ContCarSim: Continuous Carousel Simulator documentation

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Index

1. Process description

The carousel reproduced by the simulator is sketched in Figure 1. A schematic P&ID of the process is provided in Figure 2, with the legend of the equipment reported in Table 1. Figures 1-2 and Table 1 also report the sensors and controllers network implemented in the carousel simulator.
The unit can continuously process an inlet slurry stream into a dry crystals cake. The slurry system considered in the simulator is composed by pure paracetamol crystals in a mother liquor composed by pure ethanol. The carousel features five cylindrical ports, each one of 15 mm diameter, which allow a maximum hold-up of 10 mL. The ports are embedded in a main cylindrical body, aligned to five processing stations (Stations 1-5). For illustrative purposes, in Figure 2 the stations are represented as vessels in series (V-101-V-105), although the actual layout of the carousel is as in Figure 1. Stations 1-4 present a filter mesh at the bottom (F101-104). Station 5 is, instead, open at the bottom for cake discharge, which is enabled by the action of a pneumatic piston (not shown). The pressure gradient for filtration and drying is provided by a compressor (P101), connected to the top section of all the stations, whereas all stations are maintained at atmospheric pressure on the bottom section.
The carousel operates in cyclic mode: processing cycles, during which every port processes batch-wise the material therein contained, are alternated to carousel rotations, during which the ports containing the material being processed are moved to the following station. Carousel rotations are logically represented in the P&ID as material streams, whose flows are controlled by FC-101. The alternating processing cycles and carousels rotations are interrupted when significant mesh fouling is

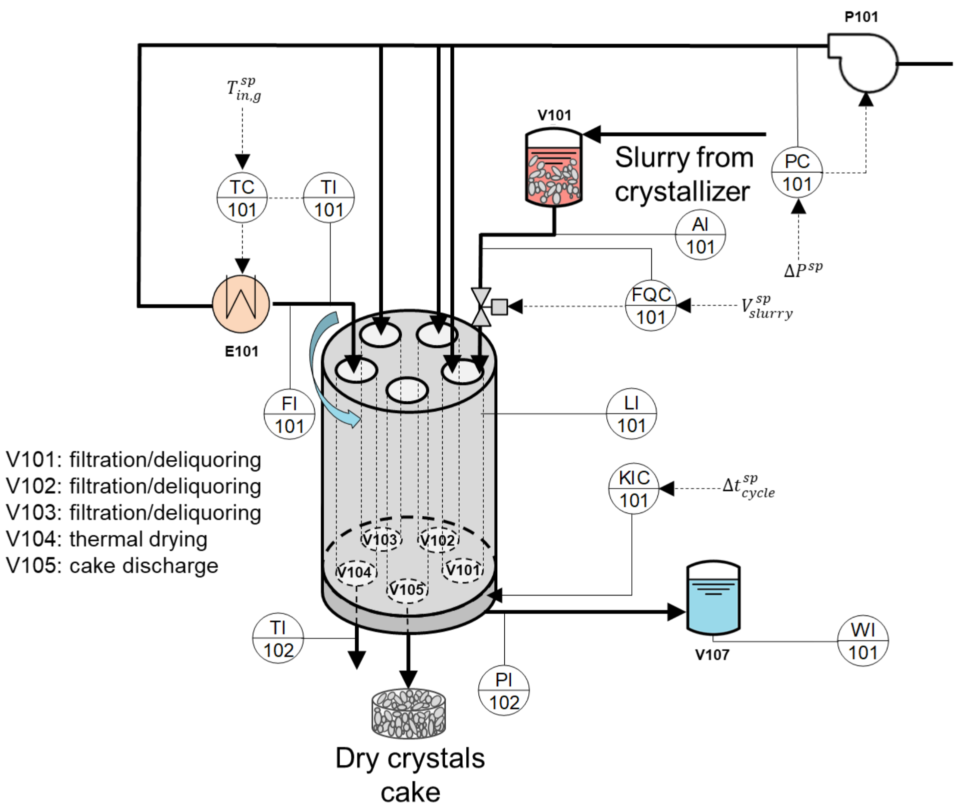

Figure 1. *Schematic drawing of the carousel for continuous integrated filtration-drying of crystallization slurries mimicked by the simulator. Filter meshes are placed at the bottom of V-101-V04 (i.e., processing stations 1–4). Station 5, instead, is open for cake discharge. In physical carousels, controllers FQC-101 and KIC-101 are routines of the programmable logic controllers of the unit.*

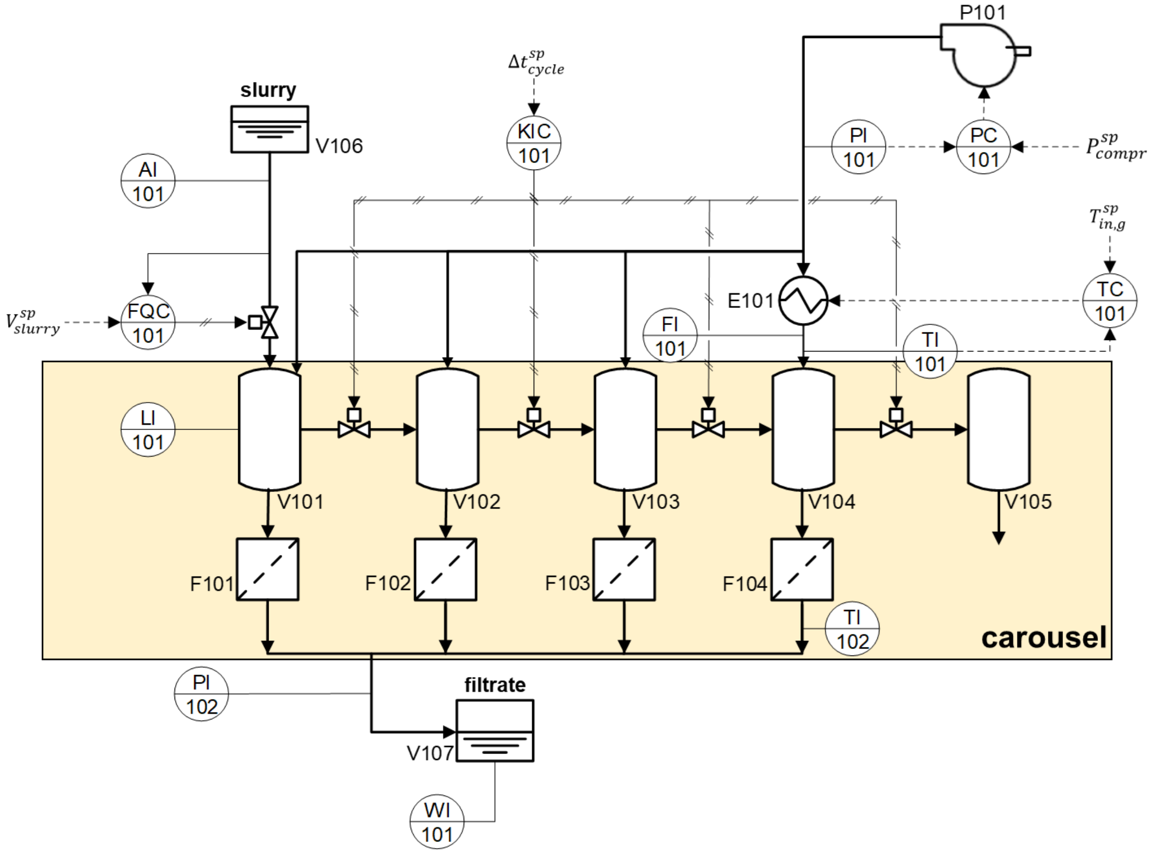

Figure 2. *Logical P&ID of the carousel illustrated in Figure 1. The equipment legend is reported in Table 1.*

detected: a cleaning-in-place cycle is then triggered. In this case, the material already loaded in the carousel ports is regularly processed during the following cycles, but no more slurry is loaded into the first station. Hence, at every cycle following cleaning-in-place initiation, an increasing number of ports will be empty. When all ports are empty, all meshes are automatically cleaned by sending a cleaning solvent into the carousel. In the simulator, mesh cleaning is assumed to occur instantaneously.

Stations 1-3 are dedicated to filtration and deliquoring, while in Station 4 thermal drying is carried out. In Station 5, only cake discharge occurs. Slurry processing occurs as follows. The crystallization slurry is fed to Station 1 at the beginning of every cycle, by keeping the valve between the slurry tank (V-106) and Station 1 open. After slurry feeding, a subsequent filtration step starts in Station 1, and it continues until filtration ends. If a carousel rotation is triggered before filtration finishes, filtration will continue in Station 2 (and, possibly, in Stations 3 and 4). During filtration, the liquid contained in the slurry is filtered out of the port by the action of the pressure gradient generated by P101, and stored in filtrate collector V-106, while the crystals are retained on top of the filter mesh, leading to cake formation. We distinguish between actual filtration, when there is a slurry hold-up on top of the cake being formed, and the subsequent deliquoring, during which the sole remaining liquid is the one retained inside the cake pores. Upon deliquoring, the liquid in the cake pores is mechanically displaced out of the cake by the action of the pressure gradient, until a certain pore saturation equilibrium is achieved. Filtration duration depends on the cake properties and on the pressure gradient itself. Depending on filtration duration, the cake can be partially deliquored in Stations 1-3, or it might even enter Station 4 with some slurry hold-up (drying cannot be properly conducted in this situation, which should be avoided). Thermal drying is performed in Station 4 by flowing a hot air stream through the cake.

