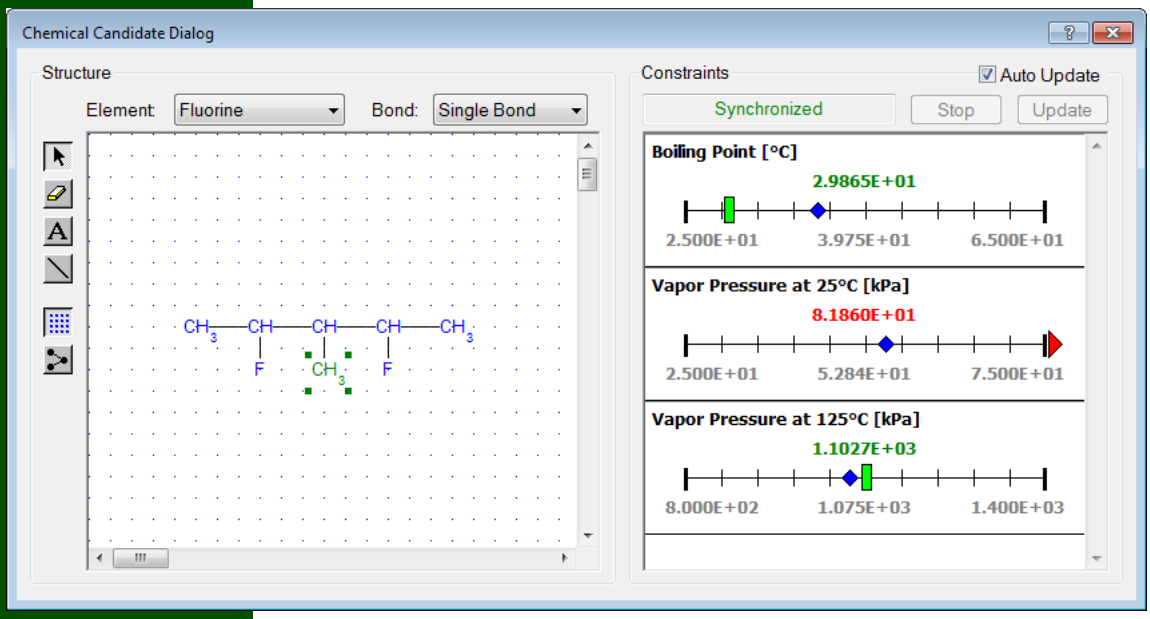
SYNAPSE®

CHEMICAL PRODUCT DESIGN



Computationally search thousands of molecular structures and mixture formulations to find those that satisfy design constraints

Today's chemical products must not only possess superior performance but also low toxicity and environmental compatibility, while being safe and highly innovative. Satisfying all these often conflicting constraints is a challenge for product designers. Synapse is a software tool which greatly assists in the design of better chemical products.

Design Solvents, Fuel Additives, Coatings, Heat Transfer Fluids, Adhesives, Lubricants, ...

Synapse is an advanced chemical product design software tool giving you a radically new approach for designing molecules and formulations that possess desired physical properties. You first enter constraints, such as the need to form an azeotrope with water, minimum solubility limits, maximum volatility and minimum flash point. Synapse then generates thousands of candidate molecules computationally assembling each candidate's molecular structure atom by atom. Mixture formulations are similarly generated by choosing from hundreds of possible components and enumerating thousands of compositions. Synapse finally estimates the physical properties of each of these candidates and evaluates each design constraint identifying those candidates which satisfy all design constraints.

Synapse has been used to design many chemical products including new solvents, aircraft deicing fluids, novel heat transfer fluids, jet fuel additives and improved rocket fuels.

