



# CC-Steady State - Reacs Section

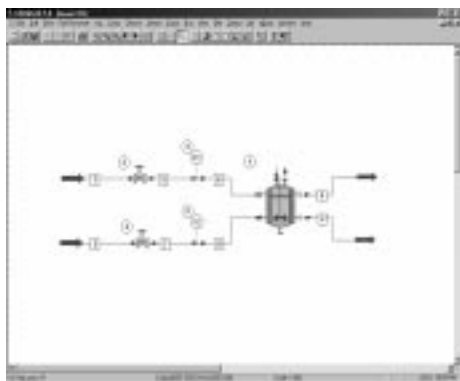
## Batch Reactor Software

### You don't have to be an expert to use CC-ReACS

The PC on your desk can now be used for highly accurate simulation of batch reaction processes without the time-intensive learning curve that would generally be expected with complex-software.

That is because CC-ReACS builds models using a simple but comprehensive input system with intelligent dialog boxes, on-line data checking and context sensitive help. There is no special input language.

So the most powerful, flexible and advanced batch process modeling software available today is actually easy to use. It was designed specifically for the batch chemical industry by a team with experience in chemistry, chemical engineering and process control.



### From experiment to production

CC-ReACS's flexibility makes it the ideal simulator for all stages of the design process, from laboratory experimentation through scale-up, yield optimization, hazard analysis and control. It can model vessels ranging from laboratory glassware or reaction calorimeters to pilot or production scale reactors under a

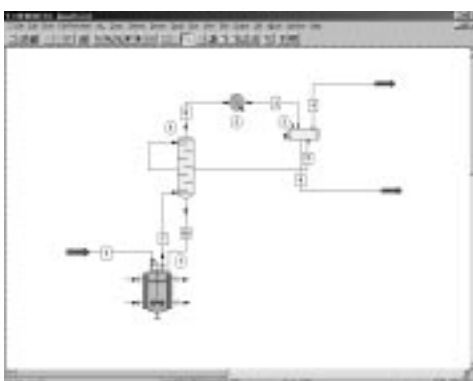
wide range of operating conditions. The cost savings that can be achieved by improving the results of your pilot plant, or by going directly from table top to full scale, can be significant.

Special options allow the chemical system to be separated from the plant model so the chemist can study the behavior of the reacting system under adiabatic or isothermal conditions.

Engineers can swiftly carry out scale-up calculations by building upon this model. A wide range of alternative production routes and operating strategies can be examined in detail, and extensive thermal safety studies can be implemented.

### Technical Power

CC-ReACS offers an impressive list of features, which makes it possible to simulate almost any chemical system in any reactor. This is accomplished by combining a unique interface which understands the process chemistry with a sophisticated reactor model that contains options for multiple jackets, internal and external coils, and heat exchangers. CC-ReACS simulates batch, semi-batch or continuous reactor operation using a flexible sequencing and PID control system.



### Reactive Distillation

Together with Chemstations' fully integrated dynamic distillation model, CC-DCOLUMN, CC-ReACS can rigorously simulate combined reactor/distillation systems.

This feature offers equilibrium based or mass transfer based simulation for packing trays.

With this powerful combination, CC-ReACS gives you a head start in tackling reactive distillation problems.

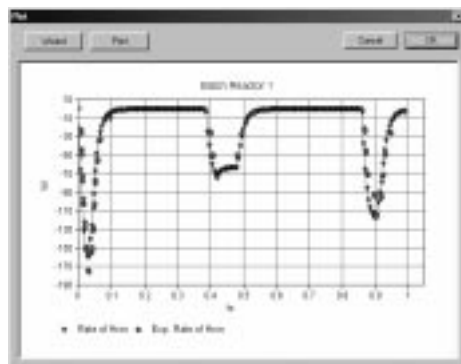
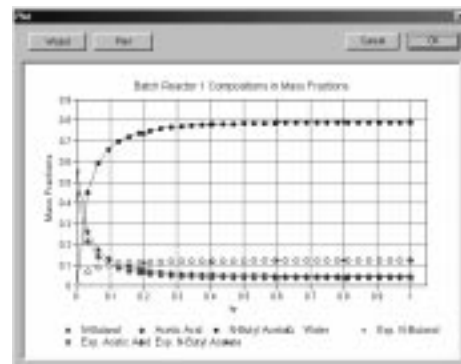


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Chemical companies worldwide, from leading multinationals to small-scale manufacturers, are already using CC-ReACS. With the continually increasing pressures of yield optimization and plant safety, there's never been a better time to have the most comprehensive batch reaction simulator working for you.

