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1 **Methods for traceability in food production processes involving** 2 **bulk products**

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13
14 **Keywords:** traceability, batch dispersion, food processing, compartmental models

15 16 **Abstract**

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

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

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

35

36 Nomenclature

37

$\mathcal{L} = \{'A', 'B', 'C', \dots\}$	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
$\gamma^A(X)$	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

39 **1. Introduction**

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

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

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

66 One possible approach to minimise recalls consists in separating the lots as much as possible
67 within the plant. In the case of fluids, for instance, the use of different containers and
68 cleaning between two product batches is a viable solution to allow distinct separated batches
69 identities. In particular, cleaning-in-place procedures, which involve pumping water and
70 detergent through the production equipment, besides guaranteeing high hygienic standards, is

71 seen as the good procedure to strictly guarantee that the different batches cannot contaminate
72 each other. Indeed, there are situations where the complete and absolute segregation of
73 different lots supply lots is mandatory. This is the case, for instance, with products subject to
74 religious specifications (e.g. Kosher or Halal certification), for military supply contracts, and
75 where products are subject to very particular safety issues and constraints. In most other
76 cases, these cleaning procedures, besides representing a high cost for the company in terms of
77 energy, manpower, and cleaning agents, become undesirable, especially in the case of
78 continuous production systems (such as, e.g., milk production in a dairy) where continuous
79 flow of liquid/granular raw material, without even minimal interruptions, is necessary to
80 maintain the production.

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

88 Moreover, with types of bulk products, it is very difficult to associate any kind of label,
89 marker or identifier that could directly identify the different lots. Recently, some markers
90 based on Radio-Frequency Identification (RFID) technology have been developed for the
91 case of continuous granular flows (specifically, iron pellets) by Kvarnström, Bergquist, and
92 Vännman (2011). These markers allow on-line traceability of continuous flows, improving
93 previous off-line solutions based on the introduction of specific tracers into the grains, such
94 as chemical compounds or radioactive tracers; see Kvarnström and Oghazi (2008) and Lee et
95 al., (2010) for detailed discussion and references on these techniques. The situation is
96 complicated by the obvious requirement that the markers should not compromise in any way
97 the integrity and quality of the food and must be not dangerous for the consumer. Thus, any
98 RFID-based traceability system would require the development of a device for safely
99 removing the tracing devices from the final product (e.g. before grain grinding). In this
100 regard, some interesting solutions were proposed in Lee et al. (2010) and Liang et al. (2012)
101 for the specific case of grains which involve particular pill-sized food-grade tracer particles to
102 be inserted directly into grain during harvest. These tracers have printed with food-grade ink
103 a miniaturised data-matrix code carrying identity information related to product origin, and

104 are composed of materials that can be safely eaten such as sugar or cellulose. However, these
105 solutions remain principally an off-line approach, suitable for modelling and validation
106 purposes, since collecting and identifying the tracers would usually still require production
107 to be interrupted.

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

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

133 These methods have been applied to many different supply chains, e.g. for fruits (Bollen et
134 al., 2007; Riden & Bollen, 2007), meat (Barge P., Gay P., Merlino V., & Tortia C., 2013;
135 Donnelly, Karlsen, & Olsen, 2009; Dupuy et al., 2005), fish (Karlsen, Donnelly, & Olsen,
136 2011; Randrup et al., 2008), grains (Thakur & Donnelly, 2010; Thakur & Hurburgh, 2009;

137 Thakur, Wang, & Hurburgh, 2010), chocolate (Saltini & Akkerman, 2012), perishable
138 products (Li, Kehoe, & Drake, 2005; Rong & Grunow, 2010; Wang X., Li D., & O'Brien C.,
139 2009) etc.

