AIChE ACADEMY

SuperChems™ for DIERS Attributes

Mixture Properties

- Handles mixtures
- Properties databank
- Property estimation methods (thermo-physical and transport)
- Data reduction and regression
- DIPPR data transfer to SuperChems™
- Create new chemical species using a similar existing species as the model and estimate its physical properties.

Vapor-Liquid Equilibrium

- Binary T-X-Y diagrams
- Binary P-X-Y diagrams
- Flash calculations (bubble point, dew point, and many others)
- BIPS estimation using UNIFAC
- VLE/VLLE consistency checks and regression
- BIPS estimation using limited solubility, azeotropic, experimental data, and infinite dilution activity coefficients
- BIPS from the database

Chemical Reactions

- Imports output data from adiabatic calorimeters
- Handles stoichiometric reactions
- Accepts Arrhenius expressions and other user-defined forms
- Handles supercritical systems
- Reaction definition module

Vessel Options

- Vertical vessel with user-defined heads
- Horizontal vessel with user-defined heads
- Spherical vessel

- Rectangular vessel
- Abnormal heat input: User-defined heating and cooling
- Abnormal heat input: cooling/heating jackets
- External fire: Choice of NFPA-30, API-520, API-2000
- External fire: Credit for less exposure to fire when the equipment is physically blocked from fire
- Calorimetry
- Insulation
- Internals
- Water exposure

Piping Layout

- Piping segment, valves, and fittings
- Rupture disk and buckling pin
- Pressure relief valve
- Control valve
- Reducer/expander
- Pump/compressor/turbine
- Orifice

Flow and Source-Term Models

- Liquid-vessel dynamics
- Two-phase/universal vessel dynamics
- Gas/vapor-vessel dynamics
- Handles one piping at a time
- Liquid flow in piping
- Two-phase/universal flow in piping
- Gas/vapor flow in piping

Dynamic Flow

- DIERS coupling equation
- Bubbly, churn-turbulent, user-specified
- Vapor/Gas
- Two-phase (flashing, non-flashing/frozen, etc.)
- Bottom-vent/subcooled
- Homogeneous-equilibrium flow

- Slip-equilibrium flow
- DIERS coupling equation options
- External streams input to the vessel

Flow in Pipes (NetFlow)

- % Inlet pressure drop for pressure-relief valves
- % Backpressure for pressure-relief valves
- Physical properties of flowing material along the pipe
- Thrust force along the pipe
- Slug force on elbows (with user calculations)

Reporting

- Individual model tabulated results
- Individual model graphs
- Spreadsheets for all individual model graphs