

# Supplementary information for: Steady-state time series data with and without anomalies from a continuous distillation mini-plant

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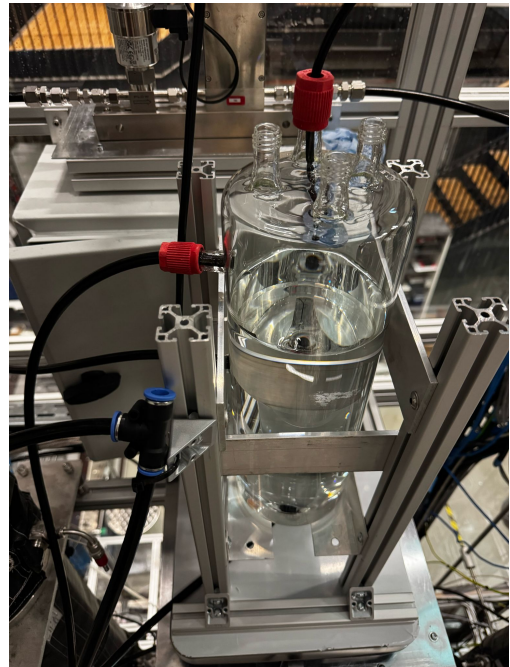
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## S1 Mini-plant setup information

Figure S1 gives a combined overview of the continuous distillation plant and the decanter that was augmented.



(a) Continuous distillation mini-plant.



(b) Decanter.

**Figure S1:** Combined overview of the continuous distillation plant and decanter.

Table S1 provides an overview of the upper and lower limit specifications of the continuous distillation plant.

**Table S1:** Specifications of the continuous distillation plant

Parameter	Lower limit	Upper limit
C1 operating pressure/kPa	1	200
C2 operating pressure/kPa	2.5	100
Reflux ratio/g g <sup>-1</sup>	0	1
C1 operating temperature/K	293.15	473.15
C2 operating temperature/°C	293.15	473.15

Table S2 gives an overview of the different sensors in the continuous distillation plant, the associated P&ID labels, the related suppliers, and the precision of these instruments. Table S3 provides detailed nomenclature on the P&ID labels.

**Table S2:** Sensor Information

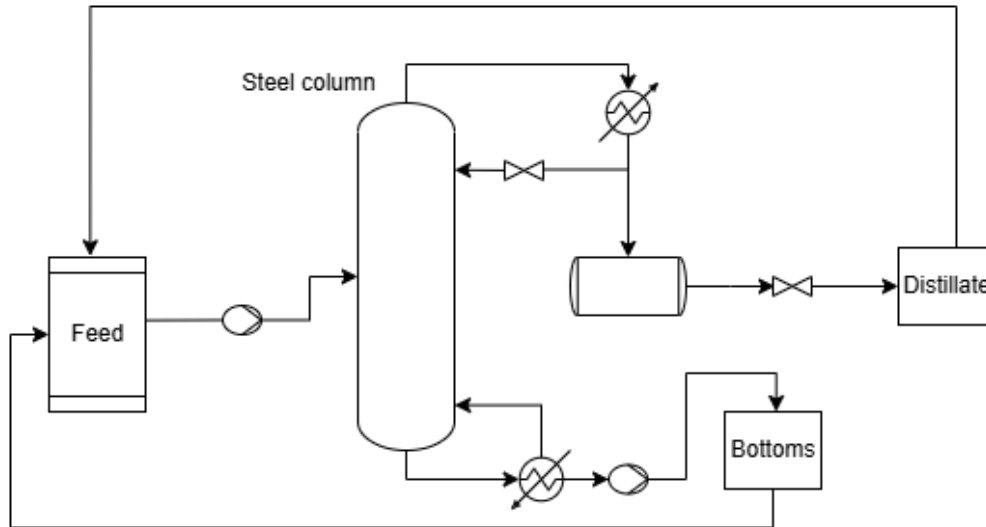
Sensor	P&ID labels	Sensor Model	Supplier	Precision
Flow indicators	F101, F102, F103, F104	Miniflow	Coriolis	±0.05 %
Level sensor	PDIC101, PDIC102, PDIC201, PDIC202	PD-33XEi	Keller	±0.05 %
Membrane pump	P101	EXBb G0613SS10A420	Prominent	±0.01 %
Pressure	PIC101, PIC201	Typ266AST	ABB	±0.04 %
Pumps	P102, P107, P201, P202	1A-A/3-19/D-SS, 1MA-A/6/D-SS	Gather	±0.005 %
Temperature	T101, T102, T104, T106, T108, T110, T112, T114, T115, T201, T202, T204, T206, T208, T210, T212, T215	Pt-100 (GTF103-Ex)	Greisinger	±0.15 °C
Thermostats	TH101, TH102, TH103, TH201, TH202, TH203	CC-202C, CC304-B, HTS 3, HTS 5	Huber	±0.02 °C
Weighing scales	A101, A102, A103, A106, A107, A203	DE	Kern	0.1% to 0.5%

