School of Chemical and Process Engineering
FACULTY OF ENGINEERING AND PHYSICAL SCIENCES
UNIVERSITY OF LEEDS

Experimental validation of Pulsed Sieve-plate Extraction Column models

International Solvent Extraction Conference
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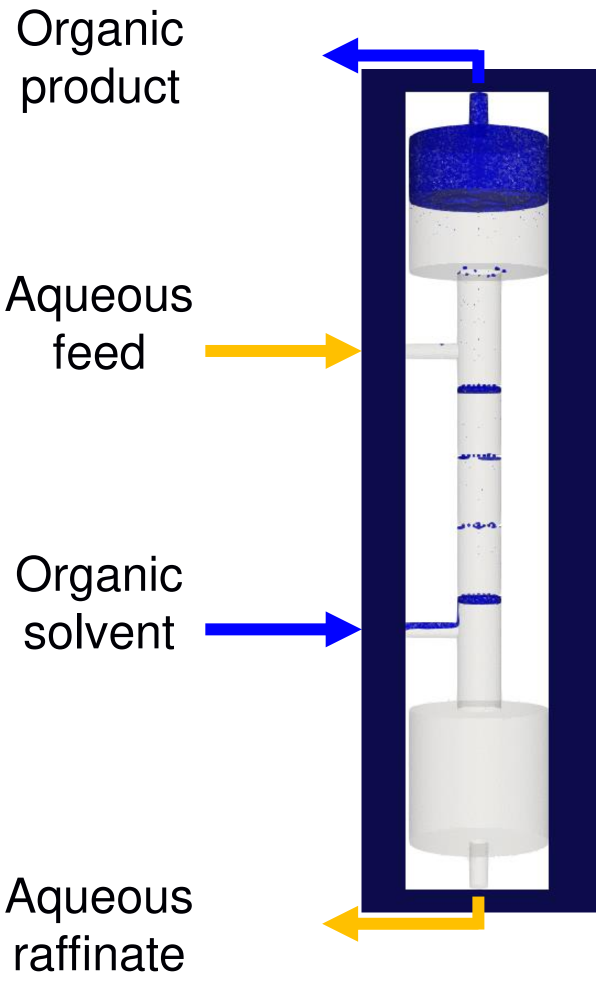
PULSED SIEVE-PLATE EXTRACTION COLUMNS

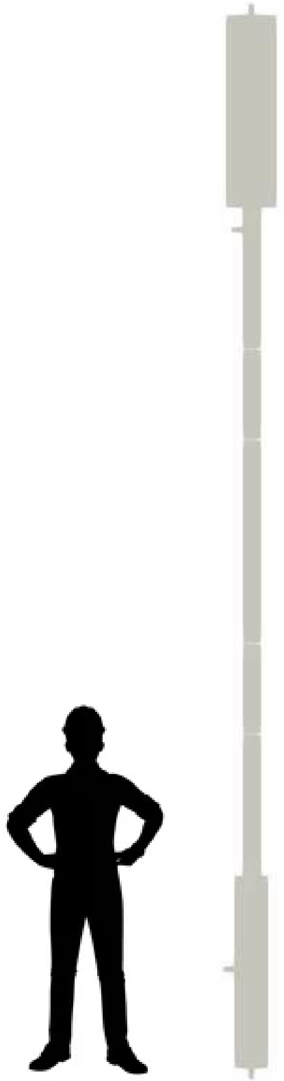
- Counter-current liquid-liquid extraction unit operation.
- Advantages:
  - No moving parts
  - Can operate with solids
- Disadvantages:
  - Empirical correlations are poor and not general.
  - Pilot plants and expensive.
- Can we develop a generalised approach to design?



VALIDATION DATA (Garthe, 2006)

- 4.5 m tall, 80 mm diameter, PSEC.
- Absorption of acetone from water by toluene.
- 17 experiments.
- 10 different operating conditions.
- Measurements:
  - Dispersed phase holdup
  - Mean droplet diameter
  - Aqueous axial solute concentration
  - Solvent axial solute concentration

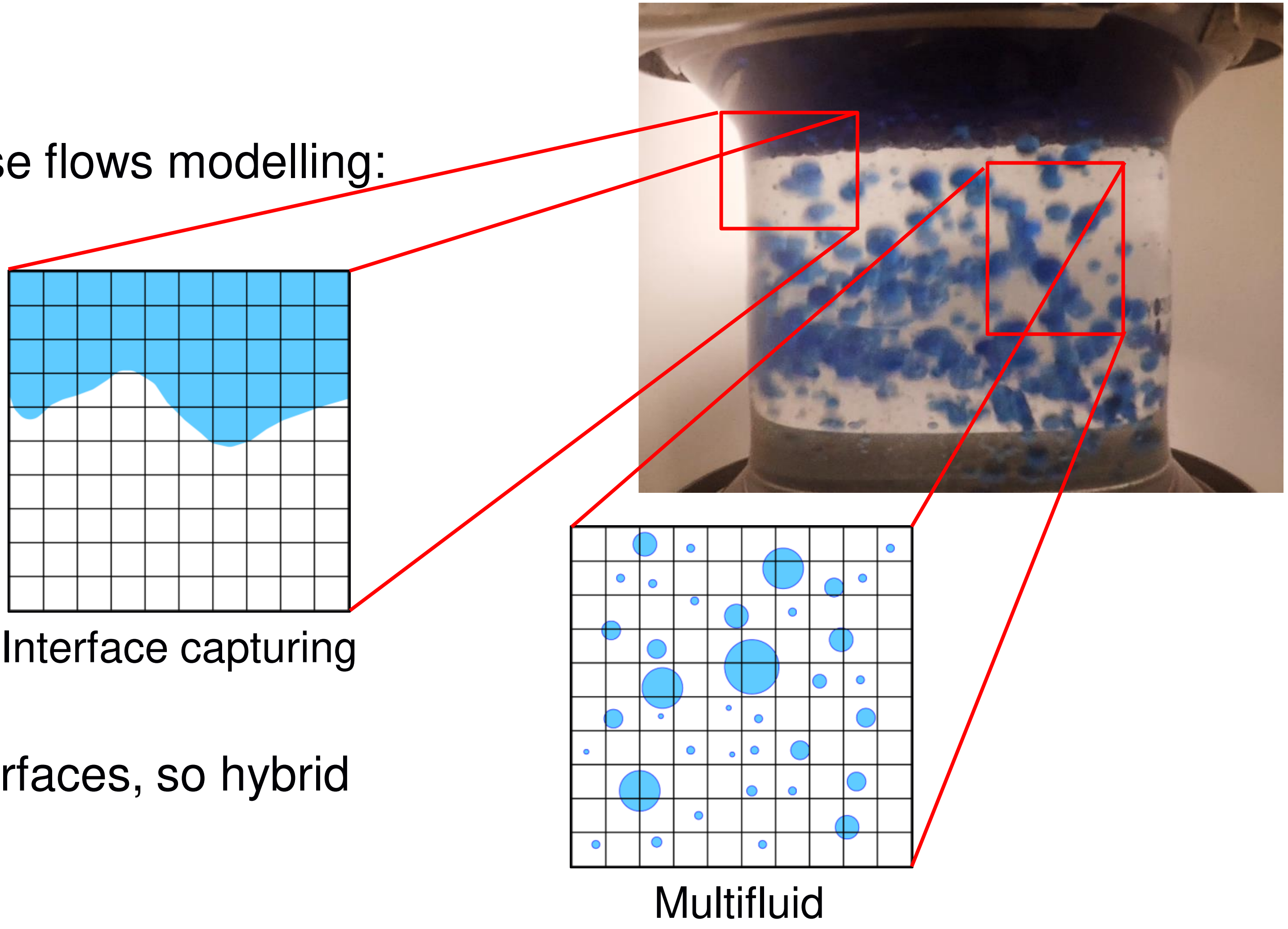
Parameter	Value
Aqueous flow rate (L/hr)	40-93
Solvent flow rate (L/hr)	48-112
Total flow rate (L/hr)	88-205
S:A ratio	1.2
Pulse velocity (cm/s)	1-2
Dispersed phase holdup (%)	7.2-36
Sauter mean droplet diameter (mm)	1.8-2.6
Aqueous feed solute concentration (mol/L)	0.885-1.02
Solvent feed solute concentration (mol/L)	0.505-0.716
Mass transfer direction	Aq. to Sol.



