

Design of Batch Scheduling

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www.chemstations.com

Agenda

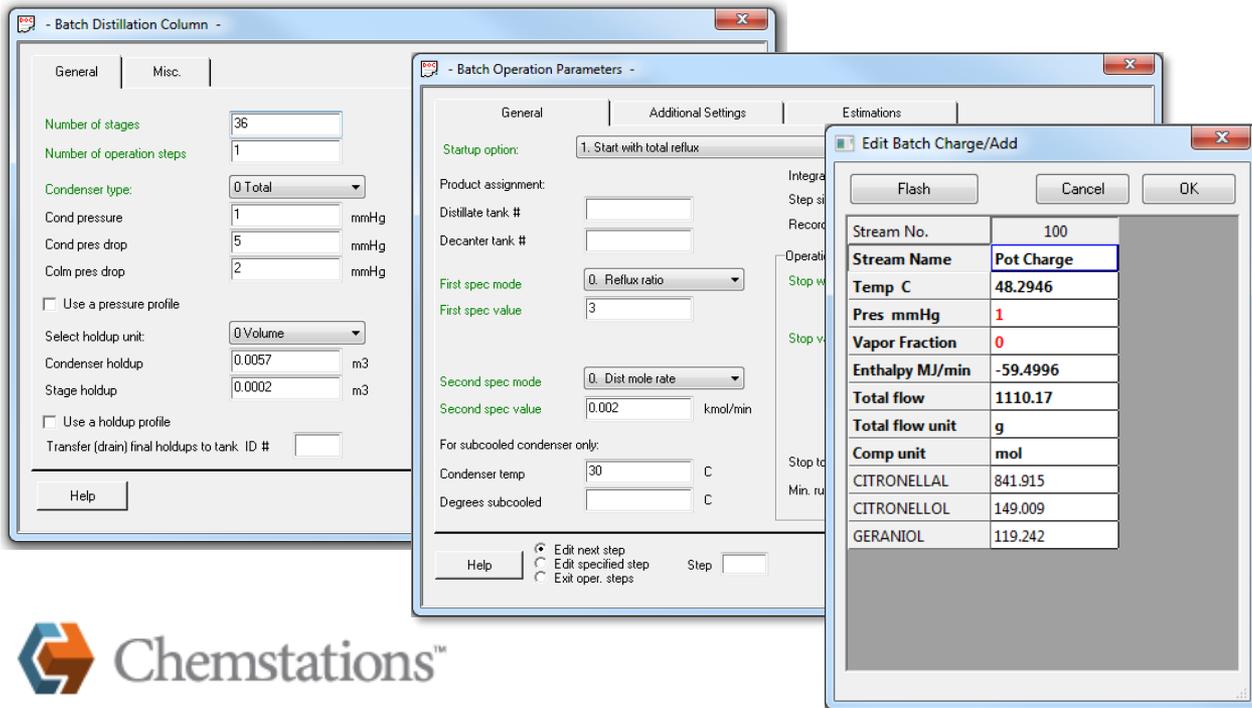
- Current practices in design of batch scheduling
- Improvements made possible with
 - Rigorous modeling methodology
 - Microsoft Excel™ to drive a schedule in a simulator
- Example using CITRON (new process)
- Example using WINTEK (existing optimization)
- Summary & suggested procedure

Current practices in design of batch scheduling

- Methods
 - Best guess & experience
 - Lab scale & pilot scale testing
 - Use a basic simulation
- Pros
 - Fast
 - Fairly easy
 - Gives a basic time and heat duty analysis
- Cons
 - Suboptimal schedule times
 - Might not account for equipment/process limitations
 - Difficult to do safety analysis until after process is running

CITRON (current practice)

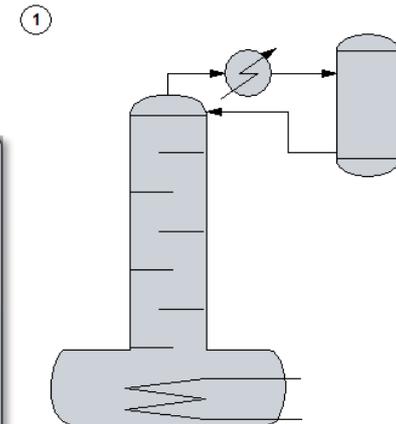
Recover 120 kgs of 99.9999% pure Citronellal from 170 kgs essential oil using a 500L pot still with a 10ft packed column.



The screenshot displays three overlapping windows from the Chemstations software:

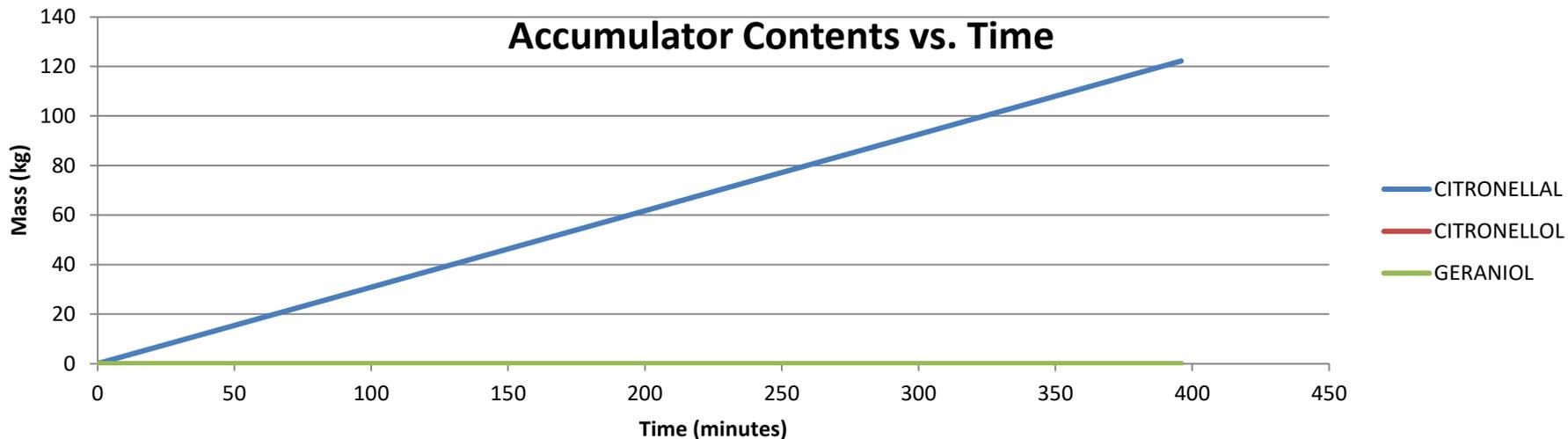
- Batch Distillation Column -**: Shows configuration for a distillation column with 36 stages, 1 operation step, and various holdup and pressure settings.
- Batch Operation Parameters -**: Shows the start-up option set to "1. Start with total reflux" and various specification modes for reflux ratio and dist mole rate.
- Edit Batch Charge/Add**: A table showing the composition of a batch charge.

