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Combined Semi-continuous and Discrete Simulation Model to Optimize a Decaffeination Process Based on Supercritical CO_2

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This article deals with a complex simulation, including discrete and continuous events, to optimize production and logistics activities in a food plant. The application scope of this work refers to an industrial decaffeination process of coffee beans, based on a supercritical carbon dioxide extraction, executed by a semi-continuous flow of materials as well as a discrete units production. The proposed model considers the semi-continuous coffee beans flow rate representation and the secondary flow rates necessary to realize the process, as, for example, carbon dioxide and caffeine flow rates. Moreover, the process parameters, the flowing material, breakdowns and repairs, speed and accumulation, and waiting time were taken into account. The model was implemented using Arena® simulation software both for discrete and continuous processes, and Microsoft Excel for the project parameters settings and for the analysis of the outputs. The model was, then, validated, considering some plant parameters and the variation of the simulated parameters with respect to the “real case” ones; for example, we obtained an error of 1.76 % for the order fulfillment and 5.10 % for the extractors’ saturation.

1. Introduction

Caffeine is an alkaloid widely known worldwide due to its presence in extensively consumed beverages, drinks and food. Despite the fact that tea is globally consumed more widely than coffee, the latter beverage is the main source of caffeine, due to its generally higher caffeine content. Numerous studies, in the last years, reported the effect of caffeine on cardiovascular diseases (Riksen et al., 2009) and on central nervous system (Nehlig et al., 1992), leading to an increasing consumption of decaffeinated coffee (Mazzafera et al., 2009). Decaffeinated coffee is widely consumed in Western countries for the previously mentioned health reasons and covers 10 % of the global coffee market (Silvarolla et al., 2004). Decaffeination methods mainly employ organic solvents, like dichloromethane or ethyl acetate, or water or supercritical carbon dioxide ($scCO_2$) (Ramalakshmi and Raghavan, 1999). Logistics activities deal with the procurement, production, storage and transportation of goods and services. The production activities incorrect scheduling can lead to not synchronized flows, which induce the operation supervisor in mistaking the estimation of the overall production lead-time. For that reason, Advanced Planning and Scheduling (APS) systems, using sophisticated algorithms, allow the scheduling of different steps in the most appropriate way (Lee at al., 2002). But, considering the uncertainty of most of the process variables, such as machine unavailability, lack of materials, variations in processing times, introduction of urgent orders, order cancellation, change in delivery dates or reprocessing due to quality, a re-scheduling activity is often required. A proper processing of variable time series, related to the plant under study, could help the formalization of each variable that, inserted in the simulation model, allow a more truthful evaluation of the expected results (Iannone et al., 2004).
Most chemical and food productions (like the decaf coffee one) involves continuous flow of materials through the manufacturing and logistics processes (Chen et al., 2002). Considering that to shut down and restart the production process is very expensive, it is desirable to plan a “three shift” production. The use of simulation

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models, which numerically reproduces the operation of a real process or system, can help the correct determination of the resources required to assess alternative strategies for logistics operations.
The simulation models can be used to reproduce both discrete and continuous realities; for example, the hydrogen production (Likkasith et al, 2014) and the acetone cleaning (Tohaneanu et al., 2014) were simulated using continuous models to optimize the process operating conditions. In some cases, the complexity of the system and the nature of the process (as in chemical industries) require the adoption of a hybrid modelling that has to include both the discrete-event and the continuous-time approach (Pritchett et al., 2000). In a discrete-event simulation, a system is modelled representing its evolution over time, using a representation in which the state variables change instantaneously at separate points in time; continuous-time simulation concerns the modelling over time of a system by a representation in which the state variables change continuously with respect to time. Some simulation packages have the capability to build hybrid discrete/continuous models; for example, Saraph (2001) developed a model that analyzed the hybrid nature of a chemical manufacturing plant.
In this work, an industrial supercritical carbon dioxide based decaffeination process is analyzed by a hybrid simulation approach with semi-continuous flow of materials and discrete units' production. The proposed model considers the coffee beans flow rate representation and the secondary flow rates necessary to realize the process. The logistics phases constitute the discrete part of the process; they were modelled, considering that they are strictly related to the efficiency of the continuous part of the process, influencing the throughput rate and the production costs. The model was developed in order to optimise the operating costs, varying the plant parameters and the master production plan.