Garthe, D., 2006. *Fluiddynamics and mass transfer of single particles and swarms of particles in extraction columns*

MODELLING MULTIPHASE FLOWS

- Two traditional approaches to multiphase flows modelling:
  - Interface-scale averaging
    - Multifluid (Eulerian) models
    - Generally used for dispersed flows.
    - Droplets are smaller than cells
  - Interface-scale resolving
    - Interface capturing models
    - Segregated flows
    - Mesh is smaller than interface scales
- PSEC exhibits both small and large interfaces, so hybrid method necessary.



De Santis, A., Colombo, M., Hanson, B.C. and Fairweather, M., 2021. A generalized multiphase modelling approach for multiscale flows. *Journal of Computational Physics*, *436*, p.110321.

GENERALISED MULTIFLUID MODELLING APPROACH (GEMMA)

- Developed at the University of Leeds by Marco Colombo and Andrea De Santis
- Variety of applications within multiphase flows.
- Introduces binary switch function C_a, 0 = dispersion, 1 = segregated/large-scale
- Momentum conservation:

$$\frac{\delta \alpha_k \boldsymbol{u}_k}{\delta t} + \nabla.(\alpha_k \mathbf{u}_k \mathbf{u}_k) = \frac{-\alpha\_k \nabla p}{\rho_k} + \nabla.(\nu_k \alpha_k \nabla \mathbf{u}_k) + \alpha_k \mathbf{g} + \frac{\mathbf{F}_k + \mathbf{F}_{st,k}}{\rho_k}$$

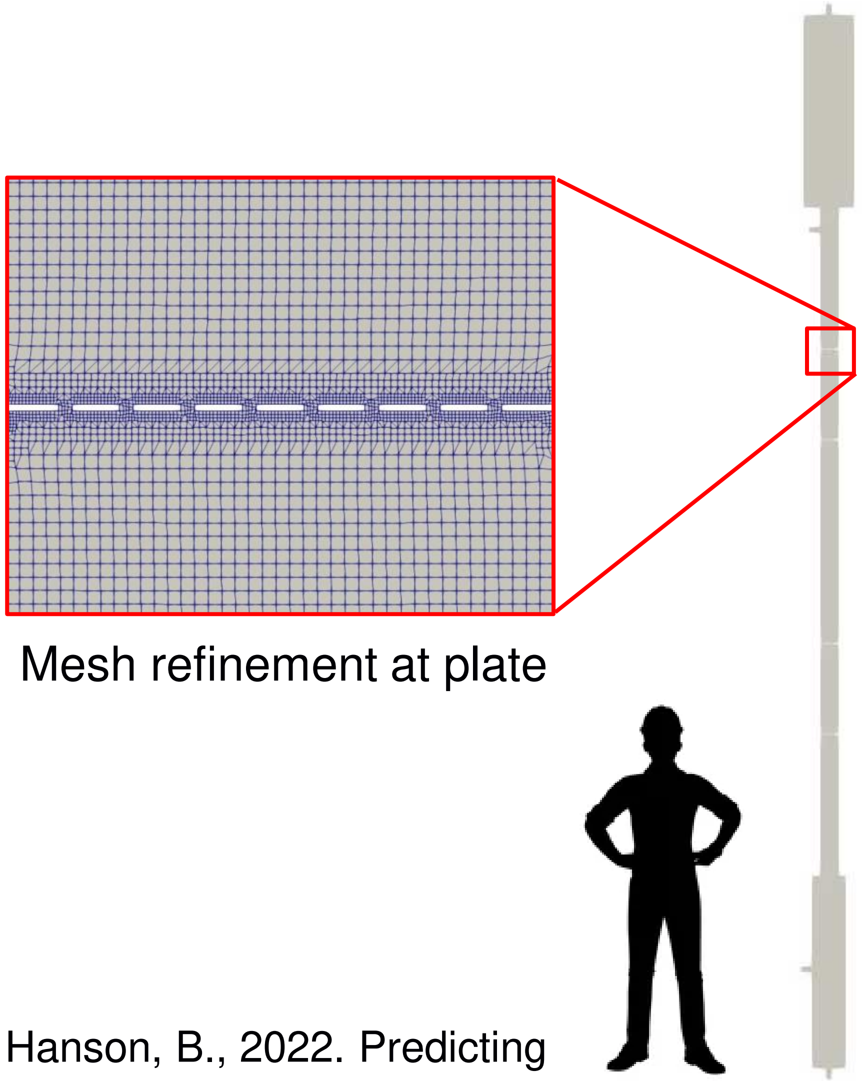
- Phase continuity

$$\frac{\delta \alpha_k}{\delta t} + \nabla.(\alpha_k \mathbf{u}_k) + \nabla.\left(\mathbf{u}_c \alpha_k (1 - \alpha_k)\right) = 0$$

De Santis, A., Colombo, M., Hanson, B.C. and Fairweather, M., 2021. A generalized multiphase modelling approach for multiscale flows. *Journal of Computational Physics*, *436*, p.110321.

NUMERICAL SET-UP

- Geometry and Mesh – 2D, 177k cells, 2mm edge length with near-wall refinement.
- Simulated physical time – 100 seconds to reach steady state, 100 seconds to collect statistics.
- Multiphase model – GEMMA.
- Turbulence modelling – RANS with k-epsilon mixture model.
- Reduced order population balance model – One Primary One Secondary Particle (OPOSPM)
- Droplet breakage – Martinez-Bazen
- Droplet coalescence – Prince and Blanch
- Momentum transfer – Schiller Naumann drag model