Stream No.	100
Stream Name	Pot Charge
Temp C	48.2946
Pres mmHg	1
Vapor Fraction	0
Enthalpy MJ/min	-59.4996
Total flow	1110.17
Total flow unit	g
Comp unit	mol
CITRONELLAL	841.915
CITRONELLOL	149.009
GERANIOL	119.242

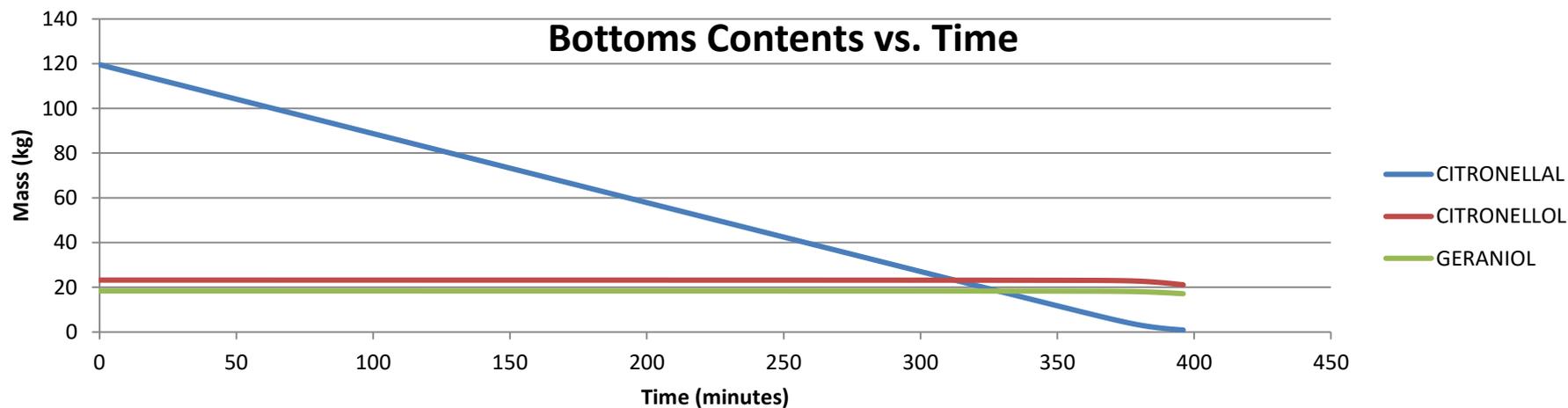


CITRON (current practice)

Accumulator Contents vs. Time



Bottoms Contents vs. Time



CITRON (current practice)

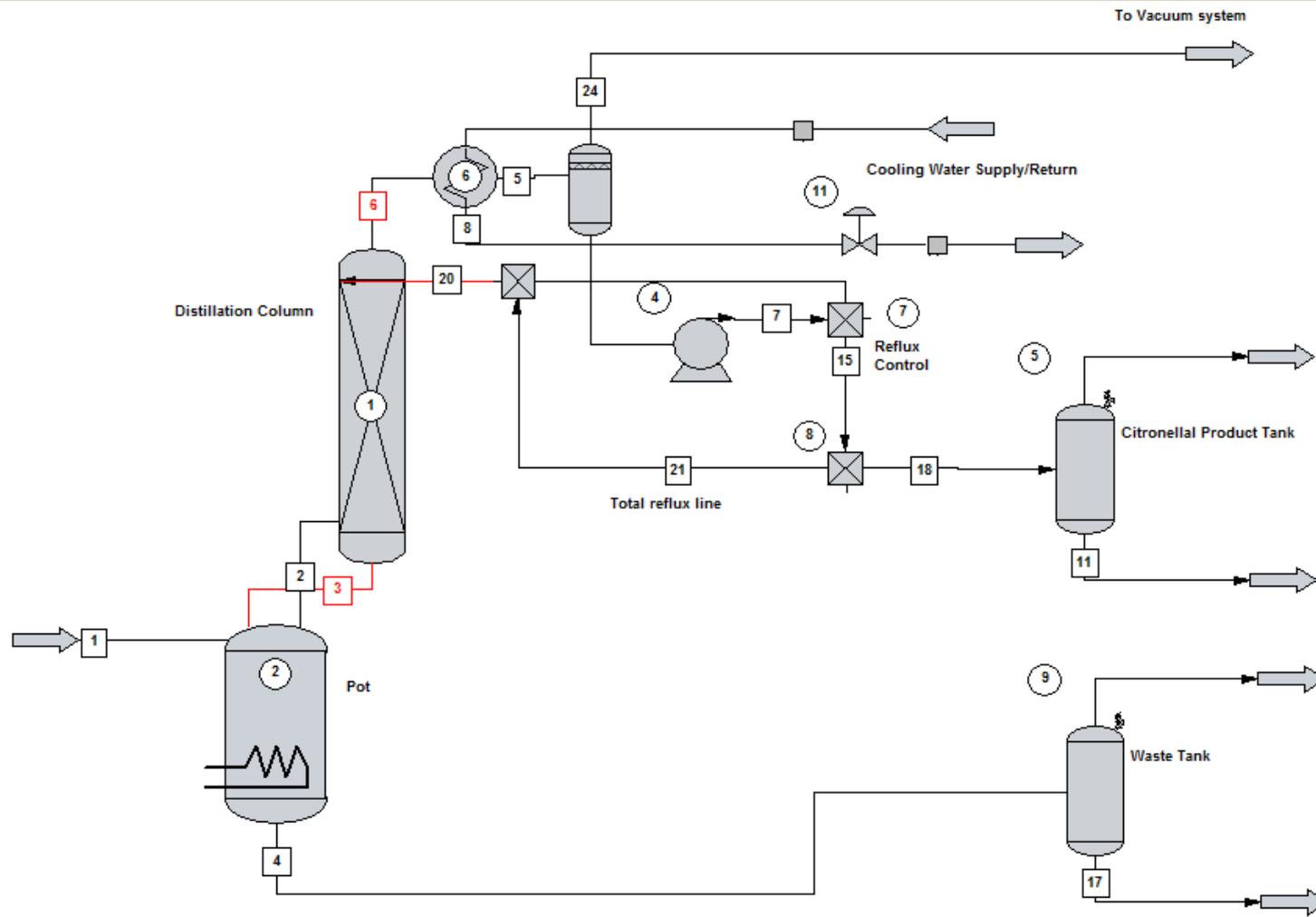
What have we learned from the model?

- Heat duty/flow/time relationship
- Basic operation steps/timing
- Limited equipment sizes and specifications:
 - Heating requirements
 - Condenser requirements
 - Column dimensions

CITRON Dynamic (advanced practice)

- Expand our previous example to include
 - Rigorous heat exchanger geometry and performance
 - Event sequencing using DATAMAP to Microsoft Excel
 - Utilities modeling
 - Column metal heat transfer
 - Heat duty / cooling water on control
 - Dry column startup to total reflux
 - Detailed engineering, e.g., nitrogen sweep on vessel, insulation, etc.