2. Overview of the production and inventory system

The plant extracts caffeine from Arabica or Robusta coffee beans using $scCO_2$. A scheme of the process is reported in Figure 1.
Decaffeination from green coffee beans typically involves four different basic steps: steaming, caffeine extracting, drying, and caffeine recovery. If an organic solvent, like dichloromethane, is used to extract caffeine, also the solvent stripping is required (Patel and Wolfson, 1972). To avoid the removing of solvent medium from the beans, $scCO_2$ is used as the extracting solvent (Vitzthum and Hubert, 1975). In the steaming step (that typically range from 1 to about 5 hours), the coffee beans are put in contact with superheated steam at elevated temperature until their moisture content is increased to 30 % by weight and, as a result, the beans swell considerably. Then, the coffee beans are charged in one of the three extractors, that is pressurized by pumping carbon dioxide until the operating conditions are reached (70 °C, 250 bar); the extracting process goes on for times in the range 5-30 hours, in order to extract 97 % of the caffeine from the beans (Zosel, 1981). Once the extraction is completed, the extractor begins a two-hour down time while it is emptied and can be charged with fresh beans. Subsequently, the stream of $scCO_2$ with the caffeine dissolved in it begins to flow at steady rate conditions through a water wash packed column, where it is counter-currently contacted with a stream of water that removes 99.5 % of the caffeine from the CO_2, considering that caffeine has a higher affinity with water with respect to $scCO_2$. The purified $scCO_2$ is pumped in the storage tank, whereas the water stream with the caffeine and a little quantity of carbon dioxide dissolved in it is depressurized through a flash operation.

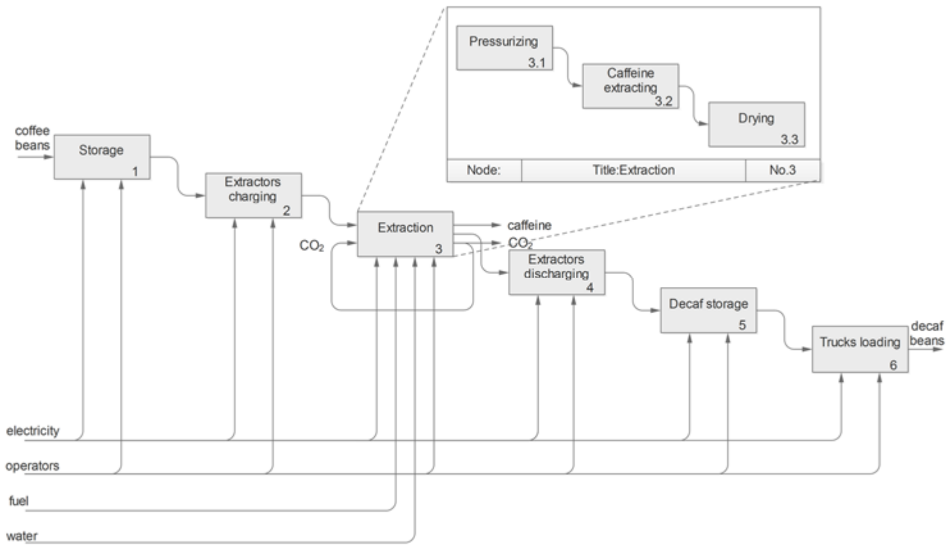

Figure 1: Scheme of the industrial production of decaffeinated coffee beans

Then, aqueous solution of caffeine is withdrawn from the extraction zone and introduced into an evaporation zone (Zosel, 1974), where, using two evaporators, the concentration of caffeine goes from 0.1 to 10 % wt/wt. Then, the mixture is cooled down using an ethylene glycol/water mixture and caffeine precipitated for crystallization.