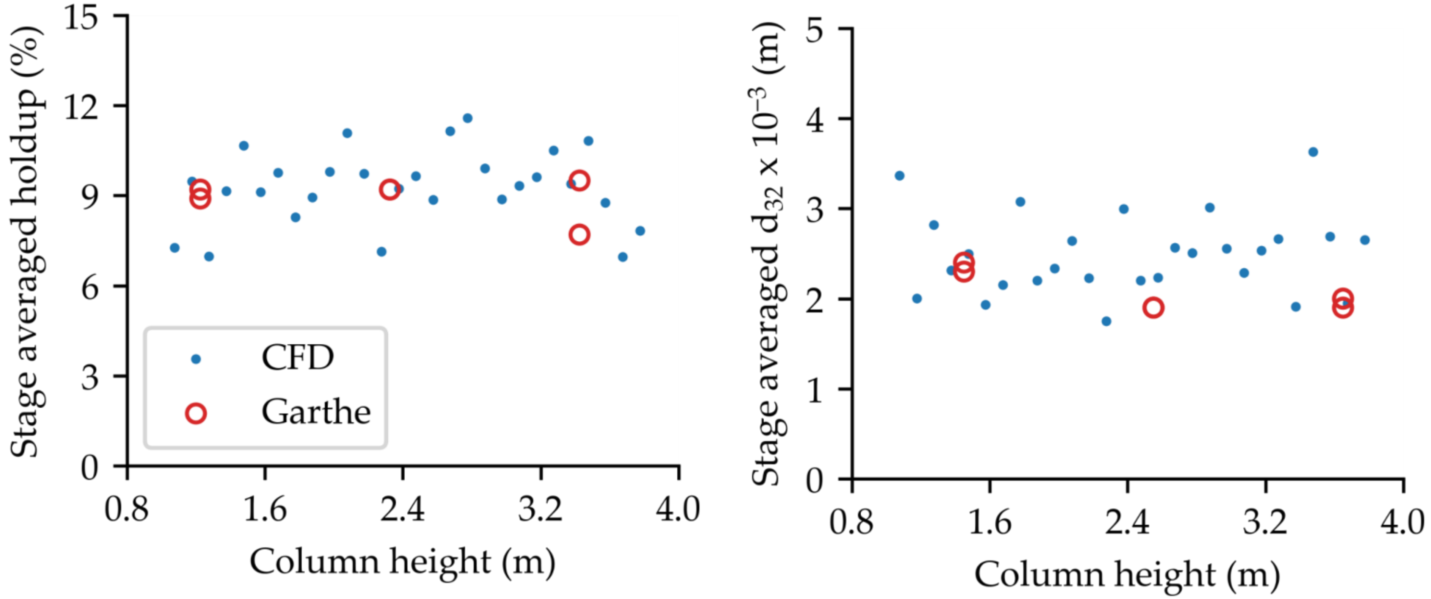
Mesh refinement at plate

Fells, A., De Santis, A., Colombo, M., Theobald, D.W., Fairweather, M., Muller, F. and Hanson, B., 2022. Predicting Mass Transfer in Liquid–Liquid Extraction Columns. Processes, 10(5), p.968.

CFD PREDICTED HYDRODYNAMICS

- Results reasonably with experimental observations:
  - 1.6% error for dispersed phase holdup.
  - 8% error for d_{32}
- Gives confidence that hydrodynamics are reasonably approximated.
- Simulation used to perform aqueous and solvent side Residence Time Distribution (RTD) study.

$$\frac{\delta(\alpha_x S_x)}{\delta t} + \nabla.(\alpha_x \boldsymbol{u}_x S_x) - \nabla^2(\alpha_x D_x S) = 0$$



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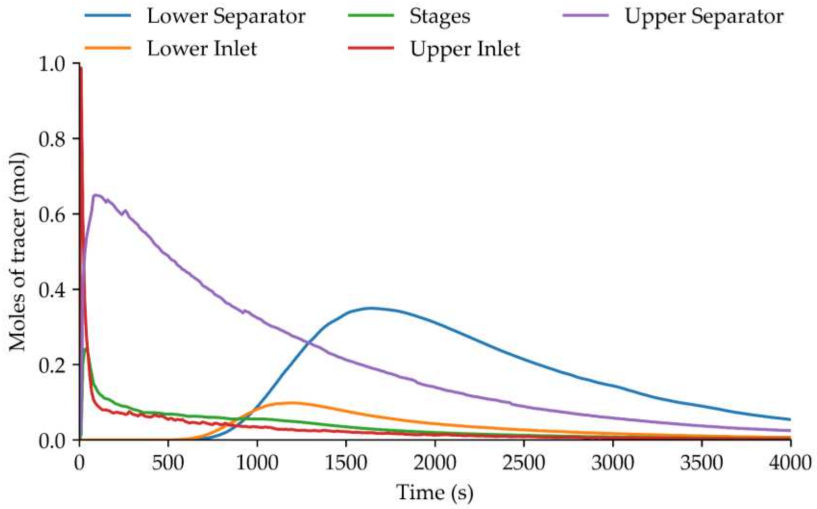
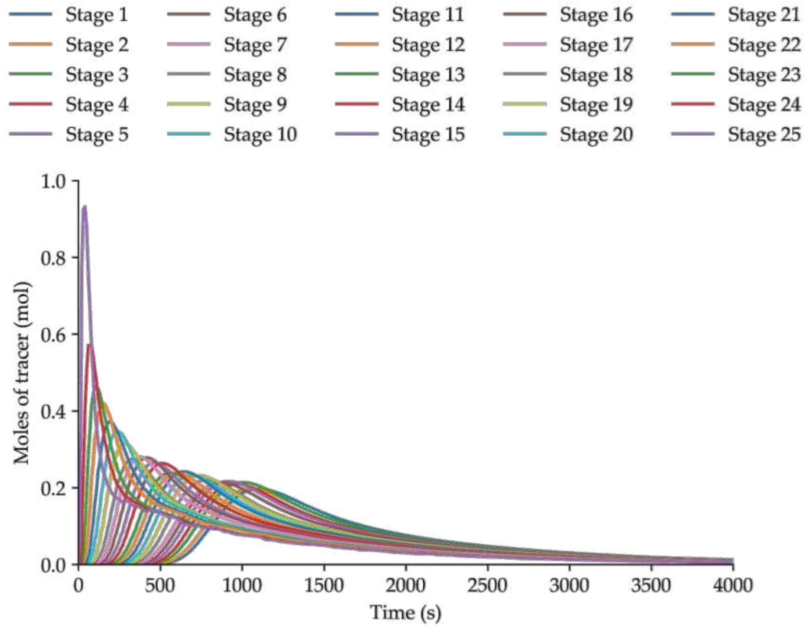
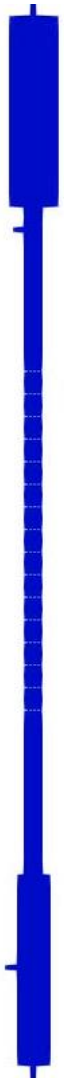
CFD AQUEOUS PHASE RTD

- Plots show moles of tracer in each zone of the PSEC with time.
- Tracer enters upper inlet and flows to the upper separator and stage 26.
- Tracer in the upper separator is well mixed and slowly returns to the upper inlet.
- Tracer in stages proceeds down the column whilst becoming axially dispersed before exiting the column.
- Long tail is associated with reservoir of tracer in upper separator.
- Implies that a large separator results in the column being slow to respond to changes in operating condition.