**Table S3:** P&ID labels and their descriptions.

<b>P&amp;ID label</b>	<b>Description</b>
B101	Feed Tank
B103	Bottoms product tank column 1
B106	Decanter upper phase tank
B107	Decanter lower phase tank
B203	Bottoms product tank column-2
C101 to C106	Column 1 parts 1 to 6
C201 to C206	Column 2 parts 1 to 6
E101, E201	Reboiler heater
E102, E202	Column head
E103, E105, E107, E109, E111, E113	Tower heating mantle column 1
E108, E208	Bottoms product cooler
E110, E210	Feed heater
E203, E205, E207, E209, E211, E213	Tower heating mantle column 2
HV101	Manual draining valve B101
HV103	Manual draining valve B103
HV108, HV109, HV110, HV111, HV112, HV113	Manual sample valve column 1
HV203	Manual draining valve B203
HV208, HV209, HV210, HV211, HV212, HV213	Manual sample valve column 2
P101	Feed pump
P102	Bottoms product pump column-1
P107	Decanter lower phase pump
P201	Decanter upper phase pump
P202	Bottoms product pump column-2
PDIC101 to PDIC103	Pressure difference indicator column 1
PDIC201 to PDIC2103	Pressure difference indicator column 2
T101	Temperature sensor reboiler column-1
T102, T104, T106, T108, T110, T112	Temperature sensor in column 1
T103, T105, T107, T109, T111, T113	Temperature sensors integrated in tower mantle
T114	Head temperature sensor
T115	Temperature sensor in bottoms product line
T116	Temperature sensor in feed line
T201	Temperature sensor reboiler column 2
T202, T204, T206, T208, T210, T212	Temperature sensor in column 1
T203, T205, T207, T209, T211, T213	Temperature sensors integrated in tower mantle
T215	Temperature sensor in bottom product

## S2 Experimental campaigns with water

### S2.1 Overview



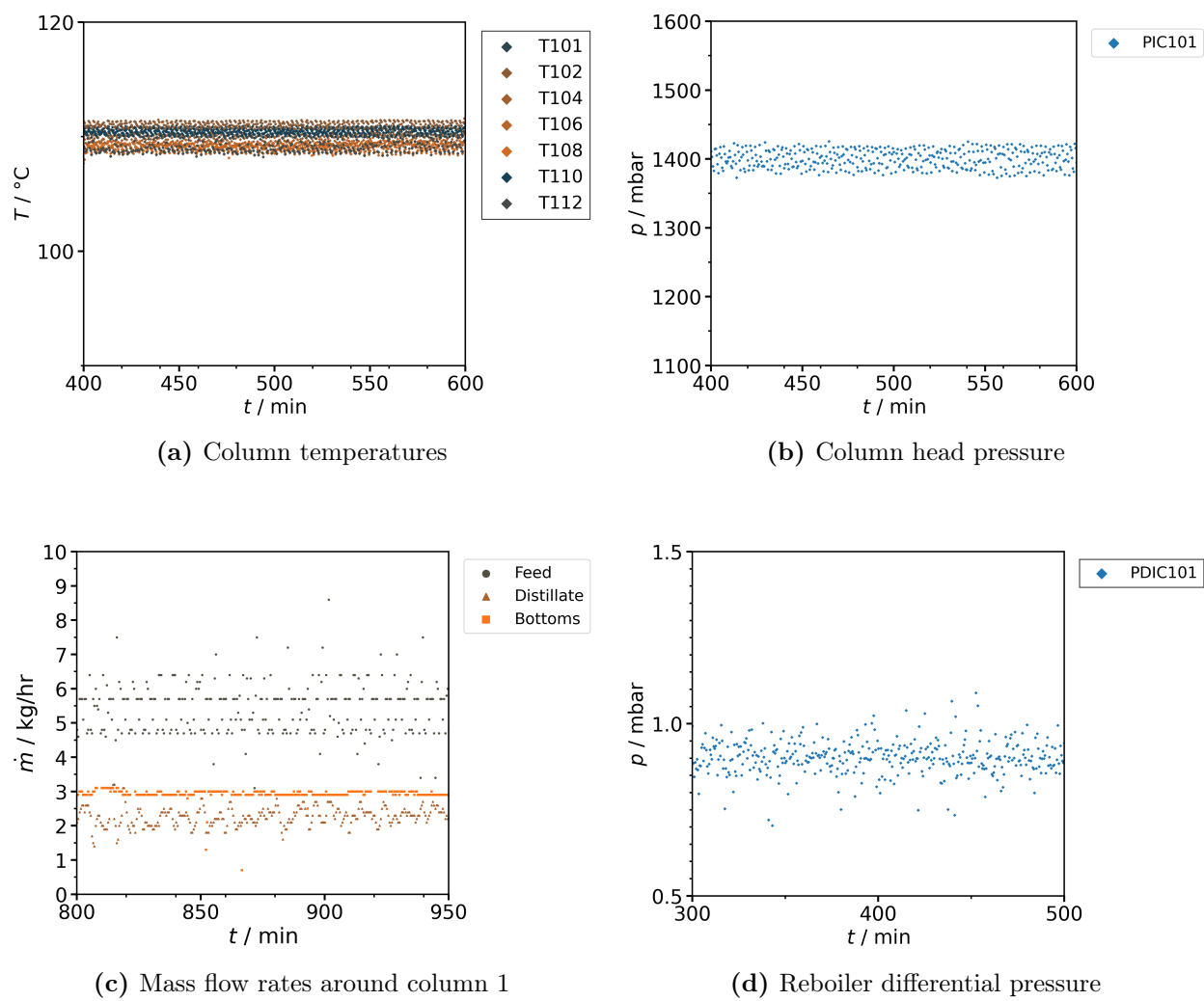
**Figure S2:** PFD of the continuous distillation plant for experiments with water.