CITRON Dynamic



Schedule of Events

- A schedule of events is made in Excel and must be connected to CHEMCAD:

The screenshot shows an Excel spreadsheet with the following data:

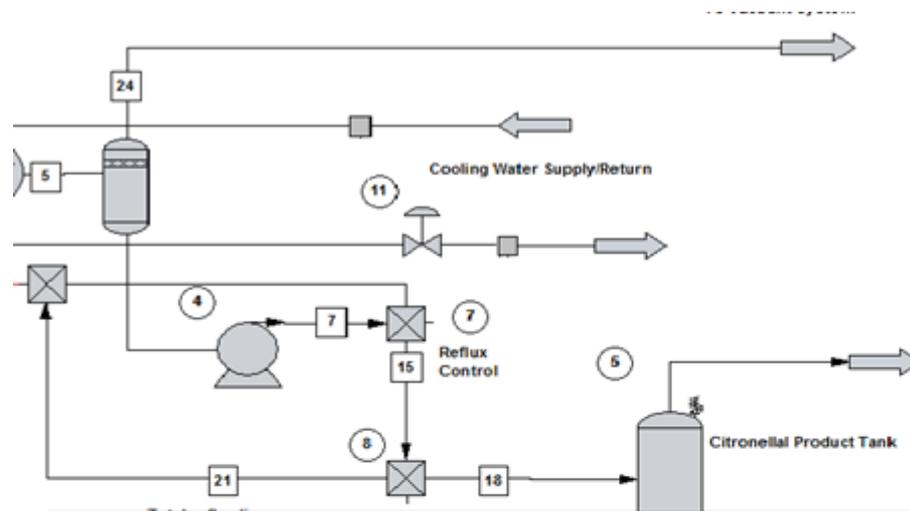
	A	B	C	D	E	F	G	H	I	J	K
6	Schedule of Events										
7	Time(min)	CW Valve mode	CW Valve Opening	Total reflux	Product Tank	Waste Tank			Notes		
8	0	4	0	1	0	0	36	0	Startup		
9	21	4	0	1	0	0	29	0	Lower heat duty		
10	25	4	5	1	0	0	29	0	Open CW Valve		
11	50	4	5	0	1	0	29	0	Switch off Total reflux		
12	473	4	5				0		Heater off, drain to tank		
13	540	4	0				0		CW off		
14											
15											
16											

CHEMCAD to Excel connection

CHEMCAD sends time information to Excel cell A2 via datamap

Excel uses time, schedule, and VLOOKUP() function to determine values of process variables

CHEMCAD collects the current time step data from row 2 of the Excel sheet and enters it into the flowsheet via datamap



File	CC Obj Type	CC Obj ID	Par ID	Component	WrkSht Cell/...	Weight	Comment
ksh...	Misc	0	Dynamic Time	<None>	A2	1.00000	Dynamic time sent to XLS
Only	UnitOp	8	Output strea...	<None>	D2	1.00000	Total Reflux
Only	UnitOp	8	Output strea...	<None>	E2	1.00000	Product tank
Only	UnitOp	8	Output strea...	<None>	F2	1.00000	Waste tank

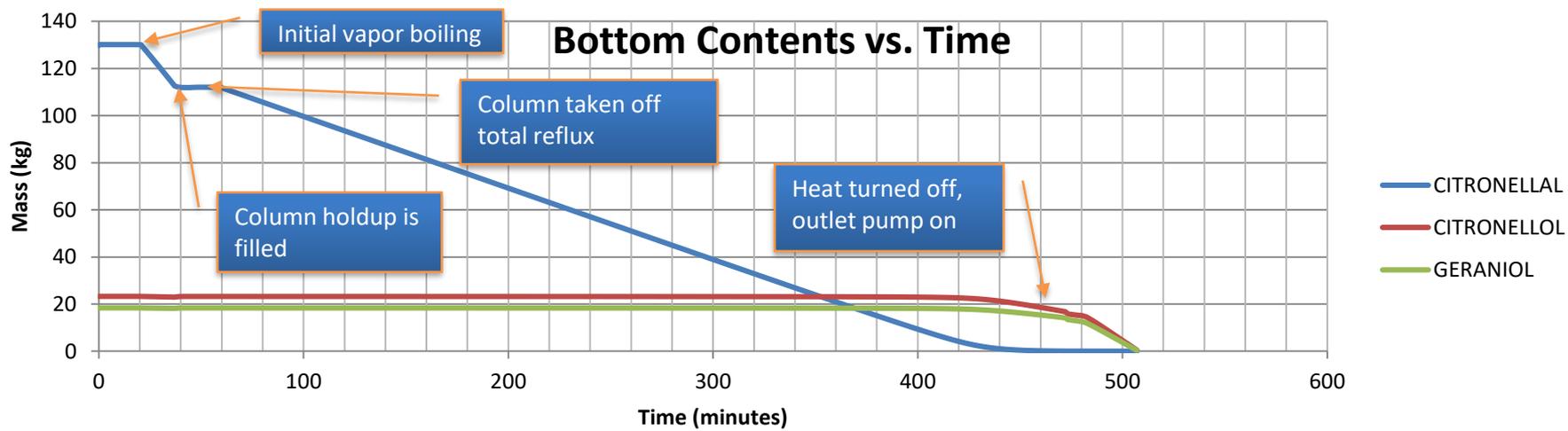
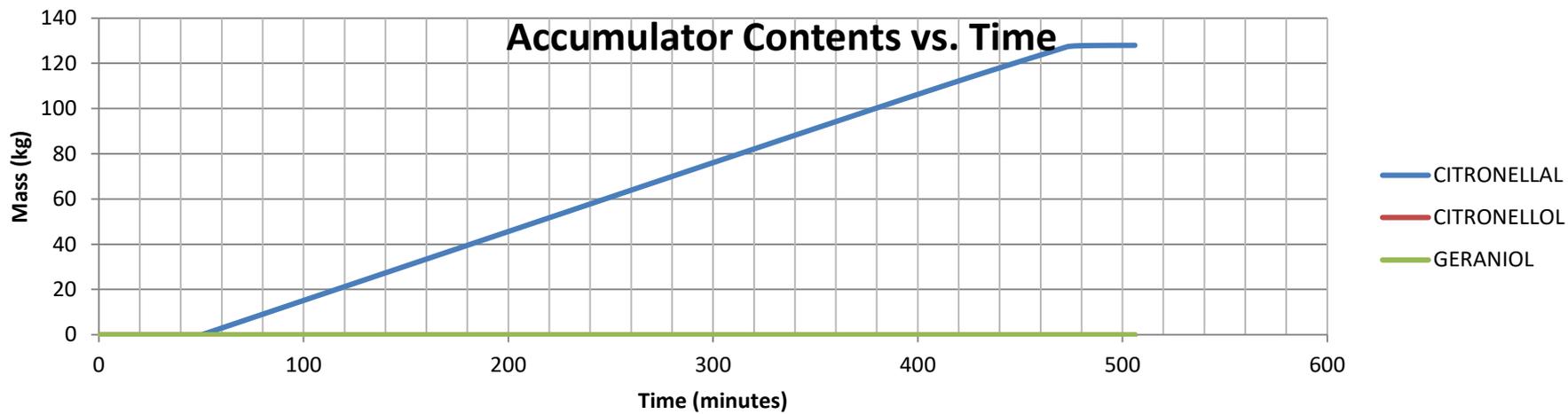
G2 fx =VLOOKUP(\$A\$2,\$A\$8:\$G\$13,7,TRUE)

