

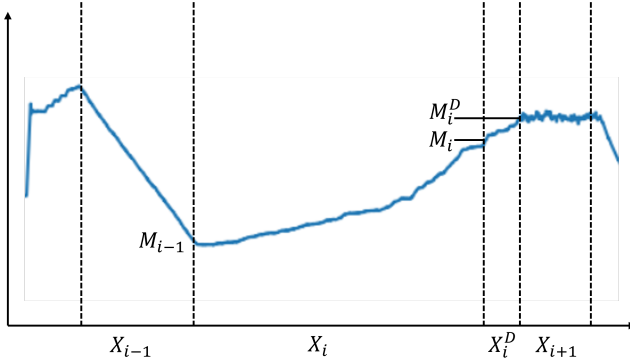
# CHAPTER 1

## Data

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In this section, we will describe and analyze the data used in this thesis. The data stems from a simulation study on a chemical batch production system and comprises six time series from which the time stamps (in hours) and level in a tank is of the most interest. The goal of this section is to describe how different phases of the production covary. The data is chosen as it resembles an actual production data set but is also implemented with what at first glance seem to be fairly realistic variation and noise in measurements. Overall, the point of this example data is to exemplify what one may encounter in a real batch production system and from this try to build a model in order to predict or quantify the behavior of the system or learn hidden (causal) structure important for optimization etc.

We define a set of phases/units  $\mathcal{U}$  that each batch comprises. In this case, units are identified with IDs 1 through 10 (with subunits such as 3.1) described further in Table 1.2. Then, for each unit, we define the stochastic variables  $X_u$  and  $X_u^D$  to be the duration and delay after a unit respectively. It is also important to keep track of the level in the tank after each unit is finished, and we thus define variables  $M_u$  and  $M_u^D$  to be the level in the tank after unit  $u$  and its associated delay respectively. As the units are executed in sequence, as is the case in this data, a simple representation of the variables can easily be visualized and is shown in Figure 1.1 below.



**Figure 1.1:** Exemplification of the variables  $X_i$ ,  $X_i^D$ ,  $M_i$ ,  $M_i^D$ .

## 1.1 Basic statistics

Initially, we present some basic statistics in Table 1.1 for batches and proceed to discuss the nature of the batches, removing outliers and faulty observations etc.

Cycle	#batch	$\mu$	$\sigma^2$	$\sigma$	$\sigma/\mu$
A	66	14.776	3.641	1.908	0.1291
B	64	15.644	3.915	1.979	0.1265
C	61	17.714	2.330	1.526	0.08617
D	60	18.069	6.922	2.631	0.1456
E	60	18.088	9.613	3.100	0.1714
F	63	17.227	7.766	2.787	0.1618

**Table 1.1:** Per cycle batch duration statistics

Each batch comprises several states. These include adding materials (IDs 1 through 4), centrifugation (ID 5), product transfer (the precipitate generated from the centrifugation, ID 6), chemical reaction (ID 7), a post operation state (Probably to let it cool down to a point where it is ready for further processing, ID 8), Cooling of the product (ID 9), material transfer (transfer the gained product before cleaning of the reaction vessel and/or prepare for the next reaction batch, ID 10). Notice that there is a total of 374 batches throughout the 6 observed cycles.

## 1.2 Incompleteness on trailing batches

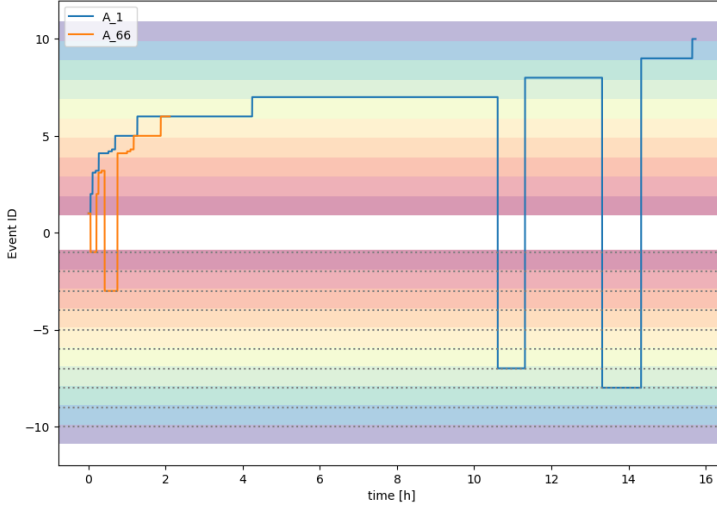
As it may be of interest to investigate the correlation structure of different metrics and variables later on, it is important to understand how each of the batches across the cycles behave. Initially, when looking through the dataset, we observe a few negative phase IDs which will need investigation. However, before we do so, we check that each of the batches actually go through all the states mentioned in [?]. Thus, we take the absolute value of the negative phase IDs to ease the analysis prior to the analysis of the negative phase IDs. After this is done, we observe that not all batches go through all the phases and that some seem to have extra phases not described by [?]. Namely, from Table 1.2, we see that IDs 3 and 4 (which are not described in [?]) have significantly fewer batches going through this phase. But perhaps even more interesting is the final 4 phases where almost all batches goes through these phases.