**Table S4:** Overall material balance example

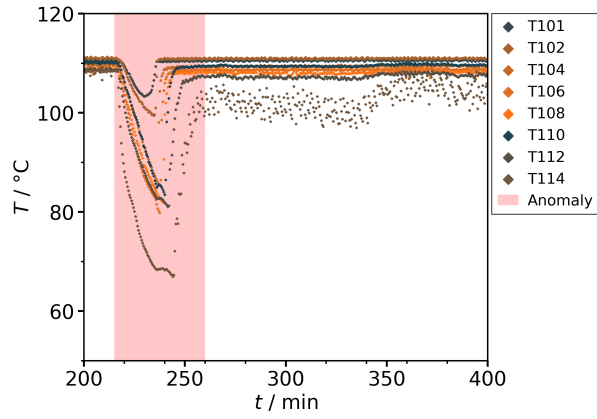
Feed flow rate (kg/h)	Distillate flow rate (kg/h)	Bottoms flow rate (kg/h)	Overall material losses (%)
5.98	2.54	2.97	7.85

Table S4 gives a sample overview of the losses encountered in column 1 during an experiment with water (operating point 001). Figure S2 represents the schematic configuration of the continuous distillation process using water. Figures S3 and S4 represent steady-state sample data with water during normal operation and anomalous operation respectively. S7 and S8 give a sample overview of the steady-state actuator data during normal operation and anomalous operation respectively.

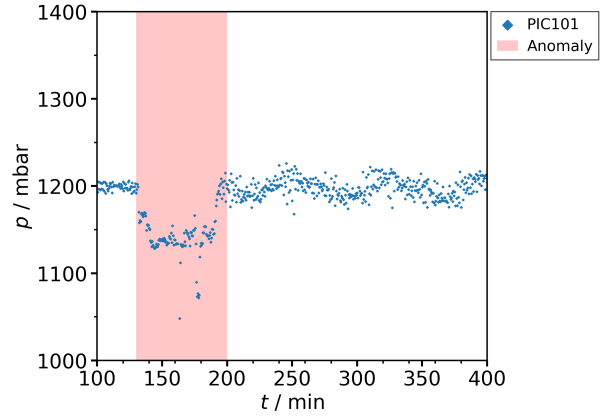
## S2.2 Time-series data sample



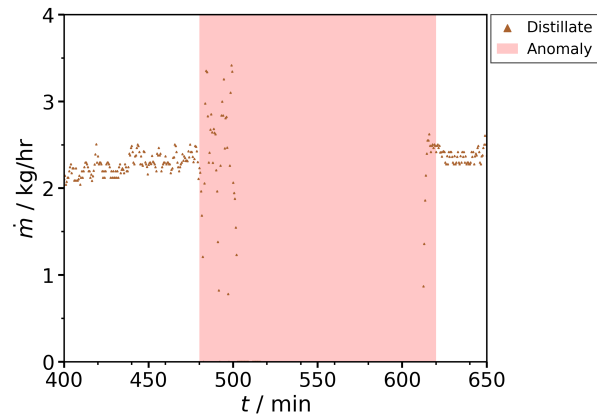
**Figure S3:** Steady state sample data with water during normal operation  
S3a, S3b, S3d - operating point 007 - train\_normal\_experiment\_001  
S3c - operating point 004 - train\_normal\_experiment\_001