3. The simulation model

Arena® simulation software is generally used to reproduce discrete processes; in this paper, we proposed a semi-continuous model to represent both continuous and discrete probabilistic process events. The simulation model receives as an input the Master Production Plan (MPP) through an Excel sheet, elaborates the data and gives back as outputs the technical and economic Key Performance Indicators (KPI), as indicated in Figure 2a. The information contained in the MPP are: customer's name; coffee type (Arabica, Robusta, blend, etc.); amount of coffee beans (kg); caffeine weight (%); caffeine extracted from the coffee beans (%); truck arrival date (date); due date (date); penalty for backlog (€ /kg day); production schedule.
The target of the model is to determine the KPI improvement as the "plant parameters" and the "operations management parameters" change. The "plant parameters" taken into account were: raw material silos number and dimensions; extractor dimension (kg); final product silos number and dimensions; operator's number. The "operations management parameters" included into the MPP are the following: production mix (coffee blend and quantity), production timetable, planned due date. The cost items considered into the model were: depreciation and amortization; maintenance costs; energy costs; workforce costs; backlog costs.
In order to describe the modelled logistics process, the block diagrams were reported in Figure 2b. The simulator, depending on the production plan, receives as an input the orders sequence with the trucks scheduled arrival timetables. Each truck goes into the factory and takes up the weigh station in order to measure the transported coffee weight. Subsequently, it arranges near the raw materials silos and is unloaded, occupying the loading area and an operator. Once concluded that phase, the truck is weighted again and leaves the factory. The coffee discharged from the truck is charged in the raw materials silos. Each silo is charged with a unique order and only if empty. If a silo is not able to contain the complete order, another silo is required to contain the remaining part of the order. In the meanwhile, the production planner receives the production order and inserts it in the planned sequence. When the order arrives in the production unit, it is partitioned in batch depending on the extractor dimensions. Subsequently, the steaming phase starts, which lifetime depends on the coffee typology and on the caffeine percentage. The three extractors are then charged one at a time, transferring the coffee from the steaming section. The charging time is equal to one hour. Once charged the extractor, the system is pressurized and the process of extraction starts. The extraction time depends on the starting caffeine percentage, on the process pressure and temperature, on the carbon dioxide flow rate and on the quantity of water absorbed during the wetting step. Therefore, the caffeine is separated from $scCO_2$ using water and stored in a silo. The decaffeinated coffee beans are transferred in the silos assigned to the "decaf final product" (the discharging time is equal to the charging time), waiting for the trucks that have to be charged to leave the factory. The modelling of the arrival time of the truck at the factory was performed considering a probabilistic distribution that takes into account the due-date planned with the customer (a delivery delay will generate a penalty that is typical of each kind of agreement).

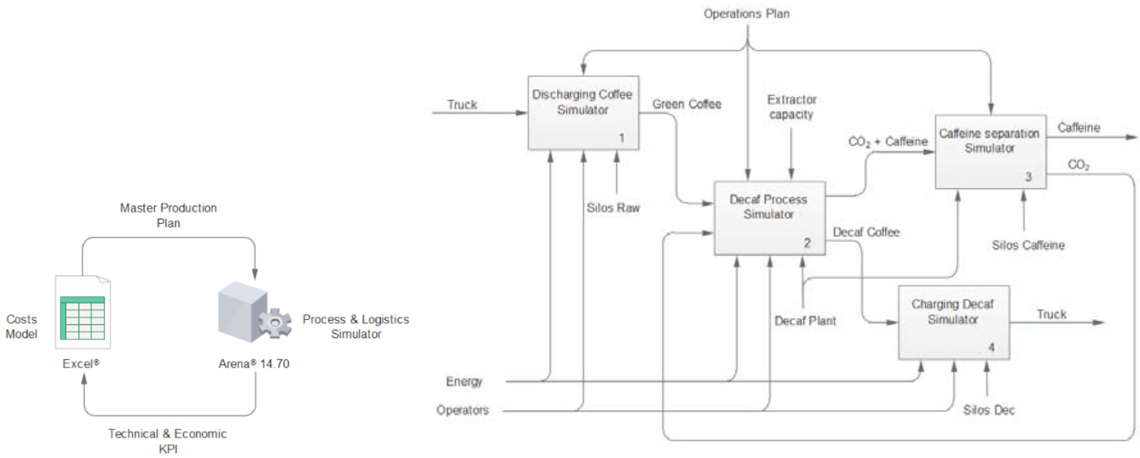

Figure 2: (left) Software structure of the simulation model; (right) block diagram of Arena® simulator

Generally, caffeine and decaffeinated coffee beans leave the factory at different times. Process times that intrinsically contain an uncertainty and/or are managed by an operator, and the plant up-time and break-down times were modelled using probabilistic distributions with parameters determined through measured data fittings and/or data directly obtained from decaffeinated coffee producers. Figure 3 shows the model flow diagram.