ID	Count	Description
1.0	374	Addition of liquid raw material Educt1
2.0	374	Addition of liquid raw material Educt2
3.0	181	Addition of liquid raw material Educt3
3.1	374	
3.2	374	Agitation
4.0	163	Waiting for field operation
4.1	374	
4.2	374	Addition of solids
4.3	374	Waiting for control operator
5.0	374	centrifugation
6.0	374	Product transfer
7.0	370	Reaction
8.0	369	Post reaction
9.0	369	Cooling
10.0	368	Material transfer

**Table 1.2:** The number of batches across all cycles that contains at least one observation for each different absolute phase ID.

Investigating when these inadequacies occur reveals that they are the last batch from each of the cycles. For example, the final batch from cycle A only goes to phase 6 (the product transfer). This can however be explained from the fact that simulation only last for 1100 hours for each cycle and is thus simply cut-off here. As we do not know if these final operations were done at the time the simulations were cut off (which is likely not the case), the final phase for each of the final batches should be disregarded. The cut-off can also be observed in Figure 1.2. Furthermore, throwing away 6 incomplete batches out of the total

374 will likely not harm the analysis and is thus thrown away as this will make the analysis much simpler later on.

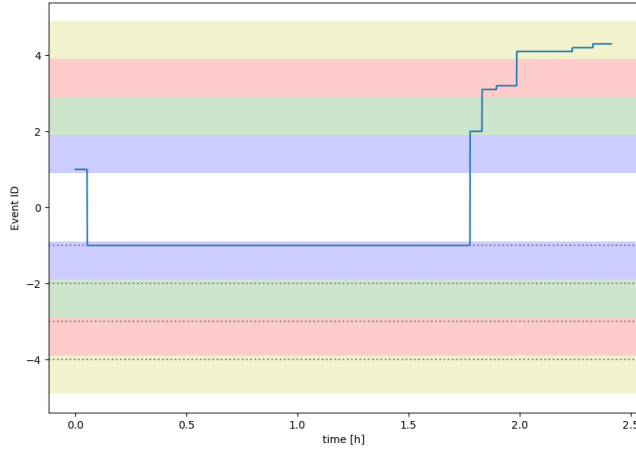


**Figure 1.2:** The first and last batch from cycle A. It is clear that the final batch is cut-off even before the current phase it finished.

After cutting of the final 6 batches, we have a total of 368 batches of which each goes through all the phases. We thus proceed to discuss the negative phase IDs in the following section, where we also discuss the first four phases.

## 1.3 Production phases

This part of the process corresponds to events tagged with ID 1 through 10 but will initially concern itself with ID 1 through 4 as much can be learned from the data set here. In Figure 1.3 an example of how the process evolves over time through the different phases is shown. Immediately, we observe something weird, namely the negative event IDs.



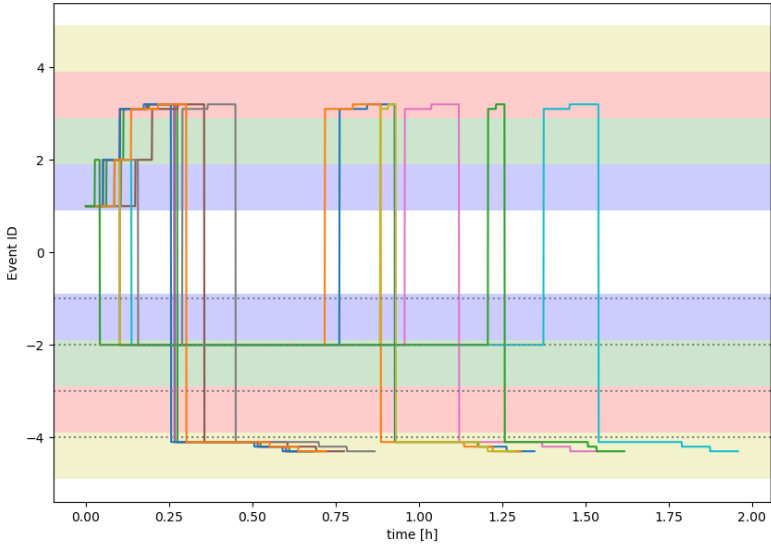
**Figure 1.3**

To see what is going on here, from data we can see that negative values occur throughout all the six cycles. More specifically, for each negative phase observed, we log in which cycles this occurs. The result is shown in Table 1.3. Notice that -4.1, -4.2 and -4.3 only show up in cycle F, which from [?] is known to be the only one with wrongly labelled phases. We thus suspect that this is indeed the case for these labels and might just have supposed to be the original 4.1, 4.2 and 4.3. To see if nothing funny goes on with these values, these batches are plotted as in Figure 1.3 in Figure 1.4.

