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Abstract

In food processing plants, raw materials are fed into the system in different *supply-lots* of product, and are processed through different stages. In these stages, raw or intermediate materials are mixed or combined together, and physico-chemical and/or microbiological processes such as heating, concentration, pasteurisation etc. take place. In this setting, traceability consists of the ability to determine for each portion of intermediate or final product, in any part of the plant, its relative composition in terms of supply-lots fed into the system as well as of new lots generated during the production process.

Traceability becomes particularly difficult in the very common case when bulk products, such as liquids or grains, are involved in the production chain. Current traceability practices are in most cases unable to directly deal with bulk products, and typically resort to the definition of very large lots to compensate the lack of knowledge about lot composition. As demonstrated in recent food crises, this over-bounding approach has weaknesses in clearly identifying, immediately after risk assessment, the affected product lots, leading to unavoidably wide, expensive and highly impacting recalls.

Motivated by these considerations, this paper presents a novel approach to manage traceability of bulk products during production, storage and delivery. It provides a tight definition of lots in terms of their composition and size, thus allowing strict control of the production and supply chains.

Nomenclature

$\mathcal{L} = \{$'A', 'B', 'C', ...$\}$	Ordered list of possible S-lots entering the system
ℓ	Cardinality of $\mathcal{L}$ (number of S-lot)
n	Number of compartments
t	Time variable [s]
$c(X)$	Composition of product X
$\gamma^{\mathrm{A}}(X)$	Percentage of product coming from S-lot A present in product X
$d(X,Y)$	Composition-distance between products X and Y
δ	Threshold level of homogeneity
FDA	US Food and Drugs Administration
FIFO	First-in first-out
$\|\|x\|\|_\infty$	ℓ_∞-norm of vector x
$\|\|x\|\|_\infty^W$	Weighted ℓ_∞-norm of vector x
w_L	Risk-factor
$m_i(t)$	Mass in the i-th compartment at time instant t [kg]
$m_i^L(t)$	Fraction of the mass $m_i(t)$ containing material from S-lot L [kg]
$\dot{m}_i^L(t)$	Time derivative of the mass fraction $m_i^L(t)$ [kg s^{-1}]
$q_{ij}(t)$	Mass flow from compartment j to compartment i at time t [kg s^{-1}]
$q_{i0}(t)$	Mass flow entering the i-th compartment at time t [kg s^{-1}]
$q_{0j}(t)$	Mass flow leaving the j-th compartment at time t [kg s^{-1}]
$q_{IN,i}(t)$	Sum of incoming mass flow $q_{ij}(t)$ in compartment i at time t
$q_{OUT,i}(t)$	Total outflow from the i-th compartment
Q	Flow matrix collecting the q_{ij}'s
RFID	Radio-Frequency Identification

S-lot	Set of units of homogeneous raw materials that enter the system from outside
S_i	Cross-section of compartment *i*
$H_i(t)$	Height of material in compartment *i* at time t
ρ	Product density [kg m^{-3}]
$\gamma_i^L(t)$	Percentage of S-lot L contained in compartment i at time t
$\gamma_i\ (t)$	Instantaneous composition of the material present in compartment i at time t
$\gamma_{IN,i}^L(t)$	Relative fraction of flow entering compartment i at time t that is constituted of material belonging to S-lot L only, at time t
$\gamma_i^L(h,t)$	Relative fraction of material in compartment i belonging to S-lot L at a cross-section at height h, at time t
t_{next_event}	Time of the occurrence of the next event in the algorithm for creation of homogeneous cohorts in FIFO compartments
t_{end}	Simulation end time of algorithm for homogeneous cohorts creation in FIFO compartments
Δt	Simulation time interval for the algorithm for homogeneous cohorts creation in FIFO compartments
UM	Uniform mixing

1. Introduction

The problem addressed here refers to the traceability of food products in processing plants, or part thereof, in which the raw materials to be processed are fed into the system as different supply-lots of bulk product. Indeed, many ingredients used in food industries are liquids (milk, vegetable oils, etc.), powders (cocoa, powdered milk, flour, yeast etc.), crystals (e.g. sugar, salt) or grains. These products are stored, in many cases, in huge silos or tanks, which are very rarely completely emptied, so that many lots are contemporarily kept in the same container. Throughout the plant, the supplied material is processed in one or more production lines until one or more final products are created, packed, and stored ready for sale.

Typically, the production process consists of different stages, which are usually carried out in different production stations. Some stages involve different raw or intermediate materials that are mixed or combined together, while in other stages physico-chemical and/or microbiological processes such as heating, cooling, concentration, and pasteurisation, take place. Thus, the production process generates different production lots. Whenever the stored material is drawn from a container to be delivered to a production station or to a new storage container, the retrieved material results in a combination of material from the different batches that have been previously fed into the container (International Commission of Agricultural Engineering, 1999).

In this setting, traceability consists in the ability to determine for each portion of the intermediate or final product, at any time and in any part of the plant, its composition in terms of supply-lots fed into the system. This information is crucial for identifying the amount and location of product portions affected by possible deficiencies caused by a defect in the material delivered in one of the supply-lots. Food recalls due to unforeseen problems are becoming more and more frequent: for instance, the web-site provided by the US Food and Drugs Administration (FDA), which gathers information from press releases and other public notices about recalls of FDA-regulated products, listed more than seventy cases of recalls for the first two months of 2013 (US Food and Drugs Administration, 2013).

One possible approach to minimise recalls consists in separating the lots as much as possible within the plant. In the case of fluids, for instance, the use of different containers and cleaning between two product batches is a viable solution to allow distinct separated batches identities. In particular, cleaning-in-place procedures, which involve pumping water and detergent through the production equipment, besides guaranteeing high hygienic standards, is seen as the good procedure to strictly guarantee that the different batches cannot contaminate each other. Indeed, there are situations where the complete and absolute segregation of different lots supply lots is mandatory. This is the case, for instance, with products subject to religious specifications (e.g. Kosher or Halal certification), for military supply contracts, and where products are subject to very particular safety issues and constraints. In most other cases, these cleaning procedures, besides representing a high cost for the company in terms of energy, manpower, and cleaning agents, become undesirable, especially in the case of continuous production systems (such as, e.g., milk production in a dairy) where continuous flow of liquid/granular raw material, without even minimal interruptions, is necessary to maintain the production.

The currently adopted solution for handling this problem consists in defining large lots, mainly referenced to production periods rather than to their precise composition in terms of supplied material. For instance, lots based on the production day (or even a whole week) are typically encountered. This rather conservative approach, based on the definition of large lots, has shown its weaknesses in recent cases of food recalls, when the lack of detailed information on lot composition has unavoidably led to wide, expensive and high impact recalls.

Moreover, with types of bulk products, it is very difficult to associate any kind of label, marker or identifier that could directly identify the different lots. Recently, some markers based on Radio-Frequency Identification (RFID) technology have been developed for the case of continuous granular flows (specifically, iron pellets) by Kvarnström, Bergquist, and Vännman (2011). These markers allow on-line traceability of continuous flows, improving previous off-line solutions based on the introduction of specific tracers into the grains, such as chemical compounds or radioactive tracers; see Kvarnström and Oghazi (2008) and Lee et al., (2010) for detailed discussion and references on these techniques. The situation is complicated by the obvious requirement that the markers should not compromise in any way the integrity and quality of the food and must be not dangerous for the consumer. Thus, any RFID-based traceability system would require the development of a device for safely removing the tracing devices from the final product (e.g. before grain grinding). In this regard, some interesting solutions were proposed in Lee et al. (2010) and Liang et al. (2012) for the specific case of grains which involve particular pill-sized food-grade tracer particles to be inserted directly into grain during harvest. These tracers have printed with food-grade ink a miniaturised data-matrix code carrying identity information related to product origin, and are composed of materials that can be safely eaten such as sugar or cellulose. However, these solutions remain principally an off-line approach, suitable for modelling and validation purposes, since collecting and identifying the tracers would usually still require production to be interrupted.