A	B	C	D	E	F	G	H	I	J
Time(min)	CW Valve mode	CW Valve Opening	Total reflux	Product Tank	Waste Tank	Heater Powe	Liquid drain flow		
0	4	0	1	0	0	36	0		
Schedule of Events									
Time(min)	CW Valve mode	CW Valve Opening	Total reflux	Product Tank	Waste Tank				Notes
0	4	0	1	0	0	36	0		0 Startup
21	4	0	1	0	0	29	0		0 Lower heat duty
25	4	0	1	0	0	29	0		0 Open CW Valve

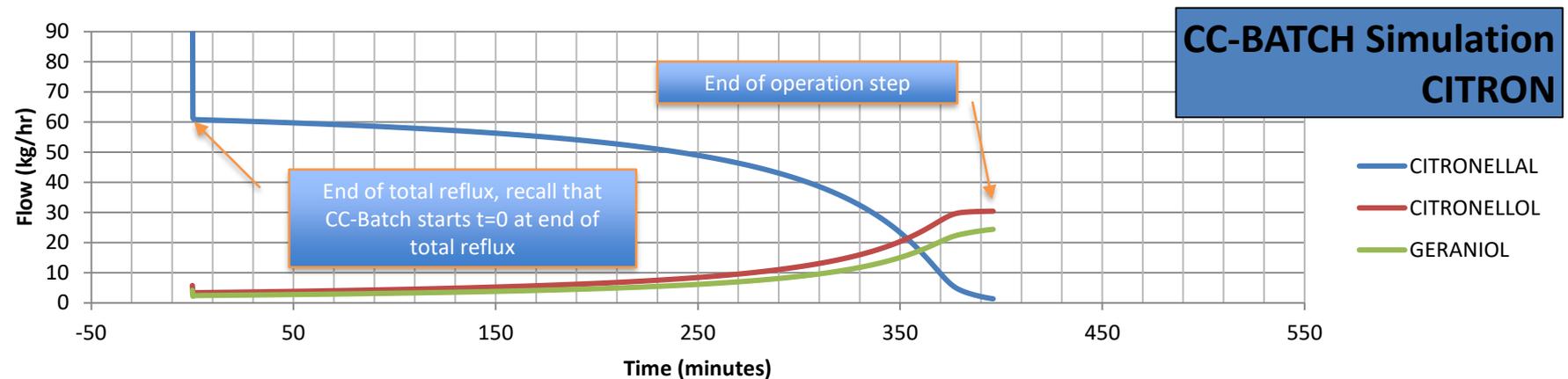
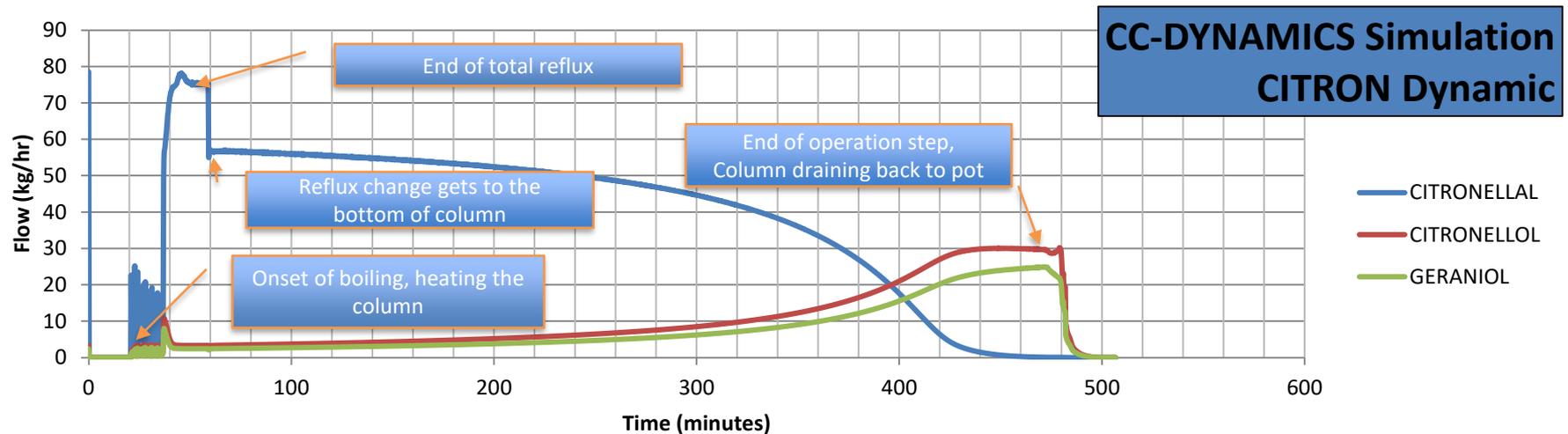
Time step sent from CHEMCAD

Duty sent back to CHEMCAD for the current time step

CITRON Dynamic Operations



Comparison of CC-BATCH and CC-Dynamics Column Bottom Flow



CITRON Dynamic Conclusions

We learned from using dynamics:

- Detailed startup procedure
- Detailed operation steps/Sequence details
- Equipment performance limitations
- Vacuum load
- Utility demands
- Equipment optimization is now possible: checking condenser capacity, vacuum system capacity, column flood %, column insulation requirements, etc.
- Higher fidelity simulation provides higher fidelity economic calculation (campaign time and costs)

WINTEK Batch Dehydration

Skid mounted solvent dehydration plant

Stripping water from a solvent stream in a two bed adsorber (mol sieve) system. One bed is active and one bed is regenerating under vacuum. Process was already built and operational before modeling analysis.

Process is scheduled with a defined sequence for opening and closing valves to allow one bed to regenerate while the other adsorbs. Rigorous equipment and piping models and pressure/flow calculation included (allows for reversible flow).