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

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

154 **2. Definitions and problem formulation**

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

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

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

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

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

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

181

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

$$c(X) \doteq [\gamma^A(X) \ \gamma^B(X) \ \gamma^C(X) \ \dots]^T. \quad (1)$$

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

$$d(X, Y) \doteq \|c(X) - c(Y)\|_\infty, \quad (2)$$

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

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

$$d(X, Y) < \delta. \quad (3)$$

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

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

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

216 Like the already mentioned case of GM and non-GM grains, there are other situations related
217 to ethical, organic, low carbon footprint, issues or subject to disciplinary or to religious
218 constraints, where lots should be maintained as much as possible separated. In such cases
219 facilities and logistics have to be designed and planned accordingly. Different management
220 strategies have been proposed to cope with this problem. They are typically based on the
221 separation of products in space, allocating specific collecting units (e.g. silos) for any
222 different lot, or they are based on the separation in time, when different lots are processed in
223 successive sessions, separated by suitable cleaning cycles (see e.g. Coléno, 2008; Maier,
224 2006).

225

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

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

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

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

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

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

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

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

277

278 **3. Modelling uniform-mixing and FIFO compartments**

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

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

286 The case of n interconnected tanks is considered, with material flowing from the outside and
287 between them. Considering a generic compartment i , it follows that there are possibly up to n
288 different mass inflows $q_{ij}(t)$, $j = 0, \dots, n, j \neq i$ entering compartment i from other $n -$
289 1 compartments, or from outside the system. So, $q_{ij}(t)$ represents the mass flow leaving

290 compartment j and entering compartment i , while $q_{i0}(t)$ represents the flow entering the i -th
 291 compartment from outside the system, and $q_{0j}(t)$, represents the flow leaving the system
 292 from the j -th compartment (this according to the standard notation used in compartmental
 293 model literature). It should be noted that the flows $q_{ij}(t)$ are bounded to be positive or zero,
 294 and cannot assume negative values. In particular, if no flow exists from compartment j to
 295 compartment i , then we assume $q_{ij}(t) = 0$. Hence, we can define the following *flow matrix*

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

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

300

301 3.1. Compartments ensuring uniform mixing

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

318 In order to describe the dynamics governing the different lots, a compartmental model is
 319 introduced, where each compartment coincides with a tank in the system. Firstly, to describe

320 the dynamic behaviour of a generic compartment i a set of suitable state variables that fully
 321 account for its status at any time is chosen.

322 In this regard, denote by $m_i(t)$ the total mass available in compartment i at time t . This mass
 323 can be divided into ℓ different sub-masses $m_i^L(t)$, one for every $L \in \mathcal{L}$, representing the
 324 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
 325 state variables that fully describe the dynamics of compartment i .

326 Then, the following quantities are defined

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

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

$$\gamma_i(t) \doteq [\gamma_i^A(t) \ \gamma_i^B(t) \ \gamma_i^C(t) \ \dots]^T, \quad (6)$$

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

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

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

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

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

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

344 *Example 1 (Complete uniform mixing)*. In order to clarify the previously presented concepts,
345 a simple system depicted in Fig. 1 is introduced. Focusing on the first part of the plant,
346 constituted by the cascade of two storage compartments (Tank 1 and Tank 2) characterised
347 by uniform mixing, considering the following situation: at initial time $t_0 = 0$ s, Tank 1 is
348 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
349 transferred into Tank 2 for 60 s. Subsequently, at time $t_2 = 80$ s, an outflow of 0.5 kg s^{-1}
350 starts from Tank 2. At $t_3 = 90$ s, an extra 70 kg belonging to S-lot 'B' is added to Tank 1.
351 Finally, at time $t_4 = 100$ s, a flow of 1 kg s^{-1} is again transferred into Tank 2 for 100 s.
352 Values of the mass flows between the three tanks over the time interval 0 - 300 s are plotted
353 in Fig. 2.

354 Assuming that the material is uniformly mixed in the two compartments, the masses $m_1^A(t)$,
355 $m_1^B(t)$, $m_2^A(t)$, $m_2^B(t)$ of material belonging to S-lots 'A' and 'B' in Tank 1 and Tank 2 are
356 reported in Fig. 3 and Fig. 4, respectively, over the interval 0 – 300 s. Figures 5 and 6 report
357 the fractions $\gamma_1^A(t)$, $\gamma_1^B(t)$, $\gamma_2^A(t)$, and $\gamma_2^B(t)$, describing the relative composition in terms of
358 S-lots 'A' and 'B' of the two flows $q_{21}(t)$ and $q_{32}(t)$, respectively. In particular, in Fig. 6 it
359 can be seen that the composition of the flow from Tank 2 to Tank 3 is continuously varying,
360 with the fraction material belonging to S-lot 'B' increasing and the that from S-lot 'A'
361 decreasing. The blue vertical lines in Fig. 6 refer to the introduction of quantisation levels,
362 which are discussed in the next section.