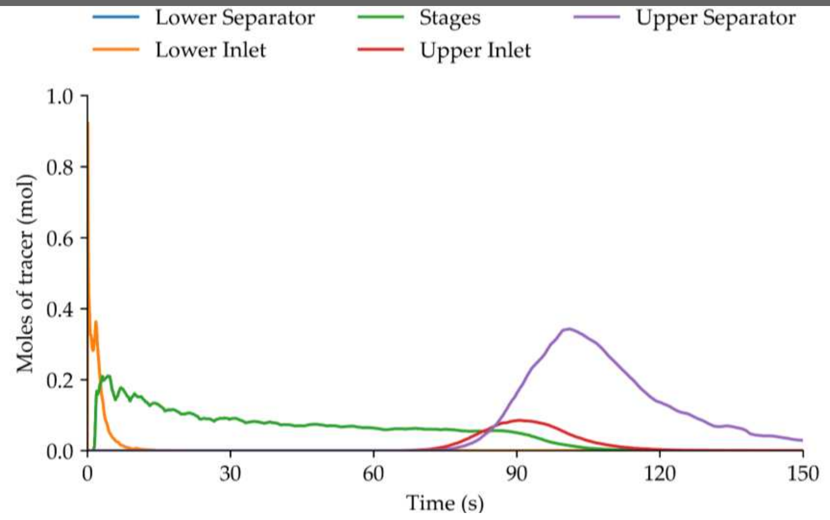


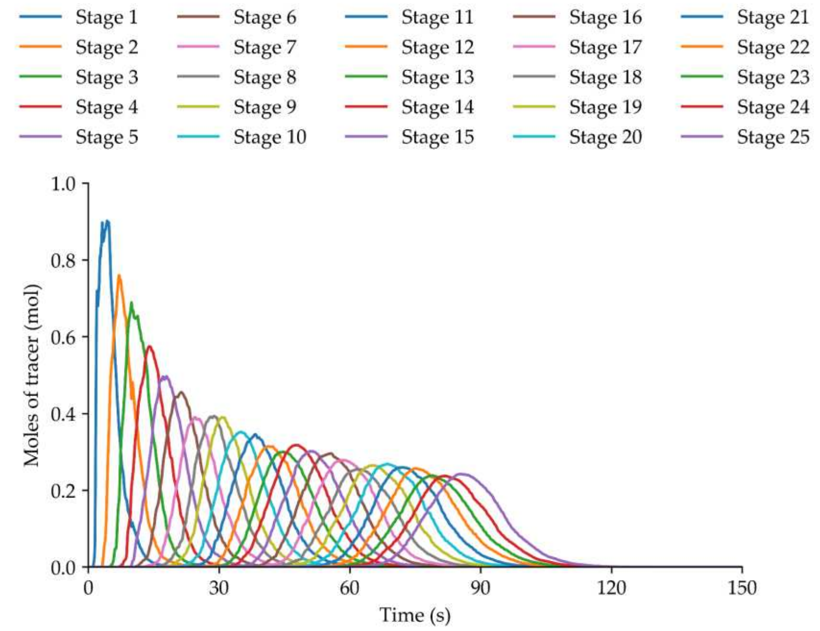




SOLVENT PHASE RESIDENCE TIME DISTRIBUTION

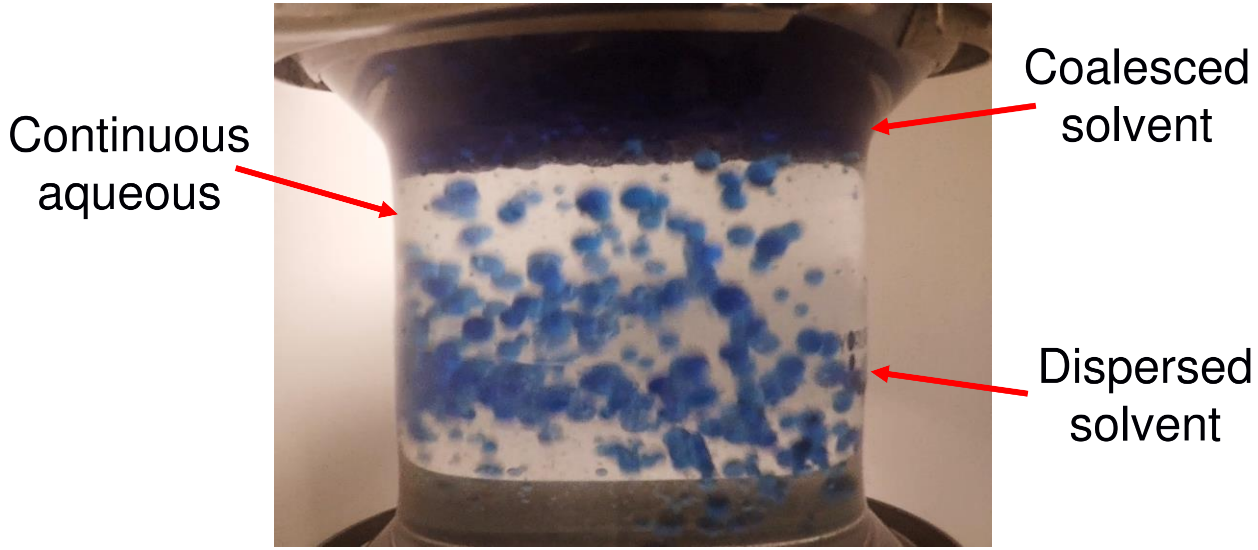
- Plots show moles of tracer in each zone of the PSEC with time.
- Tracer enters lower inlet and flows to stage 1.
- Tracer in proceeds up the column whilst becoming axially dispersed before exiting the column.
- Large peak in upper separator implies upper separator is oversized.

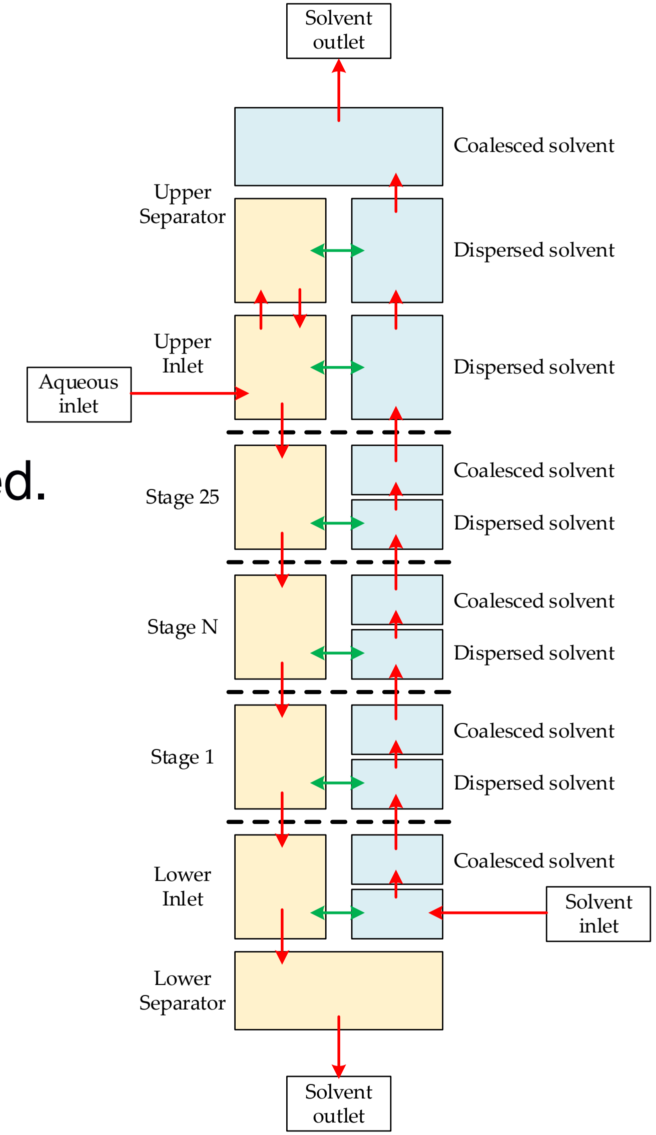




COMPARTMENT MODELLING (CM)