Table 1. *Legend of Figures 1-2, including unit operations and ancillary equipment.*

Name	Description
Unit ID	
F101-F104	Filter mesh below Stations 1-4 (respectively)
P101	Compressor
E101	Drying air electrical heater
V-101	Carousel Station 1
V-102	Carousel Station 2
V-103	Carousel Station 3
V-104	Carousel Station 4
V-105	Carousel Station 5
V-106	Filtrate collector
V-107	Slurry tank
Controllers and sensors	
AI-101	Slurry concentration sensor
FC-101	Fed slurry volume controller
FI-101	Flowmeter for drying air entering carousel ports
KIC-101	Carousel rotation controller
LI-101	Camera system measuring volume of fed slurry and cake height
PC-101	Compressor pressure controller
PI-101	Indicator of pressure provided by compressor
PI-102	Filtrate pressure indicator
TC-101	Drying air inlet temperature controller
TI-101	Thermocouple for drying air inlet temperature
TI-102	Thermocouple for drying air outlet temperature
WI-101	Scale for inferring filtrate flowrate

2 How to use the simulator

Figure 3 shows the logical structure of the simulator, while Figure 4 elucidates the set of scripts and functions that make up the simulator, together with the order and the logics with which they are called.

2.1 Inputs

The simulator inputs are reported in Table 2, and have to be set up in the script `run_carousel.m`.

Table 2. Simulator inputs.

Variable name in `run_carousel.m`	**Variable**	**UOM**	**Admissible values**
`control_mode`	Flag for selecting control strategy: 0: open-loop 1: closed-loop controller of sample case study (Section 4) Other modes can be set up by the user	-	0, 1, other values set up by user
`disturbance_scenario`	Flag for selecting disturbance scenario: (see Section 2.4) 0: normal operating conditions 1: slurry concentration ramp change 2: specific cake resistance step change	-	0, 1, 2
`total_duration`	Simulation duration	s	$[0, +\infty)$
`u_nominal.t_rot`	Nominal cycle duration	s	$[5, +\infty)$*
`u_nominal.V_slurry`	Nominal fed slurry volume	m^3	$[5\times10^{-7}, 1\times10^{-6}]$
`u_nominal.P_compr`	Nominal compressor pressure (gauge)	Pa	$[1\times10^{4}, 2\times10^{5}]$
`u_nominal.Tinlet_drying`	Nominal drying air inlet temperature	K	[293, 353]
`cryst_output.conc_slurry`	Nominal slurry concentration	kg/m^3	[50, 500]
`control_interval`	Time interval at which `run_carousel.m` is called	s	Multiples of 1
`sampling_interval`	Sampling interval for measurements and states in simulation output	s	Submultiples of 1