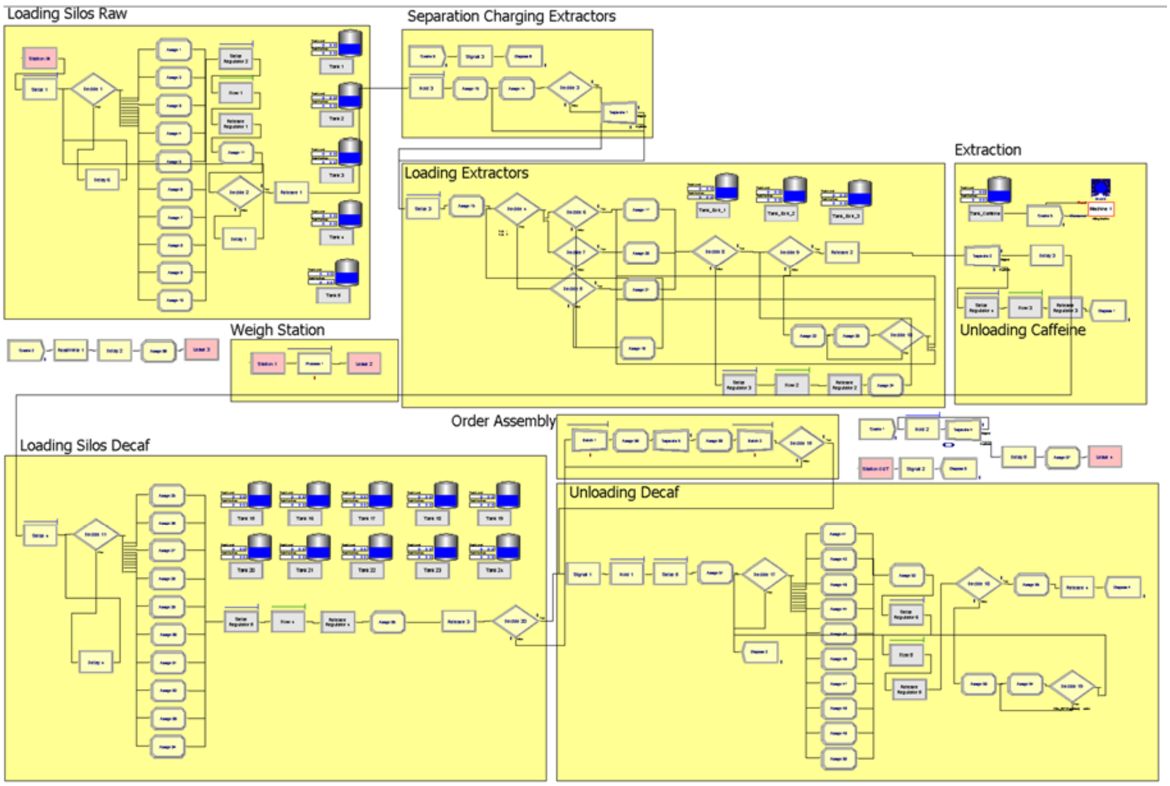

Figure 3: Model flow diagram

4. Validation

The model was validated considering an existing plant that for confidentiality obligation cannot be mentioned in the paper. In Table 1, the probabilistic distributions and the parameters used in the model are reported.

Table 1: Probabilistic distributions and parameters; M.U. = measure unit; MTBF = mean time between failures; MTTR = mean time to repair.

Process	Distribution	M.U.	Parameters
Truck arrival	Poisson	unit	mean=1.16
Silos “Raw”: MTBF	Weibull	h	λ= 1,000, k= 1.5
Silos “Raw”: MTTR	Log-Normal	h	μ=3.2, σ=1.4
Production delay	Normal	h	μ=1.2 , σ=0.5
Extractor: MTBF	Weibull	h	λ= 100, k= 1.5
Extractor: MTTR	Log-Normal	h	μ=1.7, σ=1.2
Pump: MTBF	Weibull	h	λ= 500, k= 1.5
Pump: MTTR	Log-Normal	h	μ=1.2, σ=1.1
Time in the weight station	Triangular	h	min=3, mean=5.6, max=10
Truck charging delay	Exponential	h	μ=2.3
Silos “Dec”: MTBF	Weibull	h	λ= 1000, k= 1.5
Silos “Dec”: MTTR	Log-Normal	h	μ=4.6, σ=0.8
Caffeine separation from water	Triangular	%	min=0.953, mean=0.971, max=0.985

In Table 2, data concerning the real case and the logistics characteristics of the production plan are reported.

Table 2: Technical and logistics parameters.