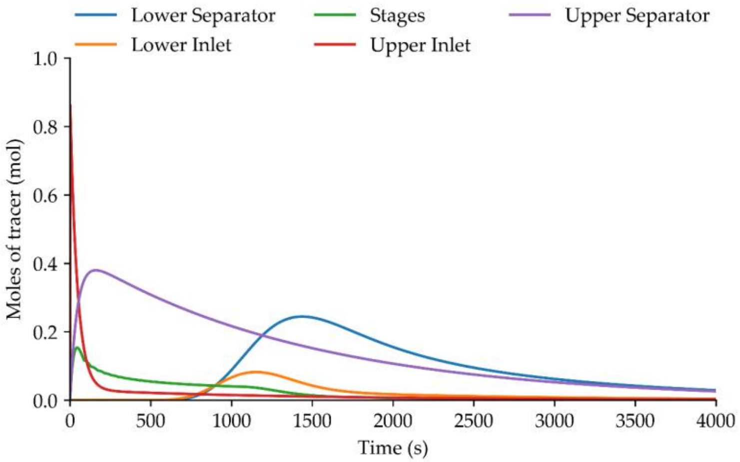
- Spatial zones are broken down into compartments.
- Each compartment is represented using a Continually Stirred Tank Reactor (CSTR).
- Flows between compartments are specified.
- Individual phenomena such as mass transfer is specified as needed.

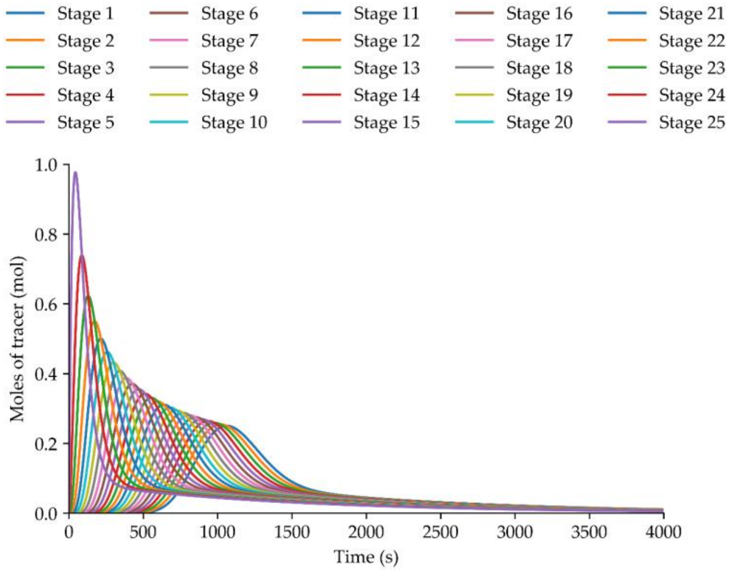


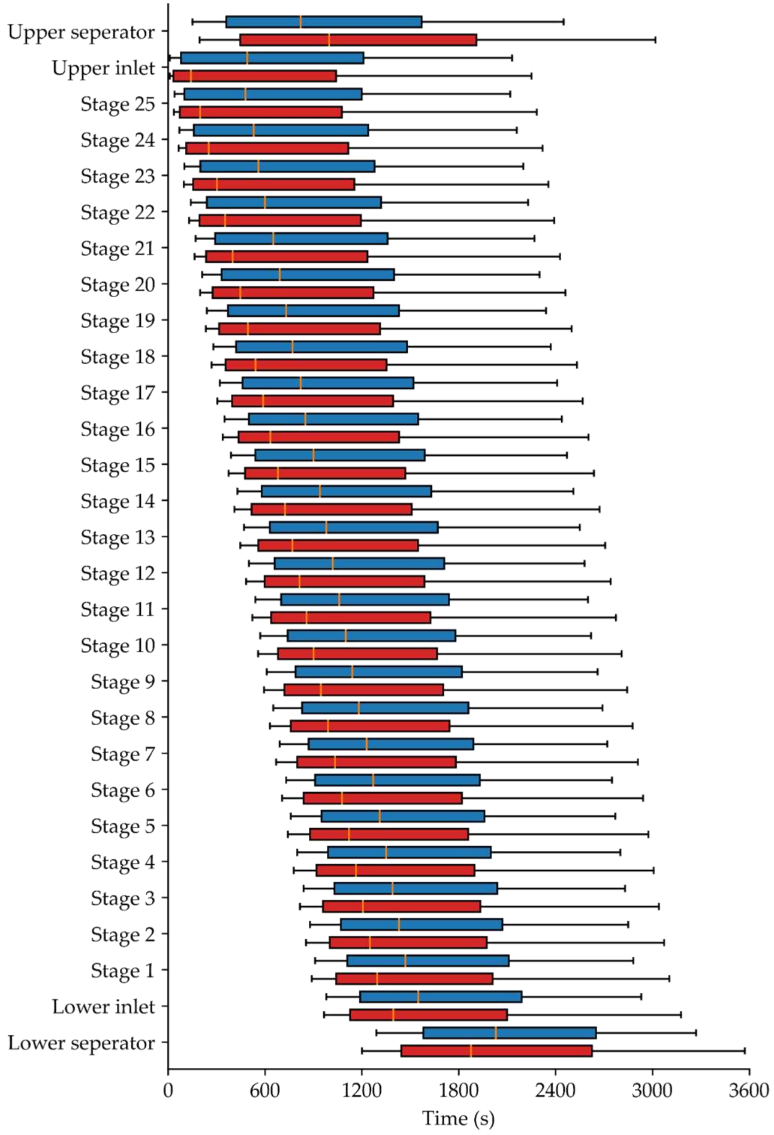


CM AQUEOUS PHASE RTD

- Visual comparison of RTD curves show general characteristics are represented.
- Box plots show CFD (blue) and CM (red) 10th, 25th, 50th, 75th and 90th percentiles of RTD curves grouped by zone.
- Shows good agreement for all zones.
- CM model is slightly early. Possibly as I have not modelled inlet pipe.