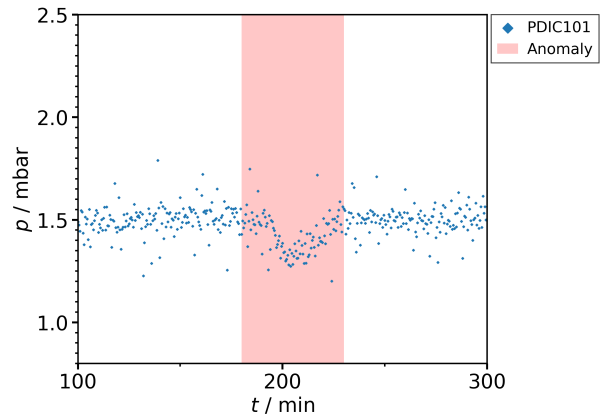
(a) Column temperatures



(b) Column head pressure



(c) Distillate mass flow rate



(d) Reboiler differential pressure

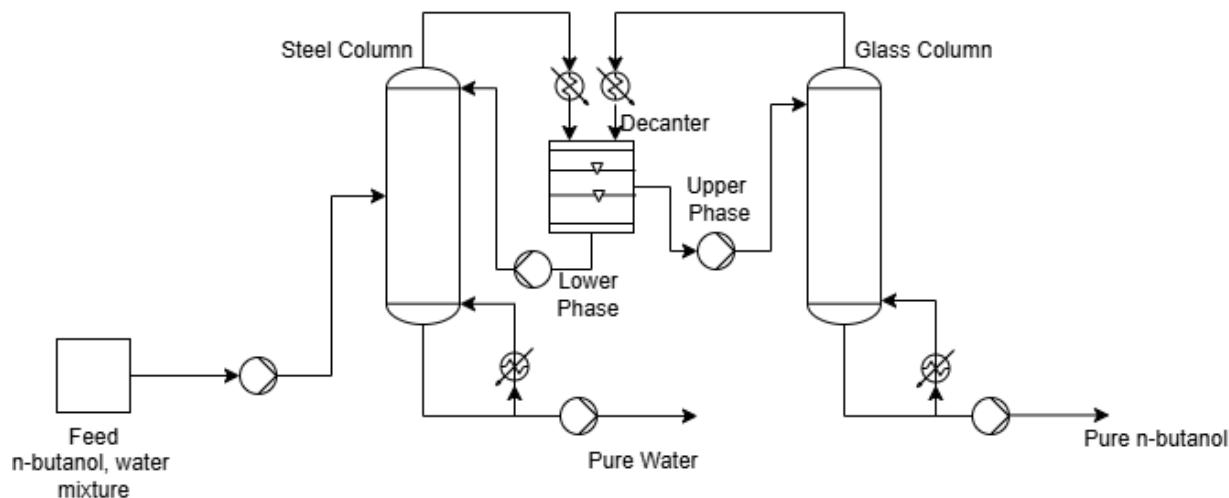
**Figure S4:** Steady state sample data with water and column-1 representing anomalies

S4a, S4b - operating point 001 - test\_anormal\_experiment\_001

S4c - operating point 005 - test\_anormal\_experiment\_001

S4d - operating point 007 - test\_anormal\_experiment\_001

## S3 Experimental campaigns with n-butanol and water



**Figure S5:** PFD of the continuous distillation plant for experiments with n-butanol and water.

Figure S5 represents the schematic process flow diagram of the mini-plant setup for experiments with n-butanol and water.

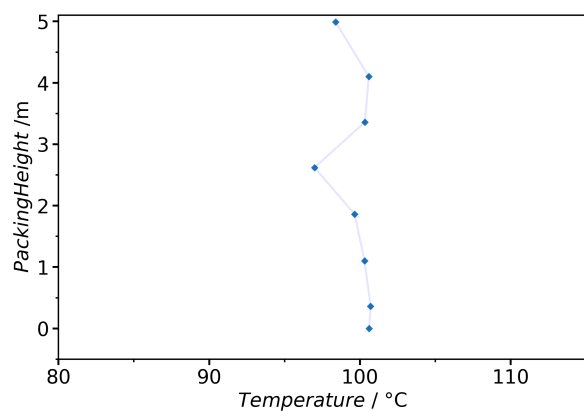
### S3.1 Sample concentration and temperature profiles

Figure S6 represents the temperature profiles from the temperature sensor measurements and concentration profiles generated by online analysis as a function of packing height during operating\_point\_003. Table S4 gives a sample overview of the losses encountered in column 1 during an experiment with n-butanol and water (operating point 003).