***MUST BE AN INTEGER**

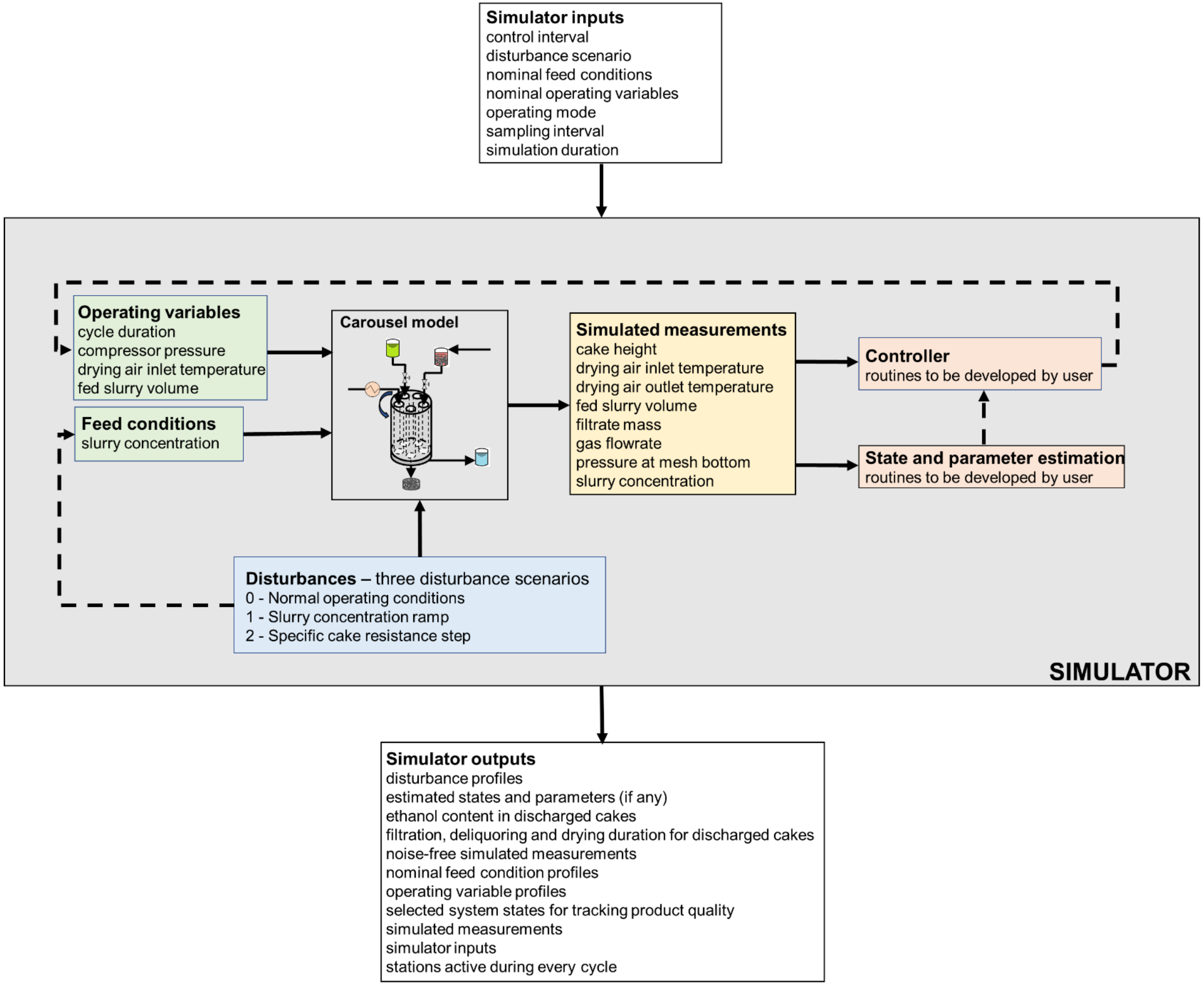

Figure 3. *ContCarSim: schematic elucidating the logical simulator structure.*

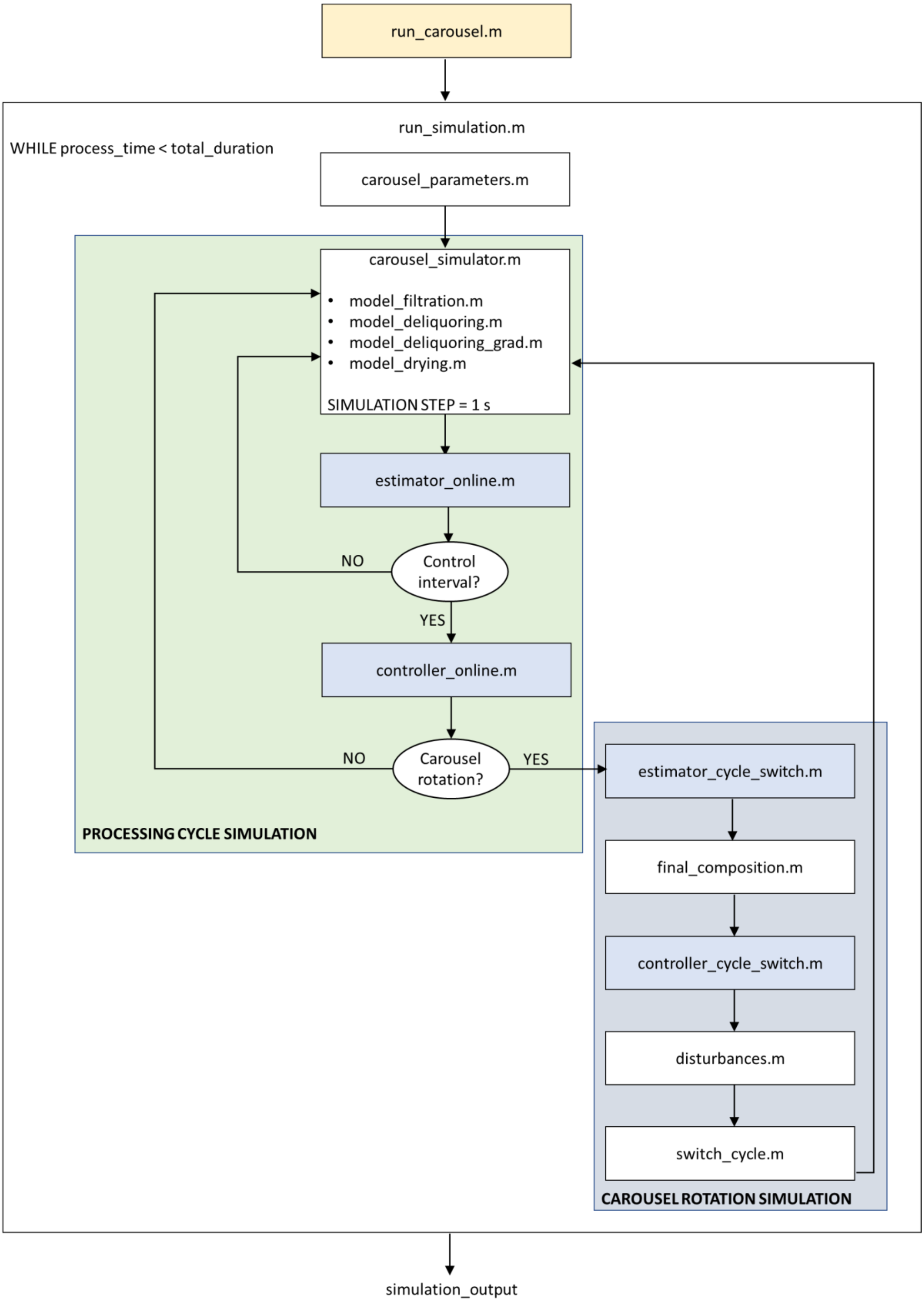

Figure 4. *ContCarSim: computational structure of the simulator, showing the logics and the order with which the functions and scripts of the simulator are called. Yellow: script to be (optionally) edited with desired operating settings and then run. Blue: functions that can be edited for modifying the control strategy.*

2.2 Simulation execution

The simulation is initialized by running the script `run_carousel.m`, after having set up the desired inputs. The simulation is carried out as shown in Figure 4. Function `run_simulation.m`, handling the simulation routine, is automatically called. The parameters of the model are automatically retrieved from function `carousel_parameters.m`.

Then, the simulation of the first processing cycle begins. The `carousel_simulator.m` function is called for simulating 1 s of carousel operation. The `estimator_online.m` function is then executed. By default, `estimator_online.m` is an empty function, but it can be modified by the user for setting up parameter and state estimation routines.

Afterwards, carousel operation is simulated again for a duration of 1 s with `carousel_simulator.m`, or, if the control interval specified by the user has been achieved, the `controller_online.m` function is called, to update the value of the operating variables as specified by the control laws implemented in `controller_online.m`. The operating variables are (Figures 1-2):

- The set-point of the inlet drying air temperature $T_{in,g}^{sp}$;
- The set-point of the slurry volume fed to the carousel at every cycle V_{slurry}^{sp};
- The set-point of the cycle duration Δt_{cycle}^{sp};
- The set-point of the pressure provided by the compressor P_{compr}^{sp}.

Within the default control mode 0, the process is operated at open-loop. Therefore, the set-points of the lower-layer controllers (FQC-101, PC-101, TC-101, and KIC-101) coincide with the nominal values set by the user (Table 2). If closed-loop routines are implemented, the lower-layer controllers set-points are instead adjusted during carousel operation, based on the control laws implemented in `controller_online.m`.
The drying air inlet temperature ($T_{in,g}$), the pressure provided by the compressor (P_{compr}), and the cycle duration (Δt_{cycle}) are assumed to be perfectly controlled, namely the actual responses perfectly track the relevant setpoints. The fed slurry volume (V_{slurry}) is instead subject to Gaussian fluctuations around the set-point, to reflect the behavior of real life carousels, as outlined in Section 2.4. Moreover, for cycles during which V-101 is empty due to the cleaning-in-place routine, V_{slurry} is automatically set equal to zero. Function `controller_online.m` also contains a sample closed-loop control routine (control mode 1), illustrated in the sample case study (Section 5).

Functions `carousel_simulator.m`, `estimator_online.m`, and `controller_online.m` are subsequently called until the cycle time reaches the current cycle duration Δt_{cycle}. At that point, the following functions are called:

- `estimator_cycle_switch.m`: by default an empty function, that can be modified by the user for setting up parameter and state estimation routines;
- `final_composition.m`: calculates the composition of the discharged cake, if there is any, and stores other variables that are outputs of the simulator;
- `controller_cycle_switch.m`: updates operating variables following control laws set up by user. The default implementation acts only on V_{slurry}, setting it to zero for cycles in which V-101 is empty, and to the nominal fed slurry volume set up in `run_carousel.m` in all the other cases;
- `disturbances.m`: updates the value of the disturbances for the following cycle;

- `switch_cycle.m`: handles the carousel rotation routine.

Subsequent processing cycles and carousel rotation routines are simulated, until the set total process duration is reached. At that point, the simulation is terminated, and the simulation output object (`simulation_output.mat`) is generated.

2.3 Outputs

The structure of `simulation_output.mat` is elucidated in Table 3. Note that `simulation_output.mat` is generated only if at least one cake has been discharged by the carousel, namely if a large enough total process duration has been specified, compared to the set cycle duration.

The fields of `simulation_output.mat` correspond to the simulator outputs in Figure 3:

- `states`, storing the value assumed by selected system states during the simulation;
- `measurements`, storing the process measurements collected from the sensors reported in Figures 1-2 and Table 1;
- `measurements_nf`, storing the noise-free values of the process measurements;
- `disturbances`, containing the values assumed by the disturbances during the simulation (Section 2.4);
- `operating_vars`, storing the profiles of the operating variables;
- `x_estim`, containing the states and parameters estimated through `estimator_online.m` and `estimator_cycle_switch.m`;
- `feed`, storing the nominal slurry concentration profile during the simulation;
- `cakes_proc_times`, reporting the filtration, deliquoring and drying duration undergone by all the cakes discharged from the carousel;
- `final_content`, listing the ethanol mass fraction in all the discharged cakes;
- `active_stations`, summarizing which stations where active during which carousel cycle (as outlined in Sections 1, 2.4 and 4, certain stations are alternatively empty during carousel operation, due to the cleaning-in-place routine);
- `settings`, containing the settings that were specified in `run_carousel.m` before initiating the simulation.

Of all the simulation outputs, the only ones available in physical carousels are those contained in the `measurements` **field**.

To retrieve the actual value of the variables affected by disturbances from the simulation output:

- **fed slurry concentration**: the actual concentrations of the slurries fed to the carousel in all cycles are obtained from the product of:
  `simulation_output.disturbances.c_slurry` with
  `simulation_output.feed.c_slurry_nom_vector`;
- **drying kinetic parameter and heat transfer coefficient** between cake and air during drying: the nominal values of the parameters vary during every cycle, following the drying model presented in the companion paper, and are not provided in the simulation output. The multiplicative coefficients acting as disturbance, varying at each cycle, are accessible from `simulation_output.disturbances`;

Table 3. Structure of `simulation_output.mat`. `n_cycles` = total number of initiated carousel cycles.