Figure 1.4 shows that nothing weird is going on except for the negation of the sub phase's ID. The same can be said for the remaining of the cases where phase ID -4.1, -4.2 and/or -4.3 is used. We thus conclude that these may simply be wrongly labelled thus we convert every such instance to its absolute value and continue with this modified data set from this point on.

Event \ Cycle						
	A	B	C	D	E	F
-1						
-2						
-3						
-4						
-4.1						
-4.2						
-4.3						
-5						
-6						
-7						
-8						
-9						
-10						

**Table 1.3:** Occurrences of negative phases IDs. It is observed that sub phases 4.1, 4.2, 4.3 only occur in cycle F which is known to be the only cycle with wrongly labelled phases.



**Figure 1.4:** 13 of the 48 batches with at least one of the sub phases 4.1, 4.2 4.3 negative.

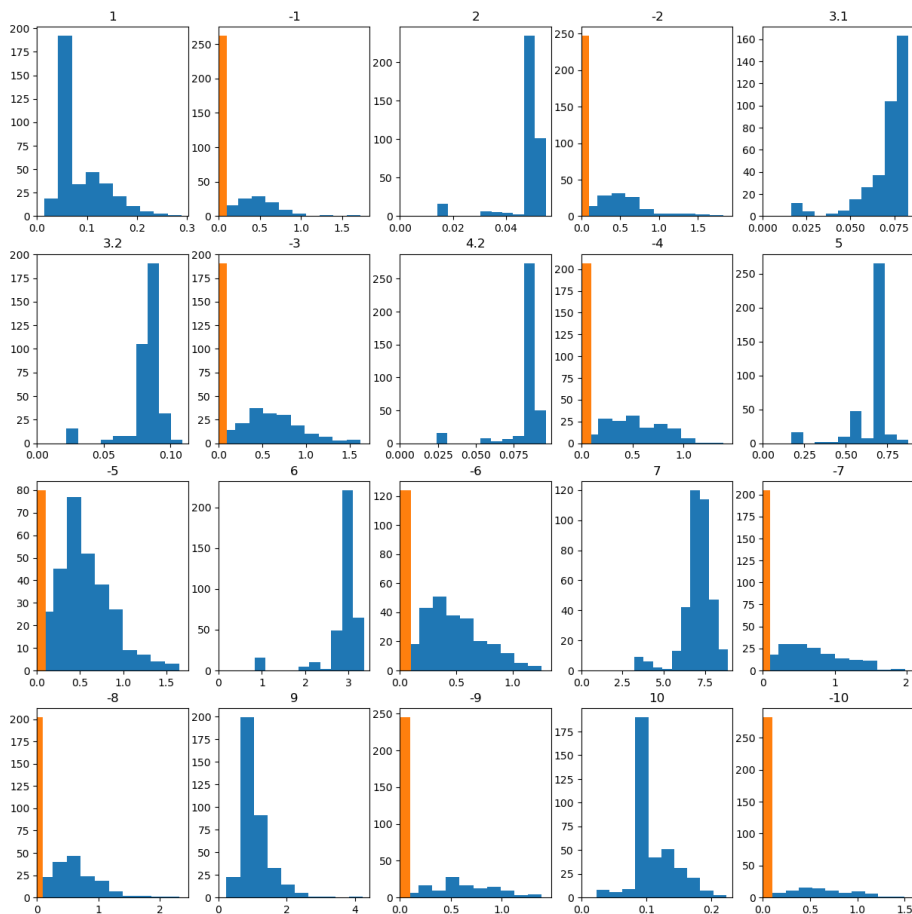
Having converted the above sub phase IDs we summarize the current situation in regard to negative phase IDs in the following table, Table 1.4. Now all the remaining occurrences of negative phase IDS does not seem to exhibit any structure from looking at Table 1.4. We thus proceed to understand what is going on with the remaining negative phase IDs.

Event \ Cycle	A	B	C	D	E	F
-1						
-2						
-3						
-4						
-5						
-6						
-7						
-8						
-9						
-10						

**Table 1.4:** Occurrences of negative phases IDs. It is observed that sub phases 4.1, 4.2, 4.3 only occur in cycle F which is known to be the only cycle with wrongly labelled phases.

When plotting different batches, it is clear that the negative phase IDs only occur at the end of a phase e.g. -1 only happens after 1 and so on. This together with the fact that -3 and -4 also only happen after 3.1, 3.2 and 4.1, 4.2, 4.3 respectively (and we never see a phase labelled 3 or 4) indicate that the negative phase IDs could very well correspond to delays at the end of a phase, which both makes sense from a production point of view but also from [?] where they note that all simulated cycles have been implemented with delays.

At this point, it would seem that the labels of the processes are understood for phases 1 through 10 corresponding to the actual production in each batch. Thus, we proceed by searching relationships and otherwise quantifying the durations of each phase, both delays and duration for each of the phases. As a beginning, histograms for each of the phases and delays are plotted in Figure 1.5. Notice that phases 4.1, 4.3 and 8 are not shown, this is because they always last 15 min, 5 min and 2 hours respectively with the only derivation being in machine precision either when loaded or during calculations. Furthermore, notice that for the negative IDs i.e. the delays, the orange bar. This bar represents the cases where no delay was observed which is thus modelled as an atom at 1.



