ADVANCED PROCESS MODELING FORUM 2014

Batch optimization

Getting more value from your models

Pieter Schmal – Application Engineer

Batch processes

- Batch/semi-batch processes contribute substantially to several key sectors
  - Specialty and fine chemicals
  - Agrochemicals
  - Pharmaceutical APIs
  - Consumer products and food
  - …
- Advantages
  - A single multipurpose facility can manufacture many products
  - Higher operating flexibility than continuous manufacturing plants
  - Ability to respond to fluctuating markets and rapidly advancing technologies
  - New products may be introduced to existing facilities without significant capital investment

Challenges – Design

- Determine the physical configuration of the plant
- Minimise capital cost
- Scale up with confidence
    - reduce pilot plant experimentation
- Optimise recipe - e.g.
    - maximise production/yield
    - maximise quality
    - minimise raw material, energy consumption
    - manage impurities

Challenges – Operational

- Training of operators
- Troubleshooting
- Reacting to changes in raw material
- Increase asset utilisation
- Minimise batch to batch variability
- Lower maintenance and operating costs
- Consideration of environmental or safety issues

Modelling needs

- Intrinsically transient processes ➔ dynamic models
- Complex recipes ➔ modelling of operating procedures
- Large number of time-varying degrees of freedom + many constraints ➔ dynamic optimisation

➔ Benefits

- accelerate time-to-market
- reduce technological risk
- increase profitability
- gain better understanding of the process

So what is the difference with steady-state optimization?

- Dynamic optimization requires specification of the control profile
  - Control vector parameterization
    - Type of approximation
    - Number of control intervals

  -> tougher problem to solve, but not so much for a gPROMS user

- Batch operation frequently based on heuristic recipes.

- Two bridges to cross in an organization
  - Mathematical modelling
  - Optimization

Two bridges

- Mathematical modelling
  - ProcessBuilder gives you a wide range of unit operations that can be readily used
  - If needed custom models can be developed
  - Parameter estimation can be used to increase fidelity in the models
- gPROMS platform does rigorous optimization that can handle:
  - Any type of objective
  - Both discrete and continuous decision variables
  - Different type of constraints
    - Equality and inequality constraints
    - End-point, interior-point and path constraints
  - Both steady-state and dynamic problems

Once you have crossed the first bridge...

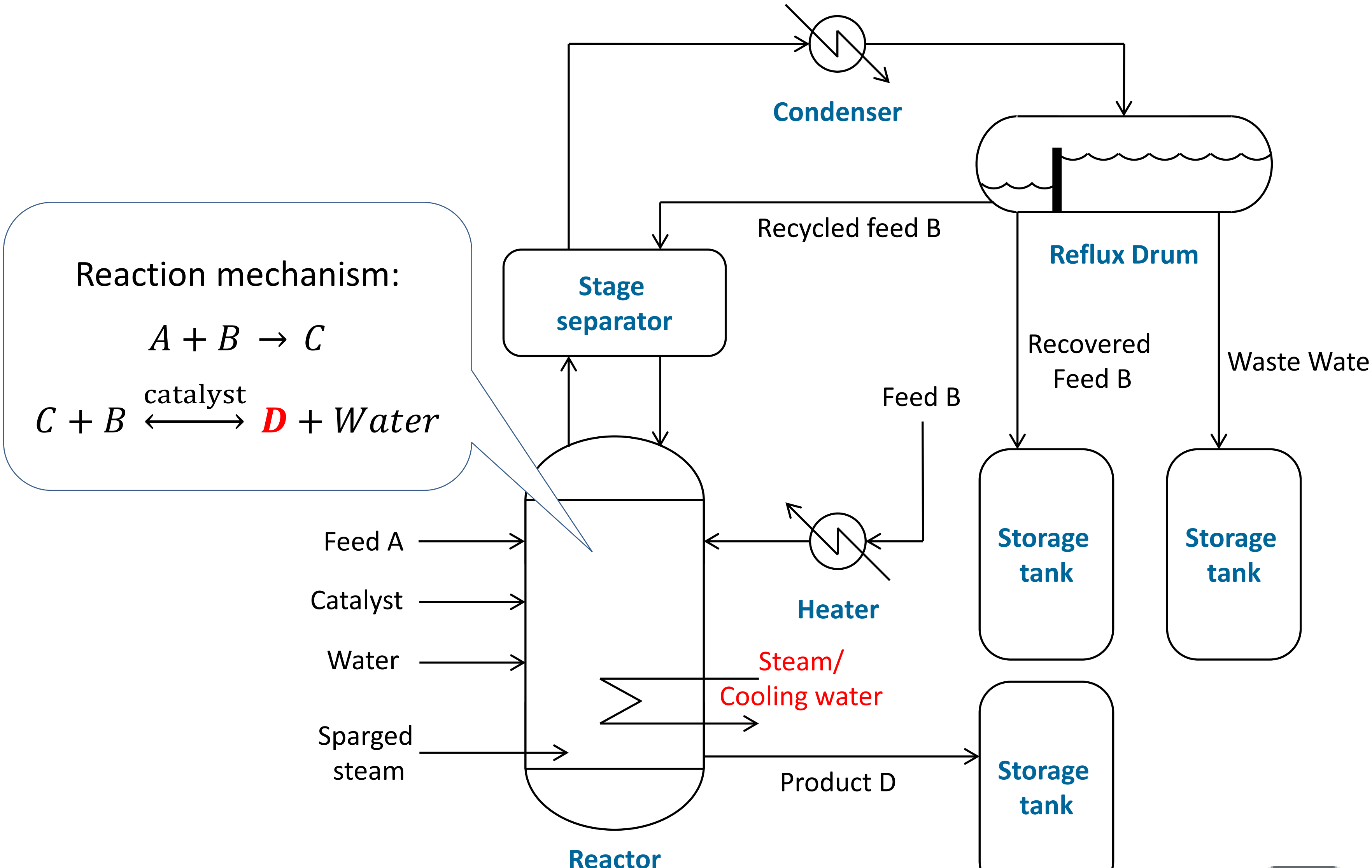
- You can use the model for
  - In a flowsheet to investigate the bigger picture
  - Operator training
  - Scenario testing
  - Soft-sensing
  - Better understanding the process
  - Other processes/products
  - A web-interface for non-modellers/flowsheeters
  - Optimization
    - Operational
    - Design
    - Safety
    - …

Models contain a lot of information and therefore value that can best be extracted by using rigorous optimization

Case Study #1: Chemicals

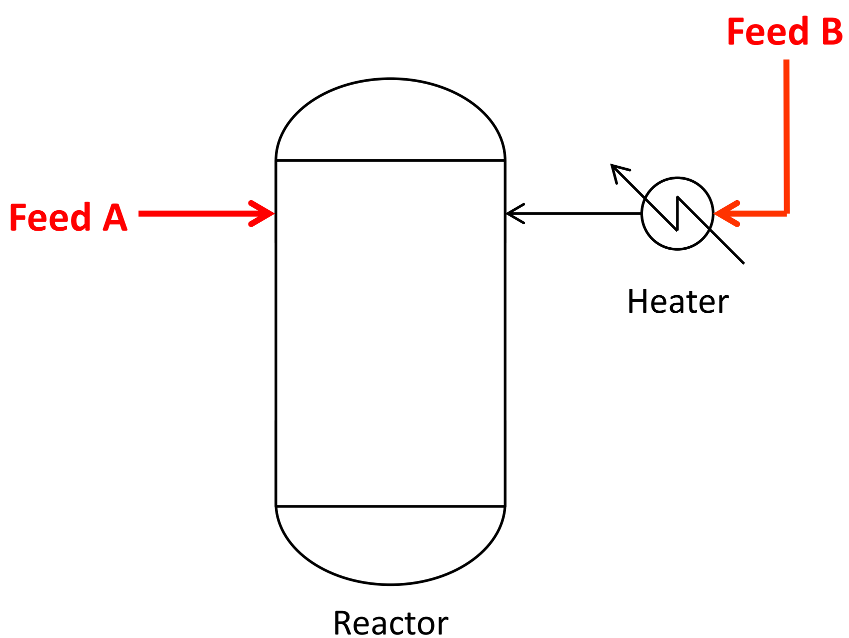
Batch esterification reaction

Overview


Reaction mechanism:
$A + B \rightarrow C$
$C + B \xleftrightarrow{\text{catalyst}} D + Water$
Condenser
Reflux Drum
Recycled feed B
Stage separator
Recovered Feed B
Waste Water
Feed B
Storage tank
Storage tank
Feed A
Catalyst
Water
Sparged steam
Heater
Steam/ Cooling water
Product D
Storage tank
Reactor

Recipe step #1 – Charging material

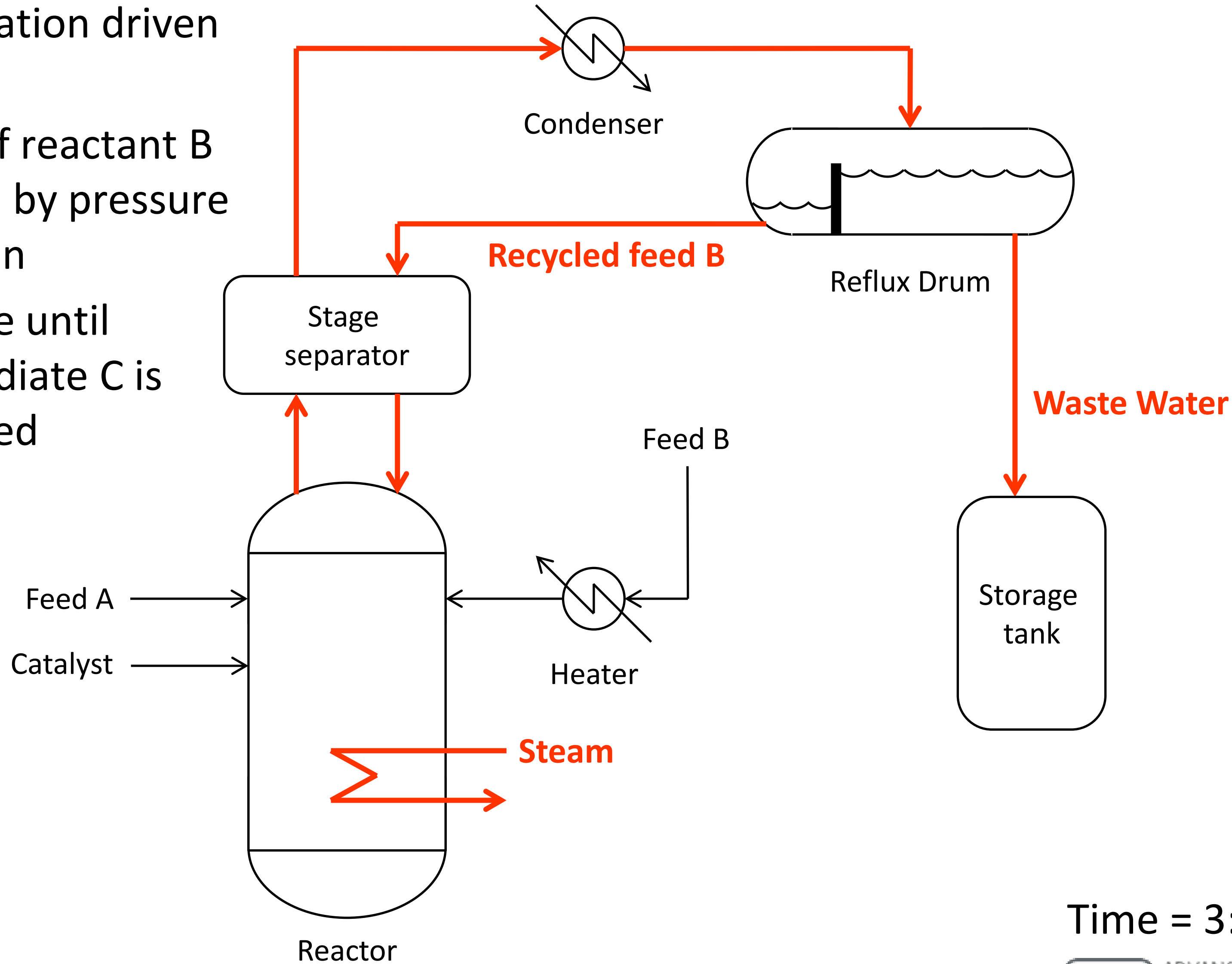
- Charge reactor with materials



Time =0:07 (h:m)