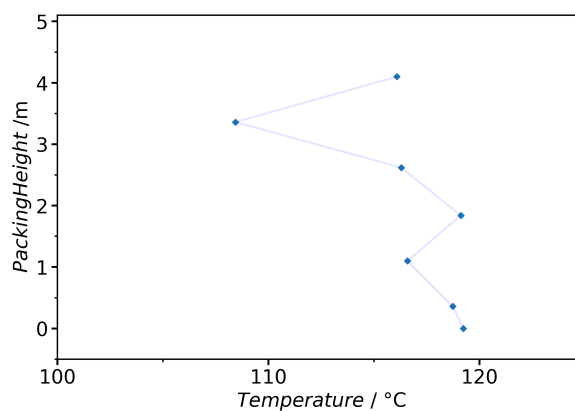
**Table S5:** Overall material balance sample for n-butanol and water

		Feed	Bottoms column 1	Bottoms column 2	Overall losses (kg/h)
Mass fraction (g/g)	n-butanol	0.075	0.003	0.995	0.142
	water	0.925	0.997	0.005	0.098
Overall mass flow rate (kg/h)		3.75	3.38	0.13	0.24

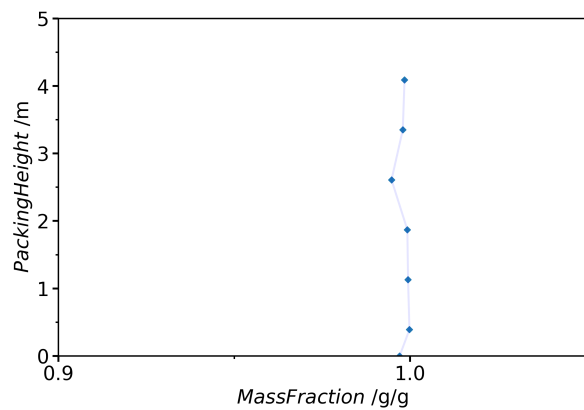
An overall material loss of 6.4 % was observed with respect to the input feed stream for the above experiment.



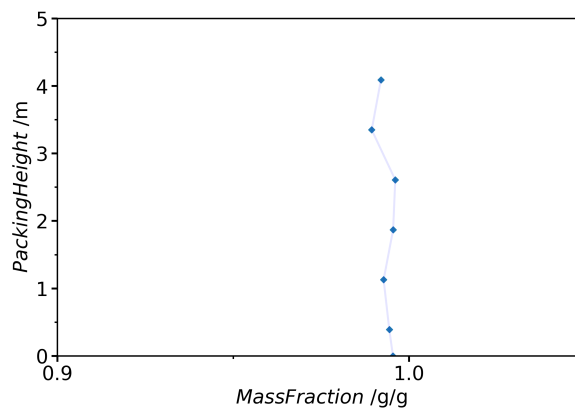
(a) Steady state temperature profile in column 1



(b) Steady state temperature profile in column 2



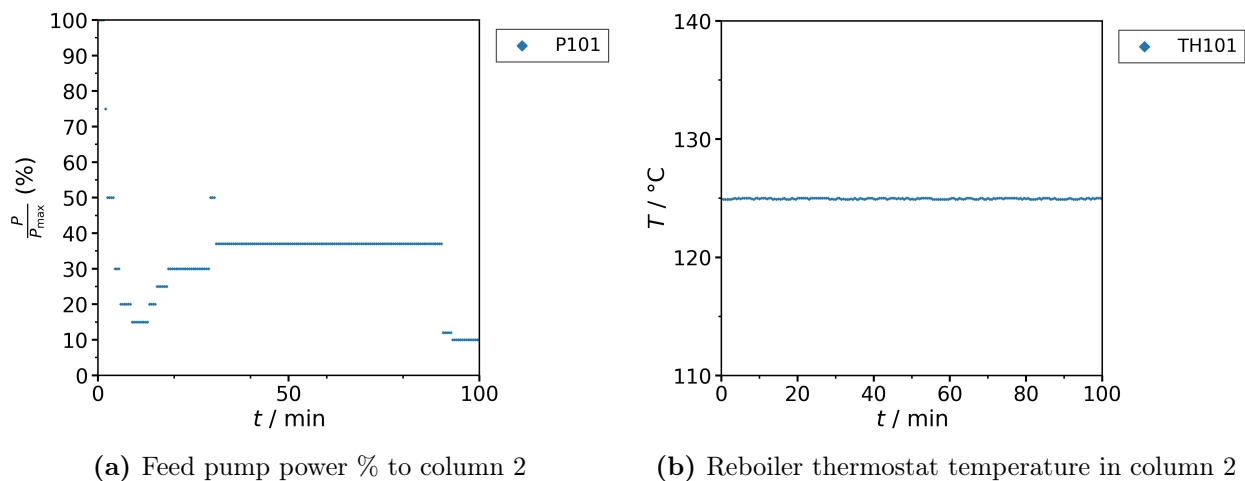
(c) Steady state water concentration profile in column 1