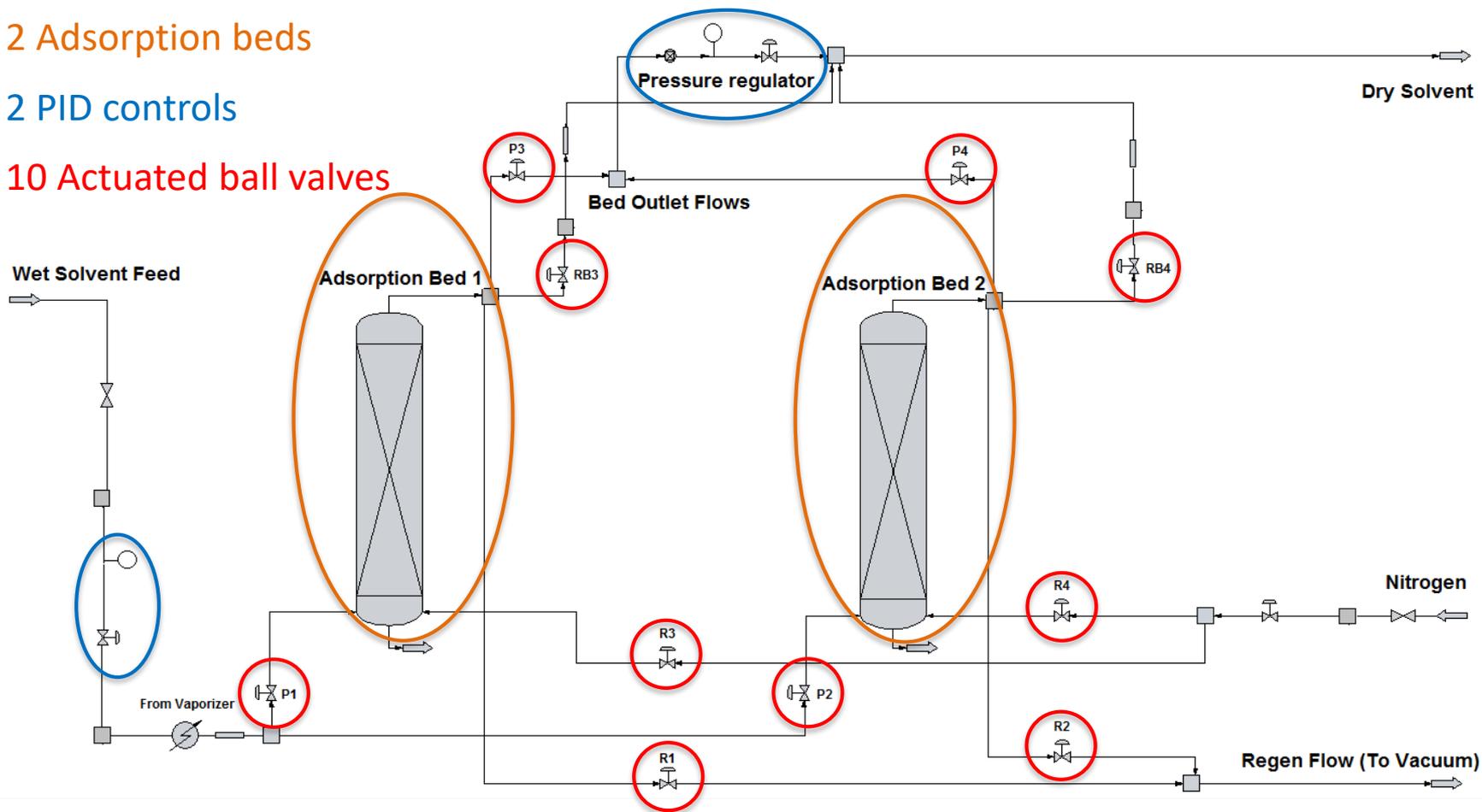
Rigorous simulation allows us to simulate effect of malfunction (RB3 blowdown valve malfunction)

WINTEK Process Flowsheet

2 Adsorption beds

2 PID controls

10 Actuated ball valves



WINTEK Datamap and Schedule

1								
2								
3					New	Embed		
4	Excel Workbook Path:	A_BREA_SIEVE_DLL_201.xls			Browse	Open		
5								
6	Excel Worksheet Name:	Sheet1						
7								
8								
9								
10	Map Rule	CC Obj Type	CC Obj ID	Par ID	Component	WrkSht Cell/...	Weight	Comment
11	To Worksheet ...	Misc	0	Dynamic Time	<None>	A2	1.00000	Dynamic time(Min)
12	To CC Only	UnitOp	26	Controller out...	<None>	D2	1.00000	P1
13	To CC Only	UnitOp	11	Controller out...	<None>	E2	1.00000	P3

VLOOKUP Function to get P1 signal at current time step

Time step sent from CHEMCAD

P1 signal sent back to CHEMCAD for the current time step

Schedule of time events
Each row is at a different time.

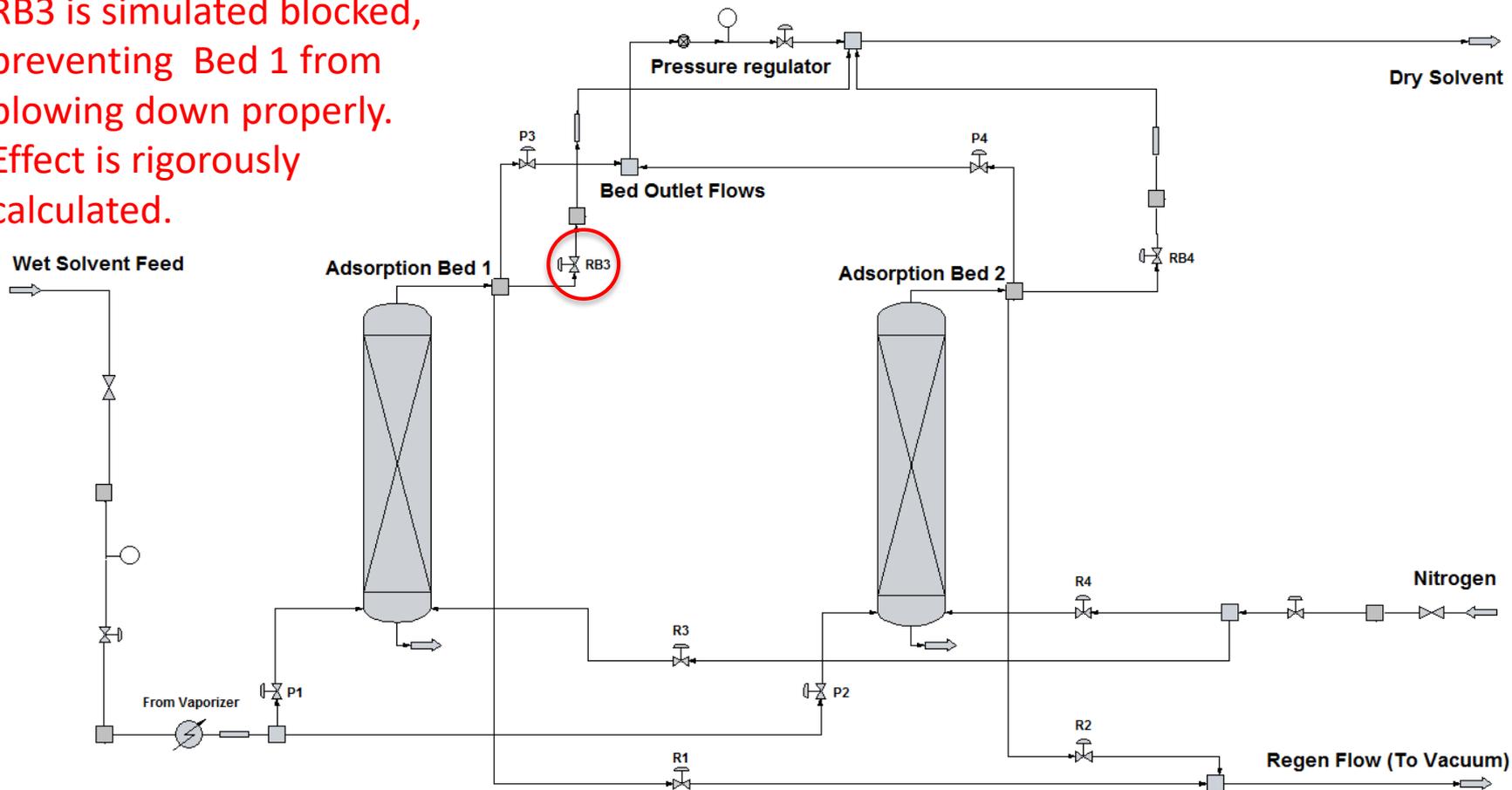
Schedule of P1 actuation signal at different times

fx =VLOOKUP(\$A\$2,\$C\$7:\$P\$27,2,TRUE)