Recipe step #2 – Esterification

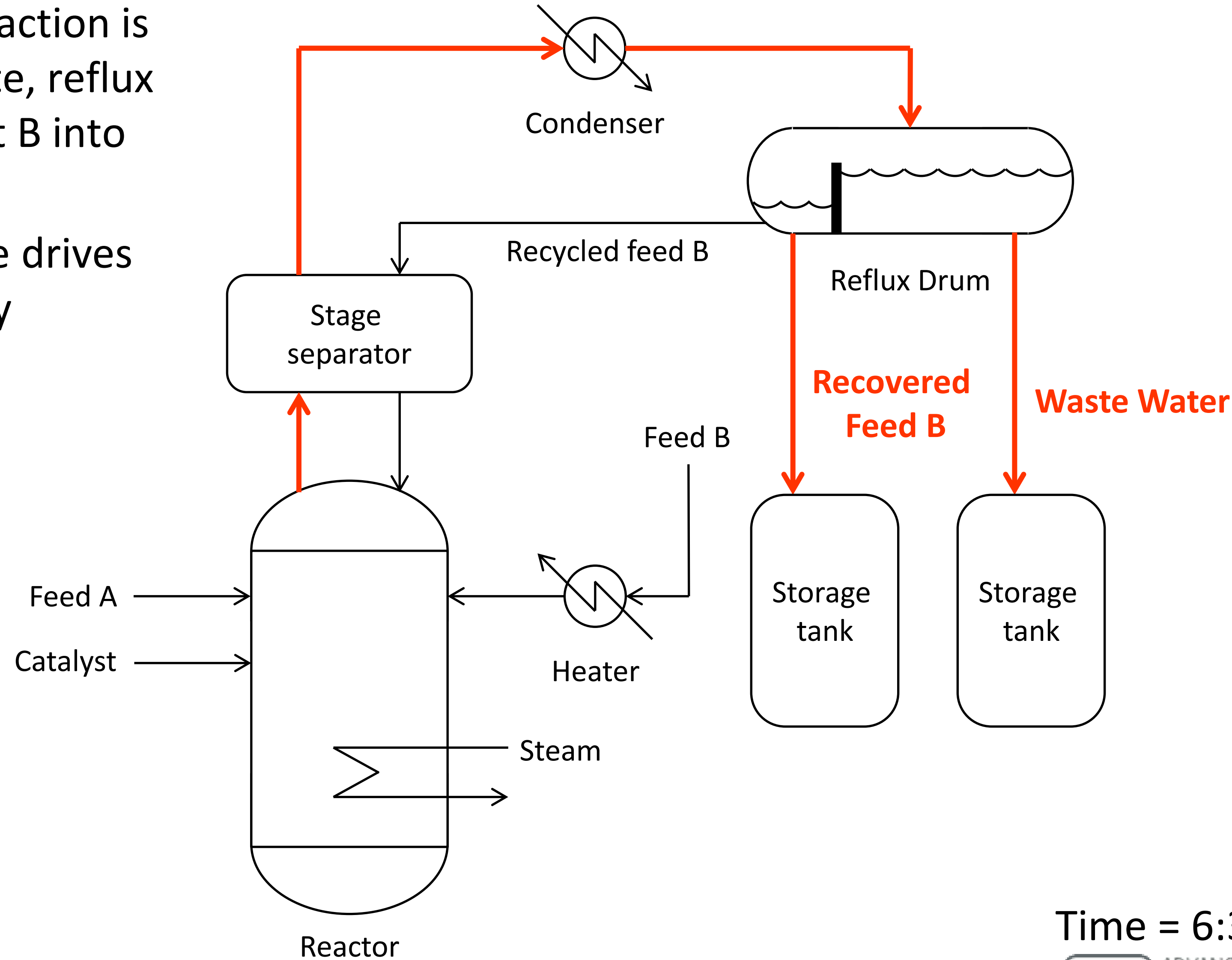
- Esterification driven by heat
- Reflux of reactant B is driven by pressure reduction
- Continue until intermediate C is consumed



Time = 3:20 (h:m)

Recipe step #3 – Stripping

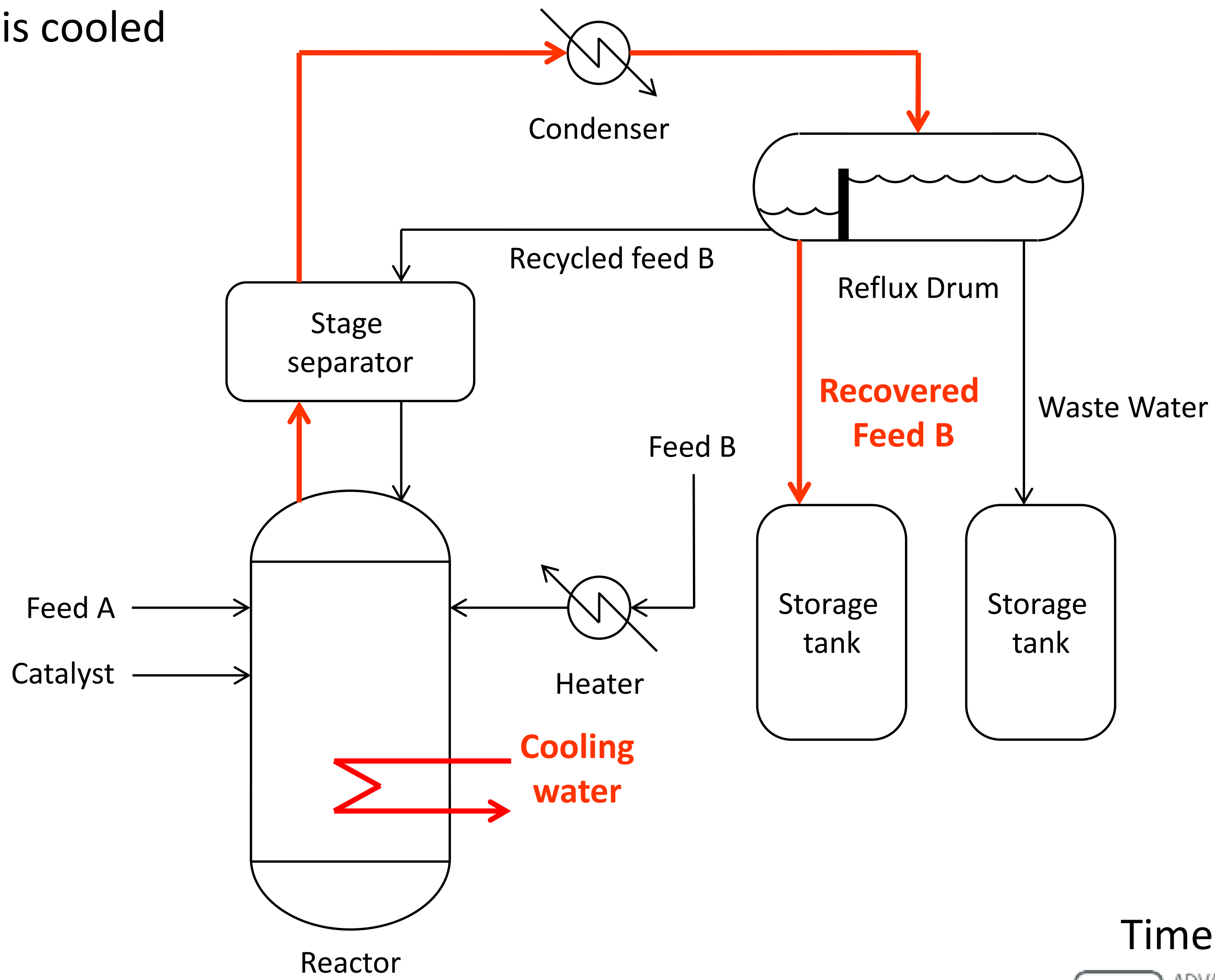
- Once reaction is complete, reflux reactant B into storage
- Pressure drives recovery



Time = 6:35 (h:m)