To the best of our knowledge, the problem of the traceability of fluid products in the case of continuous processing was first addressed by Skoglund and Dejmek (2007), who used dynamic models and simulations to identify the changeover of liquid lots in a pipe. The presence of portions of flow consisting of the partial mixing of two subsequent lots led to the introduction of the concept of fuzzy traceability. An interesting approach has been also proposed by Bollen, Riden, and Cox (2007) and by Riden and Bollen (2007), who considered the case of apples processed in a packhouse. Apples, supplied to the packhouse in bulk bins, are moved in bulk (water dump) to the grader that handles individual fruits and directs them into packaging lines. At the end of these lines the fruits are placed into homogeneous packs (in terms of colour or size). During their flow in the water dump and subsequently in the packaging lines, some mixing among different lots of apples occurs. Even if apples are discrete items, their fluidised flow can be similar to the flow of small particles. In their first paper, Bollen et al. (2007) developed and validated a set of statistical models using the measured arrival sequence of 100 blue marker balls. The proposed models are able to assign a probability of bin origin to any individual fruit in the final packs.

The performance of a traceability system can be identified with the capability of limiting the quantity of final product to be recalled to avert a food safety crisis (Dabbene & Gay, 2011). However, current methods to precisely estimate the amount of product that has to be discarded in the case of a recall are available only for the case where discrete lots of product are processed (Dabbene, Gay, & Tortia, 2013; Dabbene & Gay, 2011; Dupuy, Botta-Genoulaz, & Guinet, 2005). The quantity of product to be recalled, to which a recall cost is associated, may depend on many factors, among which is the size of the batches that have been individually tracked and managed by the traceability system (and hence the skill of the company in managing and maintaining segregated different batches of product), and the way the batches of different components are mixed to obtain the final product.

These methods have been applied to many different supply chains, e.g. for fruits (Bollen et al., 2007; Riden & Bollen, 2007), meat (Barge P., Gay P., Merlino V., & Tortia C., 2013; Donnelly, Karlsen, & Olsen, 2009; Dupuy et al., 2005), fish (Karlsen, Donnelly, & Olsen, 2011; Randrup et al., 2008), grains (Thakur & Donnelly, 2010; Thakur & Hurburgh, 2009;

Thakur, Wang, & Hurburgh, 2010), chocolate (Saltini & Akkerman, 2012), perishable products (Li, Kehoe, & Drake, 2005; Rong & Grunow, 2010; Wang X., Li D., & O'Brien C., 2009) etc.

To allow traceability of bulk products, a convenient model of the production plant is therefore needed, in order to provide a description of the production process in terms of mass transfer and storage at a lot level, and to enable an accurate prediction of the dynamics of each supply-lot that can therefore be conveniently tracked. The model introduced in this paper involves different mathematical tools, combining continuous-time differential equations deriving from the use of compartmental models, with discrete-event elements, such as queues. In particular, the discrete-event nature of the process originates from the asynchronous opening/closing of valves and activation of pumps controlling the flow of bulk materials.

A thorough theoretical analysis is carried out and a modelling framework based on compartmental models is derived. The problem of the determination of specific models of the two basic cases of uniform-mixing and first-in-first-out (FIFO) tanks is addressed. A simulation case study, showing the effectiveness of the proposed methodology, is proposed and conclusions drawn.

2. Definitions and problem formulation

The first step for developing the framework introduced in this work consists in providing a formal definition of lots and of lot homogeneity.

Definition 2.1 (Lot) *A* lot *is defined as a set of units of a product that are homogeneous in terms of composition and processing history*.

This definition is similar to the one reported in ISO 22005 (2008), where a lot is defined as *"set of units of a product which have been produced and/or processed or packaged under similar circumstances",* and it extends to some degree the concept of traceable unit (TRU) introduced by Kim, Fox, and Grüninger (1999). It should be noted that at this point the notions of homogeneity and composition considered in Definition 2.1 are still rather vague, and need a rigorous formalisation to be of practical value. To this end, the concept of S-lot (supply lot) is explicitly defined next

Definition 2.2 (S-lot) *An* S-lot *is defined as a set of units of homogeneous raw materials that enter the system from outside.*

More specifically, S-lots represent raw-materials or semi-processed products provided by a supplier and fed into the system as a unique lot. Note that it is assumed that the lot of raw materials entering the system is homogeneous. This is done without loss of generality, since non-homogeneous lots can be always modelled as the assembly of different homogeneous S-lots. At each instant, the traceability system should be able to determine the relative composition, in terms of S-lots, of the material present in the different intermediate production stages, with specific attention to the composition of the final products leaving the production chain.

To exemplify this, consider the case in which two different raw-materials are fed into the system and are labelled for simplicity 'A' and 'B'. Then, the relative composition of a final product X leaving the chain is given by the percentages $\gamma^{\mathrm{A}}(X)$ and $\gamma^{\mathrm{B}}(X)$ of materials 'A' and 'B' present in X. A formal definition is given in Section 3 but more generally, the composition of a product can be defined as follows:

Definition 2.3 (Composition) *Let* $\mathcal{L} = \{\text{'A'}, \text{'B'}, \text{'C'}, \ldots\}$ *denote the (ordered) list of possible S-lots entering the system. Then, the (relative)* composition *of a product* X *is defined as the vector of percentages of the different S-lots composing* X*, that is*:

$$c(X) \doteq [\gamma^{\mathrm{A}}(X)\ \gamma^{\mathrm{B}}(X)\ \gamma^{\mathrm{C}}(X)\ \cdots]^T. \tag{1}$$

The above definition is instrumental for a rigorous definition of homogeneous materials, in terms of composition, which in turn represents a fundamental step towards a rigorous treatment of the traceability problem for the case of bulk materials. To this end, the composition-distance between two products X and Y is introduced as follows:

$$d(X,Y) \doteq ||c(X) - c(Y)||_\infty, \tag{2}$$

where $||x||_\infty \doteq \max_{L=1,\ldots} |x_L|$ denotes the ℓ_∞-norm of vector x. Note that composition-distances different from Eq. (2) can be introduced: for instance a weighted-norm version, with $||x||_\infty^W \doteq \max_{L=1,\ldots} |w_L\, x_L|$, can be considered in order to take into account the different risks associated with the different S-lots. In this case, the greater the risk-factor w_L, the more importance is given to S-lot L. The concept of composition distance $d(X,Y)$ allows the following rigorous formalization of homogeneity.

Definition 2.4 (Homogeneous products) *Given a threshold level δ, two products X and Y are said to be* homogeneous in composition *(up to accuracy δ) if their composition-distance is less than δ, i.e.*

$$d(X,Y) < \delta. \tag{3}$$

Note that this definition does not take into account processing history. Clearly, a homogeneous-in-composition lot, if processed in $m > 1$ sessions, splits in m distinct 'production' lots characterised by the same composition vector. The handling of these production lots, in order to trace production history and not only composition, can be performed in a completely analogous way to the one discussed in this paper, but it is not considered in the present work for sake of simplicity.

