An iOiQ Product

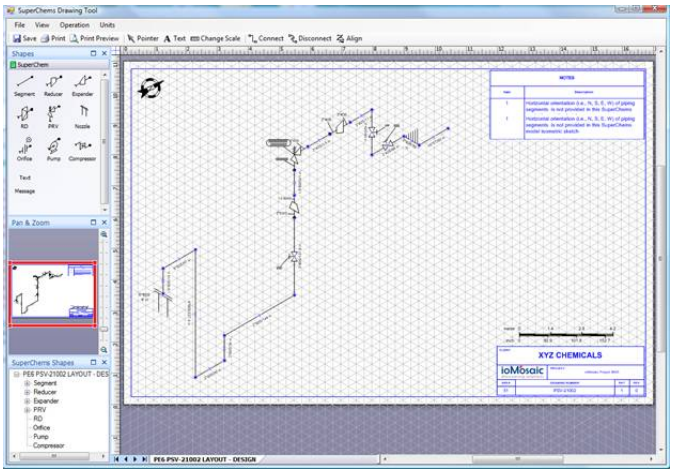
SuperChems™ Version 6.2MP

Software for Pressure Relief Design, Chemical Reactivity Assessment and Management, Consequence Analysis, And Quantitative Risk Analysis

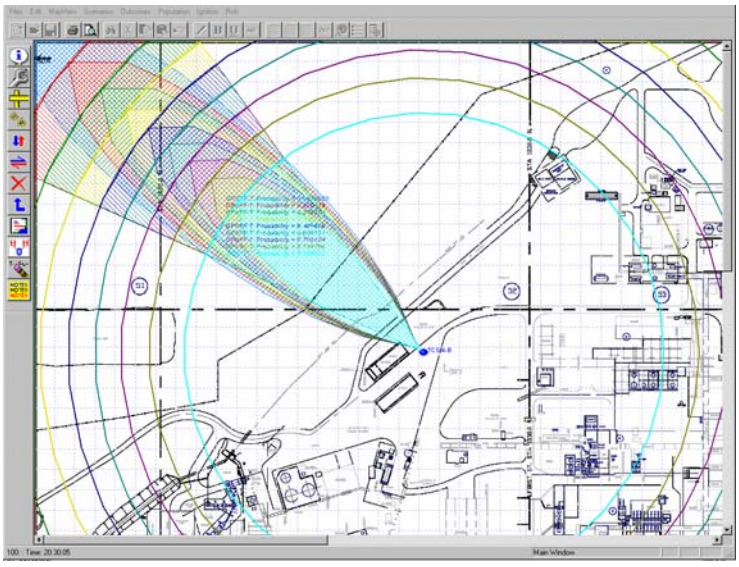
SuperChems™ Expert is a versatile software tool that provides an integrated platform for:

- *Pressure relief and Flare Systems Evaluation*
- *Risk Based Inspection*
- *Facility Siting*
- *Fixed facilities and Pipelines Quantitative Risk Analysis (QRA)*
- *Chemical Reactivity Management*
- *Fault Tree and SIS/SIL analysis with ioLOGIC™*
- *Consequence Analysis*

SuperChems™ Expert offers a variety of well validated models for single/multi-phase reacting flow, dispersion analysis, droplet dynamics, fire, and explosion dynamics. All models in SuperChems™ are true multi-component models with support for petroleum fractions and mixture toxicity.



SuperChems QRA Module



In addition, SuperChems™ provides several power productivity tools including:

- *Advanced reporting and data lifecycle management with ioXpress™*
- *Failure rates database*
- *Thermodynamic and physical properties database for more than 2800 components with complete property estimation tools*
- *Reactivity Expert*

As an equation-of-state-based program, SuperChems™ provides several benefits over existing non-equation-of-state-based methods for systems involving:

- Reactions with supercritical components
- Solution effects
- *A priori* determination of phase splitting

SuperChems™ is available in two editions: for DIERS and Expert. Its powerful engine has a proven record of handling numerous complex and unconventional systems that are not readily provided by other tools.

SuperChems™ for DIERS edition is particularly designed for the Design Institute for Emergency Relief Systems (DIERS) user group within the AIChE. Implementing DIERS two-phase technology and being empowered by SuperChems™ solid engine, SuperChems™ for DIERS is currently adopted as an industry standard tool for handling complex reactions systems and designing practical relief systems.