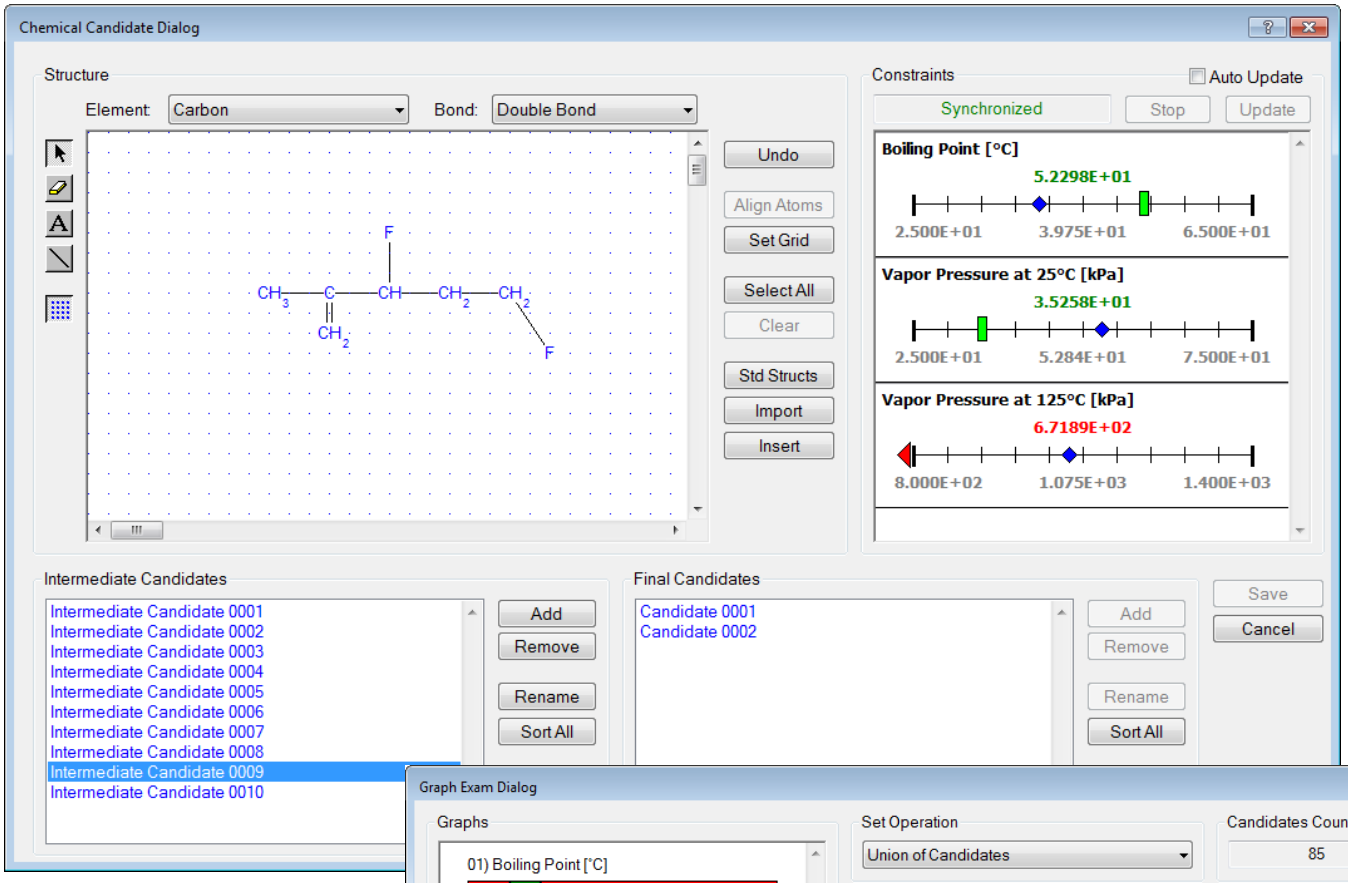
CHEMICAL PRODUCT DESIGN

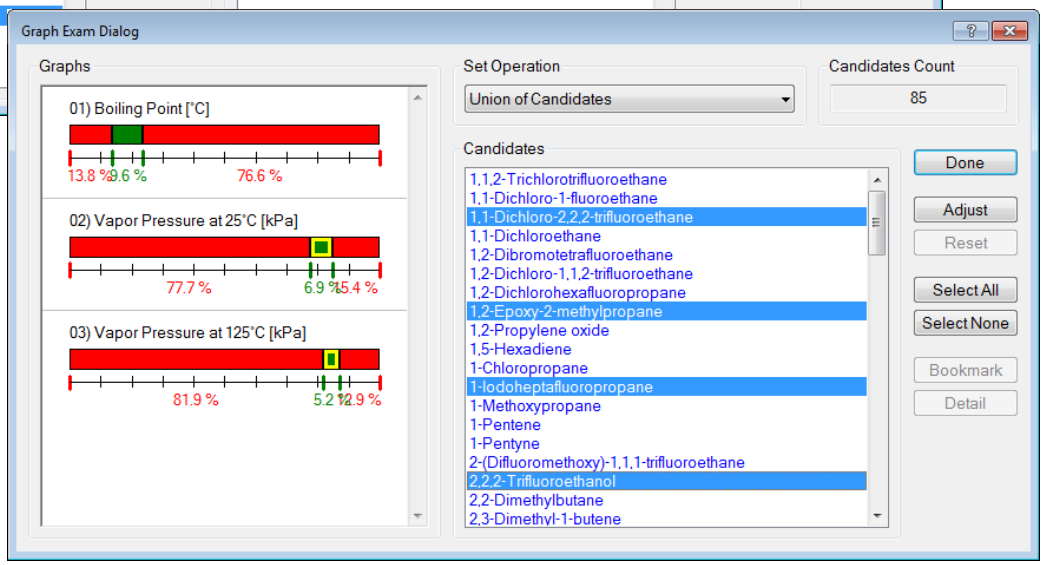
Synapse helps with the tasks needed to design improved chemical products:

1) Developing detailed, quantitative constraints on physical properties and molecular structure
2) Compiling or developing physical property estimation techniques tailored for the specific chemicals being investigated
3) Computationally generating and testing thousands of molecular structures or mixture formulations identifying those that satisfy your design constraints

GRAPHICAL DESIGN

Synapse's graphical design capabilities gives you manual control over the search for new chemical products. To design new chemicals you to simply draw candidate molecular structures. To design new mixtures you simply enter components and compositions. Synapse then estimates required physical properties, evaluates design constraints and presents the results graphically. Using Synapse's graphical design you can investigate the effect of changing your current product's structure or composition, identify conflicting design constraints and discover relationships between molecular structure and physical properties.





In a Graphical Structure Design you first specify the atoms and bonds you will use to assembly candidate molecular structures. You then specify the physical property design constraints your candidate must satisfy. As you draw your candidate's structure, Synapse evaluates each design constraint and graphically displays the results.