Note also that the introduction of the quantisation level δ is absolutely necessary when dealing with bulk products, since in principle the relative composition of the materials can vary with continuity. This approach, based on a threshold level, reflects what proposed in the EC Regulation No 1829/2003 (European Commission, 2003) for genetic modified (GM) and non-GM grains labelling. In this case, for the consumer information, these regulations require any food containing material with more than 0.9% of GM be labelled as "contains GM".

From Definition 2.4 it follows that two products, whose composition-distance is > δ, cannot belong to the same lot (according to Definition 2.1). Consequently, every time in the production process there is a change in composition greater than the selected threshold, the traceability system should be able to detect this event and keep trace of two different products (and of their specific composition). Hence, this framework provides a direct and natural way of discriminating final products and, possibly, divides them into homogeneous lots.

Like the already mentioned case of GM and non-GM grains, there are other situations related to ethical, organic, low carbon footprint, issues or subject to disciplinary or to religious constraints, where lots should be maintained as much as possible separated. In such cases facilities and logistics have to be designed and planned accordingly. Different management strategies have been proposed to cope with this problem. They are typically based on the separation of products in space, allocating specific collecting units (e.g. silos) for any different lot, or they are based on the separation in time, when different lots are processed in successive sessions, separated by suitable cleaning cycles (see e.g. Coléno, 2008; Maier, 2006).

In this work, accurate methods for tracing the composition of the product in terms of S-lots are derived using specific compartmental models. Compartmental models are mathematical models widely used to describe the way in which materials and/or energies are transferred among (and stored within) the different parts of a physical system (Godfrey, 1983). Although compartmental models have been primarily developed in biomedical engineering (the interested reader can refer to Rescigno (2001) for a short overview and a critical analysis of their use), they have been also used recently by Comba, Belforte, and Gay (2011) to describe heat-transfer phenomena in food plants characterised by mixed continuous/discontinuous flow of materials.

Indeed, in principle, a food production plant can be modelled as a set of storage compartments, each one corresponding to a storage container or to a batch processing station. Examples of compartments are tanks, vats, silos but also grain dryers, mixers, chocolate conching machines, cheese-vats etc. Material is transferred from a compartment to another either by flows, that in most cases are discontinuous (in time), or in batches. The description of these phenomena is usually simple and quite precise, since flows between compartments and masses of batches are known with good precision, and mass transfer equations are accurate. This information can be easily acquired from the plant itself, by monitoring the states of valves, pumps, conveyors, and, in general, any device that controls the flow of the material in the plant. Then, assuming that the relative composition of flows and batches in terms of S-lots is properly known, also the dynamics of such lots, in connection with the mass transfers among tanks, can be accurately determined (e.g. Skoglund and Dejmek, 2007 for the case of liquid products).

The crucial point is to know such relative composition, which is not always an easy task. In order to better understand this point, the behaviour of the compartments used to describe the production plant should be analysed, since any product flow or product batch transferring masses from compartment to compartment can be regarded as the output of a specific compartment. Only the inflow into the system of S-lots cannot be regarded as the output of a compartment, but the composition of such a flow (or batch delivery) in terms of S-lots is indeed well known.

Any compartment, whether it represents a storage unit, such as a silo, or a processing station, such as a mixer, concentrator, or heater is itself a dynamic system. It can store some quantity received over time through one or more inputs. Each one of its output flows has a suitable combination of the masses stored within it.

Assuming that the relative composition of input flows in the compartment (or batch deliveries to it) in terms of S-lots is perfectly known, then the relative composition of the outputs can be accurately computed only if the storage mechanism in the compartment is accurately known together with the laws supervising the way in which output flows are formed from the stored material.

There are at least two important and representative cases in which this happens. The first case is when all the material delivered to a compartment is instantaneously and uniformly mixed. Under this condition, referred to as uniform-mixing (UM) compartment, the relative composition of the material in the compartment in terms of S-lots is perfectly known at any time from the knowledge of the composition of the input flows (or batch deliveries). Hence, the relative composition of the output flow at any time is the same as the material in the tank at that time.

The second case is when a single-input-single-output compartment behaves as a FIFO buffer in which, however, input and output mass flows do not need to share the same intensity-time profiles. This second condition is referred to as FIFO compartment.

It should be noted that if a plant can be fully described using only UM and/or FIFO compartments, then the relative composition of any lot in the plant can be accurately derived, as detailed in sections 3 and 4, and thus lot traceability can be conveniently implemented.

3. Modelling uniform-mixing and FIFO compartments

In this section, the two important cases of UM and FIFO compartments, describing storage units or processing stations in food processing plants, are analysed, and specific models are derived.

In the following, it is assumed that a total of ℓ different S-lots are available, belonging to the set of labels $\mathcal{L} = \{\text{'A'}, \text{'B'}, \text{'C'}, ...\}$, with $\text{card}(\mathcal{L}) = \ell$. Moreover, for the sake of simplicity and without loss of generality, it is assumed that any mass that is fed to the production chain belongs to one and only one S-lot at the time it enters the system.

The case of n interconnected tanks is considered, with material flowing from the outside and between them. Considering a generic compartment i, it follows that there are possibly up to n different mass inflows $q_{ij}(t),\ \ j = 0, \dots, n, j \neq i$ entering compartment i from other $n - 1$ compartments, or from outside the system. So, $q_{ij}(t)$ represents the mass flow leaving compartment j and entering compartment i, while $q_{i0}(t)$ represents the flow entering the i -th compartment from outside the system, and $q_{0j}(t)$, represents the flow leaving the system from the j -th compartment (this according to the standard notation used in compartmental model literature). It should be noted that the flows $q_{ij}(t)$ are bounded to be positive or zero, and cannot assume negative values. In particular, if no flow exists from compartment j to compartment i, then we assume $q_{ij}(t) = 0$. Hence, we can define the following *flow matrix*

$$Q(t) \doteq \left[q_{ij}(t)\right]_{i,j=0,\dots,n}. \tag{4}$$

Formally, the matrix $Q(t) \in \mathbb{R}^{n+1,n+1}$ coincides with the adjacency matrix of the weighted graph representing the interconnections between compartments; see for instance (Godsil & Royle, 2001). Note that, by construction, the matrix $Q(t)$ is square with zero diagonal elements.

3.1. Compartments ensuring uniform mixing

Hereafter the case in which compartments describing a storage container or a processing station ensure uniform (instantaneous) mixing of their content is considered first. Note that this kind of assumption is rather common for several modelling problems, in particular when compartmental models are used (Godfrey, 1983). Moreover, the assumption of uniform and instantaneous mixing appears quite reasonable in several processes typically encountered in the food processing industry. Indeed, inside the different compartments in which the process stages are carried on, the processed material is usually mixed in a continuous manner in order to avoid settling phenomena, and to suppress possible thermal or concentration gradients. This is sometimes the case of many storage devices, for instance whenever the processed material is liquid, so that diffusion and convection motions lead over time to a uniform mixing (UM). Clearly, in real systems mixing is never purely instantaneous. However, it is in general rapid, and the mixing time-constants are usually shorter than those governing the process itself. On top of this, it should be noted that a non-uniform mixing would mainly induce errors only in the relative composition of the outflow from the compartment. Hence, whenever inflows and outflows are discontinuous and do not occur at the same time, truly uniform mixing also occurs in a real plant.

In order to describe the dynamics governing the different lots, a compartmental model is introduced, where each compartment coincides with a tank in the system. Firstly, to describe the dynamic behaviour of a generic compartment i a set of suitable state variables that fully account for its status at any time is chosen.