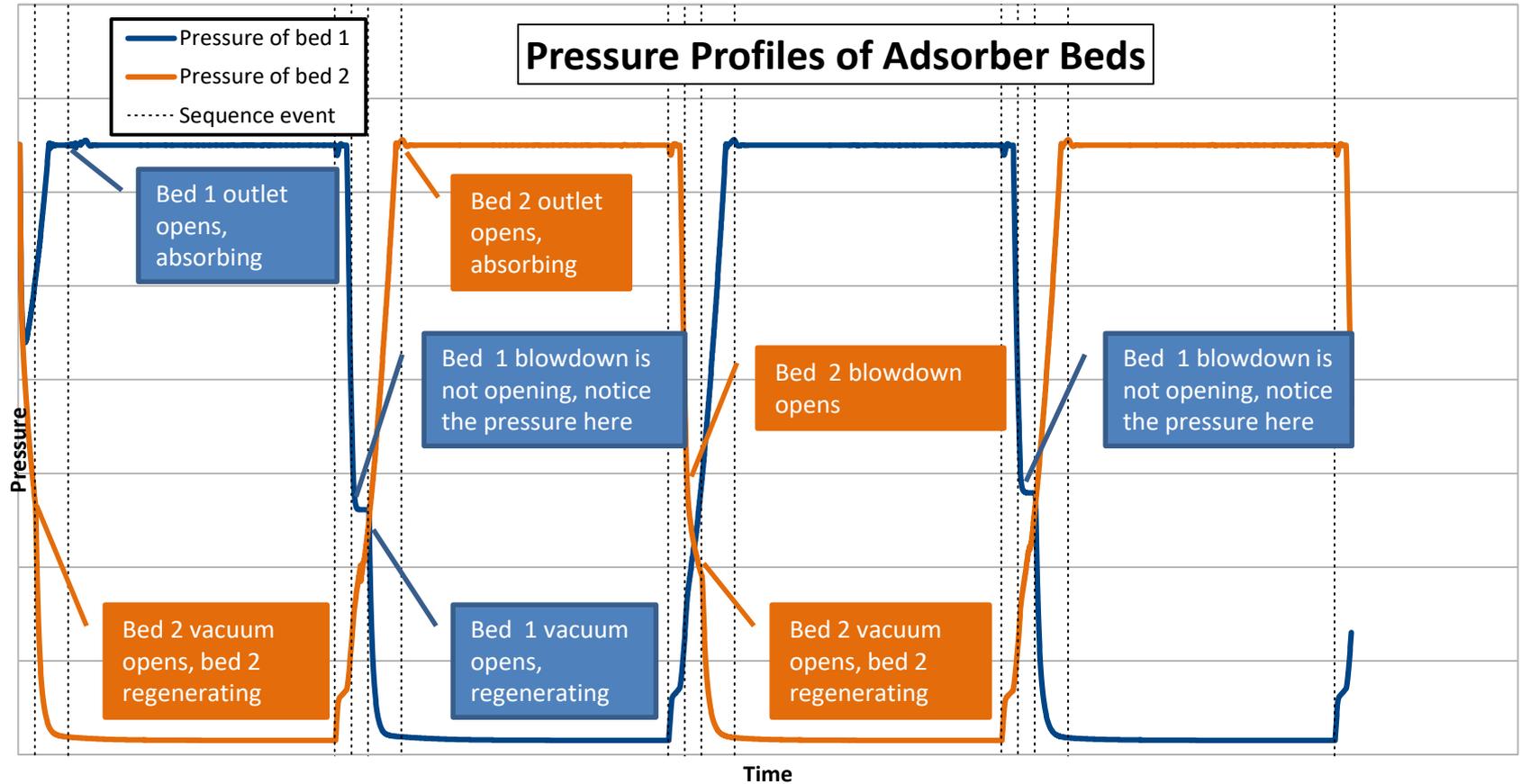
	A	D	E	F	G	H	I	J	K	L	M	R	
1	Time(m)	P1	P3	P2	P4		BV1	R1	R3	R2	R4	R	
2	20		20	4	4		4	4	4	20	20	
3													
4													
5	Schedule												
6	El. Time(s)	Interval(s)	Tstart(m)	P1	P3	P2	P4	BV1	R1	R3	R2	R4	R
7				0	4	20	4	4	4	4	4	4	4
8				3	20	20	4	4	4	4	4	4	4
9				5	20	20	4	4	4	4	20	20	4
10				5	20	20	4	4	4	4	20	20	4
11				5	20	20	4	4	4	4	4	4	4
12				3	20	20	4	4	4	4	4	4	4
13				0	4	4	20	20	4	4	4	4	4
14				5	4	4	20	20	4	4	4	4	4
15				5	4	4	20	20	4	4	4	4	4
16				5	4	4	20	20	4	4	4	4	4