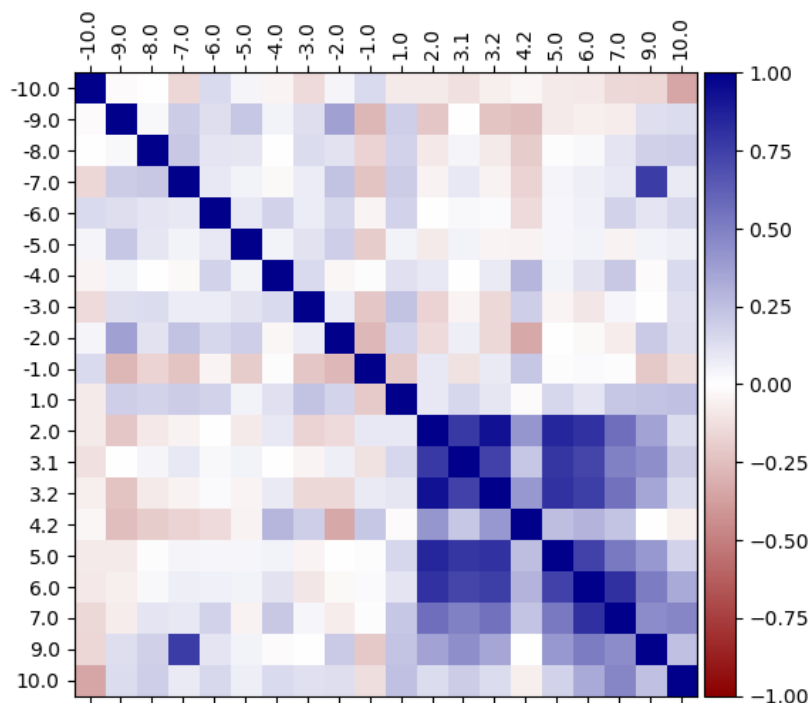
**Figure 1.5:** Histograms of all phases and delays which are non-constant.

Apart from the above comments, not much catches the eye when looking at Figure 1.5, and we thus proceed by checking if any correlation is immediately present.