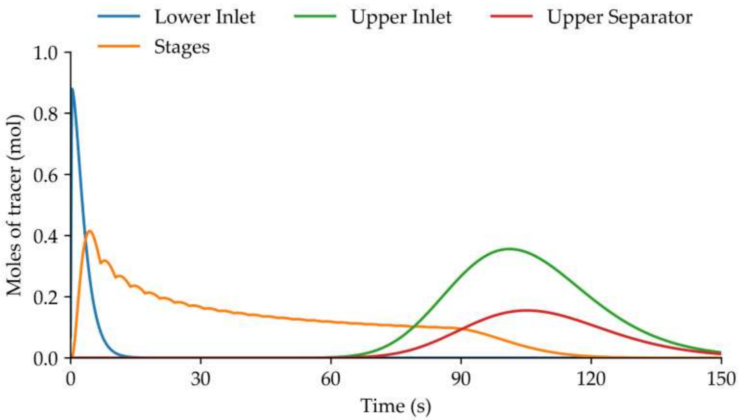


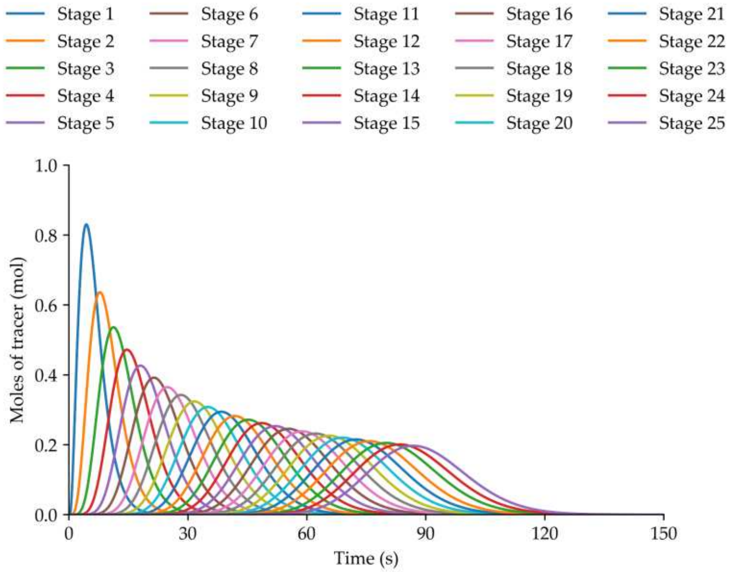


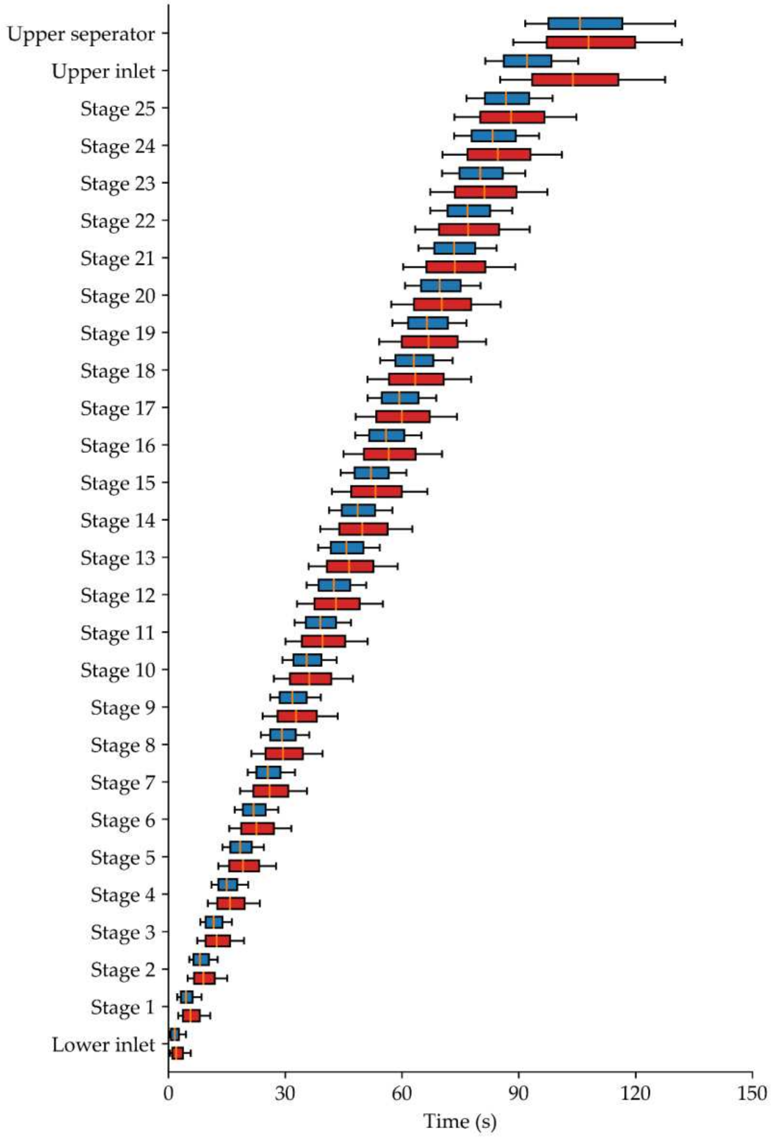


CM SOLVENT PHASE RTD

- Visual comparison of RTD curves show general characteristics are represented.
- Box plots show CFD (blue) and CM (red) 10th, 25th, 50th, 75th and 90th percentiles of RTD curves grouped by zone.
- Shows good agreement for all zones (apart from upper inlet)
- CM model is slightly more dispersed.



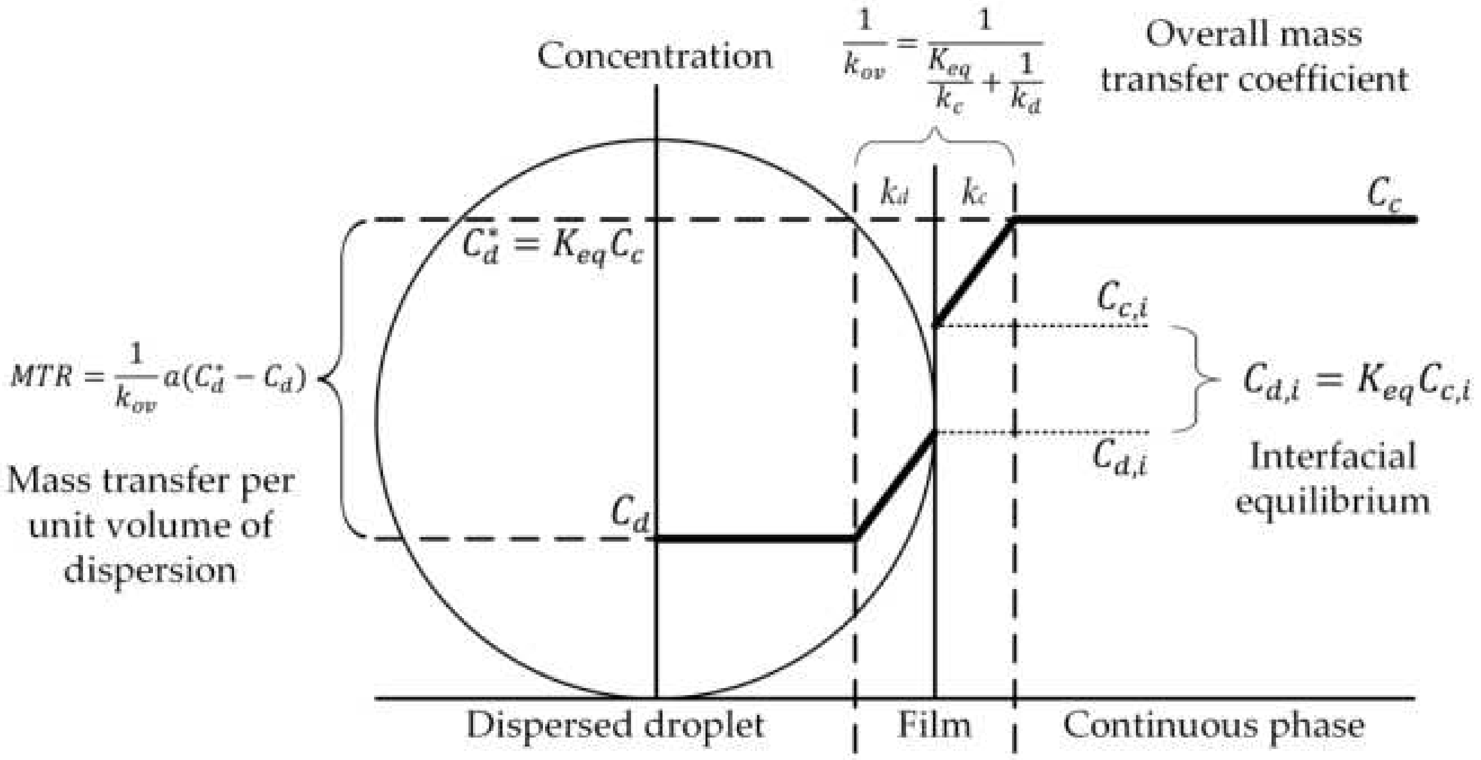




MASS TRANSFER MODELLING

- Modelled using two film theory:
  - Treybal aqueous phase mass transfer coefficient.
  - Laddah and Degaleesan solvent phase mass transfer coefficient.