(d) Steady state n-butanol concentration profile in column 2

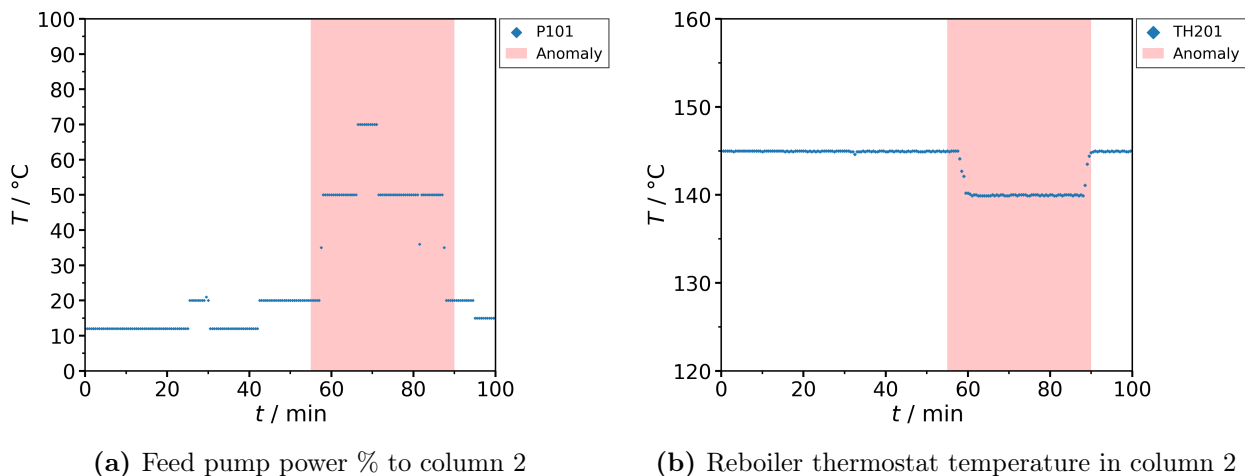
**Figure S6:** Steady state profiles with n-butanol and water

### S3.2 Sample actuator time-series data



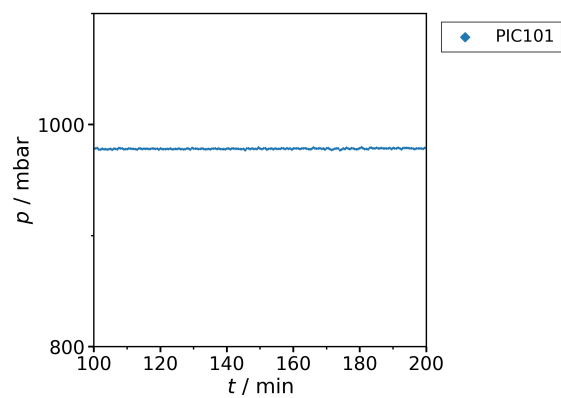
**Figure S7:** Steady state sample actuator data with n-butanol and water during normal operation - operating point 001 - train\_normal\_experiment\_001

The feed pump to column 2, as shown in S7a, is regulated by a PID controller to maintain the level of the buffer tank M106, and therefore exhibits the expected uneven profile.

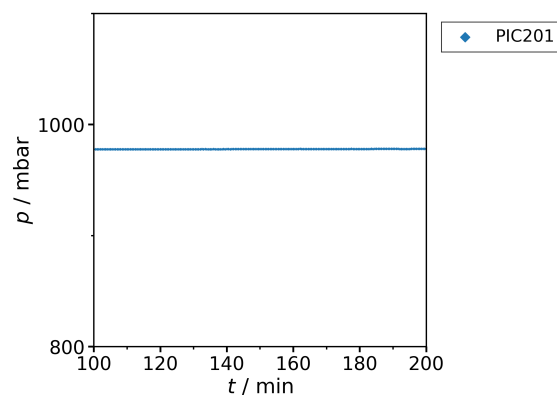


**Figure S8:** Steady state sample actuator data with n-butanol and water during anomalous operation - operating point 001 = train\_anomal\_experiment\_001