Field	Sub-field	Sub-sub-field	Variable	Description	UOM
`states`	`station1` `station2` `station3`	`cake_x`	`t`	Readings of timer reinitialized at every carousel rotation – vector, step: `sampling_interval`	s
			`S`	Average cake saturation time profile for `cake_x` in Station 1/2/3 – vector [1×length(`t`)]	-
			`w_EtOH_cake`	Time profile of average ethanol mass fraction in cake for `cake_x` in Station 1/2/3 – vector [1×length(`t`)]	-
	`station4`	`cake_x`	`t`	Readings of timer reinitialized at every carousel rotation – vector – step: `sampling_interval`	s
			`S`	Average cake saturation time profile for `cake_x` in Station 2/3/4 – vector [1×length(`t`)]	-
			`w_EtOH_cake`	Time profile of average ethanol mass fraction in cake for `cake_x` in Station 2/3/4 – vector [1×length(`t`)]	-
			`Tg_top`	Temperature of drying air at top of cake in Station 4 – vector [1 × length(`t`)]	K
`measurements`			`t_meas`	Readings of timer initialized at process onset - vector: step = `sampling_interval`	s
			`m_filt_WI101`	Readings of WI101 – vector [1 × length(`t_meas`)]	kg
			`P_PI101`	Readings of PI101– vector [1 × length(`t_meas`)]	Pa
			`P_PI102`	Readings of PI102– vector [1 × length(`t_meas`)]	Pa
			`c_slurry_AI101`	Readings of AI101– vector [1 × length(`t_meas`)]	kg/m^3
			`L_cake_LI101`	Readings of LI101– vector [1 × length(`t_meas`)]	m
			`V_slurry_LI101`	Readings of LI101– vector [1 × length(`t_meas`)]	m^3
			`Tg_in_TI101`	Readings of TI101– vector [1 × length(`t_meas`)]	K
			`Tg_out_TI102`	Readings of TI102– vector [1 × length(`t_meas`)]	K
			`Vdryer_FI101`	Readings of FI101– vector [1 × length(`t_meas`)]	L/min
`measurements_nf`	*same structure of* `measurements`				
`disturbances`			`resistances`	Vector [`n_cycles` × 4] – element (i, j) = resistance of mesh in position j during processing cycle i, for i = 1, 2, …, `n_cycles` (= total number of simulated cycles)	1/m
			`c_slurry`	Multiplicative coefficients to nominal slurry concentration – vector [1 × `n_cycles`]	-
			`V_slurry`	Multiplicative coefficients to current fed slurry set-point – vector [1 × `n_cycles`]	-
			`E`	Multiplicative coefficients to nominal cake porosity – vector [1 × `n_cycles`]	-
			`alpha`	Multiplicative coefficients to nominal specific cake resistance – vector [1 × `n_cycles`]	
			`hM`	Multiplicative coefficients to nominal mass transfer parameter – vector [1 × `n_cycles`]	-
			`hT`	Multiplicative coefficient to nominal heat transfer parameter – vector [1 × `n_cycles`]	-
`operating_vars`			`t_vector`	Readings of timer initialized at process onset – vector: step = `control_interval`	s
			`P_compr_vector`	Profile of set-points of compressor pressure (gauge)– vector [1 × length(`t_vector`)]	Pa
			`Tin_drying_vector`	Profile of set-points of drying gas temperature – vector [1 × length(`t_vector`)]	K

		n_cycle_vector	Initiated cycles counter - vector [1 × n_cycles]	-
		t_rot_vector	Completed cycles duration – vector [1 × number of completed cycles)]	
		V_slurry_vector	Set-point of fed slurry volume – vector [1 × n_cycles]	m^3
x_estim	*structure depends on routines set up in* estimator_online.m and estimator_cycle_switch.m			
feed		c_slurry_nom_vector	Profile of nominal slurry concentration – vector [1 × n_cycles]	kg/m^3
cakes_proc_times	cake_x	filtration_duration	Duration of filtration undergone by cake_x during carousel processing	s
		deliquoring_duration	Duration of deliquoring undergone by cake_x during carousel processing	S
		drying_duration	Duration of drying undergone by cake_x during carousel processing	s
final_content			Mass fraction of ethanol content in discharged cakes [1 x number discharged cakes]	-
active_stations			Vector [n_cycles x 4] – if port *j* processes material during cycle *i*, active_stations(*i*, *j*) = 1. Otherwise, active_stations (*i*, *j*) = 0.	-
settings		control_mode	Scalar	-
		disturbance_scenario	Scalar	-
		control_interval	Time interval at which control routines are called - scalar	s
		sampling_interval	Sampling interval for all sensors – scalar	s
		total_duration	Simulation duration – scalar	s
	cryst_out_nom	conc_slurry	Nominal slurry concentration in feed – scalar	kg/m^3
		x	Crystal size distribution – particles diameters	m
		CSD_perc	Volumetric crystal size distribution	%
		T	Inlet slurry temperature (equal to room temperature)	K
	u_nom	t_rot	Nominal cycle duration – scalar	s
		V_slurry	Nominal fed slurry volume - scalar	m^3
		P_compr	Nominal pressure provided by compressor (gauge) – scalar	Pa
		Tinlet_drying	Nominal inlet drying gas temperature - scalar	K

- **fed slurry volume**: the actual slurry volumes fed to the carousel in all cycles are obtained from the product of `simulation_output.operating_vars.V_slurry_vector` with `simulation_output.disturbances.V_slurry`;
- **specific cake resistance**: the actual resistances of all the processed cakes are calculated as: `simulation_output.disturbances.alpha` $\times 2.7 \times 10^9$ (m/kg)
- **cake porosity**: the actual porosities of all the processed cakes are calculated as: `simulation_output.disturbances.E` $\times 0.35$

2.4 Disturbances and disturbance scenarios

A set of disturbances is implemented in the simulator. All disturbances assume a given value of the relevant variable at the beginning of every carousel cycle, but do not vary within the same cycle. Two different types of disturbances are present in the simulator: a fouling disturbance and parametric disturbances. The simulator automatically reproduces the same disturbance pattern for every simulation, for benchmarking purposes.

A **realistic routine simulating filter mesh fouling and cleaning-in-place** is implemented in the simulator (Figure 5). The filter mesh resistances of V-101-V-104 ($R_{m,1}$, $R_{m,2}$, $R_{m,3}$, and $R_{m,4}$) are first initialized, sampling each one from $N(3\times10^9, 1\times10^{18})$ 1/m. At the end of each cycle during which some material is processed in Station i (i.e., when the station is not empty due to the triggering of the cleaning-in-place routine, described in Section 2.1), the corresponding filter mesh resistance $R_{m,i}$ increases by 2×10^9 1/m. During the first cycle of carousel operation, only the first processing station works, as no material has reached the subsequent stations, yet. It is just from the fourth cycle on that all stations V-101-V-104 will be fully operational. When the filter mesh resistance reaches a threshold value (set to 1.2×10^{10} 1/m), the mesh cleaning-in-place procedure is triggered. No additional material is loaded into the carousel for the following three cycles, which are required to complete the processing and discharge of the batches of slurry trapped into the carousel ports. Then, the filter mesh resistances are re-initialized, sampling again from $N(3\times10^9, 1\times10^{18})$ 1/m, and the feeding and fouling routines are repeated again. In practice, the described routine yields to triggering a cleaning-in-place routine every six processing cycles (Figure 5).

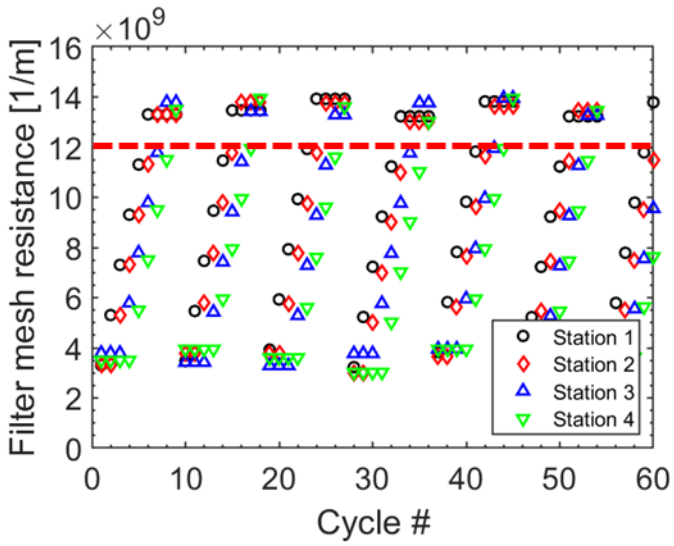

Figure 5. *Filter mesh resistances profile implemented in the simulator for the first 60 carousel cycles. The red dashed line marks the threshold filter resistance that, when crossed by any mesh of the stations, triggers the onset of the cleaning-in-place routine.*

Parametric disturbances with respect to the nominal values are set for the following variables:

- the fed slurry concentration
- the drying kinetic parameter
- the heat transfer coefficient between cake and air during drying
- the fed slurry volume
- the specific cake resistance
- the cake porosity

The disturbances are implemented in the simulator as multiplicative coefficients, **which vary at every cycle, but not during a cycle.**

Three different disturbance scenarios are available in the simulator, presenting different disturbance profiles. Note that the simulator is implemented so that the disturbances profiles are consistent across simulations in the same disturbance scenario, for reproducibility purposes. The fouling disturbance always occurs as aforementioned, while parametric disturbances follow different patterns based on the disturbance scenario:

- <u>Disturbance scenario #0 (normal operating conditions)</u>. All parametric disturbances are normally distributed;
- <u>Disturbance scenario #1 (slurry concentration ramp change)</u>. All parametric disturbances are as in normal operating conditions, except for an increase of the nominal slurry concentration by 2% per minute, starting from 5 min after the process onset and up to 25 min from the process onset;
- <u>Disturbance scenario #2 (specific cake resistance step)</u>. All disturbances profiles are as in normal operating conditions, except for a 100% step increase of the nominal specific cake resistance value, starting from 5 min after the process onset, and continuing up to the end of the process. 2.5 Setting up a control strategy

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Control strategies can be set up by the user modifying one or more of the following functions:

- `controller_cycle_switch.m`
- `controller_online.m`
- `estimator_cycle_switch.m`
- `estimator_online.m`

The input/output structure is thoroughly documented in each function. Although the functions can be freely modified, the bottom part of `controller_cycle_switch.m` and `controller_online.m`, where the updated values of the operating variables are stored and a null slurry volume for cycles in which Station 1 is empty, should not be edited.

