Applicability evaluation of AspenONE and Dynochem for solubility modeling in the pharmaceutical industry
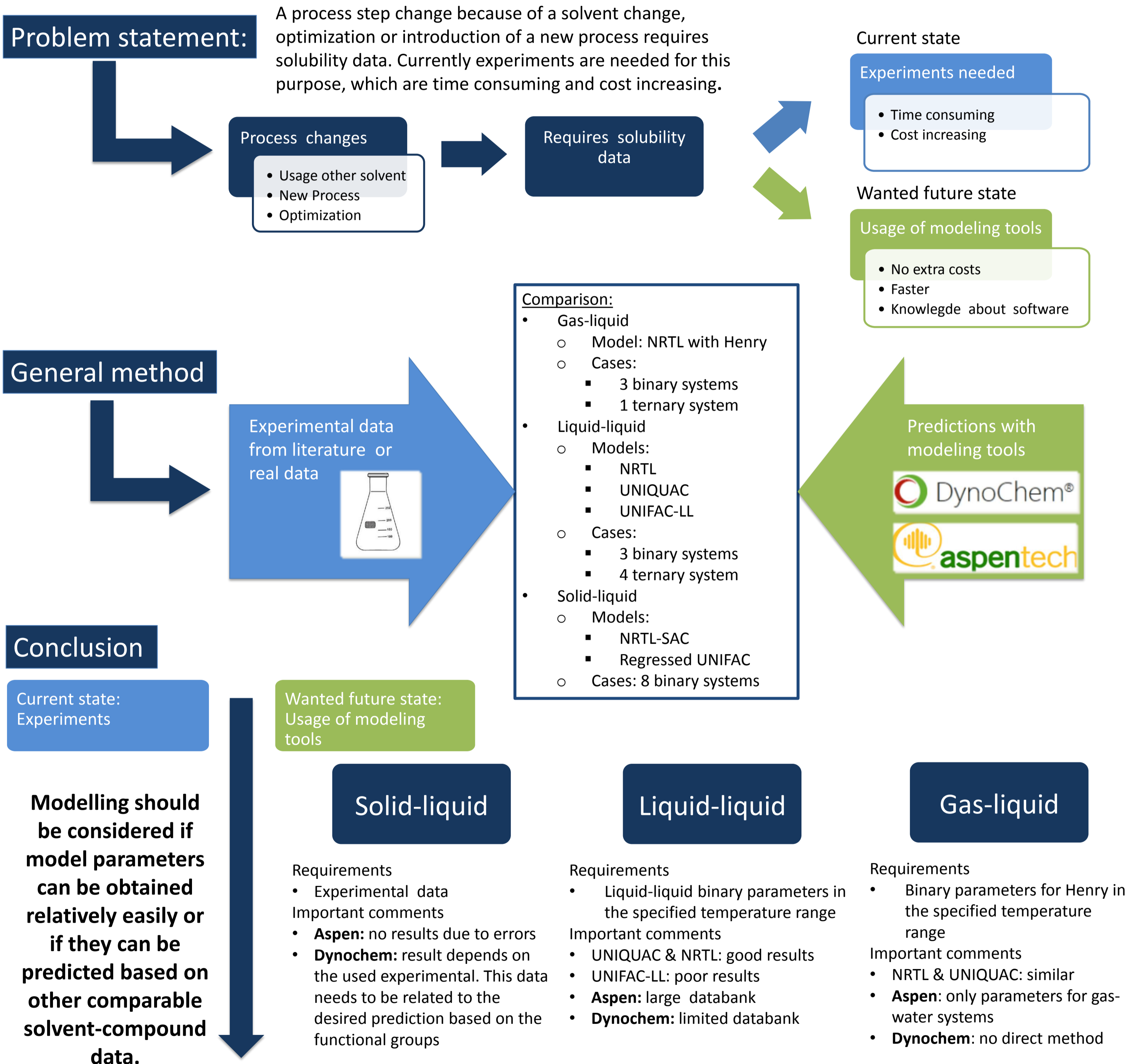
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Problem statement:

A process step change because of a solvent change, optimization or introduction of a new process requires solubility data. Currently experiments are needed for this purpose, which are time consuming and cost increasing.

Process changes
- Usage other solvent
- New Process
- Optimization

Requires solubility data

Current state

Experiments needed
- Time consuming
- Cost increasing

Wanted future state

Usage of modeling tools
- No extra costs
- Faster
- Knowlegde about software

General method

Experimental data from literature or real data

Comparison:
- Gas-liquid
  - Model: NRTL with Henry
  - Cases:
    - 3 binary systems
    - 1 ternary system
- Liquid-liquid
  - Models:
    - NRTL
    - UNIQUAC
    - UNIFAC-LL
  - Cases:
    - 3 binary systems
    - 4 ternary system
- Solid-liquid
  - Models:
    - NRTL-SAC
    - Regressed UNIFAC
  - Cases: 8 binary systems

Predictions with modeling tools

DynoChem®

aspentech

Conclusion

Current state: Experiments

Wanted future state: Usage of modeling tools

Modelling should be considered if model parameters can be obtained relatively easily or if they can be predicted based on other comparable solvent-compound data.

Solid-liquid

Requirements
- Experimental data

Important comments
- **Aspen:** no results due to errors
- **Dynochem:** result depends on the used experimental. This data needs to be related to the desired prediction based on the functional groups

Liquid-liquid

Requirements
- Liquid-liquid binary parameters in the specified temperature range

Important comments
- UNIQUAC & NRTL: good results
- UNIFAC-LL: poor results
- **Aspen:** large databank
- **Dynochem:** limited databank

Gas-liquid

Requirements
- Binary parameters for Henry in the specified temperature range

Important comments
- NRTL & UNIQUAC: similar
- **Aspen**: only parameters for gas-water systems
- **Dynochem**: no direct method

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