WINTEK Process Flowsheet: Malfunction effect

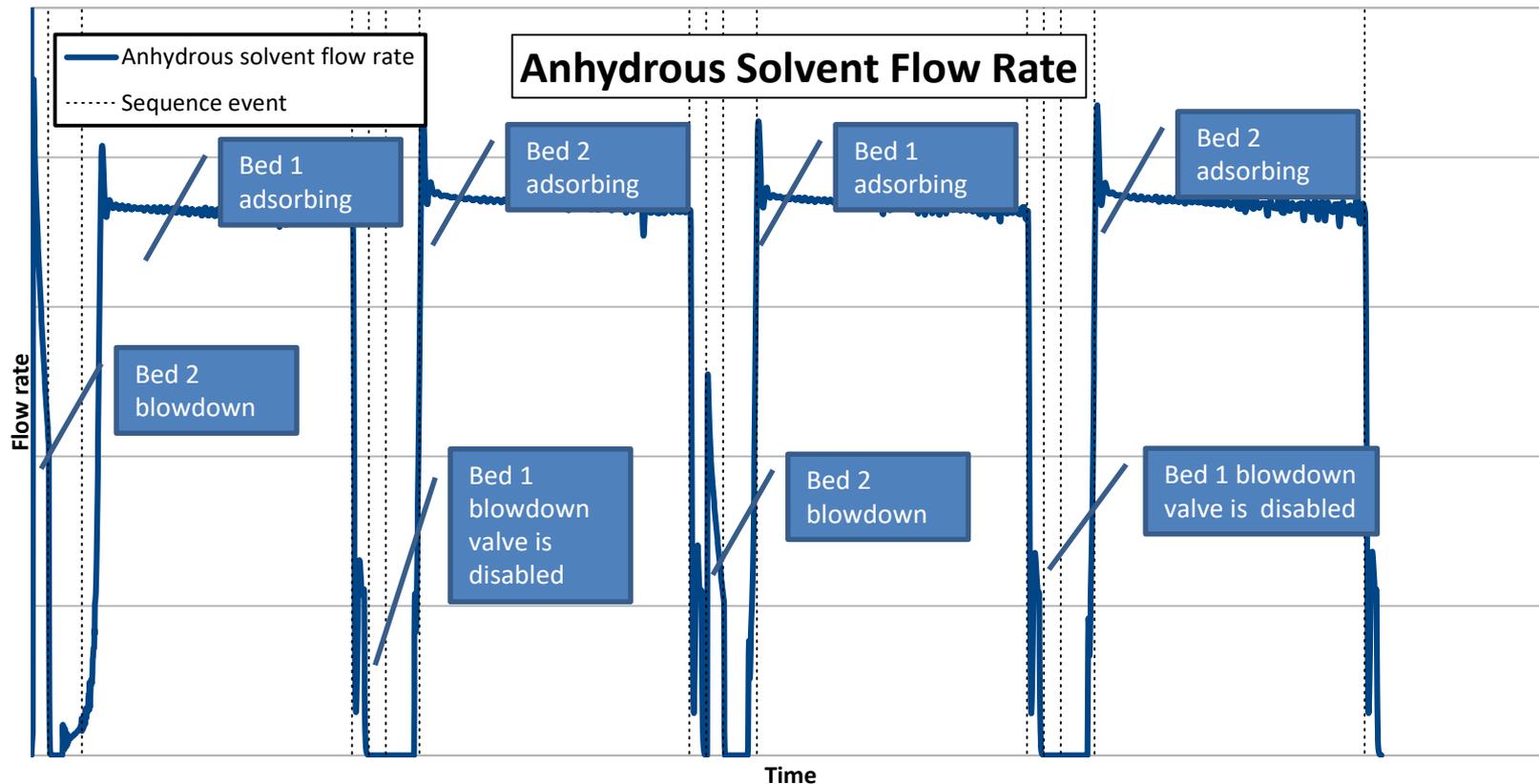
RB3 is simulated blocked,
preventing Bed 1 from
blowing down properly.
Effect is rigorously
calculated.