$$MTR = \left(\frac{1}{\frac{K_{eq}}{k_c} + \frac{1}{k_d}}\right) a\left(K_{eq}C_c - C_d\right)$$

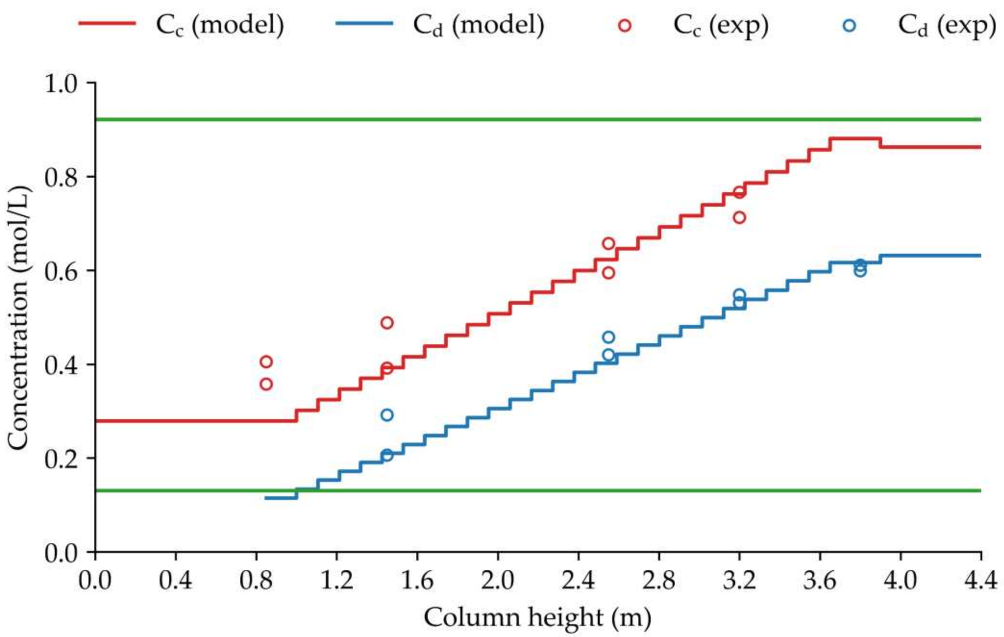


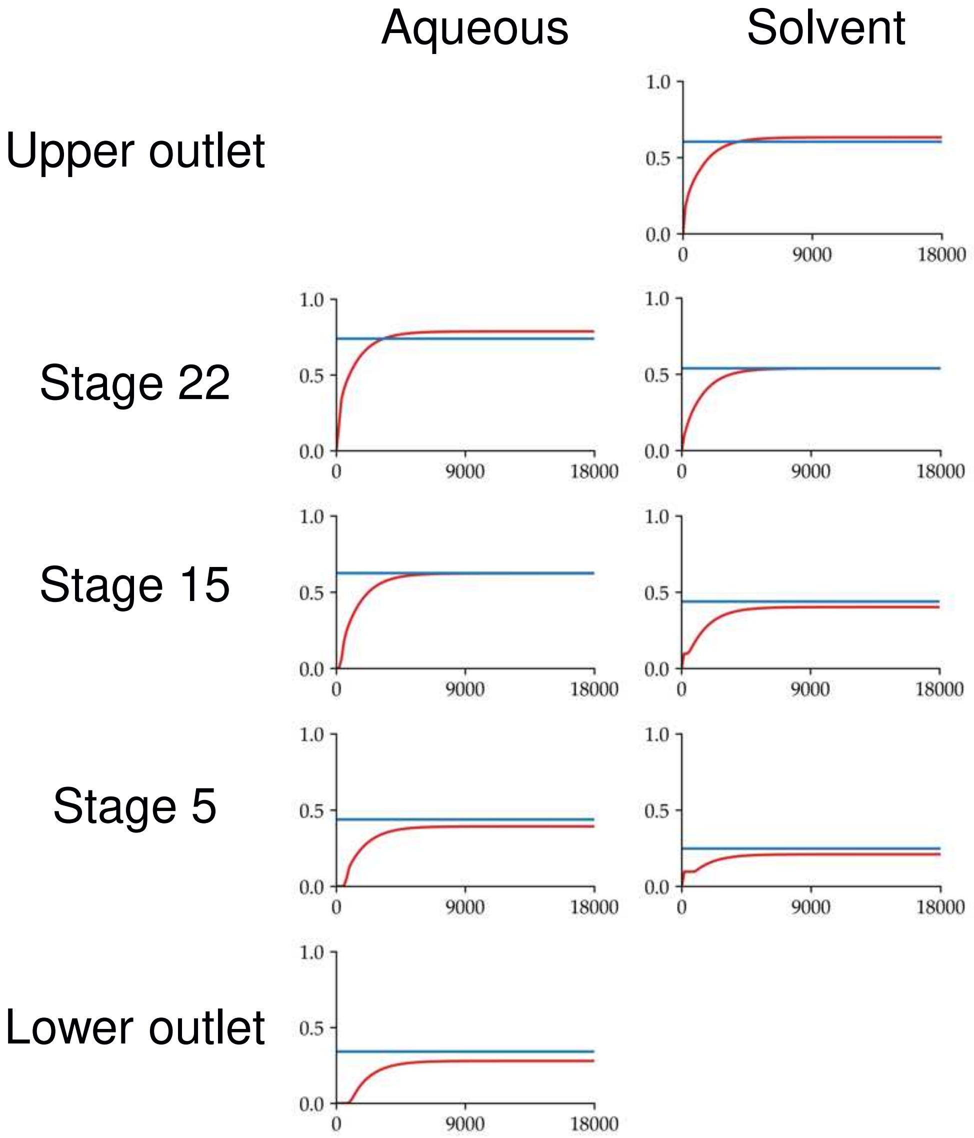
$$k_c = \frac{D_c}{d_{32}}\left(0.725 Re_{drop}^{0.57} Sc_c^{0.42}(1 - \alpha_d)\right)$$

$$k_d = 0.023\frac{U_r}{Sc_d^{0.5}}$$

MASS TRANSFER IN PSEC

- Q_{tot} = 88 L/hr, S:A = 1.2, af = 1 cm/s.
- NTU_{aq} = 1.74, HTU_{aq} = 1.61 m, Se_{av} = 24.0 %
- Error calculated to be 11.6 %.