In this regard, denote by $m_i(t)$ the total mass available in compartment i at time t. This mass can be divided into ℓ different sub-masses $m_i^L(t)$, one for every $L \in \mathcal{L}$, representing the fraction of the mass $m_i(t)$ containing material from S-lot L. The masses $m_i^L(t)$, $L \in \mathcal{L}$ are the state variables that fully describe the dynamics of compartment i.

Then, the following quantities are defined

$$\gamma_i^L(t) \doteq \frac{m_i^L(t)}{m_i(t)}, \text{ for } i = 1, \dots, n \text{ and } L \in \mathcal{L}, \tag{5}$$

denoting the fraction of S-lot L contained in compartment i at time t. Obviously, by definition, it holds that $\sum_{L \in \mathcal{L}} \gamma_i^L(t) = 1$. Notice also that, again by definition, the quantity

$$\gamma_i(t) \doteq \left[\gamma_i^{\mathrm{A}}(t)\ \gamma_i^{\mathrm{B}}(t)\ \gamma_i^{\mathrm{C}}(t) \cdots\right]^T, \tag{6}$$

coincides with the instantaneous composition of the material present in compartment i at time t.

At any given time, the mass flow $q_{ij}(t)$ is composed by masses belonging to different S-lots. In particular, it can be easily seen that the relative fraction of $q_{ij}(t)$ which is constituted by a mass-flow belonging to the S-lot L is given by $\gamma_j^L(t) q_{ij}(t)$.

The quantities previously defined allow the state equations of the mass exchange in the i -th compartment to be written as follows

$$\dot{m}_i^L(t) = \sum_{j=0}^{n} \gamma_j^L(t)\, q_{ij}(t) - \gamma_i^L(t) \sum_{i=0}^{n} q_{ji}(t), \text{ for } L \in \mathcal{L}, \tag{7}$$

where $\dot{m}_i^L(t) = \frac{\mathrm{d}m_i^L(t)}{\mathrm{d}t}$ denotes the time variation of mass $m_i^L(t)$. The first summation on the right-hand side of Eq. (7) represents the total inflow of material belonging to S-lot L entering compartment i, while the second term is the total outflow of material belonging to S-lot L leaving the compartment. Under the assumption that a uniform and instantaneous mixing takes place in all compartments of the production chain, then the whole system can be easily described by means of n different sets of Eq. (7), one for each compartment.

To show the behaviour of the introduced model in this case of complete uniform mixing, an illustrative example is presented next.

Example 1 (Complete uniform mixing). In order to clarify the previously presented concepts, a simple system depicted in Fig. 1 is introduced. Focusing on the first part of the plant, constituted by the cascade of two storage compartments (Tank 1 and Tank 2) characterised by uniform mixing, considering the following situation: at initial time $t_0 = 0$ s, Tank 1 is filled with 100 kg of mass belonging to S-lot 'A'. Then, at time $t_1 = 10$ s a flow of 1 kg s^{-1} is transferred into Tank 2 for 60 s. Subsequently, at time $t_2 = 80$ s, an outflow of 0.5 kgs^{-1} starts from Tank 2. At $t_3 = 90$ s, an extra 70 kg belonging to S-lot 'B' is added to Tank 1. Finally, at time $t_4 = 100$ s, a flow of 1 kgs^{-1} is again transferred into Tank 2 for 100 s. Values of the mass flows between the three tanks over the time interval 0 - 300 s are plotted in Fig. 2.

Assuming that the material is uniformly mixed in the two compartments, the masses $m_1^{\mathrm{A}}(t)$, $m_1^{\mathrm{B}}(t)$, $m_2^{\mathrm{A}}(t)$, $m_2^{\mathrm{B}}(t)$ of material belonging to S-lots 'A' and 'B' in Tank 1 and Tank 2 are reported in Fig. 3 and Fig. 4, respectively, over the interval 0 – 300 s. Figures 5 and 6 report the fractions $\gamma_1^{\mathrm{A}}(t)$, $\gamma_1^{\mathrm{B}}(t)$, $\gamma_2^{\mathrm{A}}(t)$, and $\gamma_2^{\mathrm{B}}(t)$, describing the relative composition in terms of S-lots 'A' and 'B' of the two flows $q_{21}(t)$ and $q_{32}(t)$, respectively. In particular, in Fig. 6 it can be seen that the composition of the flow from Tank 2 to Tank 3 is continuously varying, with the fraction material belonging to S-lot 'B' increasing and the that from S-lot 'A' decreasing. The blue vertical lines in Fig. 6 refer to the introduction of quantisation levels, which are discussed in the next section.

3.2. Compartments behaving as FIFO buffer

The case in which a generic i-th compartment behaves like a first-in-first-out buffer is surely more complex, and is discussed hereafter. Note that the FIFO model can represent several practical situations encountered in real production lines when dealing with bulk solids and powders. Indeed, there is a growing research designing specific devices and tank configurations that ensure plug-flow. Plug flow (referred also as mass flow) silos are frequently used in industrial processing because of some of their beneficial properties. Plug flow is the most productive flow because it eliminates problems such as channelling, hang-ups and flooding of powders and it prevents the formation of stagnant regions, whilst minimising caking, degrading and segregation phenomena. In silos and hoppers filled with a densely packed product, upon opening of the outlet, a narrow plug-type zone of flowing material establishes and propagates upward. Except in the proximity of the outlet, the boundaries of the plug-flow zone are nearly vertical, and the zone widens laterally and may reach eventually the walls (Waters & Drescher, 2000). The main disadvantage in designing plug-flow silos is that a steep hopper angle is required, making the silo relatively tall. Moreover, flowability characteristics of granular solids and powders depends on many factors, among which moisture content, temperature, particle size, compacting pressure, relative humidity of the interstitial and head space air and the addition of flow conditioners and anti-caking agents that can vary (Ganesan, Rosentrater, & Muthukumarappan, 2008). Some general solutions to facilitate plug flow in grain handling and drying include the use of inserts to improve material flow patterns (Wójcik, Tejchman, & Enstad, 2012), the adoption of revolving extracting screws (see e.g. Borghi, 2012; Mulmix, (2012)) and blade extractors for homogeneous bin empting and powered grain spreaders to evenly fill the silos. Nowadays, different techniques are available to measure and verify if flow conditions correspond to manufacturer's claims. For example, there is the the application of RFID tags (Chen, Rotter, Ooi, & Zhong, 2007) or of specific tracers (Job, Dardenne, & Pirard, 2009), directly introduced at the top of the silo.

A FIFO compartment can be schematically represented as a vertical cylinder of constant cross-section S_i, in which the outflow is at the bottom, i.e. at height $h = 0$, while the material inflowing the compartment enters the silo or tank from above and it is uniformly deposited at height $H_i(t)$ on top of the material that is already stored. Notice that the total level $H_i(t)$ of material stored in the pipe is in general time-varying: if the total inflow is larger than the total outflow it increases in time, while it decreases if the outflow is larger than the inflow. Obviously, it results that $H_i(t) \geq 0$ for all t and the mass stored in this i -th compartment at any time i is equal to $m_i(t) = \rho S_i H_i(t)$, where ρ is the density of the material contained in the FIFO compartment. In order to ensure a purely FIFO behaviour for compartment i, it is assumed that all the material stored in the compartment strictly moves only downwards and at the same speed, which is equal to $q_{OUT,i}(t)/(\rho S_i)$, where the total inflow to compartment i is defined as follows $q_{OUT,i}(t) \doteq \sum_{j=0}^{n} q_{ji}(t)$. Similarly, the total inflow to compartment i is defined as $q_{IN,i}(t) \doteq \sum_{j=0}^{n} q_{ij}(t)$.