WINTEK Adsorber Beds

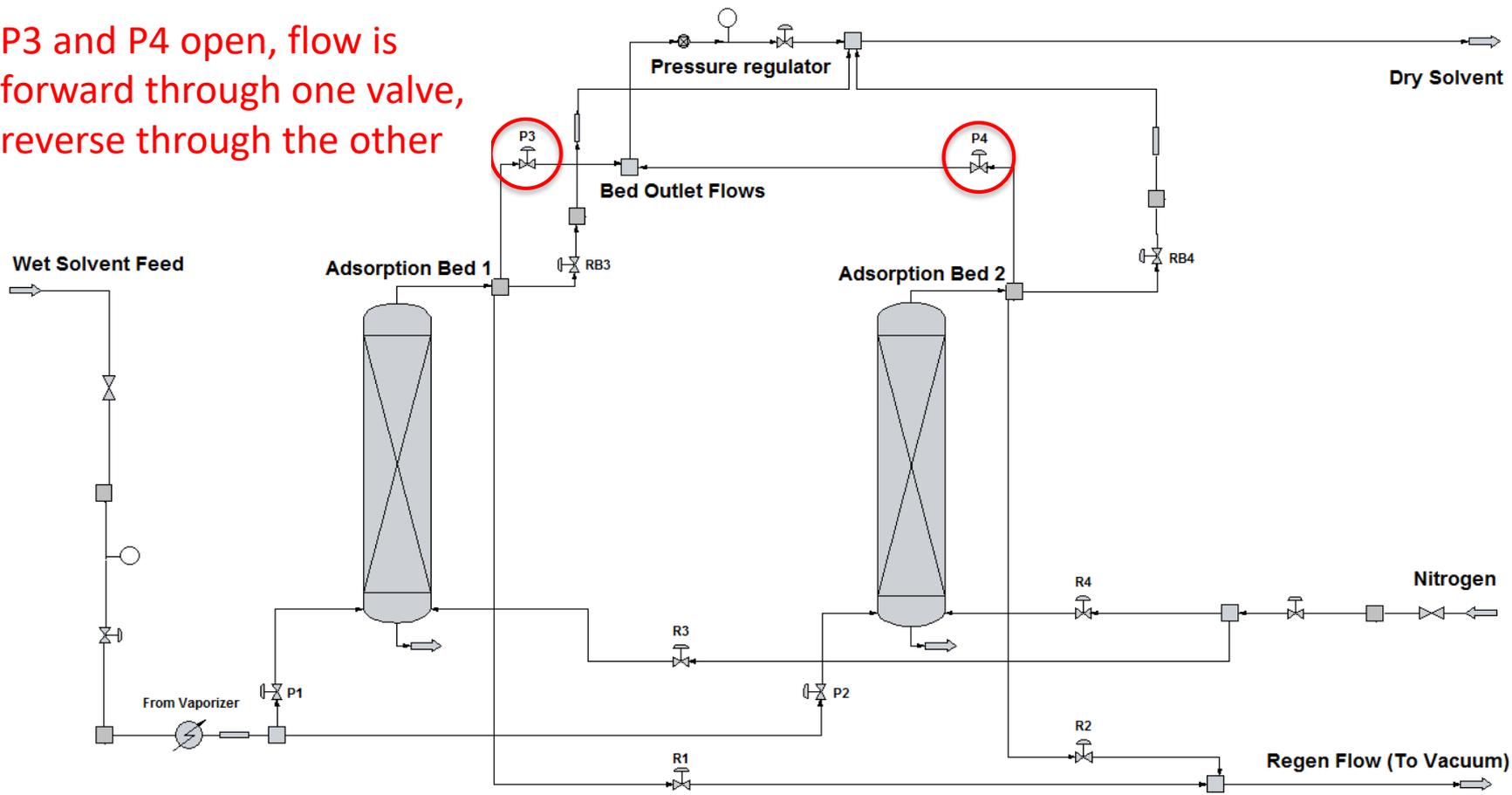


WINTEK Anhydrous Solvent Flowrate

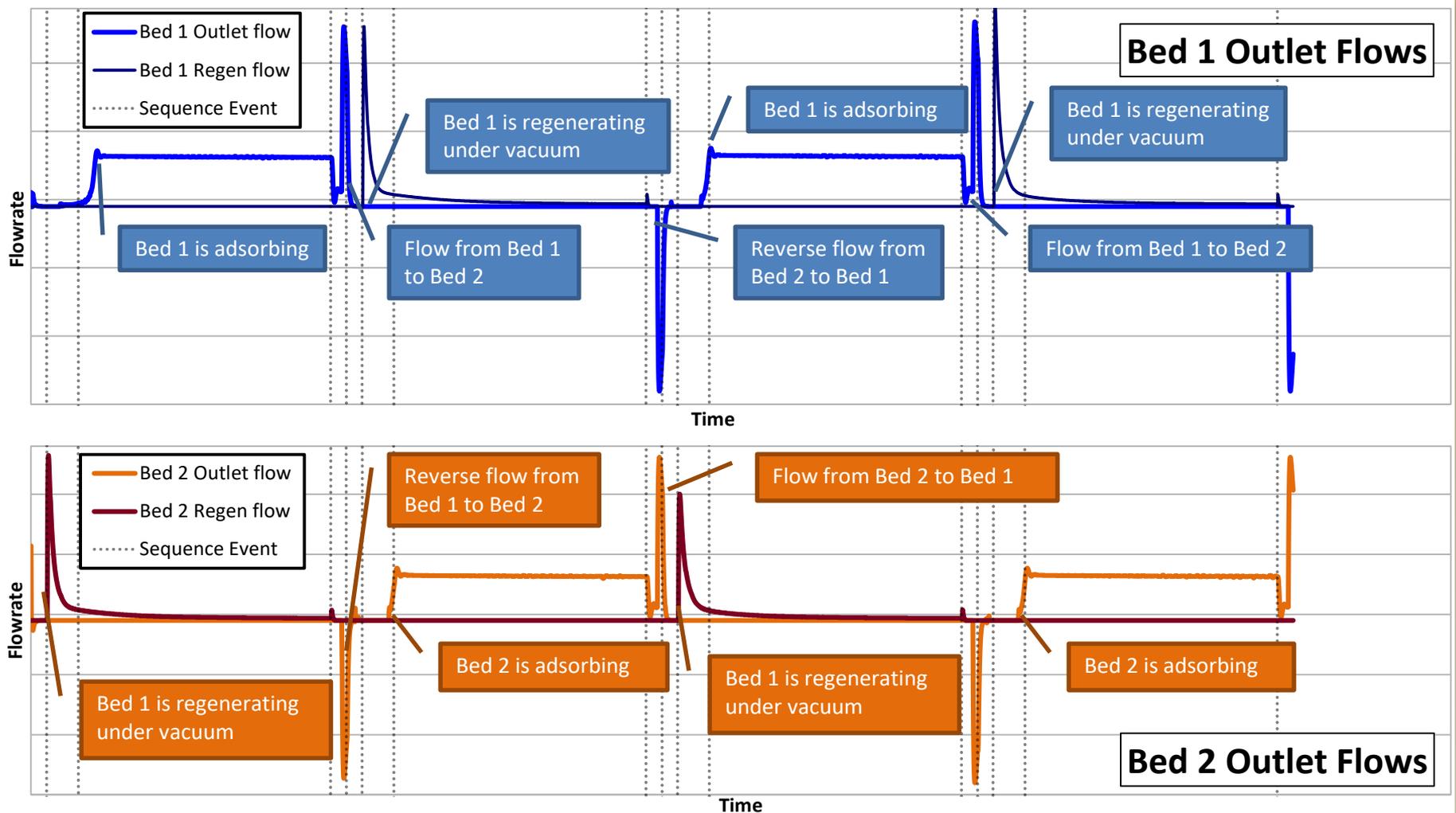


WINTEK Process Flowsheet: reversing flow

P3 and P4 open, flow is forward through one valve, reverse through the other

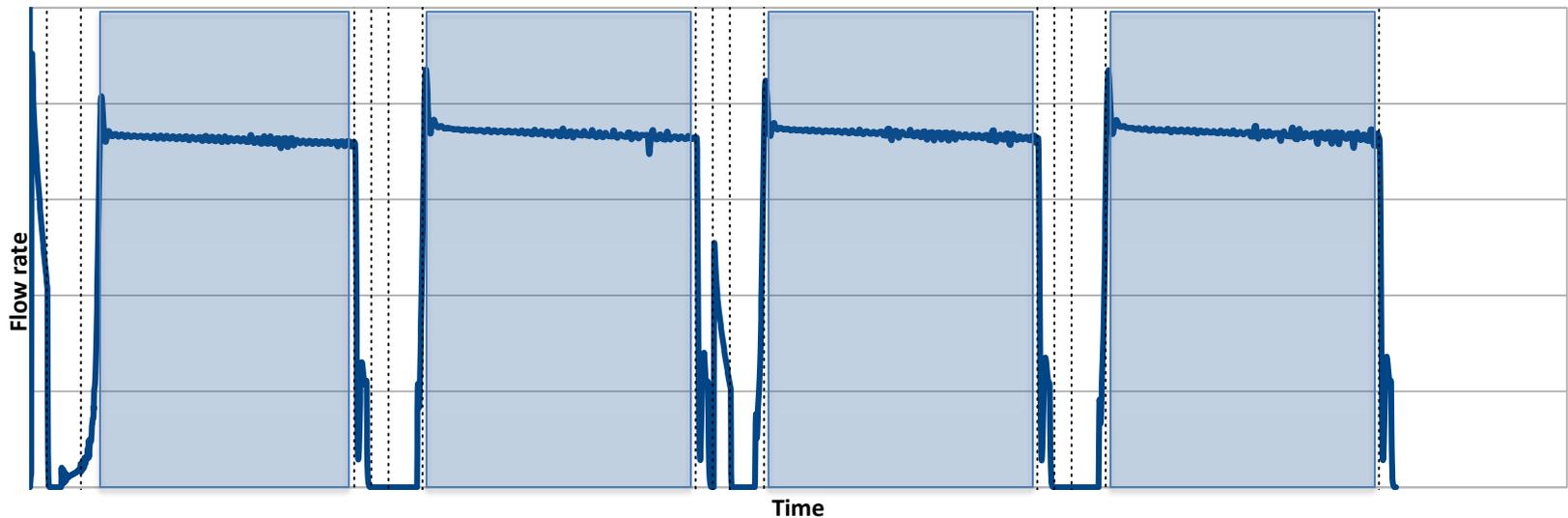


WINTEK Sequence of outlet and regeneration flows out of adsorber beds



Optimization of schedule (future)

- By using an optimization engine (either the built in engine in CHEMCAD, or an external one connected to the Excel spreadsheet) the schedule of valve events can be optimized to maximize on-stream performance (blue area of chart).



WINTEK Conclusions

What did we learn from our model?

- Discrete event scheduler with pressure and flow calculations (including reversible flow) allowed optimization of the process schedule
- Ability to identify and quantify
 - Bottlenecks
 - Sequence timing issues
 - Equipment limitations
 - Malfunction effects (bed 1 blowdown valve sticking)
 - Control loop tuning issues
- Ability to use the model for process scaling: process can be scaled up or down to meet customer requirements using the model before building/assembly
- Ability to optimize schedule of events

Suggested Procedure

1. Start with a simplified model (like CC-BATCH) to get heat duties, initial equipment sizes/specifications, and an initial timing/schedule
2. Build a rigorous dynamic model with as much detail as required (but no more than required) to solve the engineering problem (e.g., only add reversible flow if it is a concern)
3. Build an event sequence control scheme using DATAMAP and Excel starting with the information gathered in Step 1 above. Progressively improve the sequence by running the dynamic model with the scheduler

Special Thanks

Paul Winter, President and Owner

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