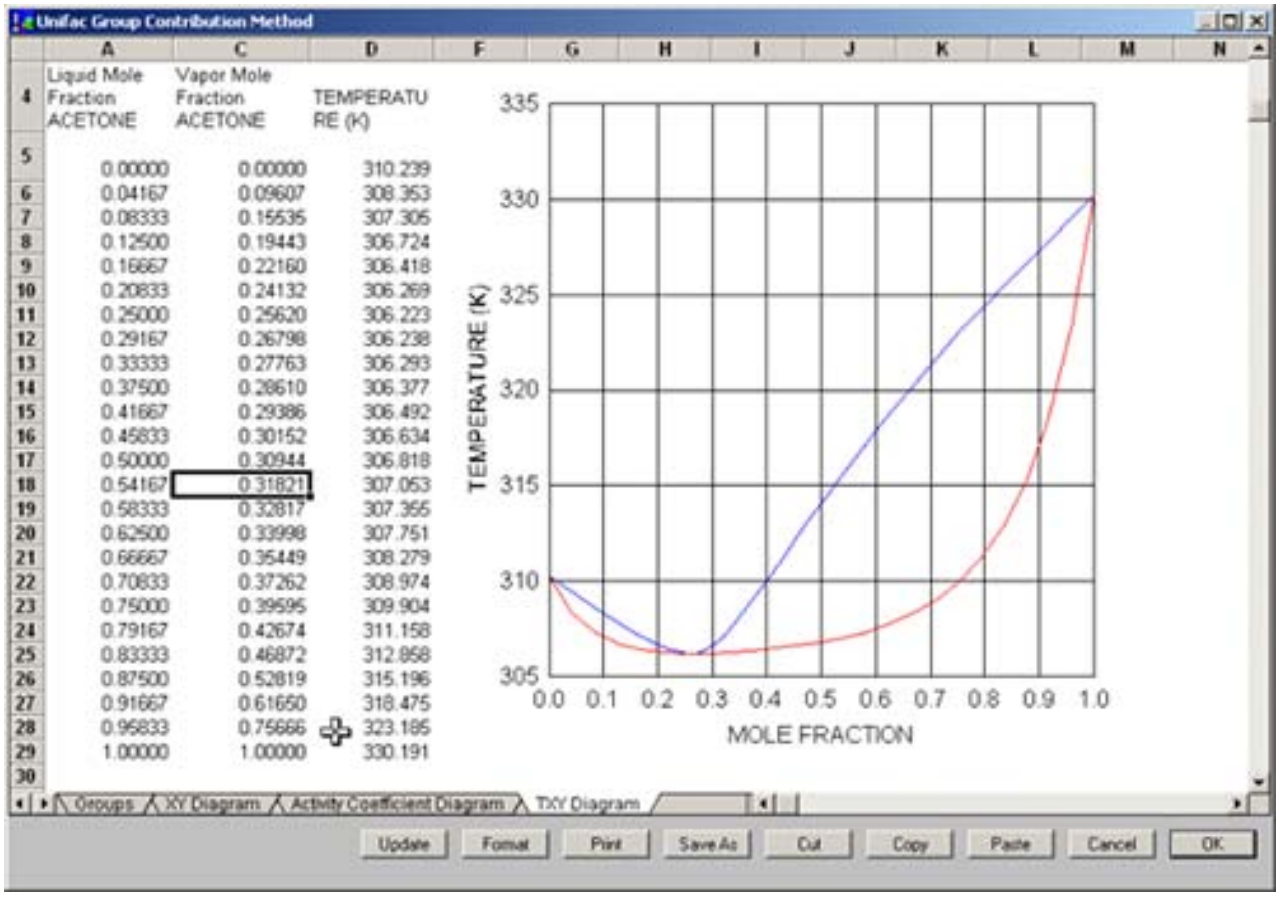
The QRA module was the major addition to SuperChems™. Users now have a full-blown QRA engine to define population; analyze failure frequencies; assess dependent failures; generate iso-risk contours; construct F-N curves; and perform consequence modeling, all within a central application. All consequence models are linked directly to user-defined site map with enhanced graphics, contours, and plots.

System Requirements

SuperChems™ runs on any Windows-compatible machine running Windows 95, Windows 98, Windows NT, Windows 2000, Windows XP , or Windows Vista. It requires about 150 MB of hard-drive space. SuperChems™ does intensive calculations and thus requires a machine with a clock speed of 1 GHz. We, however, recommend a machine with a clock speed of at least 3 GHz.

We are committed to helping our clients achieve maximum operational effectiveness, profit protection, and business value through innovative and technically rigorous approaches to process safety design.

Vapor-Liquid Equilibrium: TXY Diagram



Features Guide to SuperChems Expert and for DIERS

Features	Expert	DIERS
Mixture Properties		
• Handles Mixtures	•	•
• Properties Databank	•	•
• Property Estimation Methods (Thermo-physical and Transport)	•	•
• Data Reduction and Regression	•	•
• Mixture Flashpoint Estimator	•	
Advanced Dynamic Simulation Options		
• Interlinked Vessels (flowsheet)	•	
• Vent Header Design (single and multi-phase reaction flows)	•	
• Effluent Handling Design	•	
• Plug Flow Reactors (vapor, and two-phase)	•	
Vapor-Liquid Equilibrium		
• Phase Envelope Generation	•	
• Common Flash Blocks	•	•
• Binary T-X-Y Diagrams	•	•
• Binary P-X-Y Diagrams	•	•
• BIPS Estimation Using UNIFAC	•	•
• VLE/VLLE Consistency Checks and Regression	•	•
• BIPS Estimation Using Limited Solubility, Azeotropic, Experimental Data, and Infinite Dilution Activity Coefficients	•	•
• Simultaneous Physical/Chemical Equilibrium	•	
• Thermodynamic Stability	•	
• P-H-S Diagrams	•	
• Heat Of Solution Diagrams	•	
Reactions		
• Accepts Experimental Data Such As ARC, APTAC, VSP, and RSST Data and Reaction Types Such As Tempered, Gassy, Hybrid and Inputs	•	•
• Does Heat-up Calculations To Examine If Fire Exposure Induced Runaway Reaction Can be Avoided By Insulation	•	•
• Handles Stoichiometric Reactions	•	•
• Accepts Arrhenius pre-exponential Factor and Activation Energy for Reaction Kinetics as well as other user defined forms	•	•
• Does Free Energy Minimization to Calculate Reaction Heat and Tachometry for Systems with Unknown Kinetics	•	•
• Handles Supercritical Systems	•	•
• Considers Post-relief Reaction in Vent Piping, Effluent Handling Systems, and Exit Piping	•	
• Includes Plug Flow Reactor Models for Gas and Liquid Phase Reactions	•	
• Reaction Definition Module	•	•

