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PPBLAB: A Multivariate Population Balance Environment for Steady State and Dynamic Modeling of Solvent Extraction Columns

Motivation

State of the art:

- Extraction column design is still based on pseudo-homogeneous modelling and equilibrium stage aproaches
- Scale-up is still based on pilot plant experiments

Aim of the work:

Providing a virtual Particulate Population Balance LABoratory (PPBLAB):

- Modeling and simulating particulate systems
- Rapid one dimensional CFD extraction column simulation
- This saves time and money

PPBLAB: Particulate Population Balance Laboratory

- **New windows-based MATLAB environment for the simulation of dispersed phase flow using population balances as a modeling framework**

PPBLAB Features: (Fig. 1)

- New thermodynamics package TEA (Thermodynamics for Engineering applications) imported from CAPE-OPEN
- PPBLAB-CAPE-OPEN-UNIQUAC interaction parameter optimization tool
- PPBLAB droplet velocity model optimization tool
- PPBLAB-Dynamics tool
- Inlet feed distribution fitting tool
- PPBLAB-Report generation tool to export data in pdf or HTML format

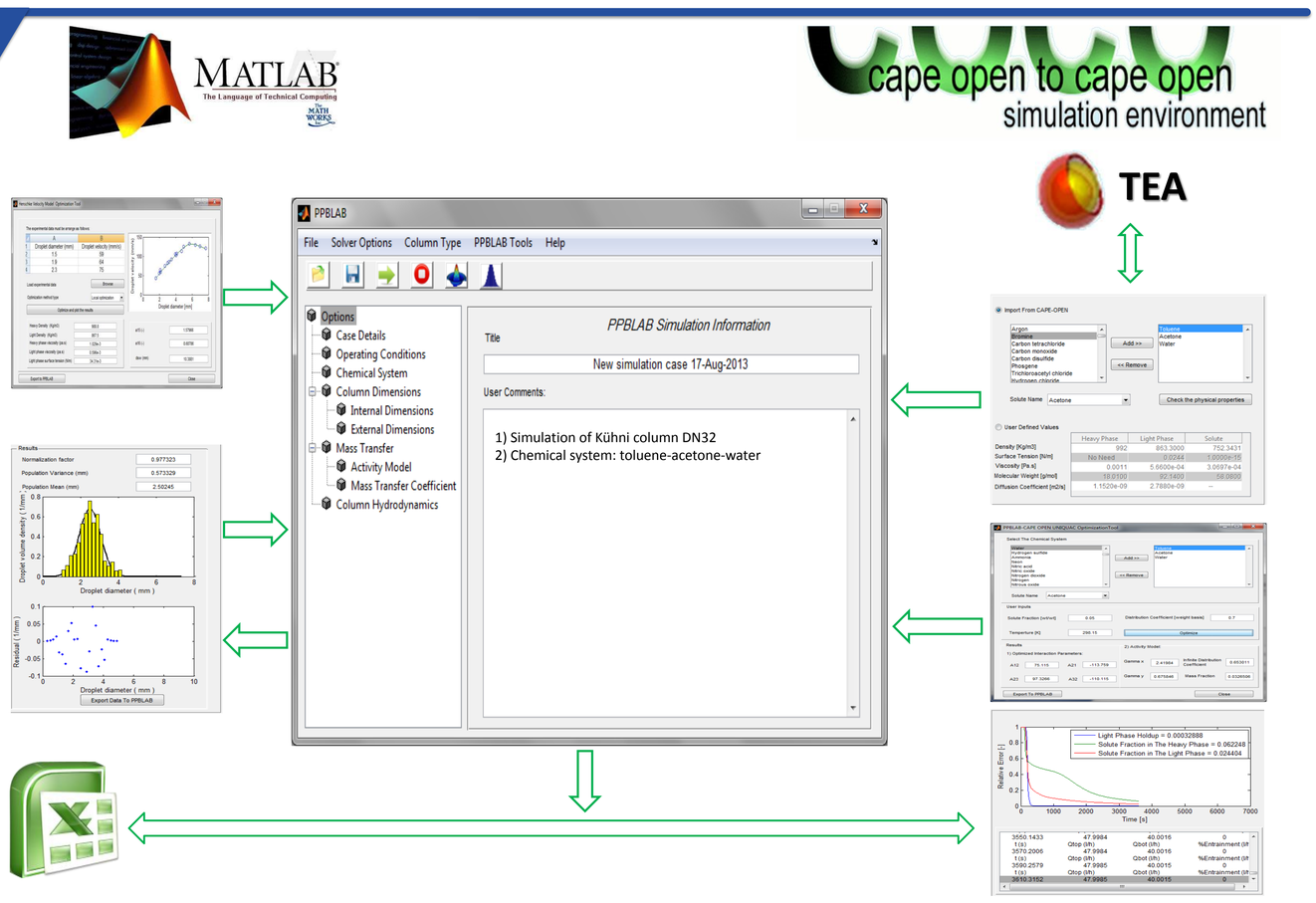

Fig. 1: PPBLAB: A population balance based software for the simulation of agitated and non-agitated liquid-liquid extraction columns.