### 1.3.1 Correlations

Lige en korrelationsmatrix



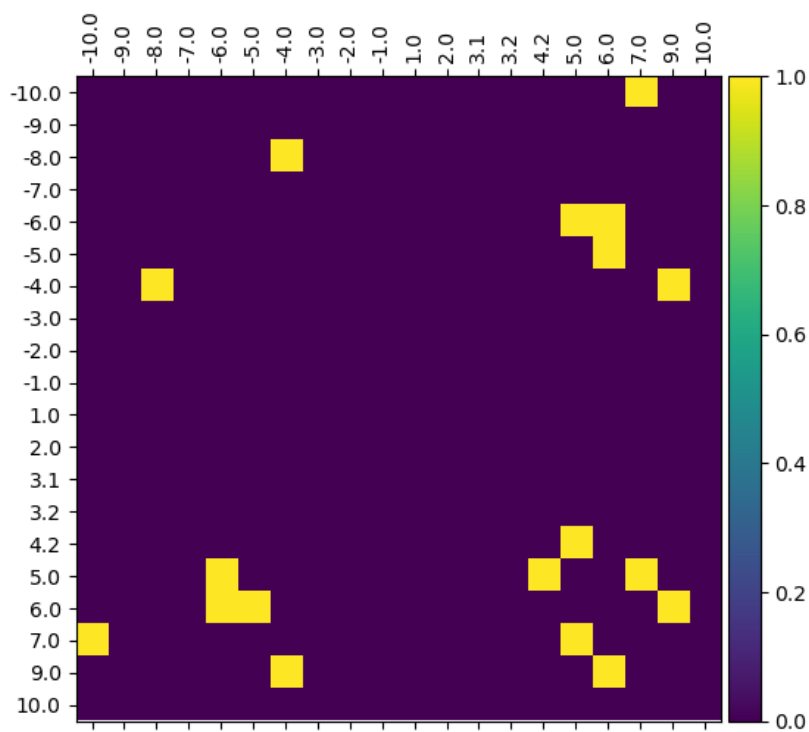


**Figure 1.6:** Correlation matrix for all phases with non-constant duration.

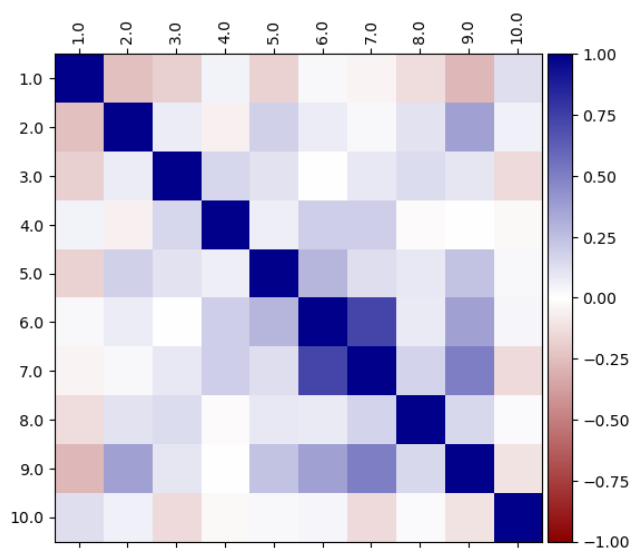
9 og 10 er ikke specielt korreleret med noget (afkøling og materiale overførsel). Ellers er 2 fremt il og med reaktionen alle korrelerede med hinanden. Eftersom rent fysisk det udvikles i tid, må handlingen i 2 påvirke de næste osv.

Umiddelbart lidt spøjst hvis delay på 7 (reaktion) skulle have noget med tiden for afkøling at gøre, især at den skulle være positiv (ville man ikke tro delay efter produktion ville afkøle mere og dermed reducere behov for afkøling, medmindre varmt steam bliver tilføjet også under delay på 7)

Herunder er samme korrelationsmatrix, dog hvor delay og phases varighed lagt sammen (også med sub phases såsom 3.1, 3.2 og -3 tilsammen bliver 3)

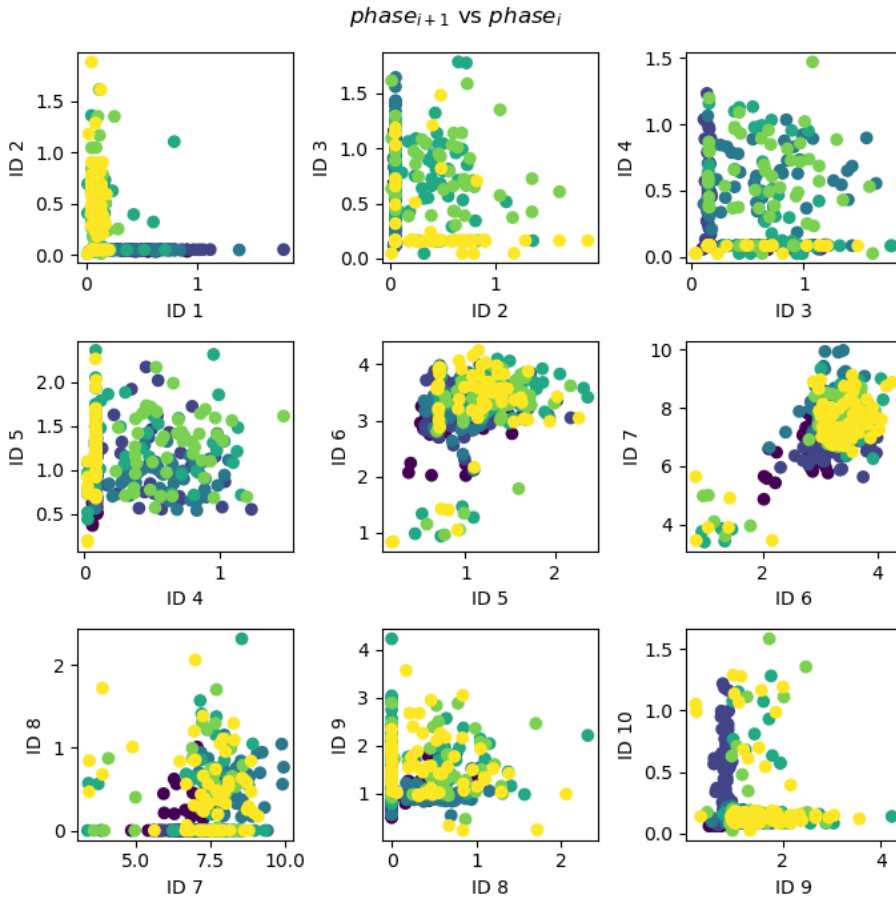


**Figure 1.7:** Permutingtest med  $\alpha = 0.05$ . Also run with less simulations but same result at 1 mil and 10k sims. The Benjamin-Hochberg procedure on the upper (or lower) triangle reveals that none of the correlations are significant.



**Figure 1.8:** Correlation matrix for all phases collapsed

Ligeledes scatter plots for superdiagonalen i ovenstående matrix. Altså phase 1 overfor phase 2, phase 2 overfor phase 3 osv. Er farvelagt efter hvilken cycle de kommer fra. Table 1.4 forklarer hvorfor nogle af de horisontale fremkommer sammen med Figure 1.5 (selve produktionstiden er ret kort sammenlignet med delay.)



**Figure 1.9:** Phases vs their next phase when collecting everything regarding a single phase into a total time duration

## 1.4 Cleaning operations

Sometimes, the vessel is cleansed. This is however not every time after a batch so might be interesting to investigate further. Initially, per cycle, the cleanings are summarized in the following table with basic statistics. As can be seen, there is quite some differences.