Note that, among all the simulation outputs, **only the process measurements are available for state and parameter estimation routines** implemented in `estimator_cycle_switch.m` and `estimator_online.m`. At the same time, **only the process measurements and potential estimated states and parameters for control routines** implemented in `controller_cycle_switch.m` and `controller_online.m`.

The default control strategies implemented in the simulator are:

- control mode = 0: open-loop operation, no estimated parameters/states;
- control mode = 1: automatic adjustment of the cycle duration (Section 2.4), no estimated parameters/states;

2.6 Simulator scripts and functions: summary

`run_carousel.m`	Script for initiating carousel simulation
`run_simulation.m`	Function handling carousel simulation schedule
`carousel_parameters.m`	Function containing simulation and model parameters
`carousel_simulator.m`	Function simulating carousel operation using filtration, deliquoring and drying models
`estimator_online.m`	Function that can be written by the user for online state/parameter estimation
`controller_online.m`	Function that can be written by the user, containing online control routines
`estimator_cycle_switch.m`	Function that can be written by the user for state/parameter estimation routines to be executed at every carousel rotation
`final_composition.m`	Function executed at the end of every cycle to calculate the composition of the discharged cake, if there is any, and for storing the value of other variables contained in the simulation output
`controller_cycle_switch.m`	Function that can be written by the user, containing control routines to be executed at every carousel rotation
`disturbances.m`	Function that sets the value of the disturbances for the following cycle (e.g., filter mesh resistance, Gaussian fluctuations, …)
`switch_cycle.m`	Function containing carousel rotation simulation routines, such as material transfer from one port to the following one
`model_filtration.m`	Function simulating filtration (ODE model)
`model_deliquoring.m`	Function simulating deliquoring with design charts (approximate method called when cake is very small, i.e. with height below 0.3 mm)
`model_deliquoring_grad.m`	Function simulating deliquoring (PDE model)
`model_drying.m`	Function simulating drying (PDE model)

Script to run for starting the simulation with the desired settings: `run_carousel.m`

Functions to edit for changing the control strategy:

`controller_cycle_switch.m`, `controller_online.m`

`estimator_cycle_switch.m`, `estimator_online.m`

3 Quality-by-design and quality-by-control challenges

The simulator proposed in this study can be used for testing different control strategies within the quality-by-design and quality-by-control frameworks.

The general objective of the process is delivering dry cakes meeting the target quality, namely a residual ethanol content (critical quality attribute) below 0.5 wt%. This is achieved by setting suitable values for the operating variables, for a given inlet slurry concentration (critical material attribute of the process).

Following the quality-by-design jargon, the critical process parameters are identified as V_{slurry}^{sp} and Δt_{cycle}^{sp}, since they significantly impact the residual ethanol in the discharged cake. $T_{in,g}^{sp}$ and P_{compr}^{sp}, instead, are identified as the control variables, which affect the product quality to a smaller extent, compared to the critical process parameters.

Control routines can be implemented in the simulator for adjusting the desired values of the operating variables (set-point of the relevant controllers), as outlined in Section 2.5. The simulator also features blocks specifically dedicated to the implementation of state and parameter estimation routines. Note that, although the simulator makes the values of multiple outputs available, only the simulated measurements can be used by the developed control and estimation routines (Figure 3), as in real life carousels.

The following specific challenges are envisioned for the simulator:

1. Open-loop operation: determination of operating points delivering the target product quality and description of the design space of the unit;
2. Implementation of state estimators, soft sensors, and real time parameter estimation routines for monitoring key process variables, such as the ethanol content in the cake being dried and the resistance of the filter meshes;
3. Implementation of (model-free and model-based) control routines for automatic adjustment of the control variables (i.e., $T_{in,g}^{sp}$ and P_{compr}^{sp}) to meet the target product quality in response to disturbances (in disturbance scenarios 0-2) and/or to changes in the inlet slurry concentration. Description of the design space of the unit with such closed-loop routines in place;
4. Implementation of (model-free and model-based) control routines for automatic adjustment of the critical process parameters (i.e., V_{slurry}^{sp} and Δt_{cycle}^{sp}), to meet the target product quality in response to disturbances (in disturbance scenarios 0-2) and/or to changes in the inlet slurry concentration;
5. Repeating Tasks 3-4 with the additional objective of maximizing the slurry throughput, namely the amount of crystals processed by the carousel in a given timeframe, in disturbance scenarios 0-2.
6. For benchmarking purposes, we define the specific objective of implementing closed-loop control routines acting on V_{slurry}^{sp} and Δt_{cycle}^{sp} to maximize the cumulative mass of the cakes (meeting the target quality) discharged by the carousel in 1 hour of operation in disturbance scenarios 0-2, with $c_{slurry}^{nominal}$ equal to 250 kg/m^3, $T_{in,g}^{sp}$ fixed to 323 K, and ΔP^{sp} fixed to 1E5 Pa. The additional objective of assessing the optimal nominal slurry concentration for maximizing the throughput with the other conditions fixed can also be addressed.

In addition to the listed tasks, the simulator can also be used for generating data for data analytics studies, or for benchmarking fault detection, identification and diagnosis methodologies.

4 Sample case study

We consider a sample case study with the objective of designing a control strategy for Δt_{cycle}, following the operating conditions proposed in challenge #6 (Section 3). We propose three control strategies (#1-3). The only difference between control strategies #1-3 is the way in which Δt_{cycle} is adjusted: all the other operating variables are always kept at their nominal values (Table 4). Control strategies #1-2 run also Δt_{cycle} at open-loop, maintaining it at its nominal value. Instead, control strategy #3 features a closed-loop control system that automatically regulates Δt_{cycle}. No state or parameter estimation routines are set up. Overall, nine simulations of 30 minutes of carousel operation are carried out: each one of the three control strategies (#1-3) is tested in all the three disturbance scenarios (0-2) of the carousel (Section 2.4). The simulator inputs are summarized in Table 4. The implemented control strategies are coded in the default `controller_cycle_switch.m` and `controller_online.m` functions of the simulator.

Table 4. *Case study: simulator inputs set in* `run_carousel.m`.

Input	Value	Units
Control mode	Control strategies #1,2: 0 Control strategy #3: 1	-
Control interval	1	s
Nominal slurry concentration	250.0	kg/m^3
Nominal drying air inlet temperature	323.0	K
Nominal fed slurry volume	3.0×10^{-6}	m^3
Nominal compressor pressure	1.0×10^{5}	Pa
Nominal cycle duration	Control strategies #1,3: 30 Control strategy #2: 45	s s
Disturbance scenario	0, 1, 2 (*every control strategy tested in every disturbance scenario*)	-
Sampling interval	0.1	s
Simulation duration	1800	s

Let us first consider the two open-loop control strategies (control strategies #1-2) for Δt_{cycle}:

- control strategy #1: open-loop control, with $\Delta t_{cycle} = \Delta t_{cycle}^{nominal}$ = 30 s;
- control strategy #2: open-loop control, with $\Delta t_{cycle} = \Delta t_{cycle}^{nominal}$ = 45 s.

Figure 6 shows the ethanol content in the discharged cakes for the simulation conditions of Table 4, with control strategies #1-2 in normal operating conditions (disturbance scenario 0); results are also plotted for control strategy #3 (to be discussed later). While with control strategy #2 all the discharged cakes meet the target quality, with control strategy #1 several cakes contain more ethanol than can be accepted. The improved performance of control strategy #2 is due to the larger cycle duration selected for this control strategy, that allows for longer cake drying.

