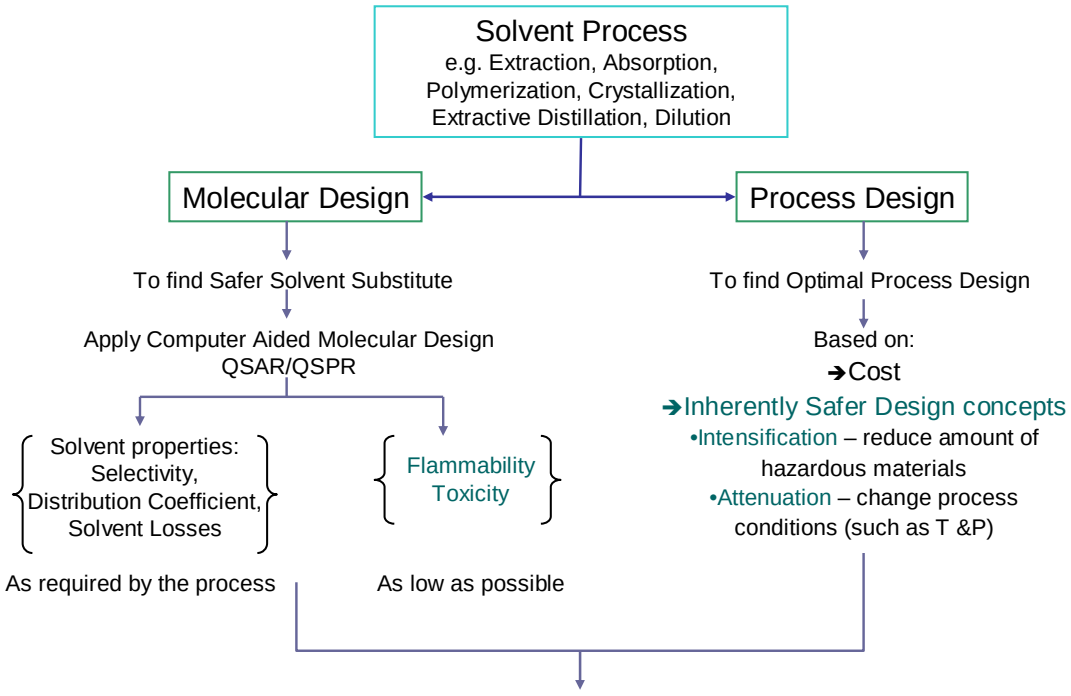
Integrating Safety Issues in Optimizing Solvent Selection and Process Design

Solvents are used in many chemical processes, but due to their hazardous nature (being highly flammable and toxic) they are involved in many accidents each year. In the course of 2006-2007, the following incidents involving solvents were recorded by the U.S. Chemical Safety and Hazard Investigation Board.

1. Synthron Facility, North Carolina, January 2006
   The reactants for a particular batch were scaled up in the polymerization unit. This caused a runaway reaction. Solvent vapors from the reactor were released to form a vapor cloud that ignited shortly afterwards.
2. CAI/Arnel, Massachusetts, November 2006
   This was a printing inks and paints facility. The solvent blend used for the process was more volatile than the individual components. The incident occurred during the night when the ventilation system had been switched off. The proximity to residential areas and offices caused a lot of property damage as a result of the explosion.
3. Barton Solvents, Iowa and Kansas, October and July 2006
   Two of the facilities for Barton Solvents were involved in solvent related incidents. One incident occurred while loading while the other one occurred in a tank storage area.

It is observed that safety is generally examined and incorporated typically as an after thought to design. This research adds safety in the conceptual phase of solvent processes – in the areas of molecular design as well as process design. The methodology has been shown in the figure below.



Molecular design enables us to select molecules based on their property requirements. Adding constraints on flammability and toxicity values generates molecules with less hazardous properties, without compromising other solvent related physical properties. Computer Aided Molecular Design (CAMD) is a well established method for the selection of chemicals based on property requirements. Generally this methodology makes use of Group Contribution Method

(GCM) for property prediction. Since the accuracy of GCM is at times questionable, in this work the applicability of Quantitative Structure Activity Relationship/ Quantity Structure Property Relationship (QSAR/QSPR) for property prediction will also be determined. The molecular descriptors used in QSPR will be selected based on their ability to predict the property and at the same time provide information about the molecular structure.

Molecular substitution alone leads to a suboptimal design. Thus, simultaneously solving a process design problem by modifying process parameters gives us more flexibility to choose optimal values. Process design parameters that can be modified to enhance process safety could be flow rates, process operating conditions, stream networking etc. Upon integration of concepts described above, this research will result in the generation of a set of suitable solvents (or blend of solvents) for a particular process along with associated costs in order to make useful comparisons. The methodology will be implemented on unique solvent applications in order to justify that it develops a safer solvent and an inherently safer process design.