Thus, the relative fraction of flow entering compartment i at time t and constituted of material belonging only to S-lot L, can be written as follows:

$$\gamma_{IN,i}^{L}(t) \doteq \frac{q_{IN,i}^{L}(t)}{q_{IN,i}(t)} = \frac{\sum_{j=0}^{n} \gamma_j^L(t)\, q_{ij}(t)}{\sum_{j=0}^{n} q_{ij}(t)}, \text{ for } L \in \mathcal{L}. \quad (8)$$

Obviously, it holds that $\sum_{L\in\mathcal{L}} \gamma_{IN,i}^{L}(t) = 1$. The following vector can also be introduced

$$\gamma_{IN,i}(t) \doteq \left[\gamma_{IN,i}^{\mathrm{A}}(t)\ \gamma_{IN,i}^{\mathrm{B}}(t)\ \gamma_{IN,i}^{\mathrm{C}}(t) \cdots\right]^{T}. \tag{9}$$

It can be regarded as the instantaneous composition of the inflow into compartment i at time t.

It follows then that also for the material stored in this compartment it is possible to derive ℓ functions $\gamma_i^L(h,t)$ that provide, at any cross-section at height h in the pipe, the relative fraction of material belonging to each S-lot L at time t. Note that these functions vary continuously with respect to the height h.The total fraction of S-lot L contained in tank i at time t can be computed integrating $\gamma_i^L(h,t)$ in the interval $[0, H_i(t)]$, that is

$$\gamma_i^L(t) = \int_0^{H_i(t)} \gamma_i^L(h,t)\mathrm{d}h \ , \text{ for } L \in \mathcal{L}. \tag{10}$$

Similarly, the total mass of material belonging to S-lot L contained in tank i at time t can be obtained as $m_i^L(t) = \gamma_i^L(t) m_i(t)$, for $L \in \mathcal{L}$.

Notice that the functions $\gamma_i^L(h,t)$, $L \in \mathcal{L}$, fully describe the state of the tank i with FIFO behaviour, which turns out to be a dynamic system with an infinite dimensional state vector. The dynamics of the tank can therefore be precisely represented only by partial differential equations. The integration of such equations, however, is usually performed numerically by approximating the system with discrete or finite elements techniques, which provide approximating models with a finite dimensional state vector (González-Montellano, Gallego, Ramírez-Gómez, & Ayuga, 2012; Ketterhagen et al., 2007).

In our case this task can be easily done directly approximating the functions $\gamma_{IN,i}^{L}(t)$, $L \in \mathcal{L}$, by quantifying them over a given number of levels. It means that the inflow relative composition is assumed to be constant over time as long as its composition does not vary more than given thresholds. Obviously the same holds also for the outgoing flow leaving the tank.

In the sequel, adopting a compartmental model terminology, the amount of material with a homogeneous composition (up to quantisation level δ), in terms of share of S-lots, that enters or leaves a compartment is called a cohort. The status of the i-th compartment with first-in-first-out behaviour is then fully described by the ordered list of the cohorts that are stored in it. Formally, the i-th compartment is hence completely described by the list

$$\begin{bmatrix} TOP \\ queued_v \\ \vdots \\ queued_1 \\ BOTTOM \end{bmatrix}_i \tag{10}$$

of cohorts contained in it. To each of these cohorts the information about its total mass and composition is associated.

Considering again the i-th compartment, if at time t the composition-distance between the inflow IN, i (entering the compartment at time t) and the material already present in the top cohort TOP, i is greater than a selected quantisation level δ, so that $d\big(\gamma_{IN,i}(t), \gamma_{TOP,i}(t)\big) > \delta$, then a new cohort is created. This newly generated cohort, with all the information that fully describes its composition, is then piled in the FIFO array. For the sake of clarity, the algorithm is schematized in Fig. 7. In particular, the differential equations in (7) are simulated (step 4 in the algorithm in Fig.7) until a new event, such as a valve opening/closing or a pump start/stop, occurs.

In order to clarify the impact of using cohorts, the dynamics of the scheme introduced in Example 1 is now analysed focusing on the third tank, schematized as a FIFO container.

Example 2. The analysis is carried out twice, using two different quantisation levels, $\delta_1 = 0.1$ and $\delta_2 = 0.02$, so that the influence of quantisation levels can be considered as well. At time $t_1 = 80$ s the valve on the connection between Tank 2 and Tank 3 is opened and a flow $q_{32}(t)$ equal to 0.5 kg s^{-1} is established. Tank 3 starts to release product out of the system at $t_2 = 110$ s, with a flow $q_{03}(t) = 0.2$ kg s^{-1}, as shown in Fig. 2. The threshold δ_1 to generate new cohorts in Tank 3 is applied on the composition of flow $q_{32}(t)$, whose relative amount of S-Lot 'A' and S-Lot 'B' is represented in Fig. 6, using $\gamma_{IN,2}^{\mathrm{A}}(t)$ and $\gamma_{IN,2}^{\mathrm{B}}(t)$ indexes. The time instants in which one of the $\gamma_{IN,2}^{\mathrm{L}}(t)$ crosses a quantisation level, with a threshold set of $\delta_1 = 0.1$, are reported in Fig. 6 with vertical lines. Masses $m_3^{\mathrm{A}}(t)$ and $m_3^{\mathrm{B}}(t)$ of material belonging to S-Lot '*A*' and to S-Lot '*B*', and the overall mass $m_3(t)$, in Tank 3 are shown in Fig. 9, that however lacks of information about the cohorts that have been generated during the filling phase with $q_{32}(t)$. For this reason, Fig. 10 is reported, in which mass content of Tank 3 is represented in three different time instants. Each cohort is characterized by a different colour, related to the relative composition in terms of S-Lot 'A' and 'B'. The influence of product quantisation in Tank 3 on the outflow $q_{03}(t)$ can be seen in Fig. 8, where indices $\gamma_{OUT,2}^{\mathrm{A}}(t)$ and $\gamma_{OUT,2}^{\mathrm{B}}(t)$ are plotted over time. Results obtained setting a threshold δ_2 equal to 0.02, are reported in Figs. 11 and 12. Note that the generated cohorts are in this case smaller and more homogeneous. A movie of this simulation example was recorded in MPEG files S1 and S2, for thresholds δ_1 and δ_2, respectively.

4. A case study: plant with both UM and FIFO tanks

In order to clarify the concepts and the procedures introduced in previous sections, a case study, consisting in seven interconnected tanks depicted in Fig. 13, is now presented. In this example, all compartments behave as FIFO buffers, with the exception of Tank 6, where an agitator ensures a uniform mixing of processed products. At time $t = 0$ s, Tanks 1 to 4 were filled with homogeneous raw material. In more detail, 100 kg of S-lot 'A' and 200 kg of 'B' was stored into Tank 1, Tank 2 was filled with 50 kg of S-lot 'C' and 200 kg of 'D', Tank 3 with 200 kg of S-lot 'E', and finally 300 kg of S-lot 'F' and 100 kg of 'G' were stored in Tank 4. Valves opening at time $t_1 = 60$ s allowed product flows $q_{51}(t) = 0.32$ kg s^{-1} and $q_{52}(t) = 0.2$ kg s^{-1} from Tanks 1 and 2 to Tank 5. At time t_2=120 s, flows $q_{63}(t)$=0.18 kg s^{-1} and $q_{64}(t)$=0.28 kg s^{-1} started from Tanks 3 and 4 to Tank 6, where the incoming products were continuously mixed. Then, at time t_3=300 s the product in Tanks 5 and 6 started flowing into Tank 7 with a rate of $q_{75}(t)$ and $q_{76}(t)$ equal to 0.3 kg s^{-1}. Figure 14 shows the evolution of the flows between storage units and processing stations over time. Adopting a quantisation level δ equal to 0.05, six cohorts of final product, characterised by different percentages of S-Lots 'A' to 'G', are generated. The simulation movie of the working plant is reported in MPEG file S3. The manner in which the S-lots spread into the plant and mixed to produce the six cohorts of final product in Tank 7 is demonstrated in Fig. 15 where the composition of each cohort is directly reported in the node. Note that this dispersion graph can be directly used to measure (and possibly to optimise) the performance of the traceability system as proposed in (Dabbene & Gay, 2011). As already remarked, the level of detail of the traceability, and therefore the number of generated cohorts, depends on the choice of the threshold δ. Simulations were performed at different values of δ ranging from 10^{-3} to 10^{-1}. Figure 16 (left) shows how the number of generated cohorts considerably increased for decreasing values of threshold δ. As expected, at increasing number of cohorts, it correspond to smaller average cohort sizes (Fig. 16, right) and more homogeneous compositions. Figure