Recipe step #4 – Cooling of reactor

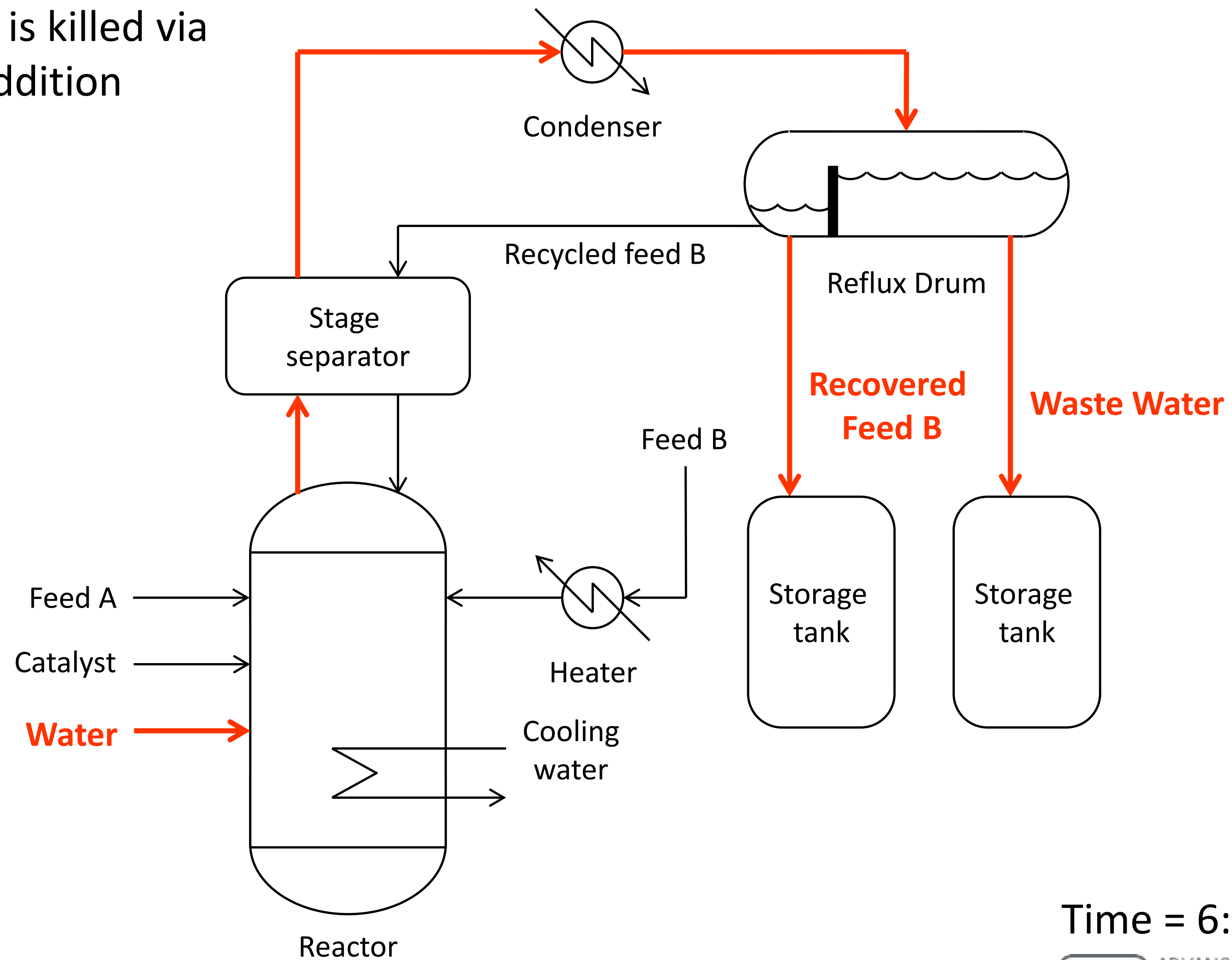
- Reactor is cooled



Time = 6:00 h

Recipe step #5 – Killing of catalyst

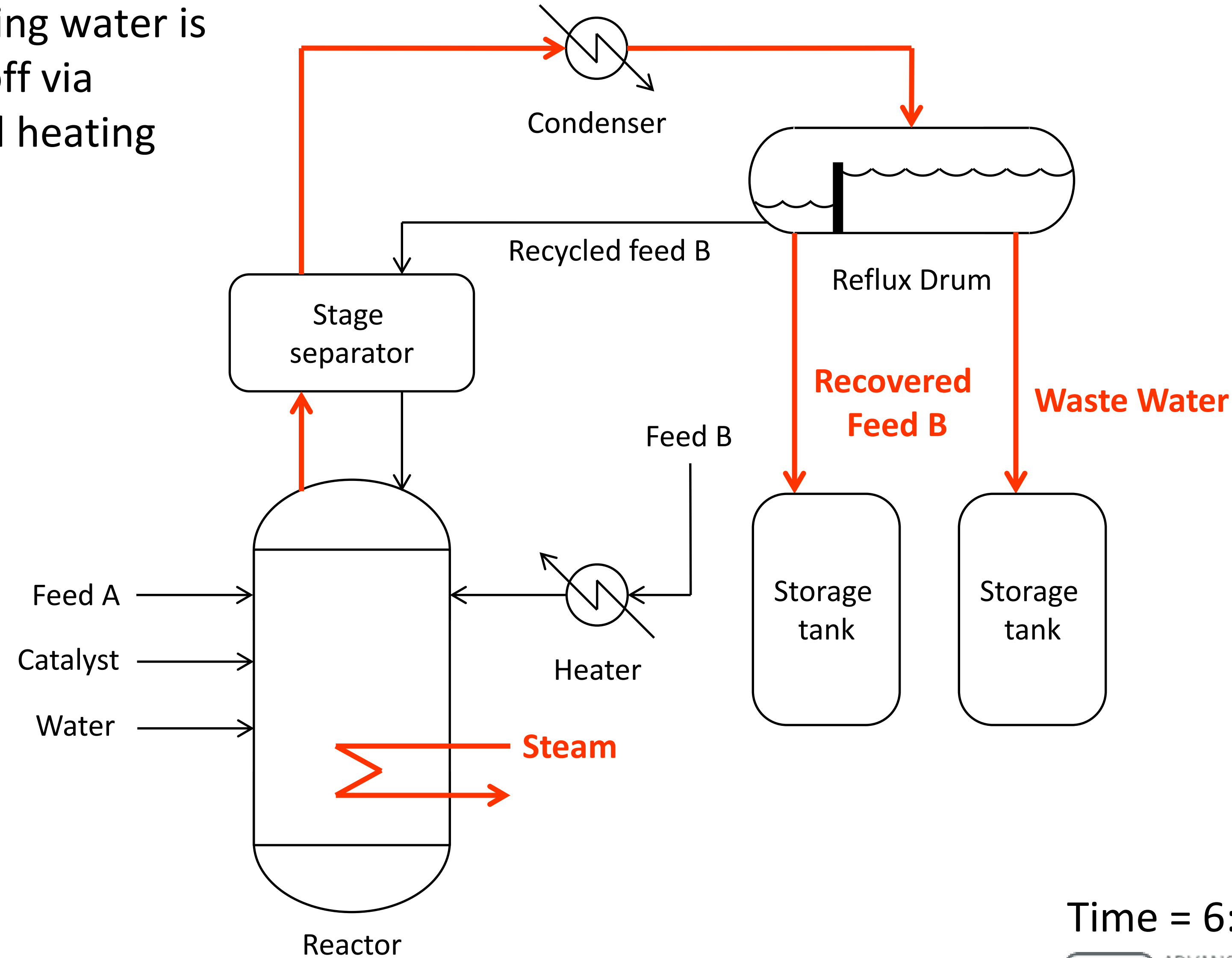
- Catalyst is killed via water addition



Time = 6:10 (h:m)

Recipe step #6 - Dehydration

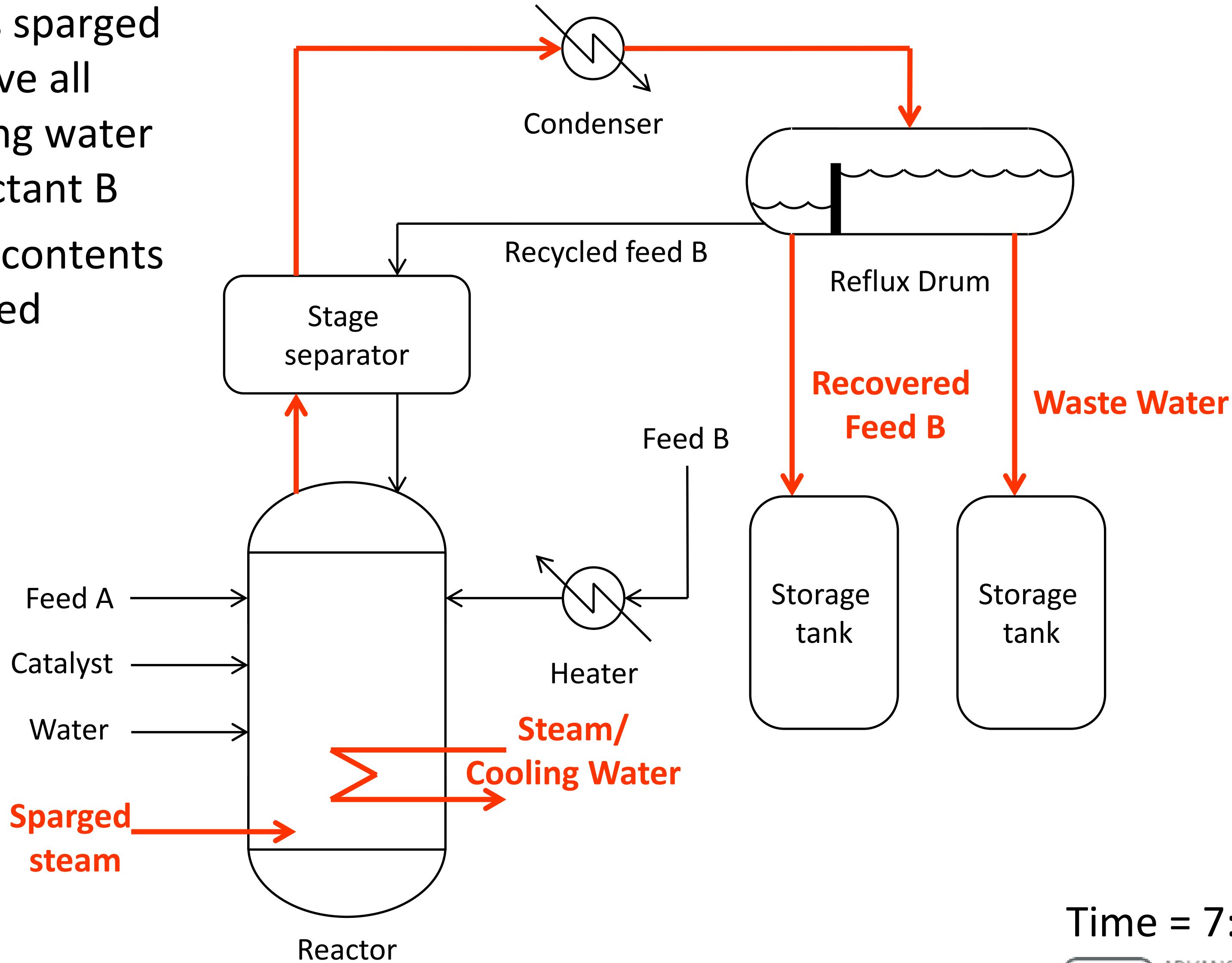
- Remaining water is boiled off via external heating



Time = 6:11 (h:m)

Recipe step #7 – Vacuum stripping

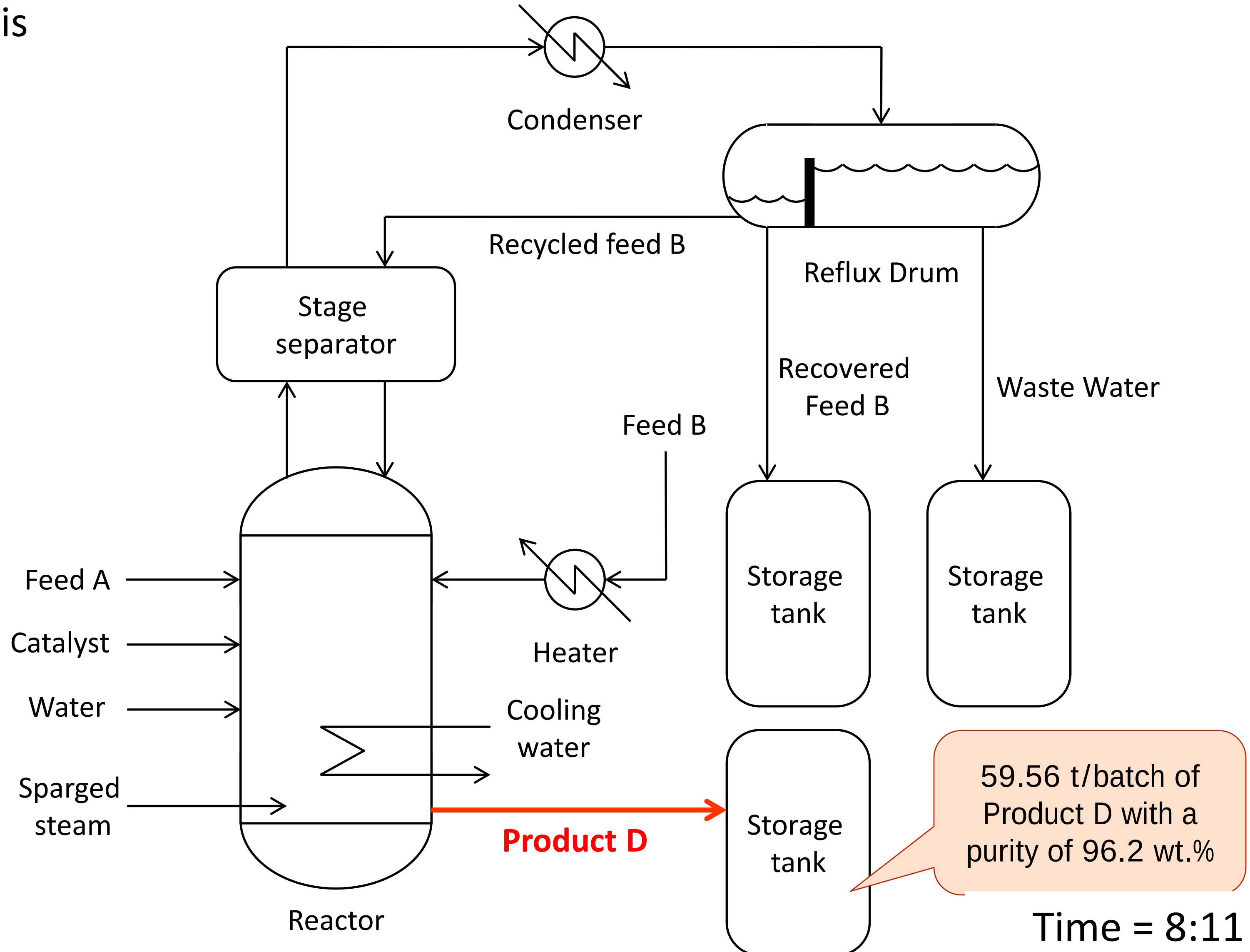
- Steam is sparged to remove all remaining water and reactant B
- Reactor contents are cooled



Time = 7:08 (h:m)

Recipe step #8 – Complete

- Reactor is emptied



Time = 8:11 (h:m)