Features	Expert	DIERS
Flow and Source Term Models		
• Liquid Flow From Vessels w/wo Piping	•	•
• Liquid Pools	•	
• Two-phase Flow From Vessels w/wo Piping	•	•
• All Gas Flow From Vessels w/wo Piping	•	•
• Two-phase Flow Expansion	•	
• Gas Flow Expansion	•	
• Piping Containing Liquids	•	•
• Piping Containing Gas/Vapor	•	•
• Piping Containing Two-Phases /Subcool Liquids	•	•
• Headers Containing Liquids	•	
• Headers Containing Gas/Vapor	•	
• Headers Containing Two-Phases	•	
• Handles Alternate Relief Path	•	
• Stream Generation From SourceView	•	•
• Ideal Nozzle Flow Liquid/Subcooled, Vapor, and 2-Phase	•	•
• Sudden Flow or Valve Closure Stacks	•	•
• Unbalanced Heat Loads	•	•
Systems Under Fire Exposure		
• DIERS Coupling Equation and Vapor/Liquid Disengagement	•	•
• QuickSize	•	•
• Choice Of NFPA-30, API-520, API-2000	•	•
• Credit For Less Exposure To Fire When The Equipment Is Physically Blocked From Fire	•	•
• Estimation Of Sprinkler Water Density To Avoid Onset Decomposition Temperature	•	•
• User Defined Heat Flux and Adjustment to Surface Area	•	•
Vessel And Pipe Flow Model Options		
• DIERS Coupling Equation	•	•
• Bubbly, Churn-Turbulent, User Specified	•	•
• Vapor	•	•
• Two-phase (flashing, non-flashing/frozen, etc.)	•	•
• Bottom-Vent/Subcooled	•	•
• Homogeneous Equilibrium Flow	•	•
• Slip Equilibrium Flow	•	•
• External Streams Input To Vessel	•	•
• Inbreathing	•	
• Thermal Expansion	•	•
Equipment Options		
• Vertical Vessel With User Defined Heads	•	•
• Horizontal Vessel With User Defined Heads	•	•
• Spherical Vessel	•	•
• Rectangular Vessel	•	•
• Jacketed Vessels	•	•

CONTINUED

Features Guide to SuperChems Expert and for DIERS *Continued*

Features	Expert	DIERS
• Elongated Vessel (pipeline)	•	•
• Heat Exchanger	•	•
Effluent handling and Vent Header Design		
• Relief Size Rating When One Vessel Releases To Another Which, In Turn, Releases To Another (vessels in series)	•	
• Simultaneous Relief Calculation Through Piping Network via Catch Tank	•	
• Optimal Cyclone Design	•	
• Optimal Separator Design (vertical and horizontal)	•	
• Stacks And Flares	•	
• Quench Tanks And Pools	•	
• Multiple Piping Segments	•	•
• Vent Header Design For Reaction And Non-reaction Flows (gas, liquid, two-phase)	•	
• Up To Three Parallel Relief Devices Per vessel	•	
• PRV Specification Sheets	•	
Dispersion Modeling		
• Indoor Dispersion	•	
• Heavy Gas Dispersion	•	
• 3D-Heavy Gas From Liquid Pools	•	
• Gas Jets	•	
• Two-Phase Jets With Aerosol Formation And Rainout	•	
• Integrated Gaussian Puff	•	
• Water Sprays And Curtains	•	
• SLAB Model	•	
Fire Modeling		
• Pool Fires	•	
• Gas Flame Jets And Flares	•	
• Two-phase Flame Jets	•	
• Vapor Cloud Fires	•	
• Fireballs	•	
Explosion Modeling		
• TNT Equivalence	•	
• Tank Overpressurization	•	
• TNO Multi-Energy	•	
• TNO Shockwave	•	
• 1D-Gas Dynamics	•	
• Semi-Confined/Vented Deflagrations	•	
• Hugoniot Curves Generation	•	
• Fragments And Projectiles Trajectories	•	

About iOiQ, LLC

iOiQ, LLC. is a leading software development company. iOiQ, LLC. Focuses on providing safety, risk analysis, and knowledge management software for business advantage. For more information about iOiQ software offerings, please visit www.ioiq.com