The most notifiable differences per batch are the number of cleanses especially when comparing to Table 1.1. For the first two cycles, the cleanses seem to be in between every batch, which is indeed also the while the later four are only sometimes. Furthermore, although the cleanses are between every batch for cycles A and B, the variances are extremely different. For the last four cycles, they seem to be grouped further, E and F are very alike while cleanses in C and D are generally longer although D has a substantially smaller variance than C.

Cycle	#ops	min	max	$\mu$	$\sigma^2$	$\sigma$	$\sigma/\mu$
A	65	1.113	3.067	1.917	0.269	0.518	0.270
B	63	1.324	1.751	1.566	0.00883	0.0939	0.0600
C	9	1.544	3.306	2.153	0.277	0.526	0.245
D	10	1.474	2.009	1.581	0.0212	0.146	0.0922
E	10	0.827	1.584	1.465	0.0462	0.215	0.147
F	10	0.748	1.610	1.466	0.0595	0.244	0.166

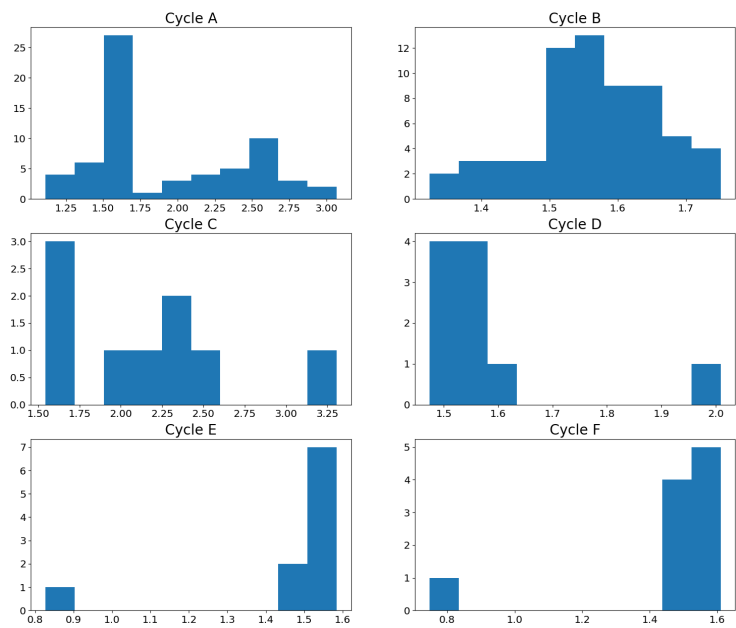
**Table 1.5:** Per cycle cleansing statistics

Cycle	A	B	C	D	E	F
$\mathbb{E}[\sum X_u]$	13.993	13.898	15.343	14.471	14.589	14.418
$\text{Var}(\sum X_u)$	0.95636	0.46587	0.76111	4.9589	4.2678	5.3545
$\sum \text{Var}(X_u)$	0.50590	0.31182	0.36667	1.8322	1.5788	1.9696
$\mathbb{E}[\sum X_u^D]$	0.96398	1.9402	2.4503	3.6050	3.7390	3.0041
$\text{Var}(\sum X_u^D)$	0.31843	0.39117	0.90187	1.2468	1.2787	1.0462
$\sum \text{Var}(X_u^D)$	0.34921	0.53198	0.74914	1.4357	1.2454	1.3099
$\mathbb{E}[\sum X_u X_u^D]$	1.9321	1.5001	4.8191	6.4225	6.0405	6.3343
$\text{Var}(\sum X_u X_u^D)$	3.7798	0.89920	16.870	22.133	12.660	16.194

**Table 1.6:** Each of the time related variables  $X_i$  and  $D_i$  and variance description.

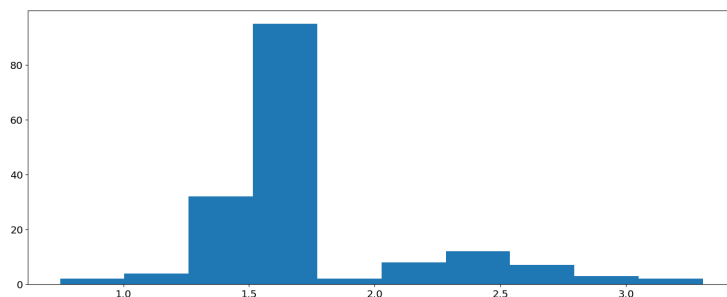
To verify these observations and potentially discovering more important facts of their probability distributions, histograms are plotted in the following Figure 1.10. We indeed again observe the likeliness between the cycles A and B, C

and D, E and F respectively. Also, for the first two cycles and more so cycle B, the cleaning times are somewhat normally distributed although cycle A has a very heavy right tail in that case. The later four cycles only have 10 observations but the mode (i.e. peak) seem to be about the same.