Batch esterification reaction

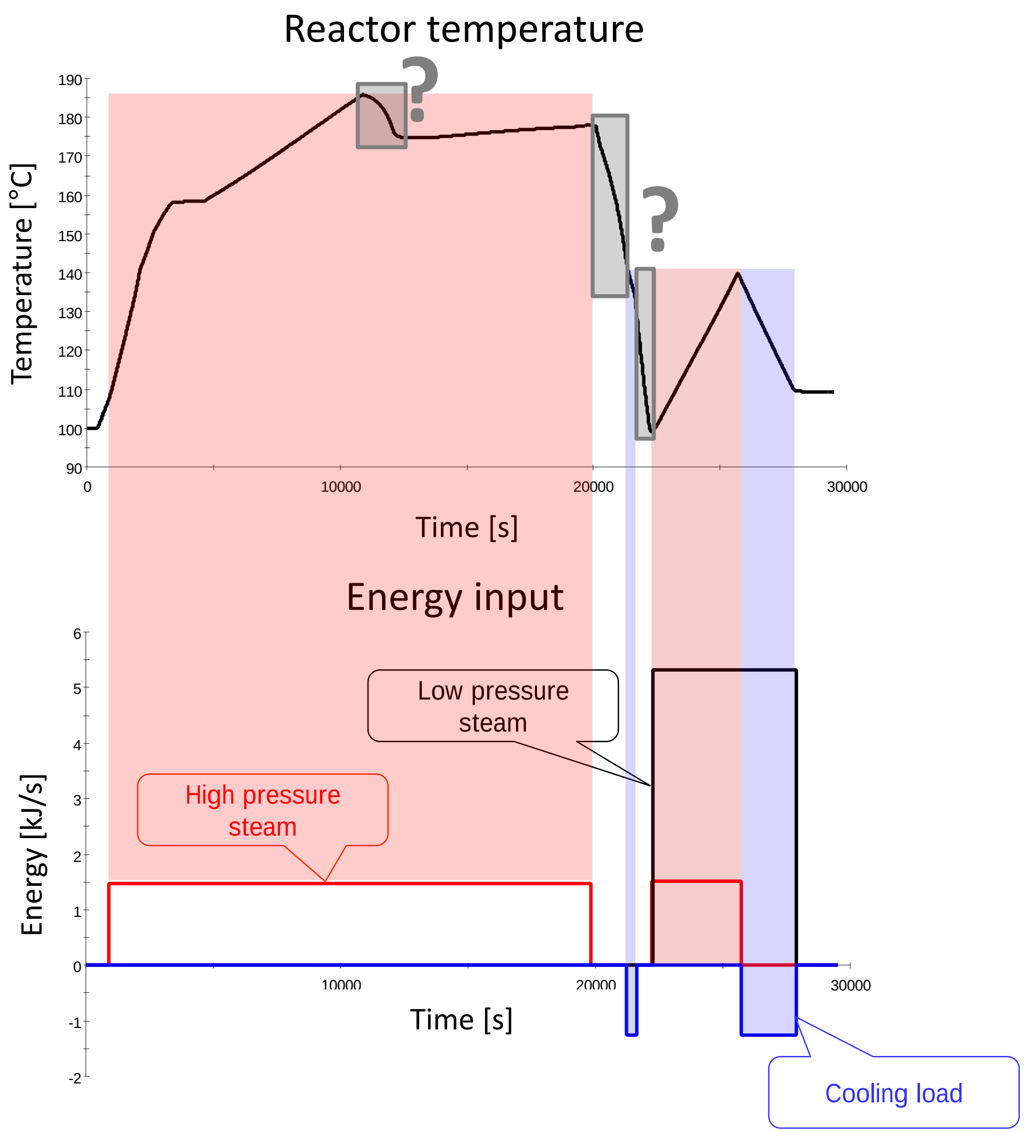
Recipe – Summary

Activity	Duration [s]	Cumulative Time [s]	Feed A [kmol/s]	Feed B [kmol/s]	Catalyst [kmol/s]	Water [kmol/s]	Low Steam [kg/s]	High Steam [kg/s]	Cooling Water [kg/s]	Pressure [bar]
Charging	420	420		0.84						0.89
	480	900	0.092							0.89
Esterification	1,020	1,920	0.092					0.11		0.89
	60	1,980	0.092		4.5×10^{-3}			0.11		0.89
	120	2,100	0.092					0.11		0.89
	540	2,640						0.11		0.89
	2,040	4,680		0.046				0.11		0.89
	6,180	10,860						0.11		0.89
	1,233	12,093						0.11		0.40
	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Stripping	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	1,104	21,204								0.03
Cooling reactor	403	21,607							0.079	0.03
Killing catalyst	600	22,207				0.14				0.03
	61	22,268						0.12		0.03
Dehydration	3,442	25,710					0.4	0.12		0.03
Vacuum stripping	2,192	27,902					0.4		0.079	0.03
Empty reactor	1,589	29,499								1

What can we do with this information in a modelling environment?

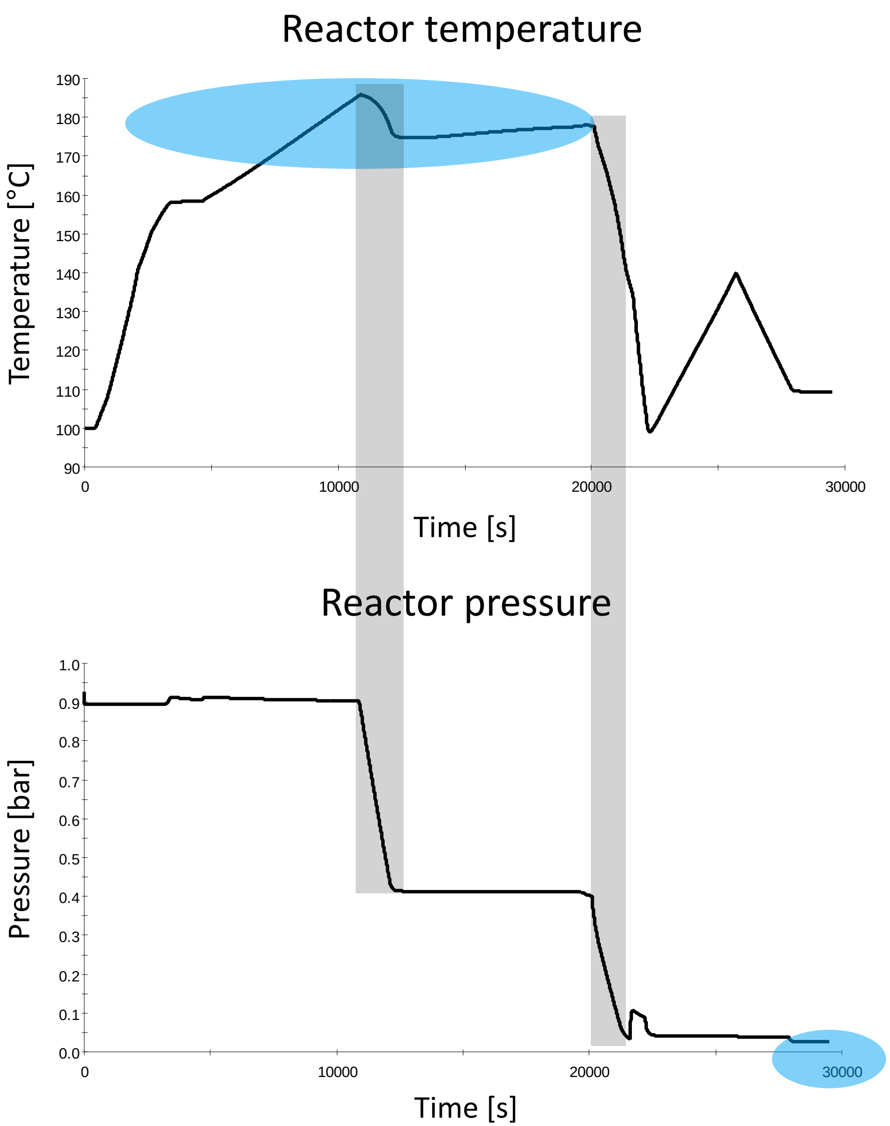
	Duration [h:m]	Feed A [kmol]	Feed B [kmol]	Catalyst [kmol]	Water [kmol]	Low Steam [kg]	High Steam [kg]	Cooling Water [kg]
Total	8:11	154.56	446.64	0.27	84	2,253.6	2,499.4	205