Parameter	M.U.	Value
Plant parameters		
Extractor capacity	kg	5,000
Extractors	unit	3
Silos “Raw”	unit	5
Silos “Dec”	unit	10
Silos “Raw” capacity	kg	34,000
Silos “Dec” capacity	kg	10,000
Operators	unit	10
Logistics parameters		
Demand/Production Capacity	%	60.3
Orders	unit	246
Operations days	days	250

Moreover, the real flow time distribution of the processed orders (246) during the 250 working days was available. In Figure 4, the comparison between the real and the simulated output data are reported. The distributions differ for the approximations due to the numerical model development. This evidence can be pointed out from the data reported in Table 3, where the main key performance indicators are shown. The automatic resources allocation to each job are not effective like the choices made by the managers. Obviously, this approximation strongly affects the delivery punctuality and, therefore, the ratio delay penalties (DP)/total costs (TC): indeed, DP/TC = 1.16 in the real case; DP/TC = 1.50 in the simulator. In any case, the model well represents the real case, if we consider that the other technical and logistics parameters (Table 3) show a maximum error lower than the 5.01 % of the real plant corresponding values.

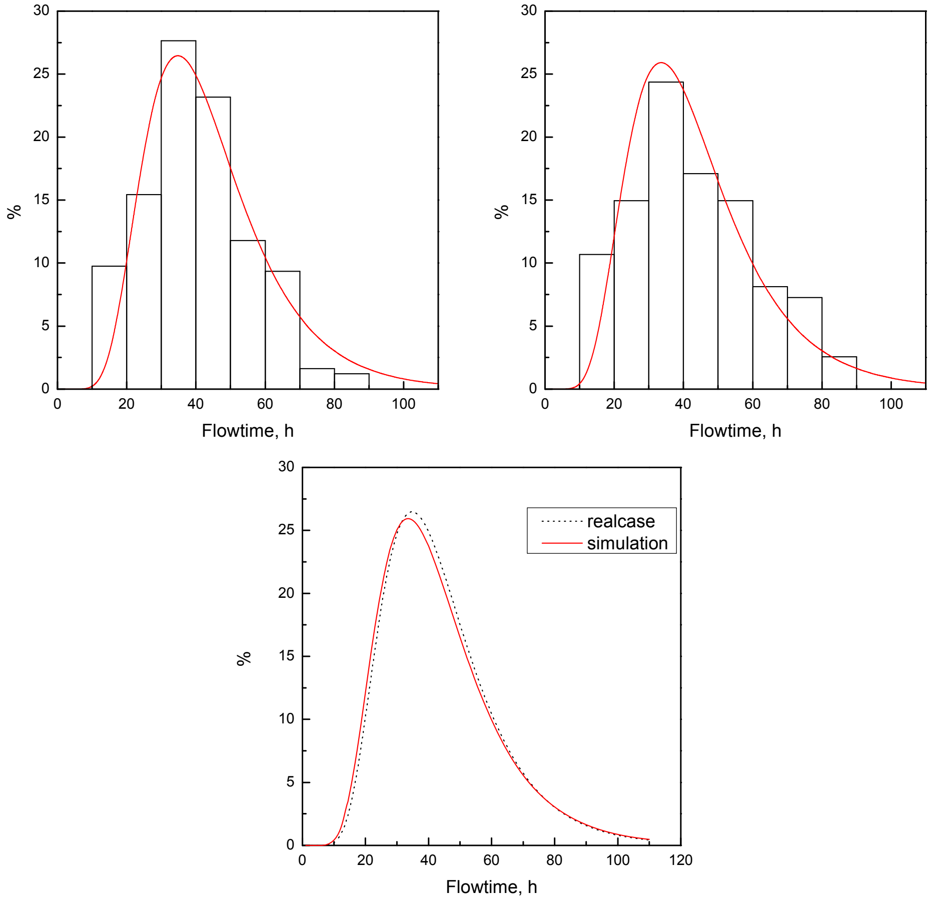

Figure 4: Flow time distributions; (left) Real case; (right) Arena® simulation; (b) comparison between the fitting distributions of the real and simulated output

Table 3: Comparison between technical and logistics parameters.

Parameter	M.U.	Real case	Simulator	Error
Order fulfillment	%	99.65	97.90	1.76
Extractors saturation	%	63.14	60.07	5.10
Silos “Raw” saturation	%	13.90	14.04	1.01
Silos “Dec” saturation	%	29.50	28.10	4.75

5. Conclusions

The simulation model shown in this paper is the first step in the developing of a decision support system to help designers and logistics managers to project a plant, considering both technical and economic aspects in a stochastic environment. Variables, like execution time distributions, failures, and sharing of resources, are rarely taken into account during the design phase, even if they substantially affect the operating performances of both chemical and logistics processes. The validation step allows the parameters tuning and, as a consequence, the check of the correspondence between real and simulated results. Nevertheless, a future improvement of the research will consider additional experimental campaigns to guarantee model response accuracy, varying the plant configuration and the assigned production plans.

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