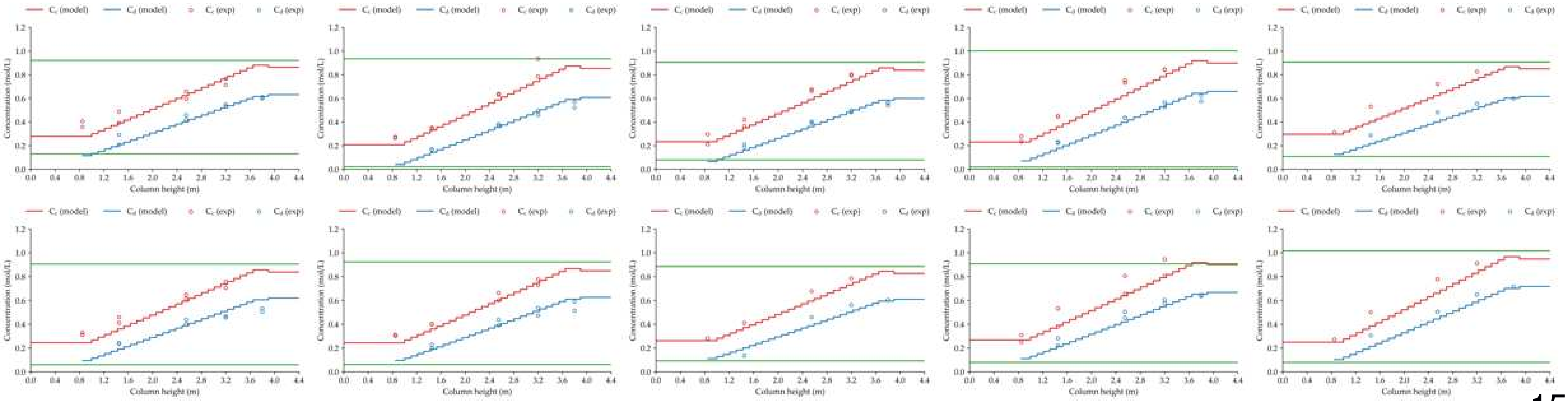
MASS TRANSFER IN PSEC

- Validation over 17 experiments, 10 conditions.
- Total error calculated to be 13.5%.
- NTU = 1.57 to 1.65, HTU = 1.69 to 1.80 m, PSEC stage efficiency = 22.9 to 29.3 %

88 L/hr | 135 L/hr | 159 L/hr | 182 L/hr | 205 L/hr

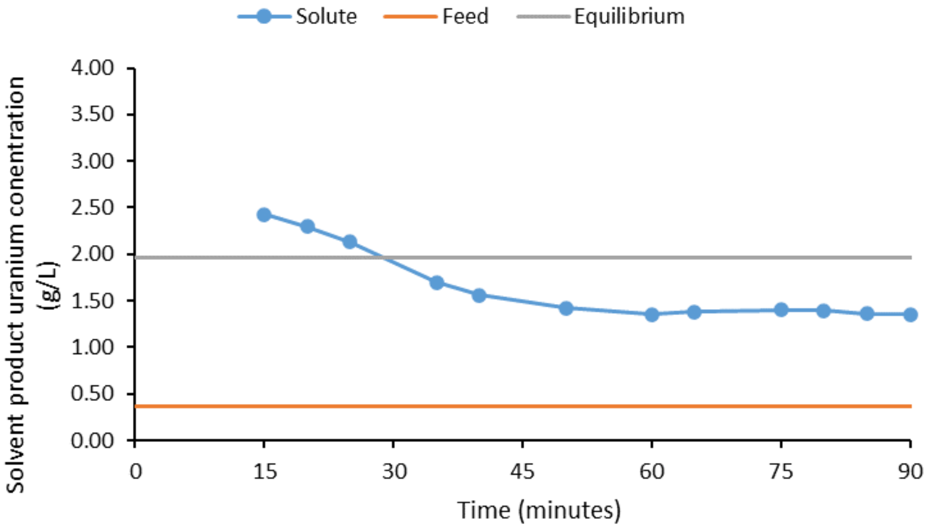
af = 2 cm/s

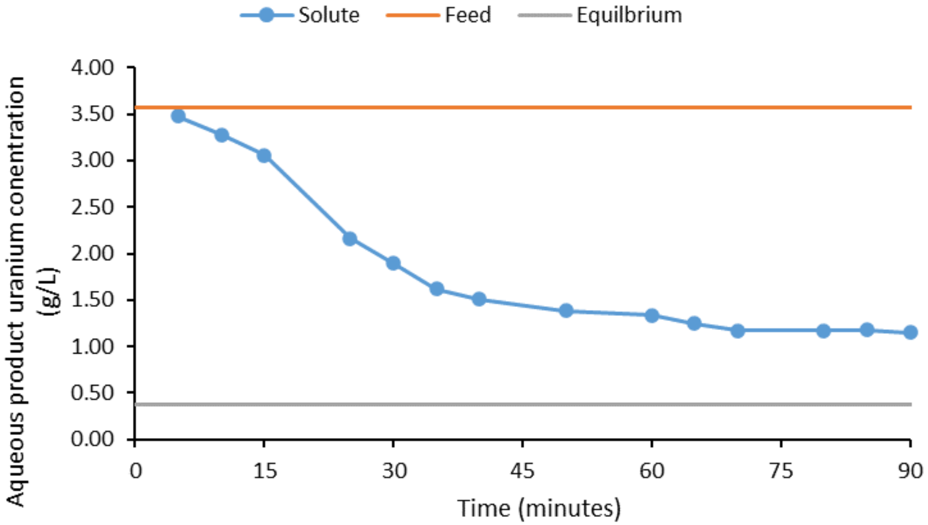
af = 1 cm/s

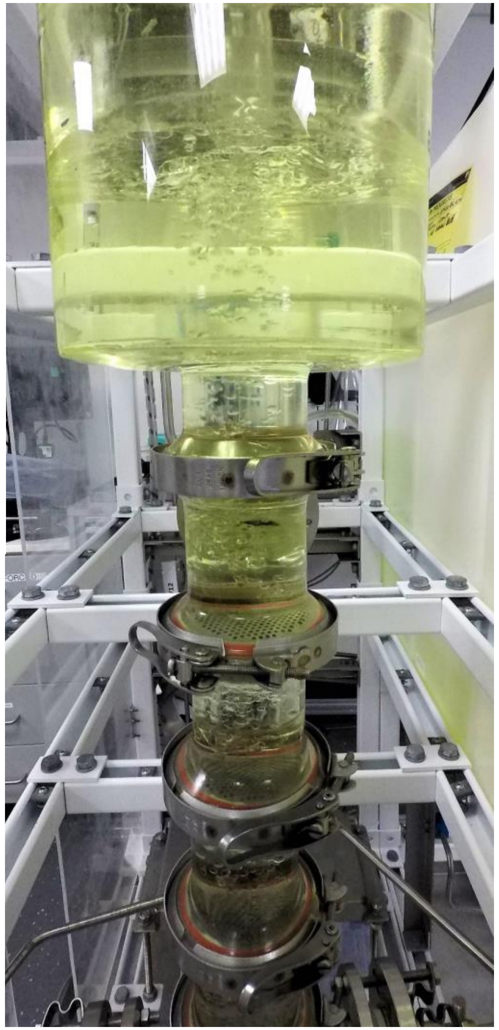


EXTRACTION OF U WITH TBP

- 6 experiments in total
- Shown:
  - Q_{tot} = 60 L/hr, S:A = 2:1, af = 0.30 cm/s.
  - NTU_{aq} = 0.70, HTU_{aq} = 0.44 m
- CM validation against data.







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AFCP
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