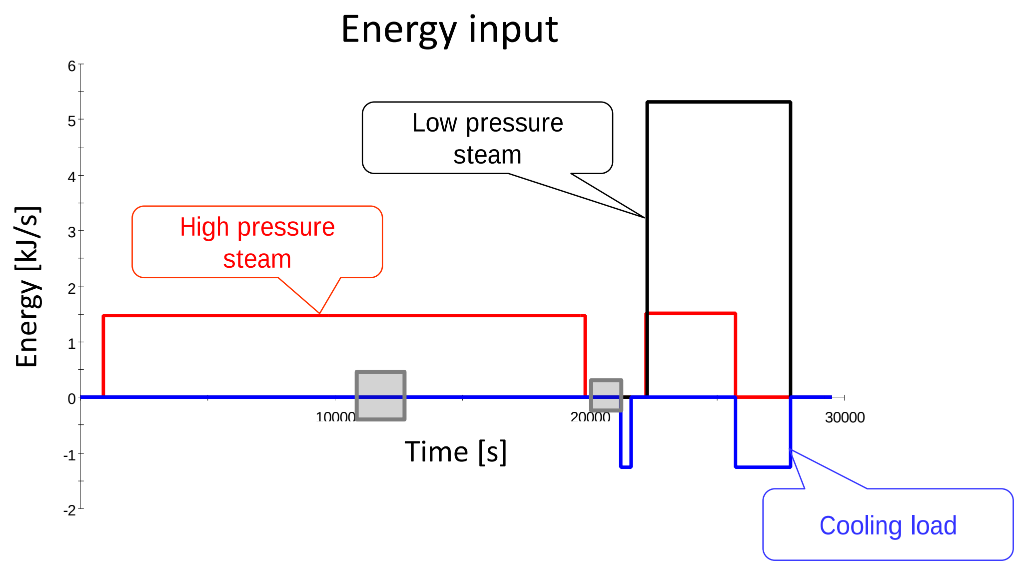
Key insights from simulation



Batch esterification reaction

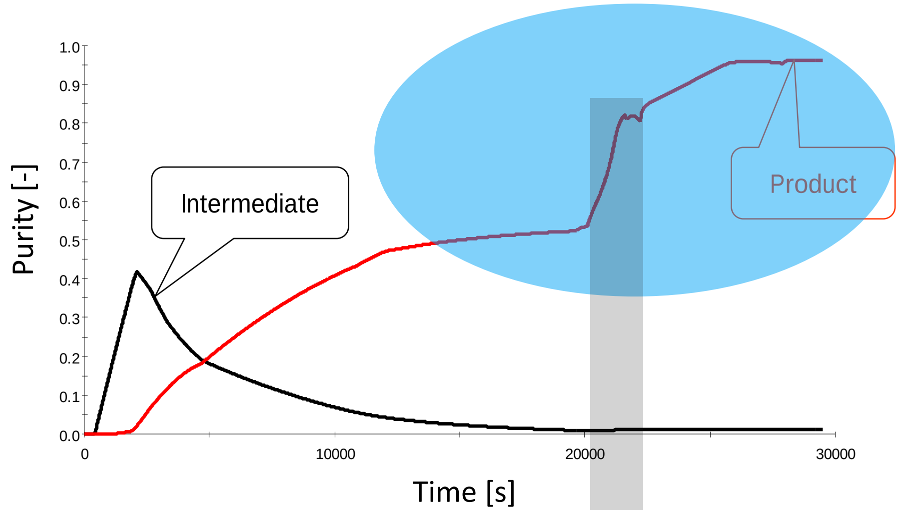
Key insights from simulation



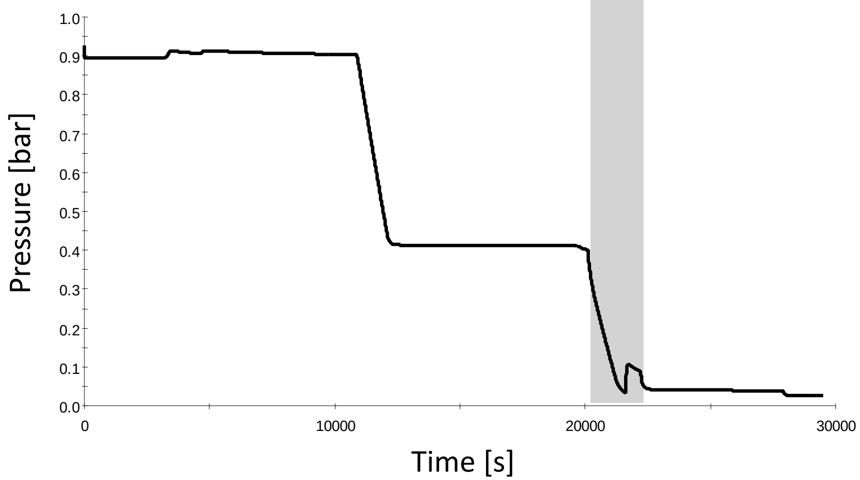


Key insights from simulation

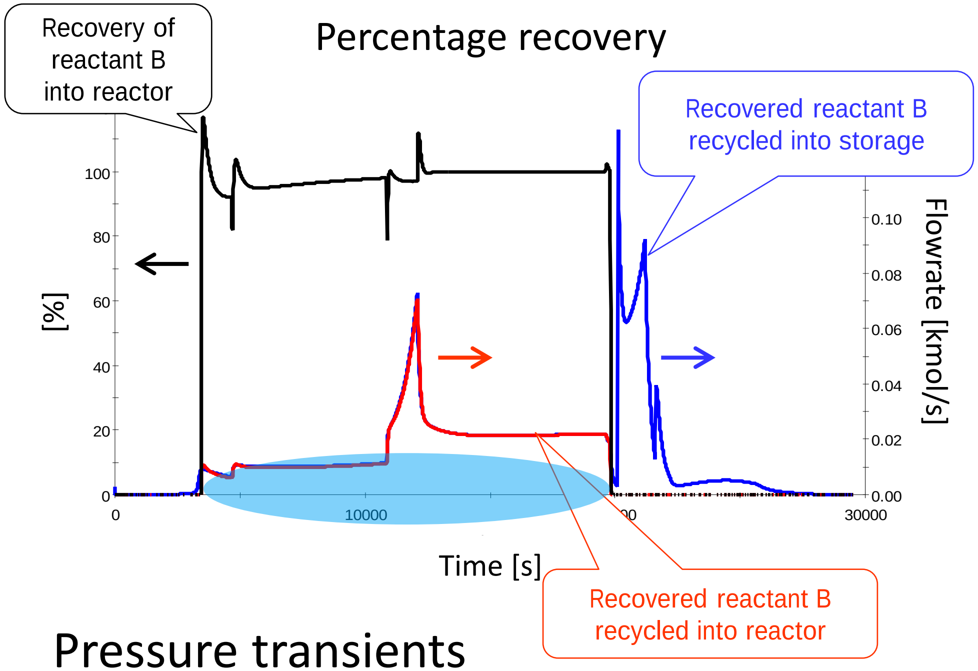
Purity profiles



Reactor pressure



Percentage recovery



Pressure transients fundamental in stripping reactant B and water

Case Study #1: Chemicals

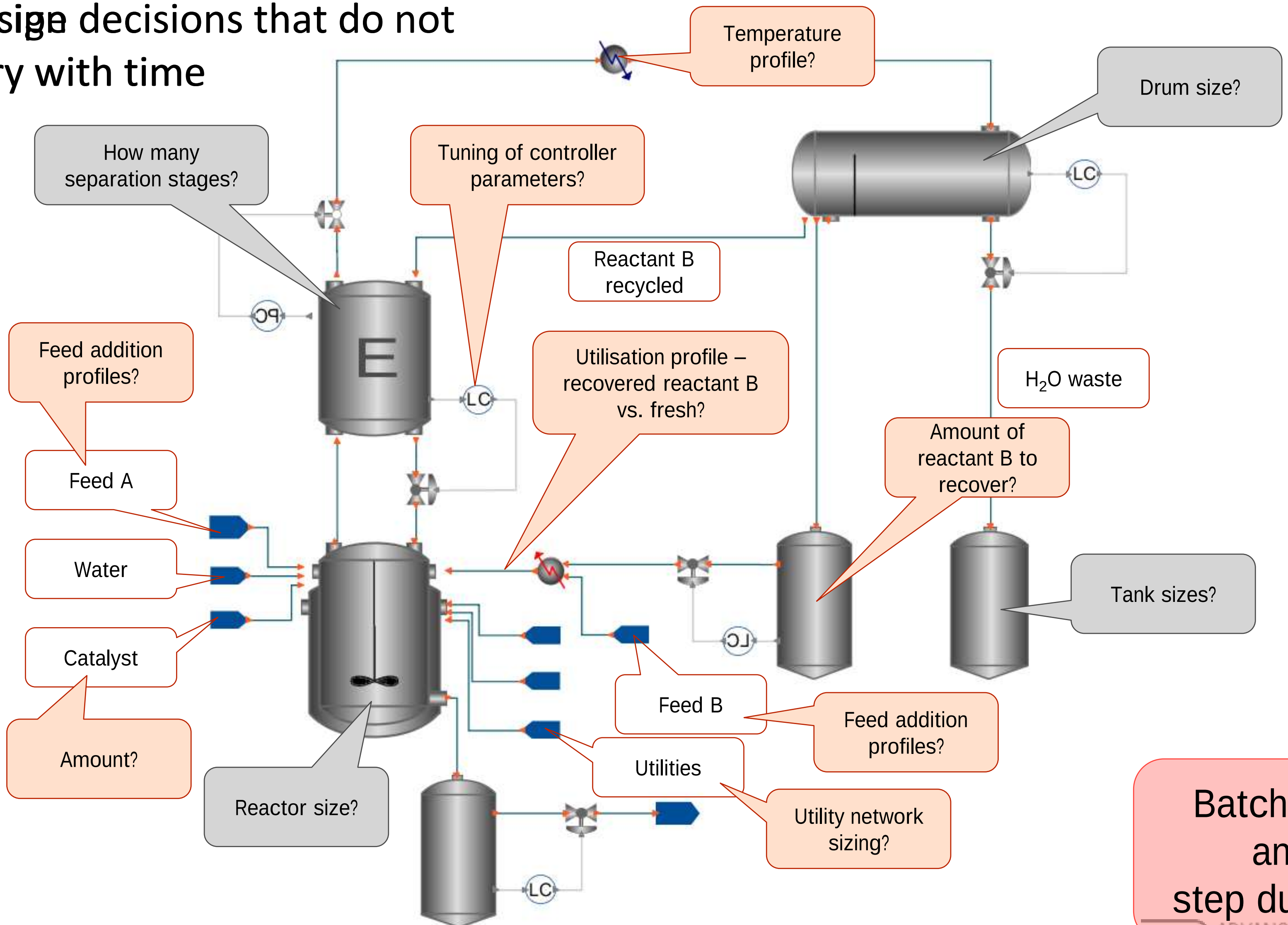
Batch esterification reaction

Optimising the recipe

- **minimise batch time,** maximise throughput
- minimise cost of raw materials & utilities
- maximise profitability
- …