### S3.3 Sample time-series data



(a) Head pressure in column 1



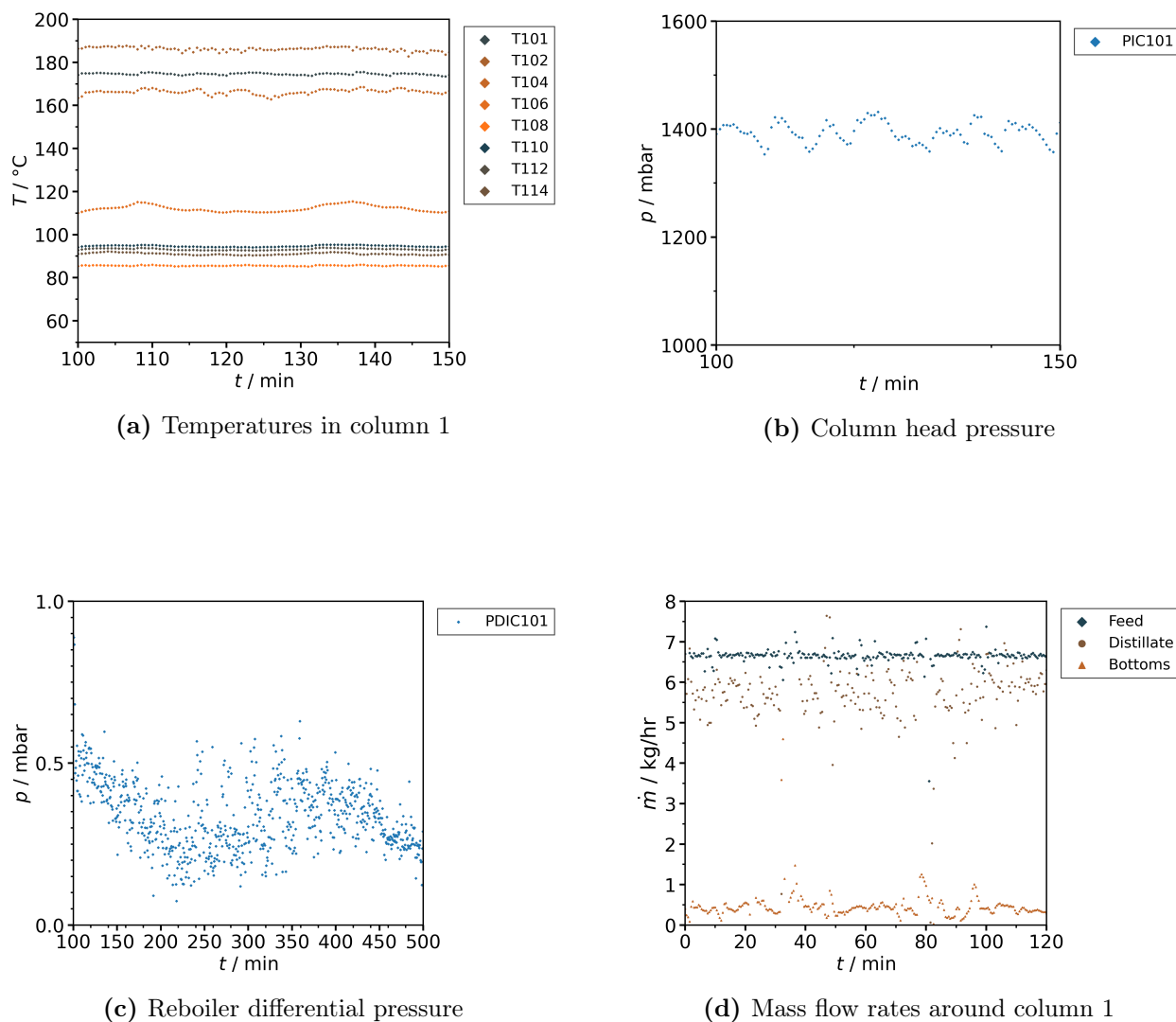
(b) Head pressure in column 2

**Figure S9:** Steady state sample data with n-butanol and water (operating point 10) during normal operation

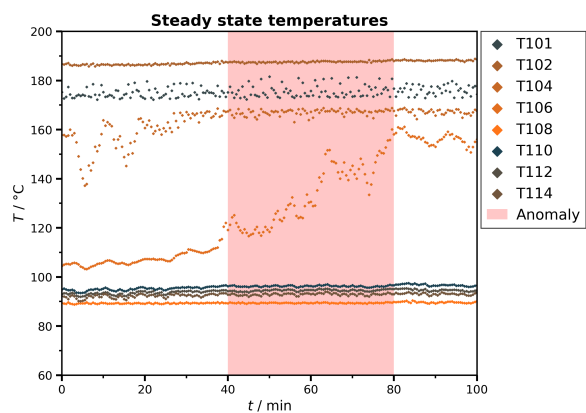
## S4 Experimental campaigns with OME

Figure S10 and S11 represent the steady state sample data from experiments with OME during normal and anomalous operation respectively.