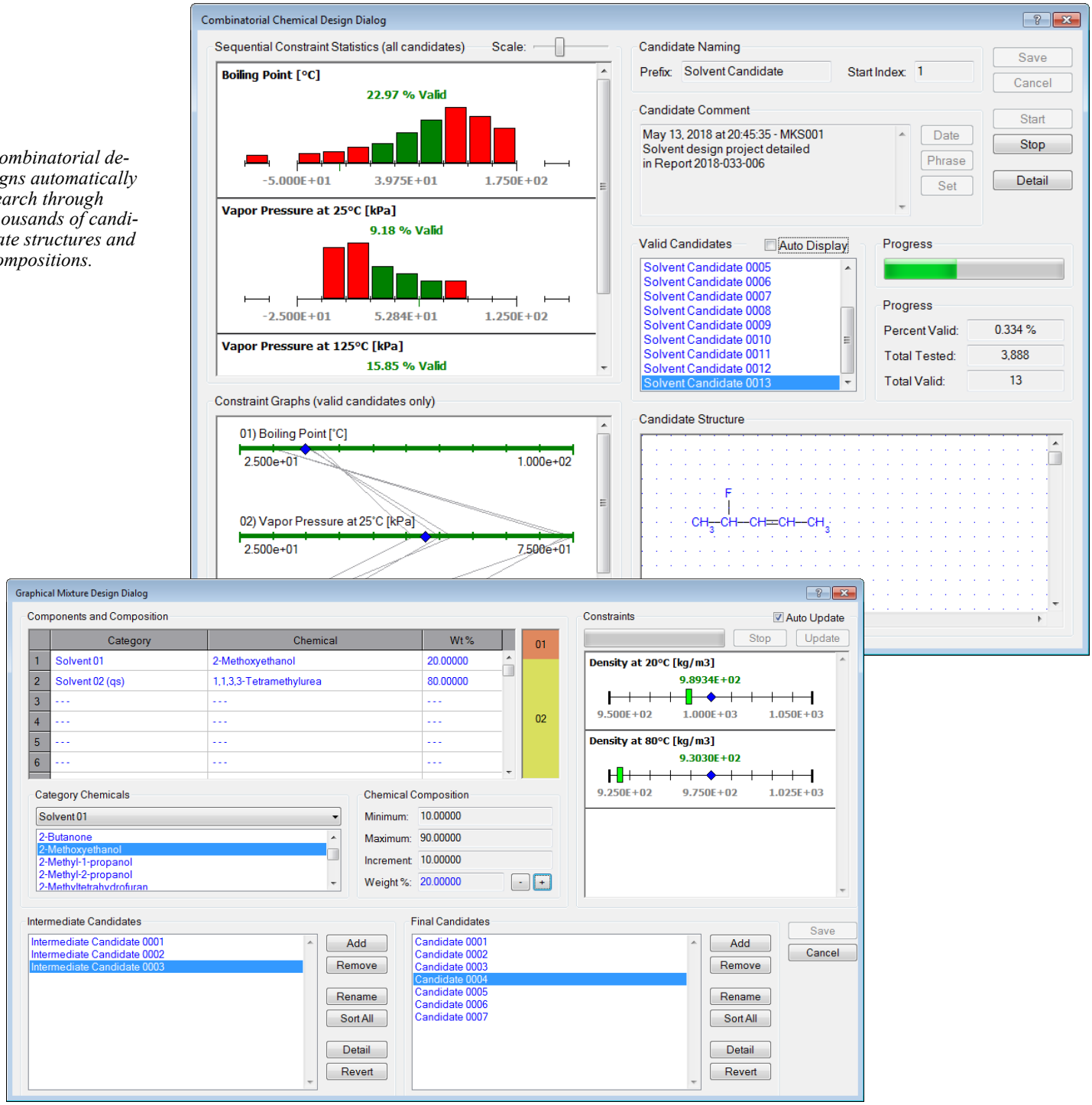
PHYSICAL PROPERTY ESTIMATION

Synapse contains hundreds of physical property estimation techniques. To estimate a chemical's or mixture's physical property, Synapse begins by collecting all applicable estimation techniques. Synapse then analyzes these techniques finding the one which is most appropriate for your entered compound. If Synapse requires other properties to perform the estimation it automatically repeats the previous steps to estimate the required property. Using a C-like language you can enter your own estimation techniques and thus tailor Synapse to your specific chemical product design needs.

COMBINATORIAL DESIGN

Synapse's combinatorial design capabilities enable you to automatically search through thousands of candidate products to find those that satisfy design constraints. Synapse generates thousands of candidate chemicals by assembling each candidate's molecular structure atom by atom. Synapse generates thousands of novel mixture formulations by combining hundreds of components and compositions.

Combinatorial designs automatically search through thousands of candidate structures and compositions.



EXAMPLE PAST DESIGNS

- New solvents for pharmaceuticals
- Carnauba wax substitutes for use in melt-castable explosives
- Improved cloud point depressants for jet fuel
- Lubricants designed for fluorinated refrigerants
- PCM enhanced heat transfer fluids for district heating
- Environmentally friendly aircraft deicing fluids
- Non-chlorinated solvents for vapor degreasing
- Non-hazardous solvents for resist stripping
- Higher performance rocket fuels
- Improved formulations for next-generation ice packs
- CO_2 solvents that require less overall energy for separation
- Stabilizers for artificial blood emulsions

KEY CAPABILITIES

- Thorough search of candidate structures and formulations
- Graphical and combinatorial design methods
- Document constraints used for product selection and design
- Enter new chemicals, estimation techniques, components
- Capture your company's knowledge
- Examine tradeoffs between design constraints

DESIGNABLE PROPERTIES INCLUDE

- Acentric Factor
- Activity Coefficient
- Aquatic Toxicity
- Autoignition Temperature
- Biological Oxygen Demand
- Boiling Point
- Chemical Oxygen Demand
- Critical Pressure
- Critical Temperature
- Densities
- Diffusion Coefficients
- Enthalpy of Formation
- Enthalpy of Fusion
- Enthalpy of Vaporization
- Flash Point
- Freezing Point
- Gibbs Energy of Formation
- Heat Capacities
- Henry's Law Constant
- Lower Flammability Limit
- Melting Point
- Molecular Weight
- Octanol-Water Partition
- Solid-Liquid Equilibria
- Solubility Parameter
- Surface Tension
- Thermal Conductivities
- Upper Flammability Limit
- Vapor Pressure
- Vapor-Liquid Equilibria
- Viscosities
- Water Solubility

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