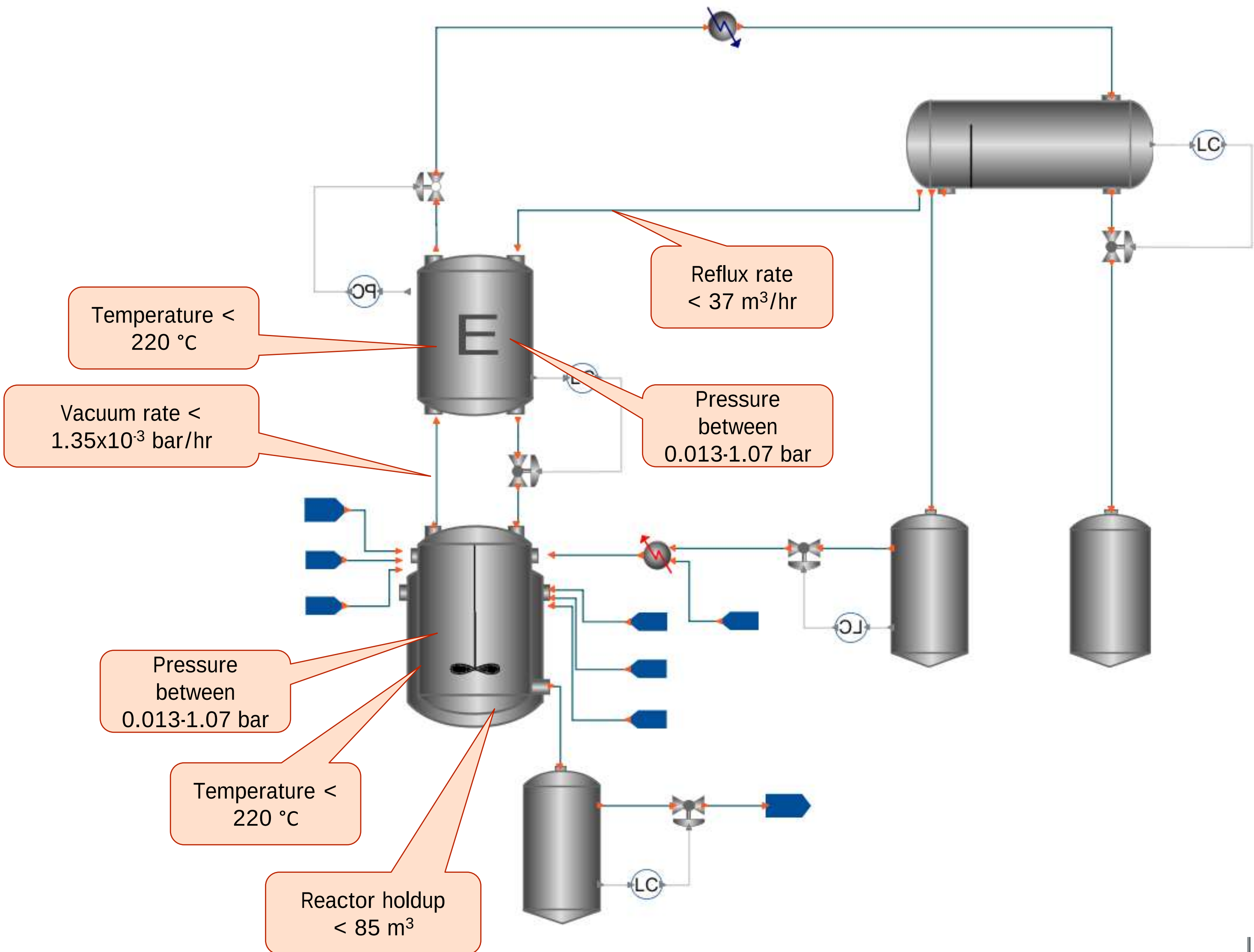
Decision variables

- Design decisions that do not vary with time

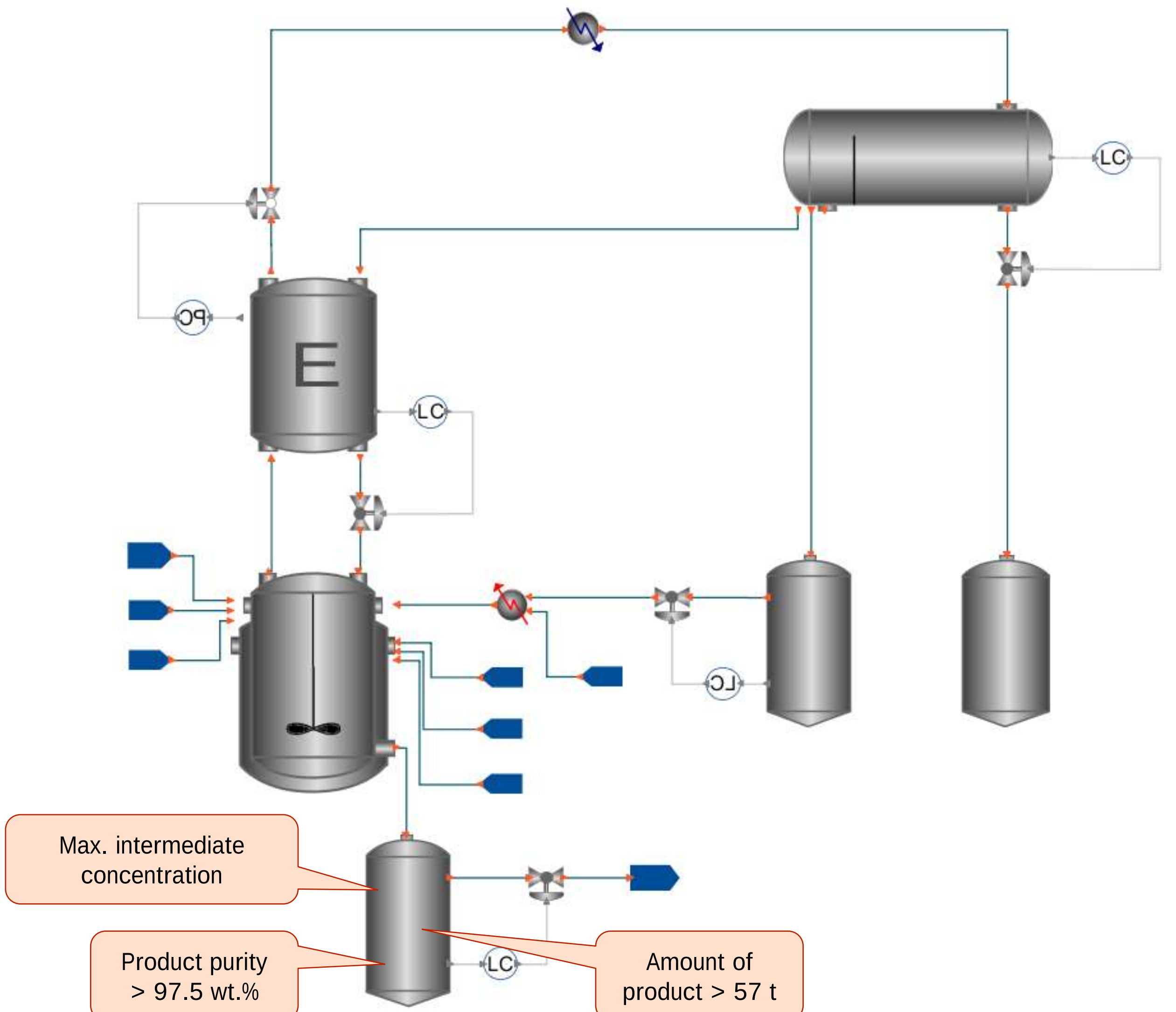


Batch time and step duration

Constraints – throughout the batch

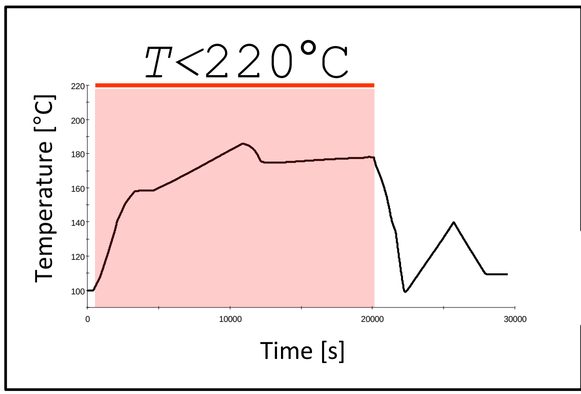


Constraints – at the end of the batch

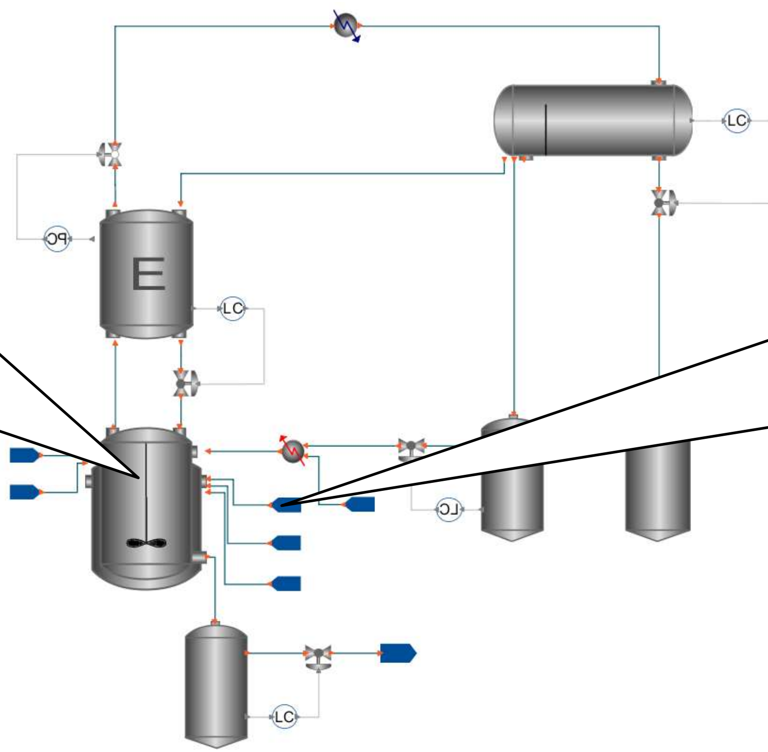


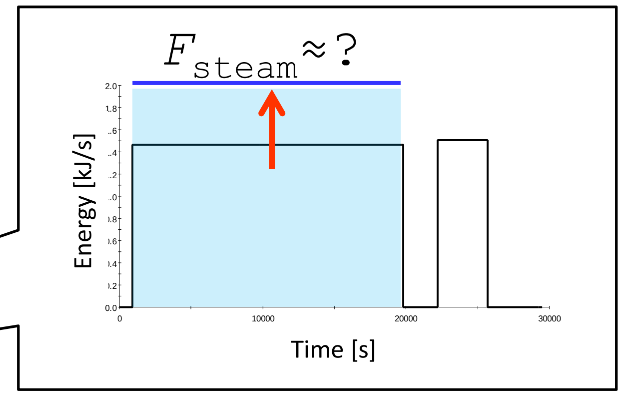
Process improvement via trial-and-error simulations

- Idea: increase temperature within the esterification stage up to the maximum limit to complete batch faster
  - achieve via incremental increases in the flowrate of high-pressure steam



Reactor temperature





High-pressure steam feed rate

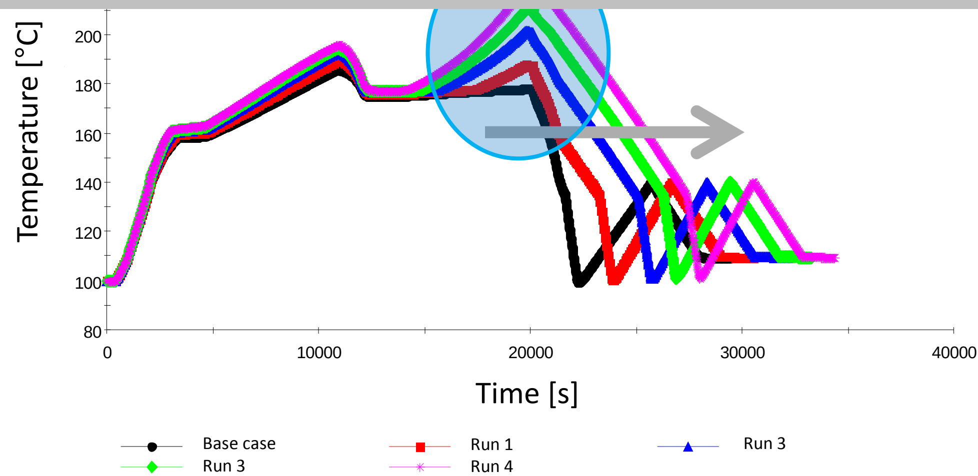
Process improvement via trial-and-error simulations

- Iteratively, we can somewhat improve from the base case

Simulation	Ave. Reactor temperature [°C]	Max Reactor temperature [°C]	High pressure steam flowrate [kg/s]	High pressure steam quantity [kg]	Product purity [wt.%]	Batch time [s]
Base case	167.22	185.76	0.11	2,126	96.2	29,499
Run 1	169.38	189.44	0.121	2,339	96.8	30,524
Run 2	172.39	201.44	0.132	2,552	97.2	32,195
Run 3	174.29	210.35	0.1375	2,658	97.3	33,286
Run 4	176.45	220.22 ✓	0.143	2,764	97.4 ✓	34,355 ✗