Table 5 clarifies the correspondence between the process time and the number of processing cycle under control strategy #2 in normal operating conditions. The stations active during each cycle are also listed (note that this piece of information is available from the simulation output; Section 2.3). For a given cycle, it is also reported the number of the cake that will form from the slurry loaded in Station 1, if any, and the number of the cake dried in Station 4 and discharged at the cycle end, if any. Note that the numbers of the discharged cakes correspond to those in Figure 6 for control strategy #2. During the first cycle after carousel start-up, only Station 1 is active, where, from the loaded slurry, cake #1 forms. Cake #1 will be discharged from the carousel only at the end of the fourth cycle, after having being processed in Station 2-4 during, respectively, cycles 2-4. From the

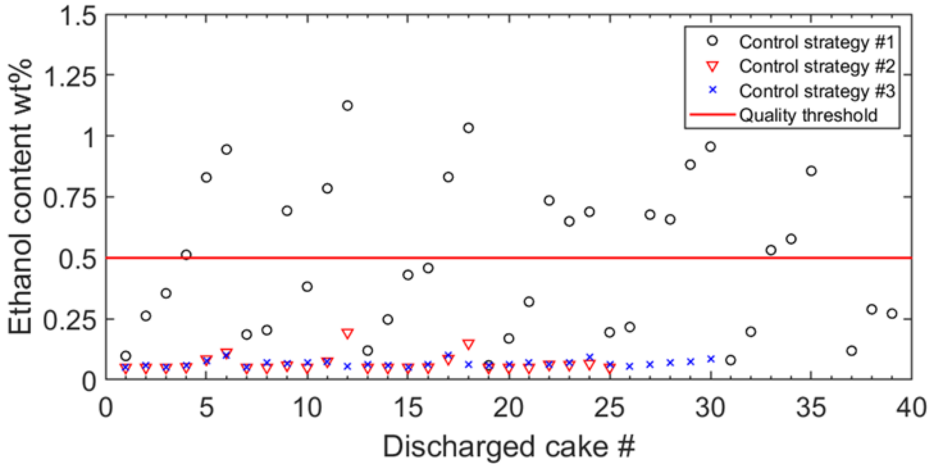


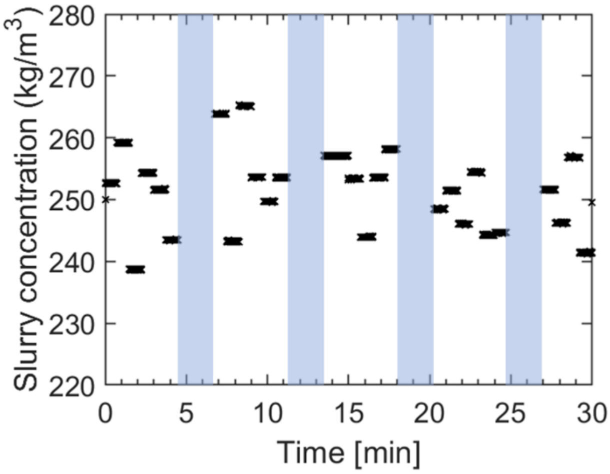
Figure 6. *Case study: ethanol content in discharged cakes under control strategy #1-3 in disturbance scenario 0 (normal operating conditions).*

process onset, cycle 4 is the first one during which all the stations of the carousel are filled, and operate simultaneously. At the end of cycle 6, the resistance of the filter mesh of Station 1 crosses the threshold value (Figure 5) that triggers the cleaning-in-place procedure. Hence, during cycle 7, no slurry is loaded in Station 1, which remains inactive. During cycle 8, the ports corresponding to both Stations 1 and 2 are empty, while during cycle 9 only Station 4 is active. At the end of cycle 9, the cake just dried in Station 4 is discharged, and all ports remain empty. The filter meshes are cleaned (instantaneously, as assumed in Section 2.4), and from cycle 10 the carousel is started-up again, with the same schedule followed at the process onset. The same processing-cleaning routine is followed until the process finishes.

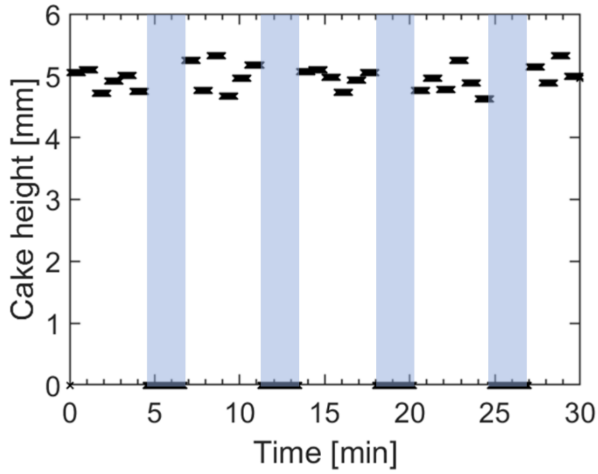
Table 5. *Case study: control strategy #2 in disturbance scenario 0. Correspondence among process time, cycle number, and stations active during every cycle. For every cycle, it is also reported the number of the cake that forms from the slurry loaded in Station 1, if any, and the number of the cake dried in Station 4 and discharged at the cycle end, if any.*

Process time [min]	Cycle #	Stations active	Loaded cake #	Discharged cake #
0.00-0.75	1	1	1	-
0.75-1.50	2	1,2	2	-
1.50-2.25	3	1,2,3	3	-
2.25-3.00	4	1,2,3,4	4	1
3.00-3.75	5	1,2,3,4	5	2
3.75-4.50	6	1,2,3,4	6	3
4.50-5.25	7	2,3,4	-	4
5.25-6.00	8	3,4	-	5
6.00-6.75	9	4	-	6
6.75-7.50	10	1	7	-
7.50-8.25	11	1,2	8	-
8.25-9.00	12	1,2,3	9	-
9.00-9.75	13	1,2,3,4	10	7
9.75-10.50	14	1,2,3,4	11	8
10.50-11.25	15	1,2,3,4	12	9
11.25-12.00	16	2,3,4	-	10
12.00-12.75	17	3,4	-	11
12.75-13.50	18	4	-	12
…	..	…	…	…
27.00-27.75	37	1	25	-
27.75-28.50	38	1,2	26	-
28.50-29.25	39	1,2,3	27	-
29.25-30.00	40	1,2,3,4	28	25

The plots of the measurements collected during the simulation under control strategy #2 in normal operating conditions are shown in Figure 7. The step variations seen in most plots (e.g., in the measured slurry concentration, Figure 7a), are due to the onset of new cycles, when the carousel rotates and a new slurry batch is loaded in V-101. Time spans during which no slurry concentration



(a)



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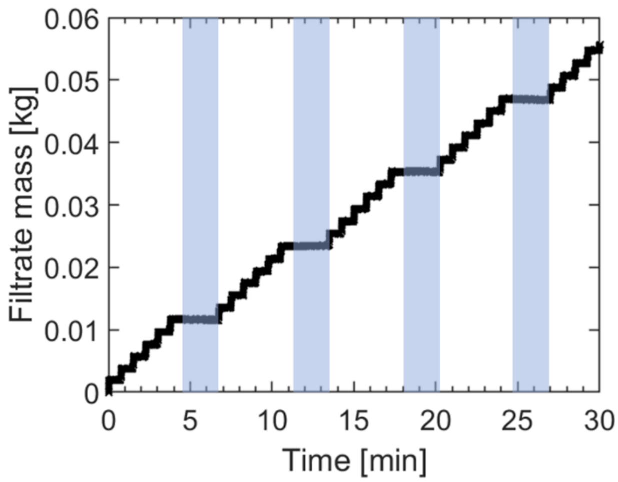

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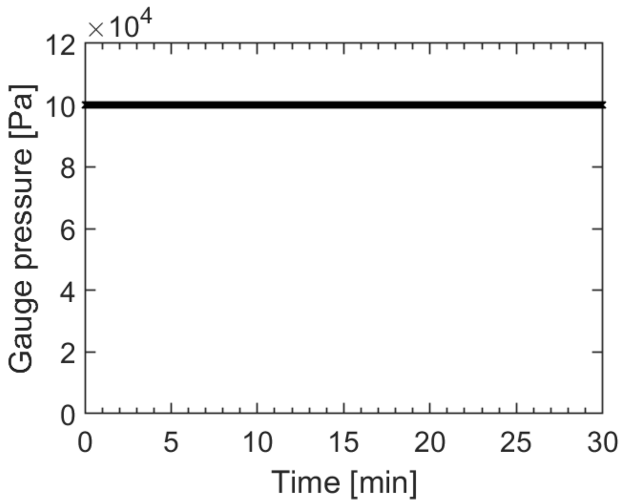

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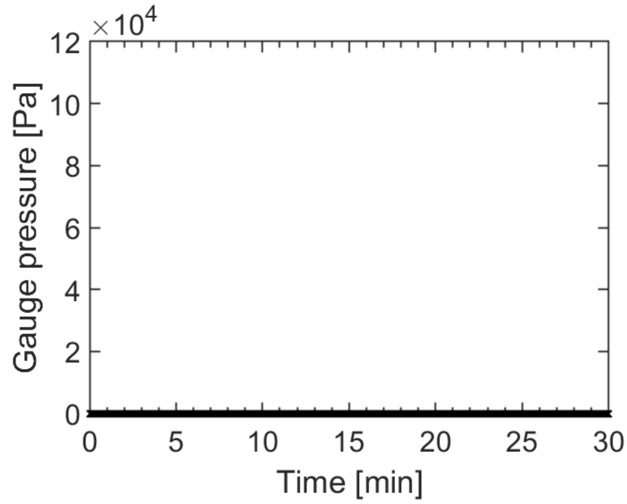

