dissolver, countercurrent decanter, centrifuge, rotary drum filter, dryer, solid separator, cyclone

Reactor Models

- Conversion & equilibrium reactors, plug flow reactor, continuous stirred tank reactor, shift & methanation reactors, boiling pot reactor, batch reactor
- Inline FORTRAN reaction kinetics, Gibbs free energy minimization

What we will make using PRO II?

- Study of the phase equilibrium of binary/ternary mixtures
- Use of the databank
- Simulation of a Flash, distillation column
- Simulation of a chemical batch or continuous reactor
- Use of the Case Study function
- Regression of the parameters of a thermodynamic model