16 shows also the masses of the largest and smallest cohort generated in each simulation of the set. These figures show that there exists a clear trade-off between the quantisation level δ and the number of different lots generated. This trade-off should be taken in due consideration by the supply chain manager in designing and optimising the traceability system.

5. Conclusions and future directions

A methodology for efficiently tackling the problem of traceability when continuously processing and storing bulk materials has been proposed. In particular, the introduced framework is particularly suitable for the management of internal traceability, i.e. during the production processes within a company. According to the key advantages provided by internal traceability, as discussed in Moe (1998), this methodology makes it possible to monitor (and thus avoid) uneconomic mixing of high and low-quality raw materials and ingredients, and provides the basis for the adoption of efficient recall procedures to minimise losses; advantages that at present are available only for the processing of discrete lots. In particular, this method allows the proper identification and definition of batches of homogeneous product, without resorting to the currently often-adopted process of oversizing the lots. In particular, the availability of precise information about the composition, in terms of lots of raw ingredients, introduces the possibility to correlate product data with raw materials and then to optimise the recipes for each final product type. Indeed, in most cases the lots of bulk product entering the company's process are subject to chemical, physical and microbiological analysis. This precise characterisation of the raw or semi-finished materials, especially for properties of products (or raw materials) that cannot be measured in real-time, can be exploited to design new and improved adaptive control strategies.

Two representative cases of product containers, namely UM and the FIFO compartments were analysed. It is however important to notice that the approach introduced in the paper can be extended to the more general case of storage compartments that do not show either UM or FIFO behaviour. Fundamental in this case is the availability of an accurate description of the dynamics governing the way the material delivered to the compartment is stored within its volume, and of the laws by which such material is combined into the output flow. The problem of experimentally determining such laws has been the subject of growing interest in the literature. See, for instance, the recent works of Ganesan, Rosentrater, and Muthukumarappan (2008), González-Montellano, Ramírez, Gallego, and Ayuga (2011), Mellmann et al. (2011), Sielamowicz and Czech (2010), and Sielamowicz, Czech, and Kowalewski (2011), which applied finite/discrete elements techniques to describe tank filling/emptying dynamics. Indeed, once the laws governing the storing and mixing phenomena taking place in the tanks are adequately modelled, these mathematical models can be directly integrated in the framework discussed so far, since compartmental models are well-suited to cope with such situations. Specific cases are currently under study, and will be the subject of further works.

Finally, in the context of the present work, the fraction of the inflow allocated to each S-lots has been considered exactly known. However, it appears possible to consider instead the case when such fraction is subject to uncertainty. For instance, this could account for situations in which the UM or FIFO models are not sufficiently accurate in describing the real behaviour of the processes or some uncertainties affect flow dynamics (for example in the case in which the flow is dependent on some product conditions like temperature, moisture content etc.). In such case, the knowledge of the real composition of the outflow is not precise, and it can be determined only up to a given tolerance. Hence, it could be important to develop a method able to determine the maximum amount of each S-lot that could be present in each compartment as well as in each flow.

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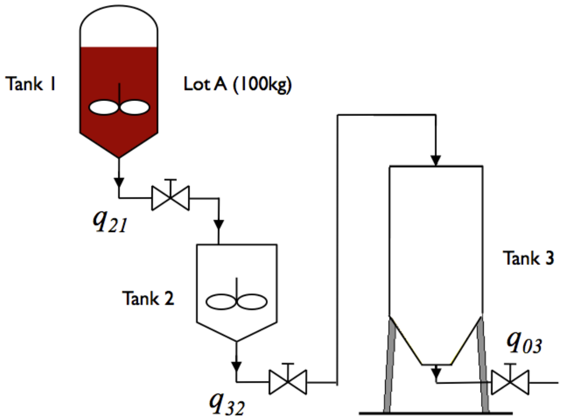

Fig. 1. Scheme of the plant in examples 1 and 2

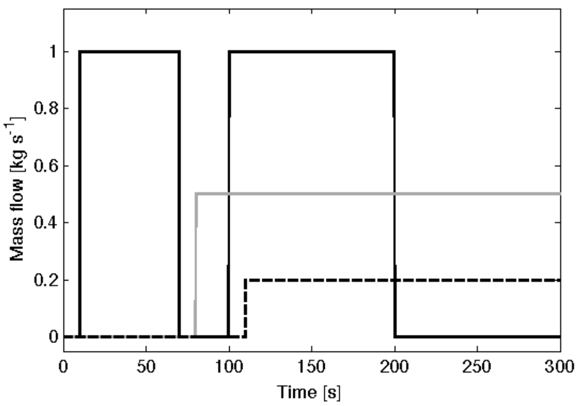

Fig. 2. Mass flow q_{21} (black solid) from Tank 1 to Tank 2, q_{32} (grey solid) from Tank 2 to Tank 3, and q_{03} (black dashed) from Tank 3 out of the system

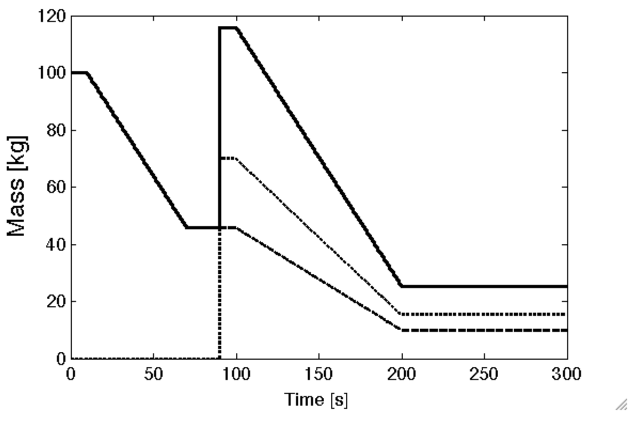

Fig. 3. Mass of product belonging to S-lot A (black dashed), S-lot B (black dotted), and overall mass amount in Tank 1 (black solid).

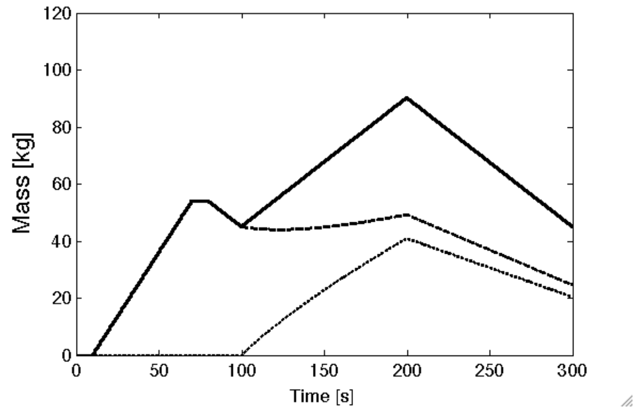

Fig. 4. Mass of product belonging to S-lot A (black dashed), S-lot B (black dotted), and overall mass amount in Tank 2 (black solid).