Numerical vs. Experimental Results:

- Dynamic simulation of a Kühni DN32 extraction column during start-up
- Axial dispersion and energy dissipation correlations are determined using 3D-CFD simulations (Fig. 2)

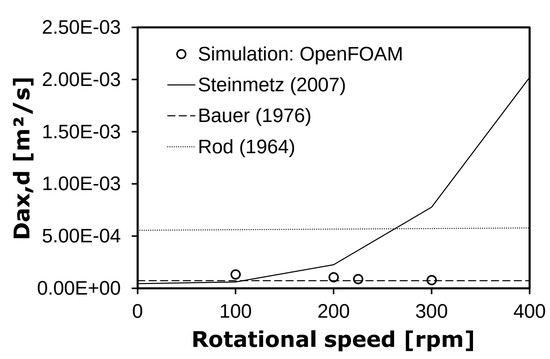

Fig. 2: The axial dispersion coefficient of the dispersed phase using 3D simulation. Upper Figure shows the results as compared to the published correlations.

- Based on the experimental droplet size distribution at the top of the column, PPBLAB predicts the dynamic mass transfer behavior along the column height (Fig. 3)

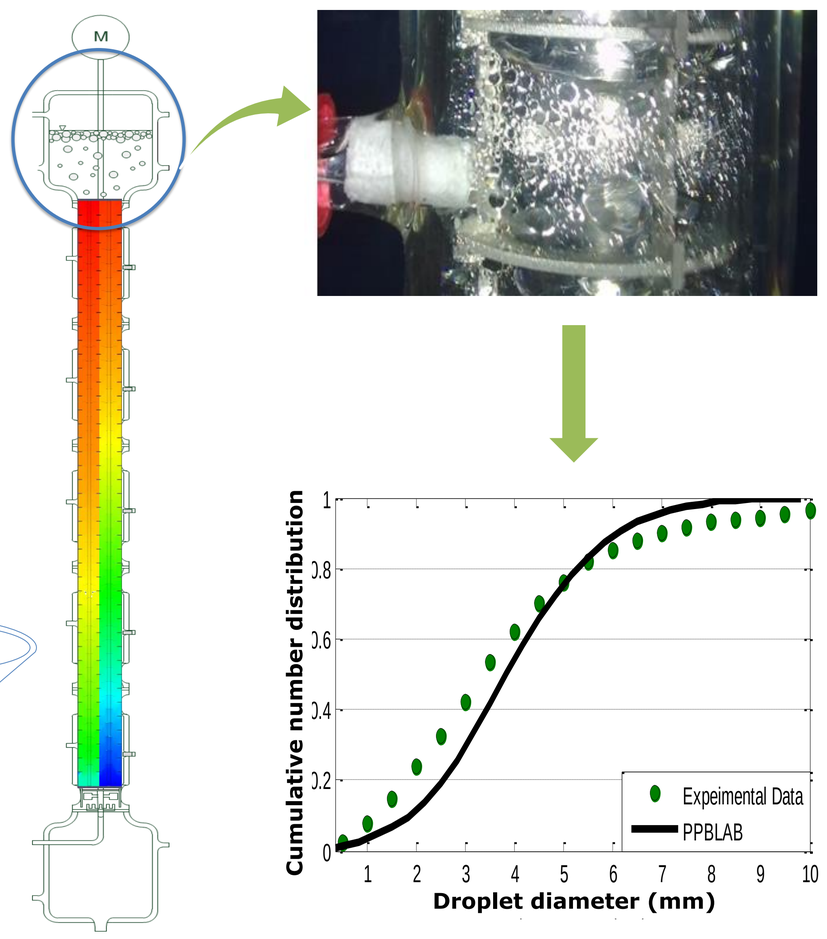

Fig. 3: Experimental droplet size distribution at the top of the column as compared to 1D PPBLAB simulation.

- Concentration profiles are measured at five positions along the column height (Fig.4)

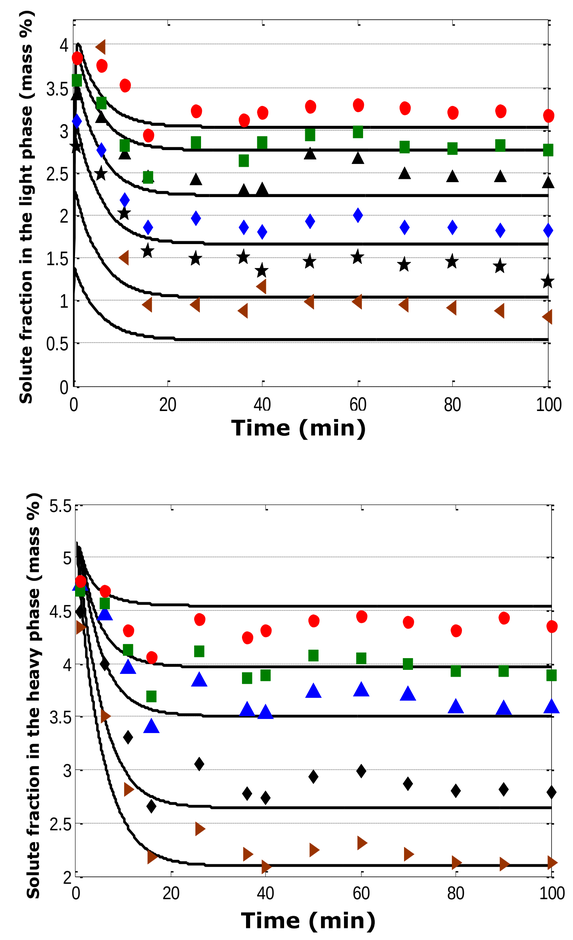

Fig. 4: 1D PPBLAB dynamic validation using transient concentration profiles along the column height.

Conclusions:

- PPBLAB is a 1D simulation software which benefits from 3D CFD simulations
- PPBLAB 1D simulation saves time and money

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