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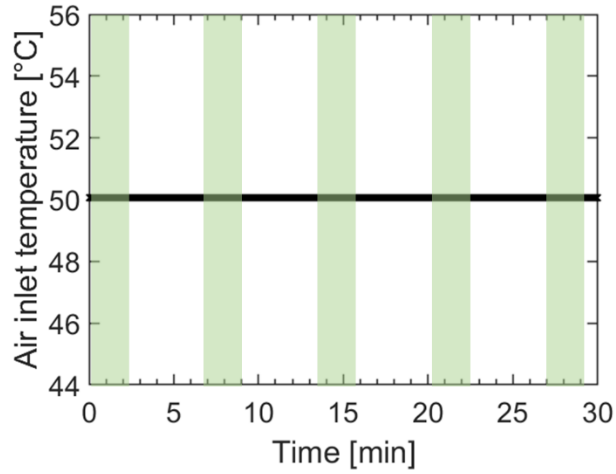

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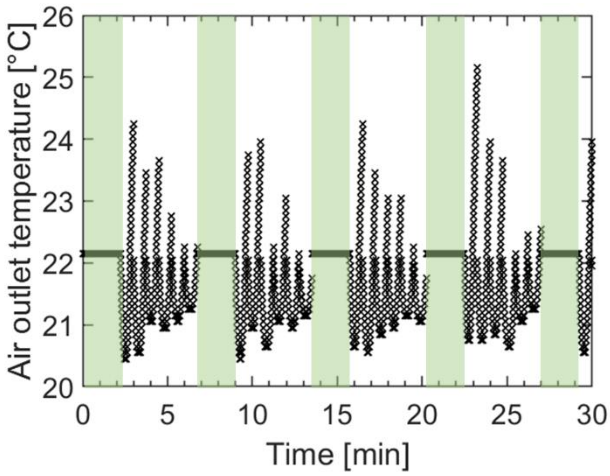

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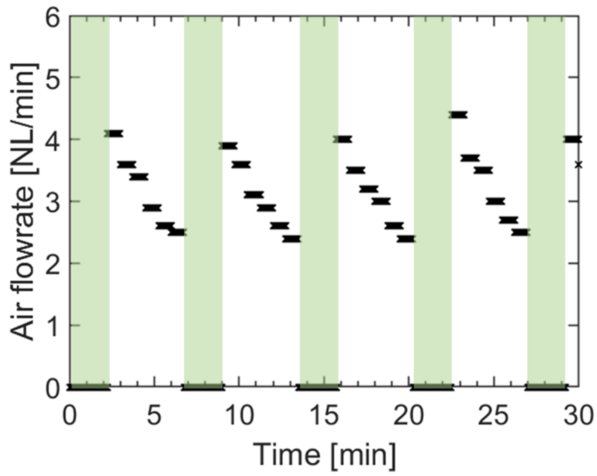

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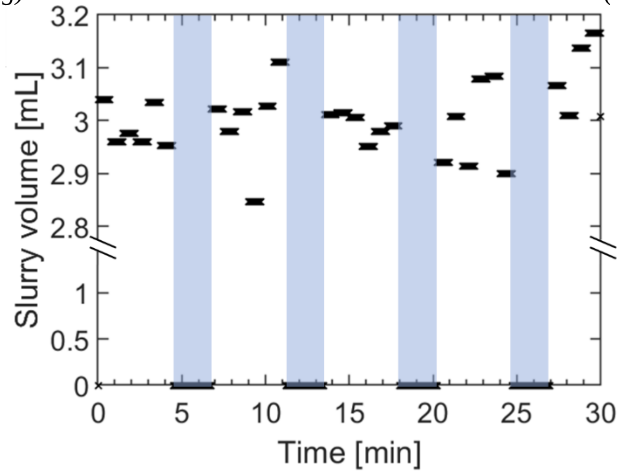


(i)

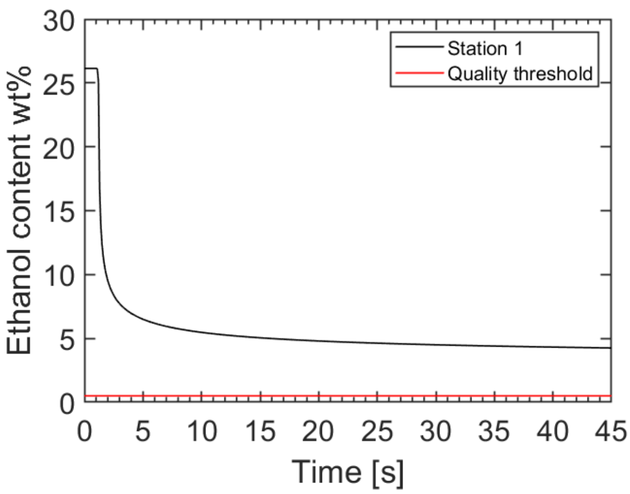
Figure 7. *Case study: measurements collected under control strategy #2 in disturbance scenario 0 (normal operating conditions). (a) slurry concentration , (b) cake height, (c) filtrate mass, (d) pressure provided by the compressor, (e) pressure at carousel bottom, (f) drying air inlet temperature, (g) drying air outlet temperature, (h) air flowrate, and (i) fed slurry volume. The shaded areas in the figures indicate the time windows during which the station relevant to each measurement is inactive: blue = Station 1, green = Station 4.*

is plotted in Figure 7a correspond to those periods of time during which the slurry concentration is null, since V-101 is empty due to the cleaning-in-place routine. Null values during the cleaning-in-place routines are also registered for the measured cake height (Figure 7b) and fed slurry volume (Figure 7h). While (small) intra-cycle variations of the measured slurry concentration are due to measurement noise (not visible in Figure 7a), inter-cycle fluctuations around the nominal slurry concentration (250 kg/m^3) are a consequence of disturbance the slurry concentration disturbance (Section 2.4). The same applies to the fed slurry volume, whose inter-cycle fluctuations (Figure 7h) around V_{slurry}^{sp} (= 3 mL) are due to fed the slurry volume disturbance. Inter-cycle variations of the cake height (Figure 10b) are, instead, due to the combined effect of disturbances on the fed slurry volume concentration, volume, and on the cake porosity.

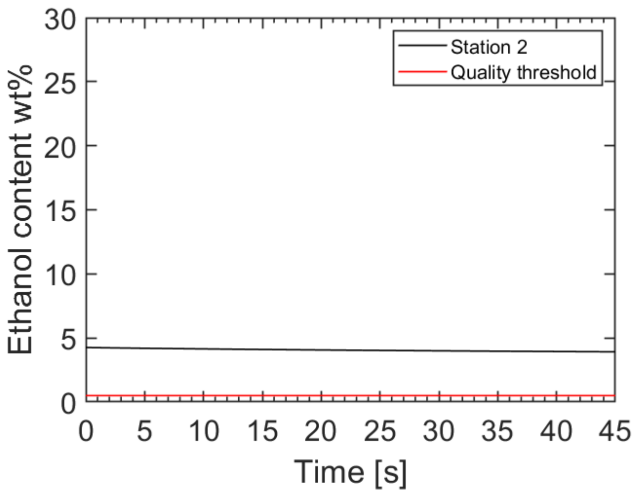
The filtrate mass (Figure 7c) presents a growing profile, as during the process the filtrate keeps accumulating in the filtrate receiver under which scale WI-101 is installed. Since there is only one filtrate collector for all ports, the signal read in Figure 10c is the cumulative filtrate from filtration and deliquoring coming from all ports. However, since the weight of the filtrate collected from filtration is orders of magnitudes greater than the one from deliquoring and, for the given operating conditions, cake filtration always finishes in V-101, most (>99%) of the filtrate collected in the receiver comes from V-101. Sharp increases in the filtrate mass are due to the onset of a new cycle, when new slurry is loaded into V-101 and starts being filtered. When filtration finishes, the filtrate mass remains almost constant, except for small changes due to deliquoring, until a new cycle is initiated. The longer periods of time during which the filtrate mass does not increase (e.g., about 4.5 to 6.75 minutes from the process onset) correspond to the time window during which V-101 is empty, due to the cleaning-in-place routine.

The measured inlet drying air temperature (Figure 7f) is constant during the simulation, since $T_{in,g}$ is operated at open-loop at its nominal value. The measured outlet drying air (Figure 7g) shows the typical inversion profile of drying processes. At the drying onset, the outlet air temperature drops, because of the large amount of heat spent for ethanol vaporization. When the ethanol content in the cake becomes lower, the drying rate decreases, and the outlet air temperature starts rising. The periods of time during which the measured air temperature is at the room value (22.1 °C) are the cycles in which no cake is being dried in V-104. These cycles are the first three ones after the process onset or mesh cleaning, and are also identified in Figure 7h as those time windows in which the air flowrate is null. The benefits of mesh cleaning are also highlighted in Figure 7h, which shows how the air flowrate decreases cycle-after-cycle after that the cleaning routine is carried out.