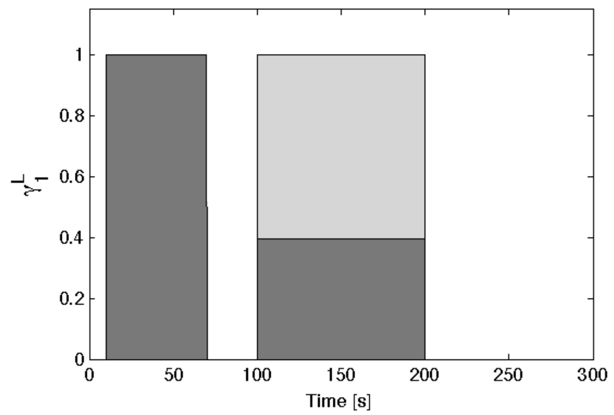

Fig. 5. Relative fractions $\gamma_1^{\mathrm{A}}(t)$ (dark grey) and $\gamma_1^{\mathrm{B}}(t)$ (light grey) of q_{21} flow constituted by mass belonging to lot of product A and B respectively. The sum of $\gamma_1^{\mathrm{A}}(t)$ and $\gamma_1^{\mathrm{B}}(t)$is always equal to 1.

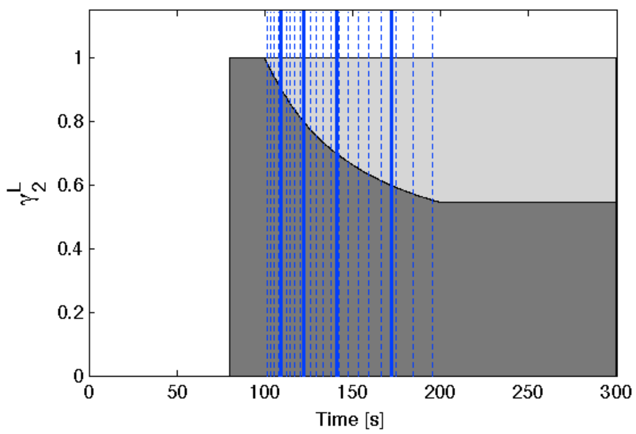

Fig. 6. Relative fractions $\gamma_2^{\mathrm{A}}(t)$ (dark grey) and $\gamma_2^{\mathrm{B}}(t)$ (light grey) of flow q_{02} constituted of mass belonging to S-lot A and B respectively. The sum of $\gamma_2^{\mathrm{A}}(t)$ and $\gamma_2^{\mathrm{B}}(t)$ is always equal to 1. Time instants in which a new cohort is generated inside Tank 3 are represented by vertical solid and dashed lines, for the two cases of quantisation level δ equal to 0.1 and 0.02, respectively.

1: $j \leftarrow 0$
2: Do
3: $t_{j+1} \leftarrow min(t_j + \Delta t, t_{next\_event})$
4: Simulate $\gamma_{IN,i}(t)$ for $t \in [t_j, t_{j+1}]$
5: For $t = t_j$ to t_{j+1} do
6: If $d\left(\gamma_{IN,i}(t), \gamma_{IN,i}(t_j)\right) > \delta$ then
7: $j \leftarrow j + 1$
8: $t_j \leftarrow t$
9: $v \leftarrow v + 1$
10: $queued_v \leftarrow TOP$
10: Create new TOP cohort
11: Goto 3
12: End
13: $j \leftarrow j + 1$
14: While $t < t_{end}$
15: End

Fig. 7. Algorithm for the creation of homogeneous cohorts in a FIFO compartment. Simulation parameters: t_{next_event} - time of the occurrence of the next event after t; t_{end} – end time of the simulation; Δt arbitrary time interval.

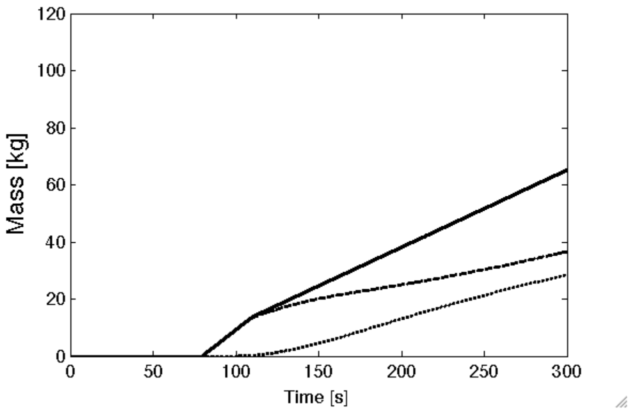

Fig. 8. Mass of product belonging to S-lot A (black dashed), S-lot B (black dotted), and overall mass amount in Tank 3 (black solid).

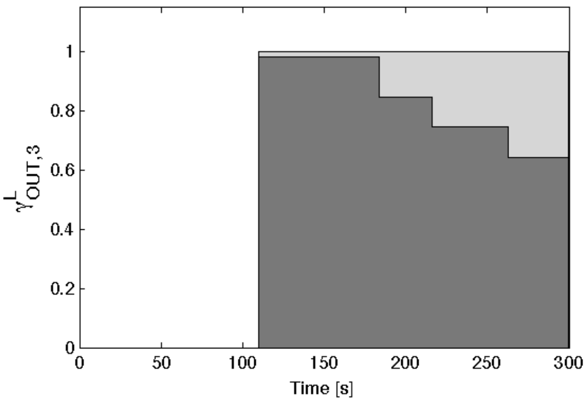

Fig. 9. Relative fractions $\gamma^{A}_{OUT,3}(t)$ (dark grey) and $\gamma^{B}_{OUT,3}(t)$ (light grey) of flow q_{03} constituted of mass belonging to S-lot A and B respectively, in the case of quantisation level δ equal to 0.1

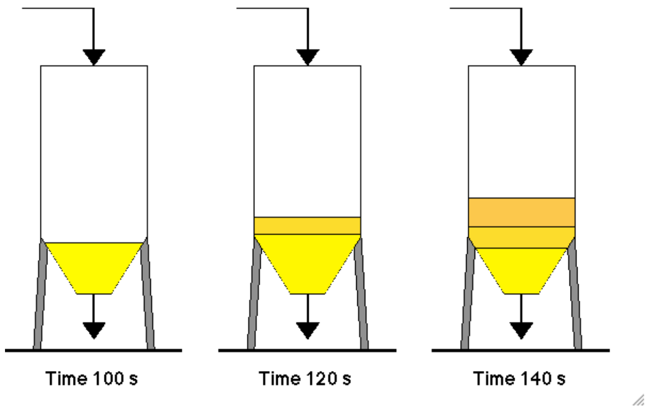

Fig. 10. Tank 3 content at t=100, 120 and 140 seconds, in the case of quantisation level δ equal to 0.1. Different cohorts are represented with colour hues proportional to the % of product belonging to S-Lot A and S-Lob B.