### Kinetic Rate Regression

CC-ReACS rate regression facility enables you to determine the rate parameters from imported experimental data. This data can be any combination of temperature, concentration, volume or heat release data from as many experiments as you have available. No other software package enables you to easily fit this much data in a single run.



### CC-ReACS gives you an edge

CC-ReACS's use throughout the design process and its ability to act as a bridge between different disciplines will accelerate the entire design process.

This, of course, leads to clear cost savings as well as the commercial advantages inherent in bringing a product to the marketplace more quickly. You'll have greater process profitability, reliability and safety.

# Batch Reactor Software

## General Features

- Interactive, menu driven input
- On-line help screens
- Extensive data checking
- Graphical Display of process equipment
- Customized reports
- On-line, real-time display of results during calculations
- Calculation interruption
- Integration into CHEMCAD flowsheets
- Flexible engineering units

## Chemical Design

- Unlimited number of species
- Unlimited number of simultaneous reactions
- Choice of Arrhenius or Langmuir-Hinshelwood rate equations forms
- Regression of kinetic process data

## Thermodynamics

CC-ReACS uses the CHEMCAD thermodynamics and physical properties system which has been used and proven in a wide range of processes for over fifteen years. This means that CC-ReACS can be rigorously applied to regular, polar, electrolyte and polymer systems as well as a wide range of less common systems. It also means that CC-ReACS users have access to the comprehensive CHEMCAD pure components and mixture databank and physical properties estimation system.

## Reactor Design

- Multiple Coils and jackets
- Service or process side heat exchangers and electric heaters
- Heat transfer rate calculation; includes calculation of process and service side film coefficients
- Vapor and liquid draws permitted
- Batch, semi-batch or continuous operation
- Vessel pressurization calculated

## Auxillary Equipment

Any unit operation may be used with the batch reactor to flexibly model the process, including: dynamic vessel, heat exchanger, mixer, divider, separator, valve, pump, etc.

## Control System

- User Specified PID loops
- Multiple ramp or step changes in setpoint
- Control of reactor or jacket temperature differential
- Level controllers
- Pressure controllers
- Cascade control
- Heat-cool-chill system with safety interlocks
- Split range controllers

## Reactive Distillation

CC-ReACS is fully integrated with CHEMCAD's dynamic distillation column simulator, CC-DColumn. It can thus model reactive distillation systems such as a column on top of a batch reactor. This and other systems are common in the chemical and specialty chemicals industries and are easily simulated using CHEMCAD.

## Kinetics Data Regression

- Can regress any combination of concentration, temperature volume and/or heat of reaction (Qr) data
- Can fit multiple experiments in a single regression analysis
- Can calculate the frequency factor, activation energy, component reaction order, Langmuir absorption parameters
- Offers a variety of numerical methods to ensure that the regression is fast, accurate and can handle stiff systems
- Accepts data from a wide range of calorimeters including the Mettler RX1 for which special features are provided.

- Graphical and tabular comparison of experimental and predicted results makes it easy for the user to evaluate the validity of the model.

## Diers Analysis Facility

For both the reactor vessel and the dynamic vessel unit operations modules, CC-ReACS provides you with a practical, comprehensive, field tested DIERS (Design Institute for Emergency Relief Systems) analysis facility. This can be used to simulate reactive and non-reactive emergency relief situations on a dynamic basis. CC-ReACS DIERS options include:

- Design and rating of relief valves and systems disks
- Bubbly, churn-turbulent, and homogeneous vessel models
- HEM,ERM, Henry-Fausek HNE, non-flashing liquid and single phase vapor vent flow models
- API-520/52, API-2000, OSHA 1910.116, and NFPA-30 fire models
- Outlet piping pressure drop calculations
- Comprehensive vessel specification capabilities
- Atmospheric and pressure vessels
- The DIERS results are included in the heat and material balance of the reactor and dynamic vessel.

## Batch Reactor Output

CC-ReACS provides graphical or tabular time histories for any stream or unit operation parameters, as well as batch reactor output that includes (among others):

- Compositions
- Pressure
- Temperature
- Heat of reaction
- Utility flowrates
- Liquid level
- Reaction mass physical properties
- Rates of formation
- Yields
- Conversions



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