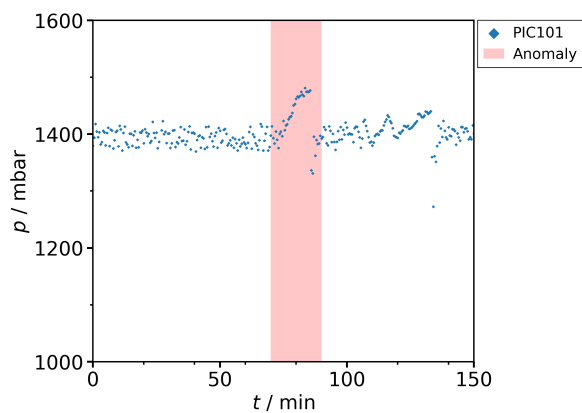
### S4.1 Time-series data sample



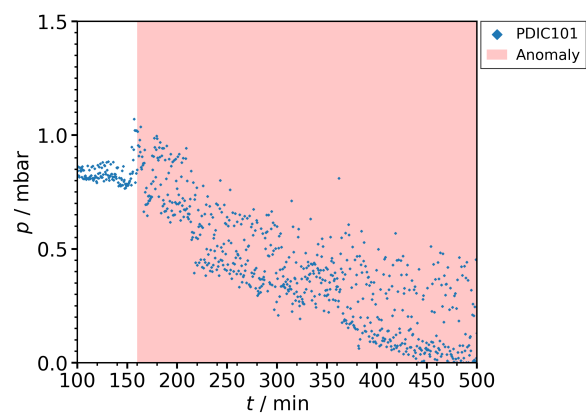
**Figure S10:** Steady state sample data with OME during normal operation  
S10a, S10b - operating point 002 - train\_normal\_experiment\_001  
S10c, S10d - operating point 001 - train\_normal\_experiment\_001



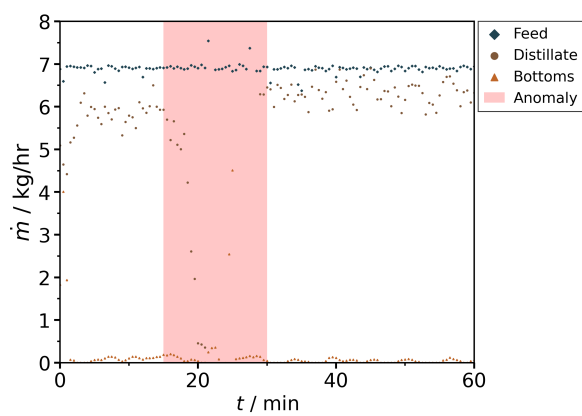
(a) Column temperatures



(b) Column head pressure



(c) Reboiler differential pressure



(d) Mass flow rates around column 1

**Figure S11:** Steady state sample data with OME during anomalous operation

S11a, S11d - operating point 004 - test\_anormal\_experiment\_001

S11b, S11c - operating point 007 - test\_anormal\_experiment\_001

## S5 Anomaly labeling scheme

For each run and at each time step, separate label columns are provided to describe the different anomaly types and their levels of detail. The “common” labels give a simple binary indication of whether an anomaly is present, while the “advanced” labels show how the anomaly develops over time, from its cause to its final effect.

- **Label (common/hard fault):** 0 or 1, indicating when a severe anomaly is present, from the beginning of its cause to the end of its effect.
- **Label (common/soft fault):** 0 or 1, showing the presence of a mild or transient anomaly.
- **Label (common/hard and soft):** 0 or 1, showing the presence of an anomaly related to the process including severe or transient anomalies.
- **Label (common/controller fault):** 0 or 1, showing the presence of an anomaly related to controller behavior rather than the process itself.
- **Label (common/all):** 0 or 1, marking the occurrence of any anomaly, regardless of severity, over the entire duration from cause to effect.
- **Label (advanced/hard fault):** 0, 1, 2, or 3, indicating the phase of a severe anomaly (1: cause active, 2: cause and effect active, 3: only effect remaining).
- **Label (advanced/soft fault):** 0, 1, 2, or 3, showing the phase of a mild or transient anomaly.
- **Label (advanced/controller fault):** 0, 1, 2, or 3, describing the phase of an anomaly related to controller behavior rather than the process itself.

## S6 Visualization website

The user can select one of the three operating scenarios, Water, n-butanol + Water, or OME, and load the corresponding dataset. For the n-butanol and water system, one can visualize the steady-state time series data or concentration profiles. If a steady-state time series is selected, one can select either training data (normal data) or test data (anomalous data). The experiments can be selected by the user. using a drop-down, which is organized by operating point and experiment index. Once the data is selected, the corresponding metadata is displayed, and the file can be visualized in a table or a plot. The users can select the variables to plot, zoom into the plot, customize the axes, select different types of time-series plots (line plot, rolling averages, heatmaps, box plots, autocorrelation, or seasonal breakdowns), and also get information on the sensor selected. If anomalous experiment data is selected, the plot also highlights the anomalous region.