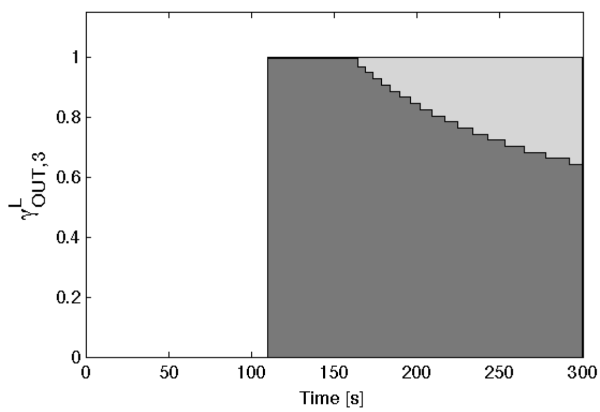

Fig. 11. Relative fractions $\gamma^{A}_{OUT,3}(t)$ (dark grey) and $\gamma^{B}_{OUT,3}(t)$ (light grey) of flow q_{03} constituted of mass belonging to S-lot A and B respectively, in the case of quantisation level δ equal to 0.02.

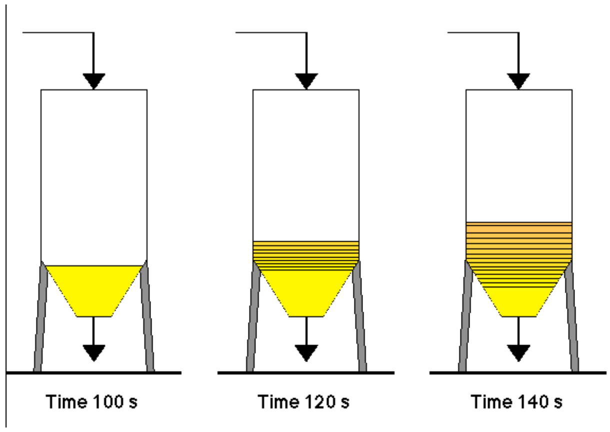

Fig. 12. Tank 3 content at t=100, 120 and 140 seconds, in the case of quantisation level δ equal to 0.02. Different cohorts are represented with colour hues proportional to the % of product belonging to S-Lot A and S-Lob B.

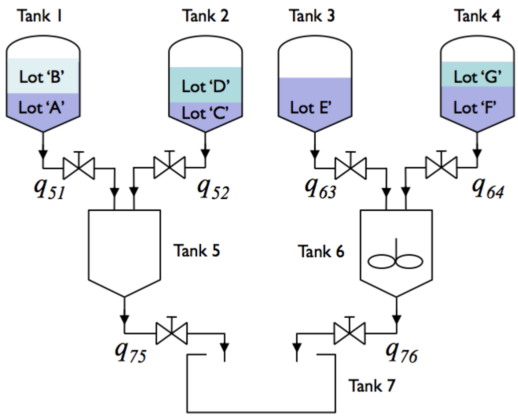

Fig. 13. Scheme of the plant in the case study at time $t = 0$

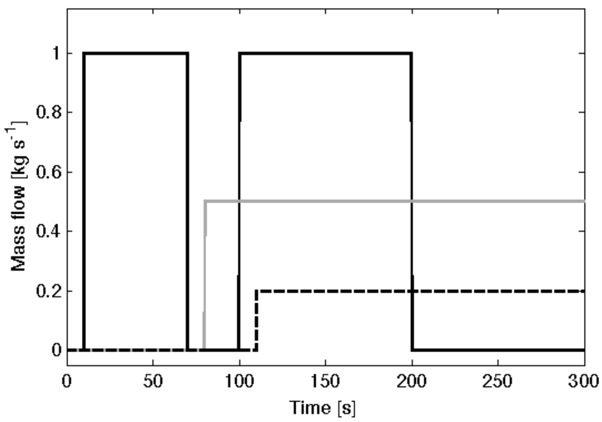

Fig. 14. Mass flows $q_{51}(t)$ (black solid) from Tank 1 to 5, $q_{52}(t)$ (grey dashed) from Tank 2 to 5, $q_{63}(t)$ (grey dotted) from Tank 3 to 6, $q_{64}(t)$ (black dashed) from Tank 4 to 6, $q_{75}(t)$ (grey solid) from Tank 5 to 7, and $q_{76}(t)$ (black dotted) from Tank 6 to 7.

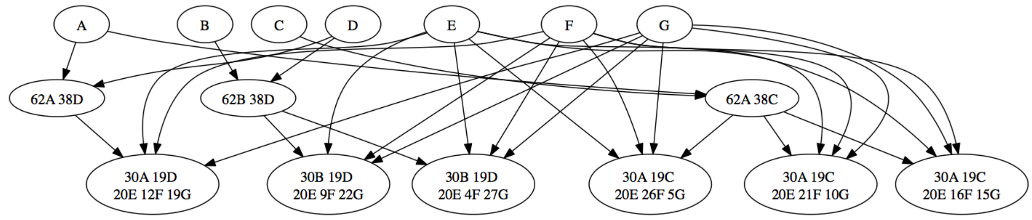

Fig. 15. Graph of the composition of the six cohorts. The label of each node in the graph reports the composition of the cohort, where the numbers express the percentage of the different S-lots (A to G).

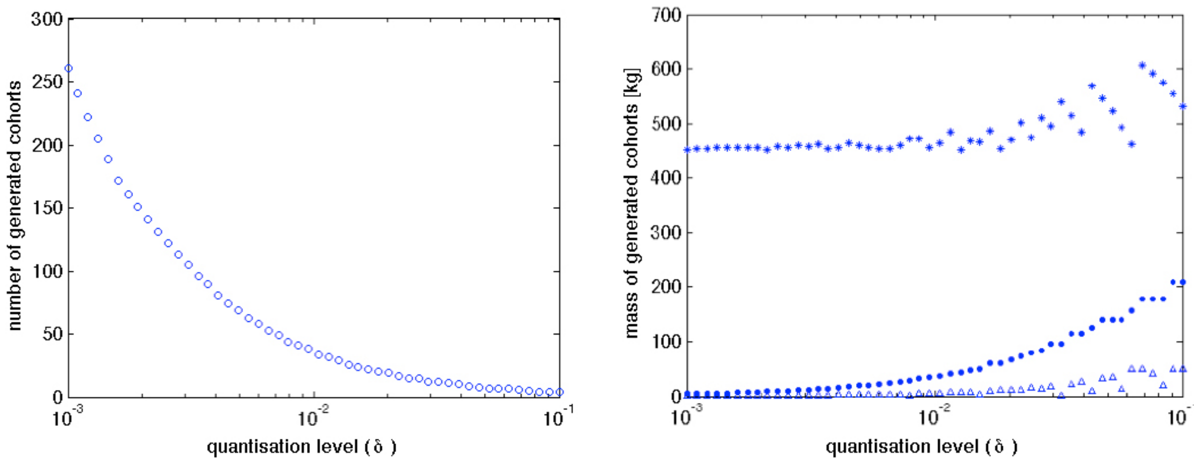

Fig. 16. Number (on the left) and average mass (dotted, on the right) of generated cohorts obtained with different quantisation levels δ ranging from 10^{-3} to 10^{-1} in Example 3. On the right, masses of the biggest ($*$) and smallest (Δ) cohort are also reported.

Highlights

- Development of a model for traceability of bulk products, like liquids, powders, crystals, or grains
- Based on compartmental models of process in terms of transfer, combination, and storage of mass
- 2 representative cases with the uniform-mixing and plug-flow behaviour described
- Method is based on formal identification and definition of lots of homogeneous product
- Results gives the basis for efficient recall procedures to minimise losses

Graphical abstract