- However, is detrimental to duration of stripping stage

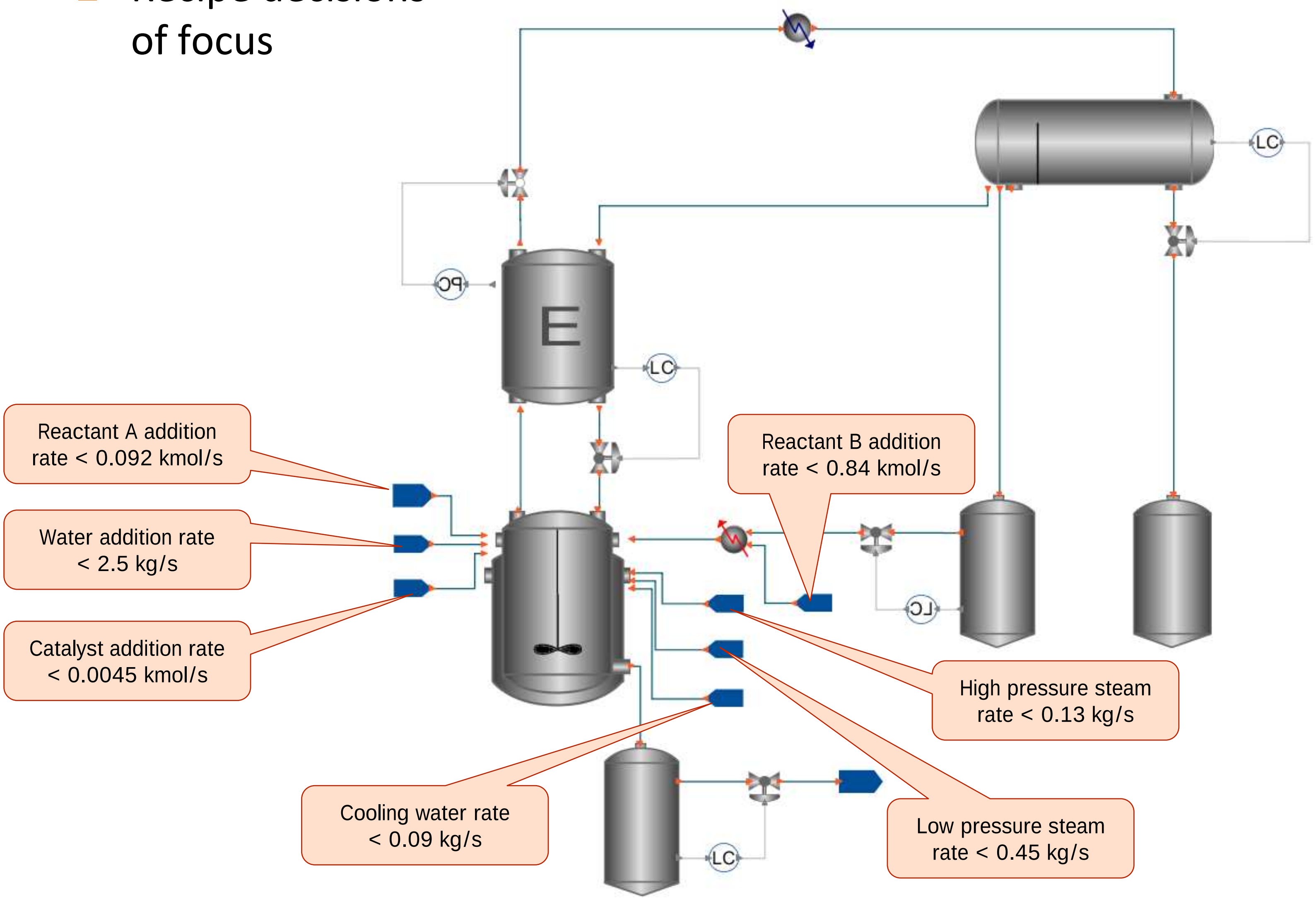
NEED RIGOROUS MATHEMATICAL OPTIMISATION



➔ ***need to consider multiple degrees of freedom simultaneously***

Dynamic optimisation of batch recipe

- Recipe decisions of focus

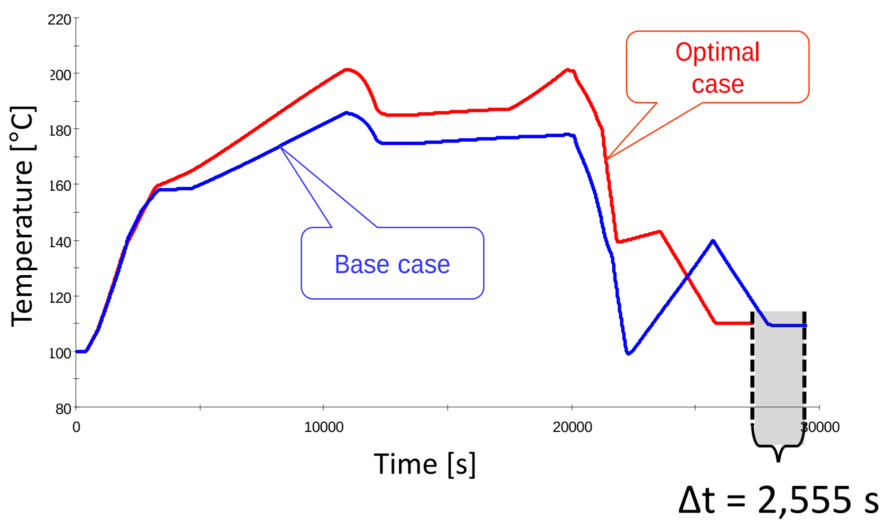


Key insights

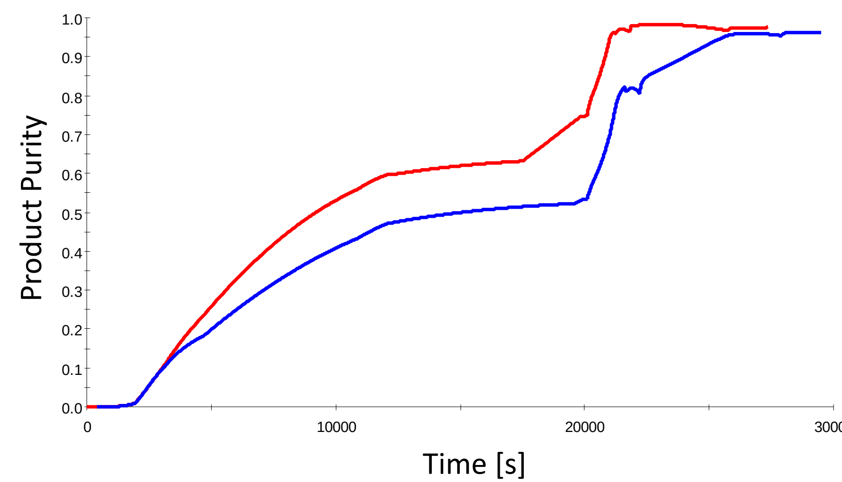
- Comparing to the approach of trial and error simulations

Simulation	Ave. Reactor temperature [°C]	Max Reactor temperature [°C]	High pressure steam flowrate [kg/s]	High pressure steam quantity [kg]	Product purity [wt.%]	Batch time [s]
Base case	167.22	185.76	0.11	2,126	96.2	29,499
Trial & error simulations	176.45	220.22 ✓	0.143	2,764	97.4 ✓	34,355 ✗
Optimisation approach	176.96	201.36 ✓	0.125	2,321	97.6 ✓	27,346 ✓

Reactor temperature



Product purity



Could we do even better?

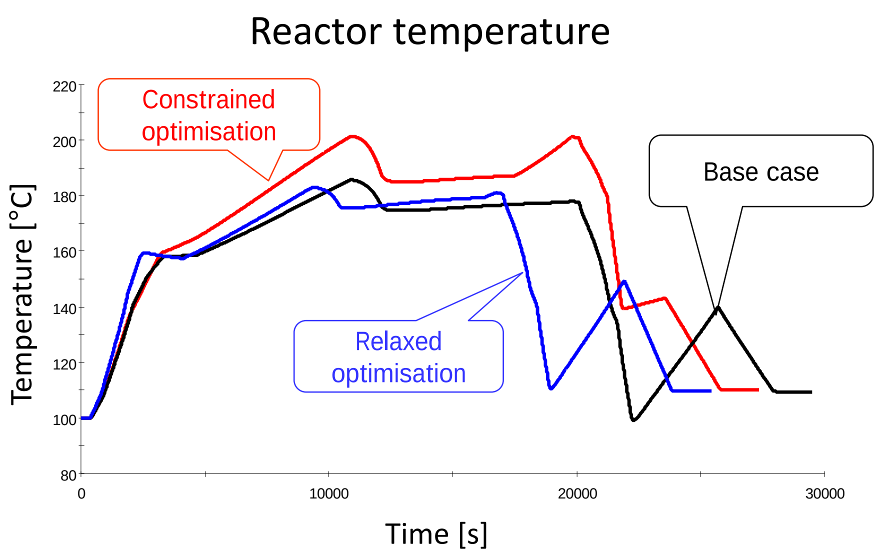
- gPROMS supplies information on the solution that can help improve the process with respect to the constraints that are on their bounds

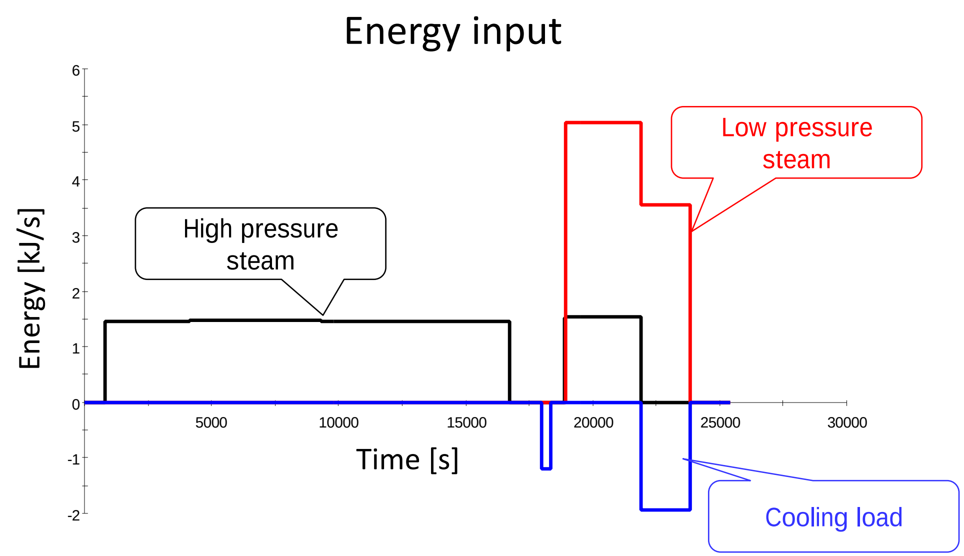
Feed_Catalyst → F			Type: piecewise constant			
Control Interval	Final Value	Initial Guess	Lower Bound Value	Lower Bound Lagrange Multiplier	Upper Bound Value	Upper Bound Lagrange Multiplier
Interval # 1	0.0000	0.0000	0.0000 *	-1.0000×10^{30}	0.0000 *	1.0000×10^{30}
Interval # 2	0.0000	0.0000	0.0000 *	-1.0000×10^{30}	0.0000 *	1.0000×10^{30}
Interval # 3	0.0000	0.0000	0.0000 *	-1.0000×10^{30}	0.0000 *	1.0000×10^{30}
Interval # 4	5.0000×10^{-3}	4.5000×10^{-3}	1.0000×10^{-3}	0.0000	5.0000×10^{-3} *	1.8207×10^{2}

Could we do even better?

- Further increase in the margin of feed material/utilities benefits greatly

Simulation	Ave. Reactor temperature [°C]	Max Reactor temperature [°C]	High pressure steam flowrate [kg/s]	High pressure steam quantity [kg]	Product purity [wt.%]	Batch time [s]
Base case	167.22	185.76	0.11	2,126	96.2	29,499
Constrained Optimisation approach	176.96	201.36	0.125	2,321	97.6	27,346
Relaxed Optimisation approach	168.72	183.03	0.112	1,792	97.1	25,421