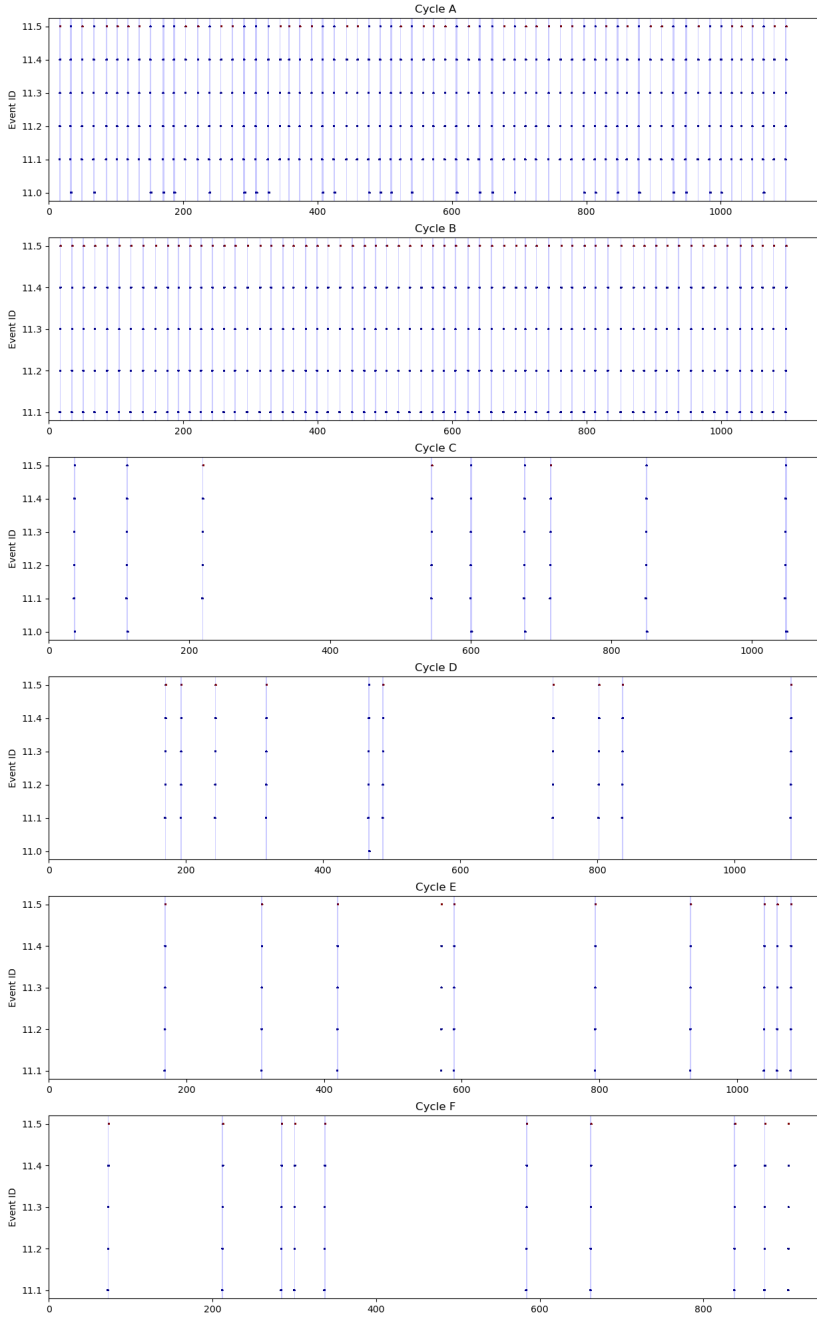
**Figure 1.10:** Each of the 6 cycles, cleaning operations histograms.

From the above observation of like modes one may want to observe the histogram of the combined set of cleaning times. In particular, under the hypothesis that the durations are actually from the same probability distributions and realized independently within each cycle a histogram of all the observations are of interest and is shown in Figure 1.11 below.



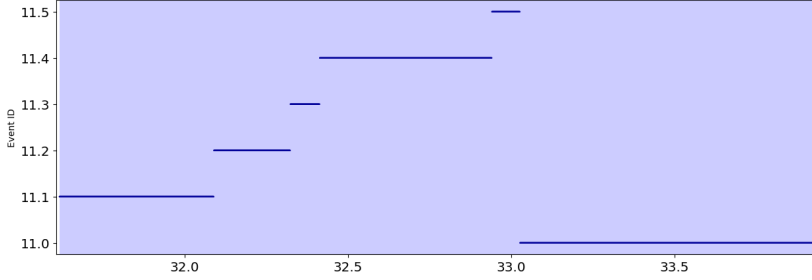
**Figure 1.11:** Combined cleaning operations histograms.

Finally, to get a better overview of the irregularities in the number of cleaning periods (mostly concerning cycles C through F), each cleaning operation is shown in the following Figure 1.12. The vertical shaded rectangles signify the period in which a cleaning operation is taking place. Furthermore, the event IDs are shown but to get a clearer view on what is going on, a single rectangle (zoomed in) is shown in Figure 1.13.



