WHAT IS MECHANISTIC CHROMATOGRAPHY MODELING?

Mechanistic modeling is based on the laws of physics and biochemical principles to predict system behavior and is the most advanced way to speed up chromatography process development, scale-up, and troubleshooting.

PROVEN BENEFITS

- Reduce experimental work
- Accelerate process understanding beyond experimental boundaries
- Reduce risk in tech transfer
- Effective root cause analysis to resolve production problems

Process development & Scale-up to production Troubleshooting

& adaptation

CAN BE USED FOR

HOW IT WORKS

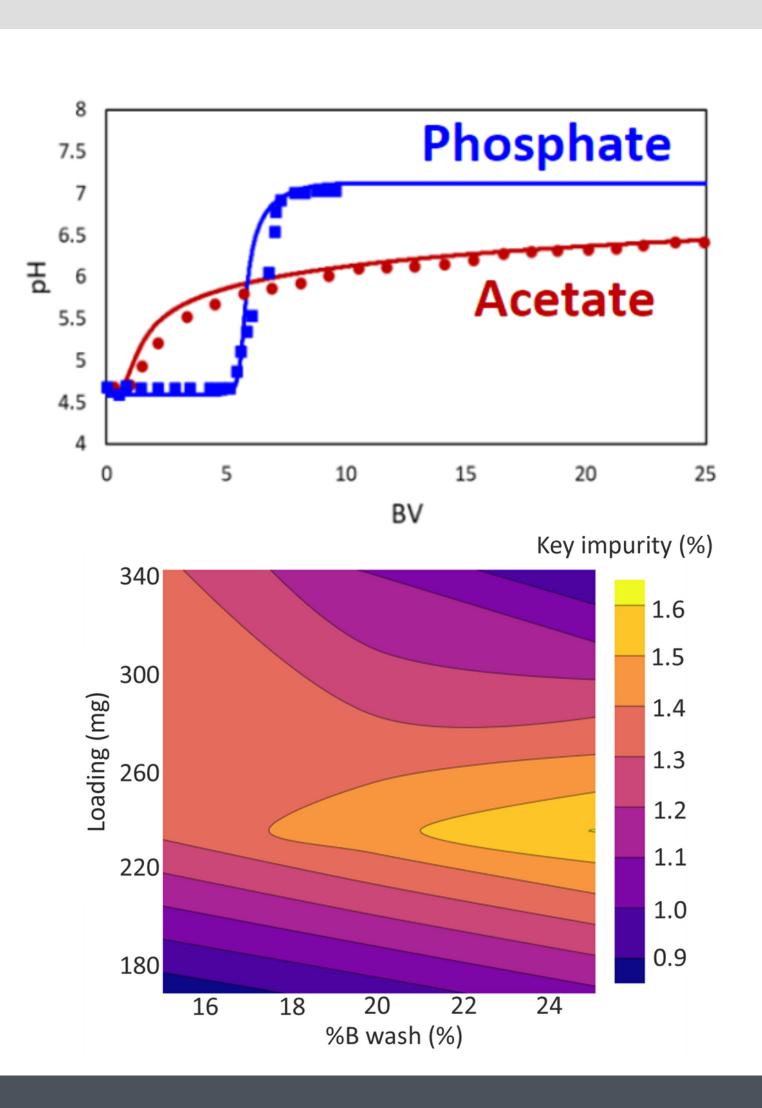
 Define list of (bio)chemical species 2. Calibrate the model with targeted experiments



- 3. Confirm the model with validation experiments
- 4. Start optimizing process performance

MECHANISTIC CHROMATOGRAPHY MODELING CAN PREDICT

- Behaviour of buffer type/salt species
- Complex ionization mechanisms
- Impact of loading, flowrate, pH, gradient slope, etc.
- pH waves within the column
- Outlet concentration profiles
- Single-column and multicolumn
- Key Performance Indicators





WHAT IS MECHANISTIC CHROMATOGRAPHY MODELING?

AND HOW DOES IT COMPARE TO STATISTICAL MODELS SUCH AS DoE?

Statistical	Mechanistic
Find patterns in existing data	Complex equations based on physical laws
Requires large experimental data set	Requires data from 5-10 experiments
Limited process understanding	Strong process understanding
Can only assess impact of parameters studied experimentally	Can predict impact of process changes beyond parameters studied experimentally
20 15 $y = 5.27x^2 - 10.73x + 6.48$ 10 10 1	100 90 80 $4C$ -MCC, $n_{col} = 4$ $4C$ -MCC, $n_{col} = 3$ $3C$ -MCC, $n_{col} = 2$ $2C$ -MCC, $n_{col} = 1$ 60 Single Column 50 0 200 400 600 800 800 800

Mechanistic models are powerful tools but getting them right is art as much as science. Ypso-lonic® was developed by chromatography experts to maximize the value of your data with a user-friendly approach that bridges the gap between defining required experimental work and achieving model predictability.

YPSO-IONIC® EXAMPLE APPLICATIONS

Comparison of single and multicolumn process for mAb capture

Impact of buffer selection on protein purification by IEX

Model for protein purification by hydrophobic interaction (HIC)

Troubleshooting of antibiotics IEX purification process

Identification of the Design Space for oligo IEX process

Quick design of a MCSGP for oligo purification