- …however, recipe requires validation through experimental analysis

Case Study #2: Pharmaceuticals

Batch crystallization process

gPROMS product family

General mathematical modelling

Model Builder

Advanced process modelling environment

Sector-focused modelling tools

Chemicals & Petrochemicals

Process Builder

Process flowsheeting

AML: GLC
AML: FBCR
AML: FT
AML: BCR
AML: TBR

Advanced model libraries for reaction & separation

Life Sciences, Consumer, Food, Spec & Agrochem

gSOLIDS

Solids process optimisation

gCRYSTAL

Crystallization process optimisation

gCOAS

Oral absorption

Power & CCS

gCCS

CCS system modelling

Fuel Cells & Batteries

gFUELCELL

Fuel cell stack & system design

Oil & Gas

gFLARE

Flare networks & depressurisation

Wastewater Treatment

gWATER

Wastewater systems optimisation

gPROMS

The gPROMS platform

Equation-oriented modelling & solution engine

Materials modelling

gSAFT

INFOCHEM Multiflash

OLI

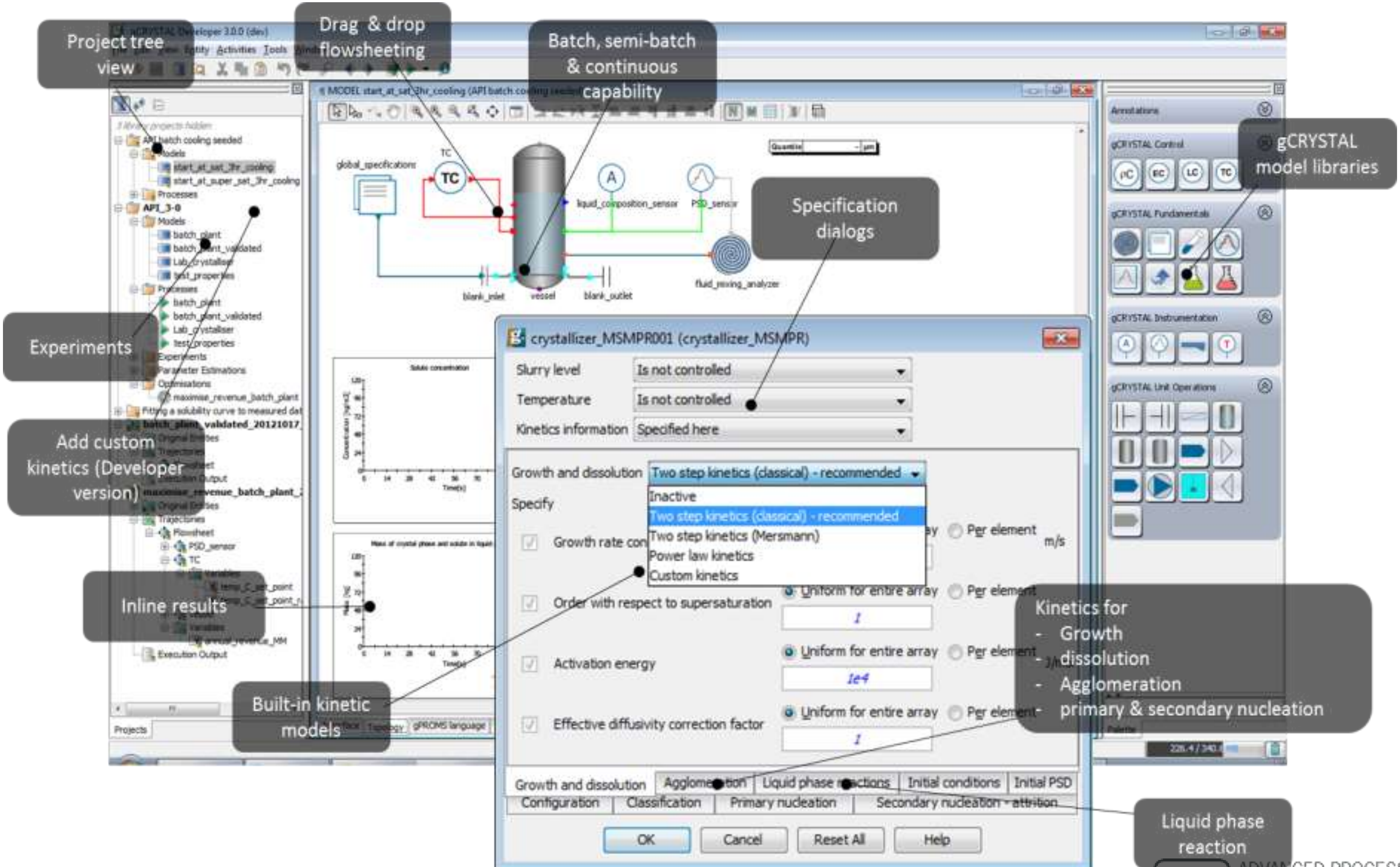
Model deployment tools

Enterprise

Objects

Deploy models in common engineering software

Modelling a batch crystallization process in gCRYSTAL

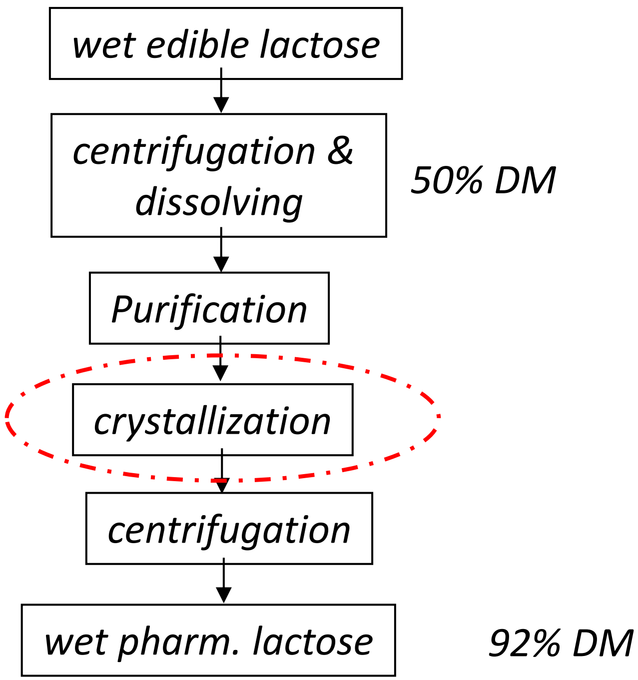


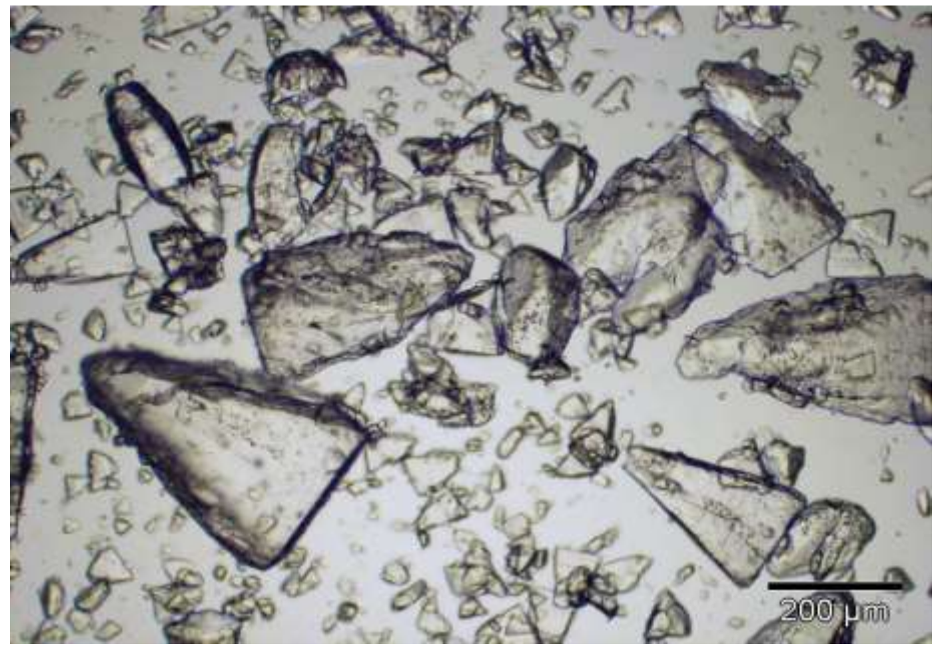
ADVANCED PROCESS MODELING FORUM 2014

Lactose production - Aims

- An application by Friesland Foods Domo for reducing batch time without degrading the crystal size distribution and purity

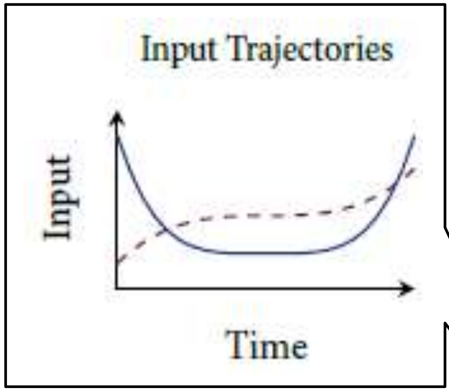
Lactose crystallization

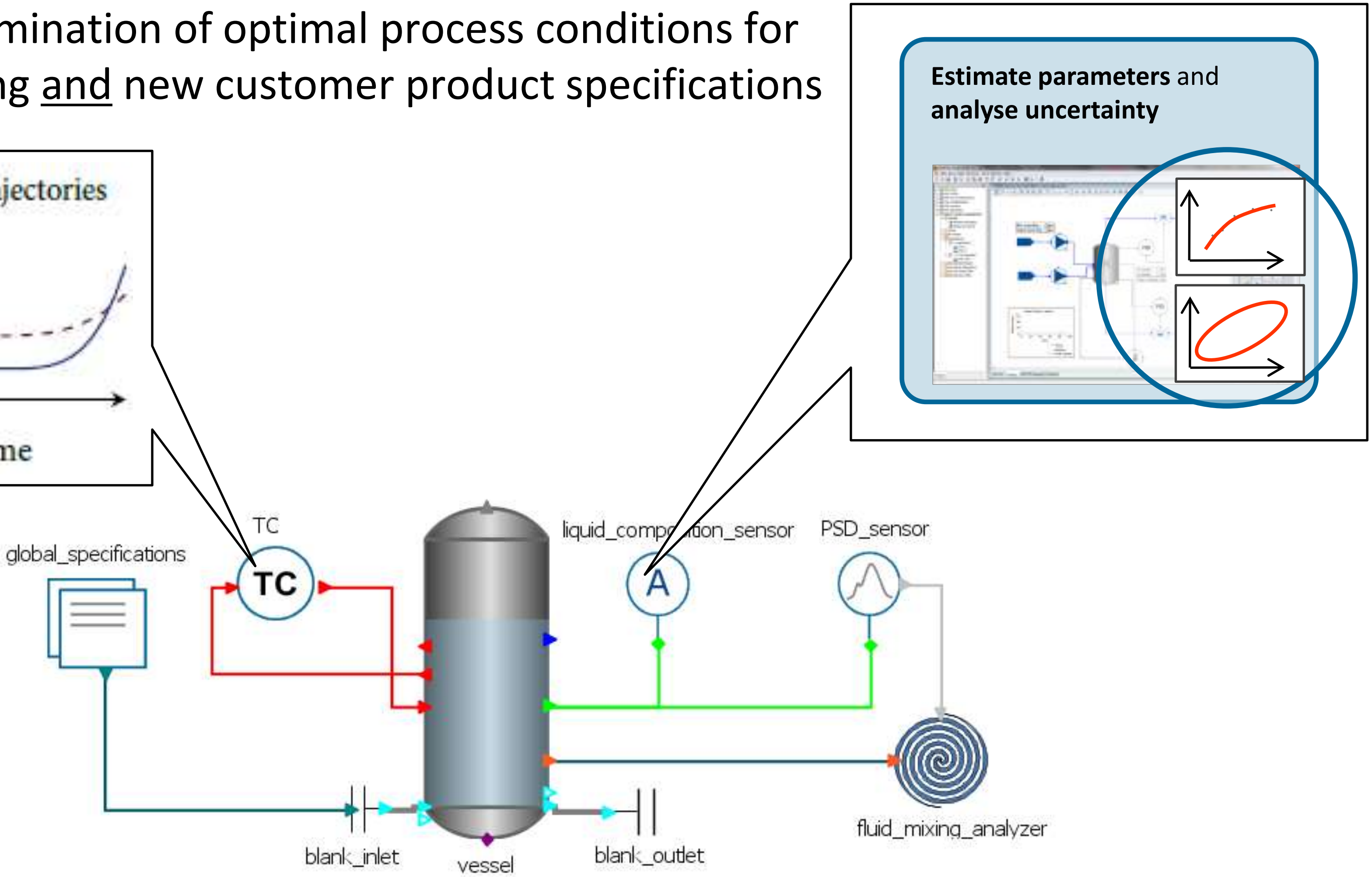




Lactose production - Activity

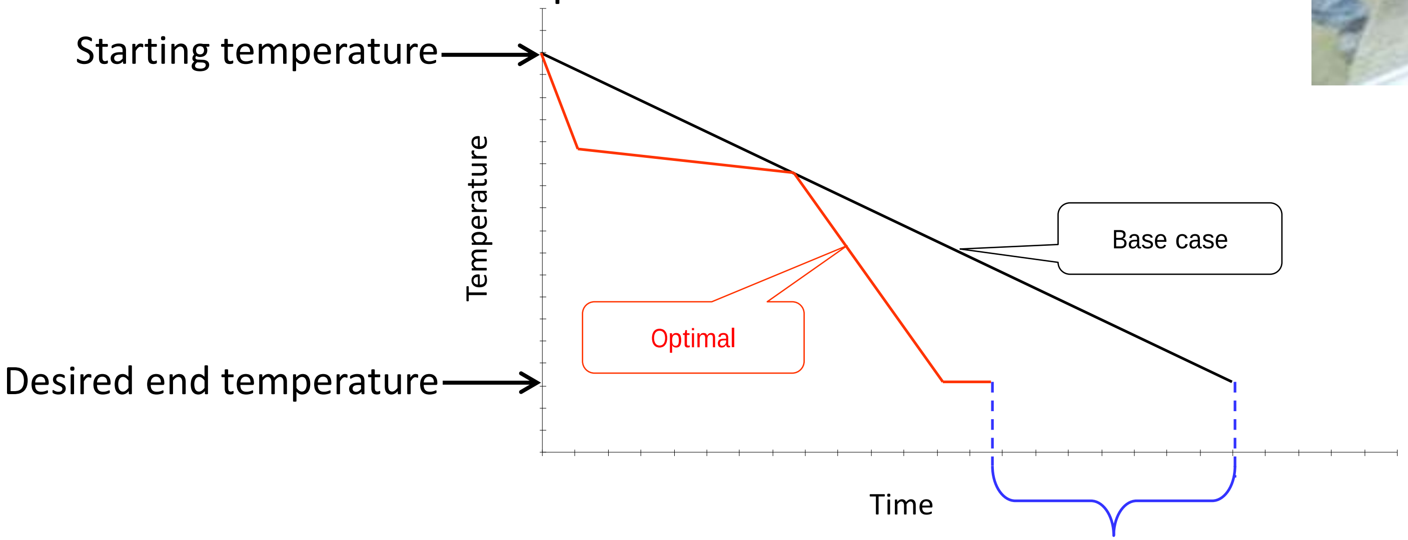
- Process optimisation
  - Determination of optimal process conditions for existing <u>and</u> new customer product specifications





Lactose production - Optimisation

- Objective
  - minimise batch time
- Decision variable
  - temperature profile during batch
- Constraints
  - same median size
  - no increase in impurities



44 % reduction in batch time

As a result, DOMO is now successfully able to meet specific customer demands regarding functional properties of lactose

Conclusions

Conclusions

- Model-based engineering of batch processes:
  1. dynamic modelling through high-fidelity model libraries or customized models
  2. modelling complex operational sequences
  3. dynamic optimisation of recipes within the degrees of freedom available to maximise a given objective

- Widely applicable workflow:
  - for batch reaction, distillation, crystallization, …

- All within the scope of state-of-the-art process modelling technology
  - challenges addressed in an efficient and user-friendly way

Thank you