**Figure 1.12:** Each of the 6 cycles, cleaning (corresponding to `BatchID = 0`). Each (Cleaning Procedure), CIP, is highlighted with an opaque interval (the blue rectangles). The dots marked with red (only ID 11.5, but not all of these are red), is if the Cleaning ID is 0.





**Figure 1.13:** A single blue rectangle zoomed in

It is observed that the observations marked with red in figure 1.12 occur exactly when that specific cleaning operation does not go to the state 11.0 after the flush of the tank (event ID 11.5) and vice versa. It is hard to conclude what this may mean, but the cleaning being in state 11.0 may indicate that the system is idle before continuing the next batch like what is observed from the other steps of the process flow. Also, it is noted that while the red dots occur nothing else is happening according to the dataset.

From a modelling point of view, the cycles C through F can be thought of as the cleansing operation having a probability of not happening or equivalently as having a duration of 0. It is thus of interest to observe what the probability of cleaning after an operation is. From Table 1.1 and Table 1.5, we that indeed for cycles A and B, the probability is 100 % when disregarding the possibility of cleaning after the final batch. Hence, we see that for the remaining cycles, the probabilities of cleaning the tank after an operation are as in Table 1.7

Cycle	% cleaning
A	100.00
B	100.00
C	15.00
D	16.95
E	16.95
F	16.13

**Table 1.7:** Per cycle probability of cleaning

Furthermore, let  $C_i$  denote whether the  $i$ th batch is followed by a cleaning of the tank or not. It is then of interest if the next batch is followed by a cleaning given whether the current batch is followed by a cleaning. In particular, we count for each of the cycles the transitions which are shown in the following tables. Notice that the number of observations is two less than the total number of batches within each specific cycle. This is due to the last batch is never followed by

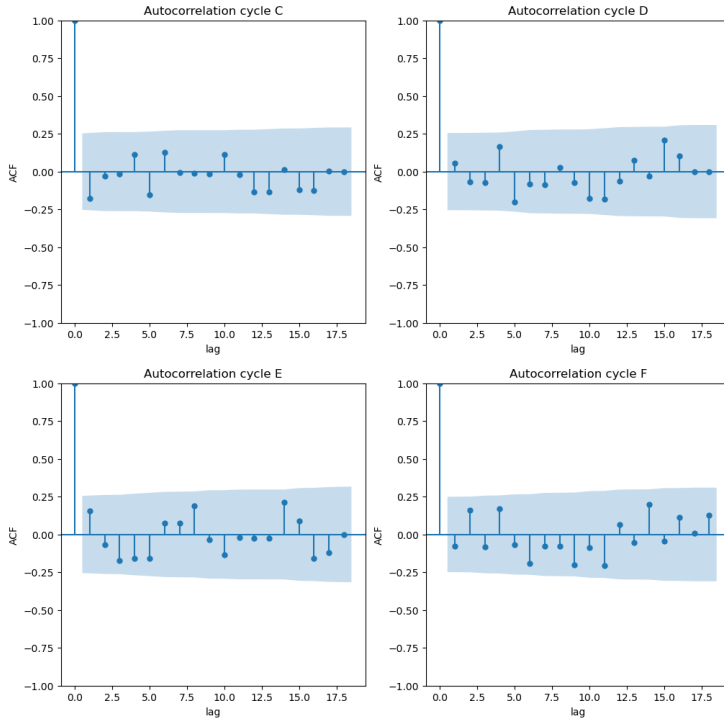
a cleaning (nor is the first batch superseded by a cleaning procedure) which results in one less observation and also due to the fact that we are logging transitions and hence lose another observation. To test for randomness, a Chi-squared test is carried out on each of the cycles to check for independence. It is observed all the cycles exhibit independence between the groups i.e. there is no statistical evidence for information is gained about if the next batch is followed by a cleaning operation given whether the current batch is followed by a cleaning operation.

$C_i \backslash C_{i+1}$		No	Yes
		41	9
No		9	0
Yes			
(a) C, $p = 0.3293$			
$C_i \backslash C_{i+1}$		No	Yes
		41	7
No		7	3
Yes			
(c) E, $p = 0.3532$			
$C_i \backslash C_{i+1}$		No	Yes
		41	8
No		7	2
Yes			
(b) D, $p = 0.6456$			
$C_i \backslash C_{i+1}$		No	Yes
		41	9
No		9	1
Yes			
(d) F, $p = 1.0000$			

**Table 1.8:** Contingency table for Cycle C-F

Thus collecting the observations from all the last four cycles, we may want to model the atom of the cleaning procedure independently of the previous batch and with a probability of 0.8375 corresponding to the cleaning procedure only being carried out 16,25% of cases.

Finally, we show the autocorrelation function for each the four cycles C-F in Figure 1.14 and note that all the ACF stay within the 95% confidence interval.



**Figure 1.14:** Autocorrelation function for each of the final 4 cycles. As can also be seen from this there seem to be no information to be gained of  $C_i$  from  $C_{i-1}$ .