**REGSOExpert**

- A wizard computer tool including 224 feasibility rules, and 326 batch azeotropic and extractive distillation processes.
- Systematic checking for each entrainer candidate for determining its feasibility to be used in rectifying or stripping batch column.
- A list of potential homogeneous and heterogeneous entrainers in an optimal time for separating A and B as any industrial mixture.

**Strategy for solvent recovery by distillation**

1. Chose entrainer candidates Ei for A + B
2. Residue curve map of ABEi
3. Topological stability: A, B, E, AB, AEi, BEi, ABEi
4. Batch distillation sequences
5. Simulation + Economic evaluation

**Industrial Applications**

- **Pressure Swing Distillation**
  - **Brabant Industry case:** Cyclopentanone (136.6°C) – Propylene Glycol Monomethyl ether (146°C)
  - **Extractive Distillation (HEBD)**
  - Chloroform (A) 61.1°C + Methanol (B) 64.5°C + Water (E) 100°C
  - USE: Extraction of bioactive substances from biological sources
  - **Acetonitrile (A) 104°C + Water (B) 100°C + Heterogeneous (E)**
  - USE: Liquid chromatography separation in pharmaceutical Industry

**REGSOExpert software algorithm**

- **Heterogeneous**
  - Mixture AB: Determination AB azeotrope or azeoAE
  - Heterogeneous phase (P, Ei)
  - Pressure swing distillation
  - azeo constant, T = 30°C
- **Ideal**
  - Azeotropic distillation
  - A + B

**Acetonitrile (A)**

- **1- Selecting Heterogeneous Entrainer with RegSOExpert®**
  - Initial List: 55 candidates from several chemical families (DIPPR database)
  - Heterogeneous E: Acetonitrile and Chloroform form unstable azeotrope with H2O

- **Simulation ProSim Batch**
  - Recovery yield (A) = 92.5%

**CONCLUSIONS**

- Pressure swing distillation is a privileged option. It doesn’t involve additional entrainer. Simple performance in one or two batch distillation columns operating at different pressures.
- Heterogeneous entrainers have a more privileged position than homogeneous. Higher number of ternary diagram match with feasible rules.
- Heterogeneous entrainers in HABD: little amount of entrainer, separatrix can be crossed by the still path, simplest batch distillation column operating at different pressures.

**General procedure to systematize the search of several alternatives enabling the separation of non-ideal binary mixtures such as pressure-swing distillation, azeotropic and extractive distillation.