The plots of the ethanol content during carousel processing for the first discharged cake (Figure 8) under control strategy #2 in disturbance scenario 0 provide additional information on the process. Note that even though the time profile of ethanol content is an output of the simulator, it is not a measurement available in real carousels. During processing in the first station (Figure 8a), the ethanol content decreases from the initial value of about 26 wt% to slightly below 5 wt%. The trait in Figure 8a at constant ethanol content (up to about 30 s from the process onset) corresponds to filtration. When filtration ends, deliquoring starts, and the liquid starts exiting the cake pores. The ethanol content in the cake quickly approaches the equilibrium value for deliquoring, and the further reduction in Stations 2-3 (Figure 8b-c, respectively) is modest. Only with thermal drying (Station 4; Figure 8d) can the ethanol content significantly decrease, eventually dropping below the acceptable quality threshold.



(a)



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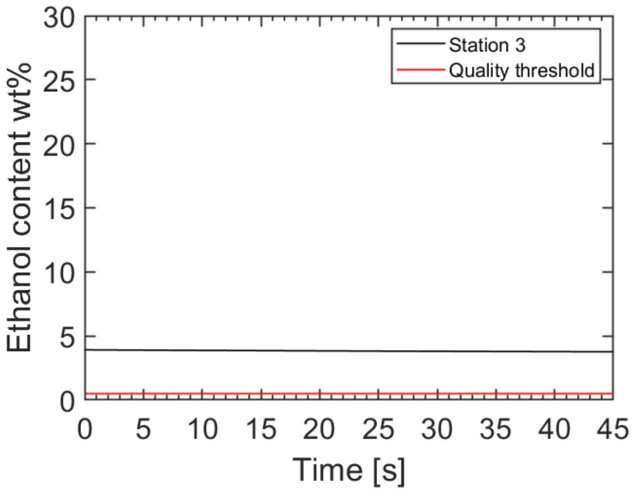

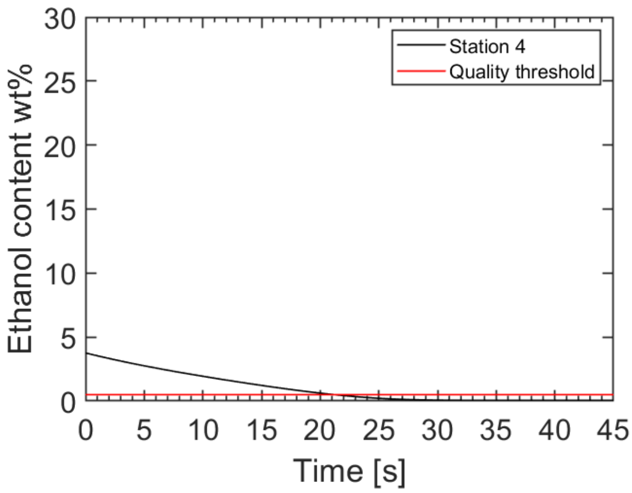

(c) *(d)*

Figure 8. *Case study: ethanol content in the first discharged cake across whole carousel processing (control strategy #2, disturbance scenario 0). (a) Station 1, (b) Station 2, (c) Station 3, and (4) Station 4.*

We now consider a third control strategy (control strategy #3), which manipulates Δt_{cycle} to terminate every cycle when the target product quality is estimated to have been achieved. Under control strategy #3:

i) For cycles in which no cake is being dried in Station 4 (V-104), $\Delta t_{cycle} =$ = 30 s;

ii) For cycles in which a cake is being dried in Station 4 (V-104), the cycle is terminated when $y_{T_{out}}$ reaches room temperature (after the temperature inversion). In practice, $y_{T_{out}}$ is used as a surrogate measurement to infer the cycle end-point at which the target ethanol content in the cake being dried is reached.

Note that, although drying is almost complete after the temperature inversion, there is no guarantee, generally speaking, that waiting for $y_{T_{out}}$ to reach room temperature is always enough to guarantee the product quality for all process and operating conditions. In this study, condition *ii)* has been designed and validated with simulations for the case study under investigation.

Control strategy #3 allows meeting the target quality for all the discharged cakes in normal operating conditions, and yields to obtaining five more cakes than with control strategy #2 in the same processing time (Figure 9). control strategy #3 leads to an improved performance also under abnormal operating conditions. When the slurry concentration is subject to a ramp increase (disturbance scenario 1; Figure 9a), control strategy #2 allows meeting the product quality specification, but under control strategy #3 one cake more is produced in the same processing time. However, under a step increase of the specific cake resistance (disturbance scenario 2; Figure 9b), control strategy #2 does not even allow meeting the target quality in most cakes, whereas control strategy #3 always lead to satisfying the target product quality.

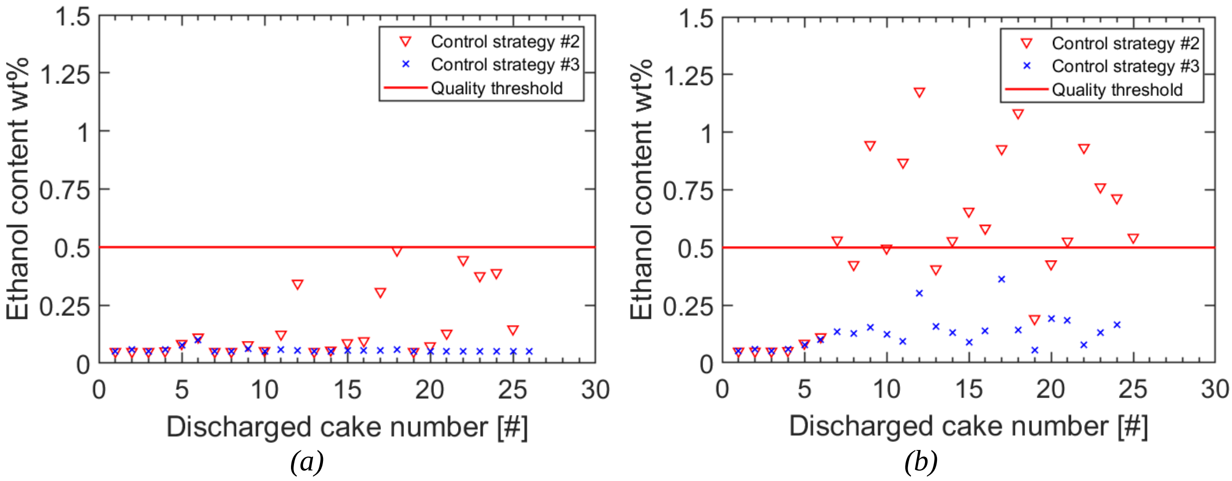

Figure 9. *Case study: ethanol content in discharged cakes under control strategies #2-3 (a) in disturbance scenario 1 (slurry concentration ramp change), and (b) in disturbance scenario 2 (specific cake resistance step change).*

The profiles of cycle duration under control strategy #3 in disturbance scenarios 0-2 are reported in Figure 10. Following Condition #1 of control strategy #3, cycles during which the dryer is empty (e.g., cycle #0-3) always present Δt_{cycle} equal to 30 s. However, when drying occurs, the cycle duration is adapted by the controller system, based on $y_{T_{out}}$. The effect is, as expected, that a larger cycle duration is selected for increasing mesh fouling conditions, as particularly evident in normal operating conditions (disturbance scenario 0). The significantly larger cycle duration needed for obtaining a cake meeting the target quality under the specific cake step disturbance (disturbance scenario 2) can be clearly assessed in Figure 10, explaining why control strategy #2 fails to deliver the target product quality in this situation (Figure 9b).

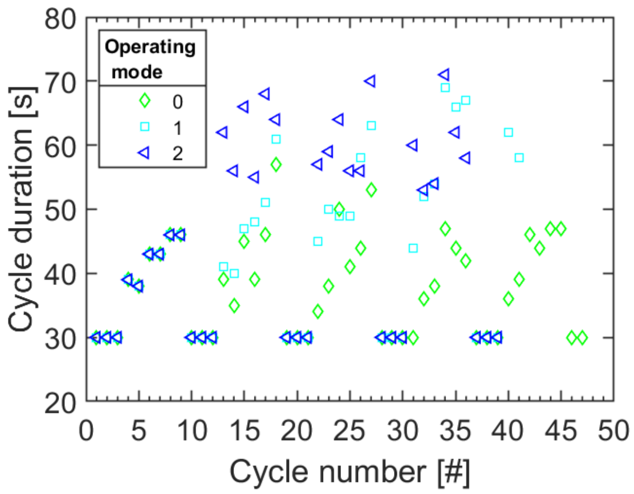

Figure 10. *Case study: cycle duration under control strategy #3 in disturbance scenarios 0-2.*