363

364 3.2. Compartments behaving as FIFO buffer

365 The case in which a generic i -th compartment behaves like a first-in-first-out buffer is surely
366 more complex, and is discussed hereafter. Note that the FIFO model can represent several
367 practical situations encountered in real production lines when dealing with bulk solids and
368 powders. Indeed, there is a growing research designing specific devices and tank
369 configurations that ensure plug-flow. Plug flow (referred also as mass flow) silos are
370 frequently used in industrial processing because of some of their beneficial properties. Plug
371 flow is the most productive flow because it eliminates problems such as channelling, hang-
372 ups and flooding of powders and it prevents the formation of stagnant regions, whilst
373 minimising caking, degrading and segregation phenomena. In silos and hoppers filled with a
374 densely packed product, upon opening of the outlet, a narrow plug-type zone of flowing
375 material establishes and propagates upward. Except in the proximity of the outlet, the

376 boundaries of the plug-flow zone are nearly vertical, and the zone widens laterally and may
377 reach eventually the walls (Waters & Drescher, 2000). The main disadvantage in designing
378 plug-flow silos is that a steep hopper angle is required, making the silo relatively tall.
379 Moreover, flowability characteristics of granular solids and powders depends on many
380 factors, among which moisture content, temperature, particle size, compacting pressure,
381 relative humidity of the interstitial and head space air and the addition of flow conditioners
382 and anti-caking agents that can vary (Ganesan, Rosentrater, & Muthukumarappan, 2008).
383 Some general solutions to facilitate plug flow in grain handling and drying include the use of
384 inserts to improve material flow patterns (Wójcik, Tejchman, & Enstad, 2012), the adoption
385 of revolving extracting screws (see e.g. Borghi, 2012; Mulmix, (2012)) and blade extractors
386 for homogeneous bin emptying and powered grain spreaders to evenly fill the silos.
387 Nowadays, different techniques are available to measure and verify if flow conditions
388 correspond to manufacturer's claims. For example, there is the the application of RFID tags
389 (Chen, Rotter, Ooi, & Zhong, 2007) or of specific tracers (Job, Dardenne, & Pirard, 2009),
390 directly introduced at the top of the silo.

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{bmatrix} TOP \\ queued_v \\ \vdots \\ queued_1 \\ BOTTOM \end{bmatrix}_i \quad (10)$$

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

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

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

445 *Example 2.* The analysis is carried out twice, using two different quantisation levels, $\delta_1 = 0.1$
 446 and $\delta_2 = 0.02$, so that the influence of quantisation levels can be considered as well. At time
 447 $t_1 = 80$ s the valve on the connection between Tank 2 and Tank 3 is opened and a flow
 448 $q_{32}(t)$ equal to 0.5 kg s^{-1} is established. Tank 3 starts to release product out of the system at
 449 $t_2 = 110$ s, with a flow $q_{03}(t) = 0.2 \text{ kg s}^{-1}$, as shown in Fig. 2. The threshold δ_1 to generate
 450 new cohorts in Tank 3 is applied on the composition of flow $q_{32}(t)$, whose relative amount
 451 of S-Lot 'A' and S-Lot 'B' is represented in Fig. 6, using $\gamma_{IN,2}^A(t)$ and $\gamma_{IN,2}^B(t)$ indexes. The
 452 time instants in which one of the $\gamma_{IN,2}^l(t)$ crosses a quantisation level, with a threshold set of
 453 $\delta_1 = 0.1$, are reported in Fig. 6 with vertical lines. Masses $m_3^A(t)$ and $m_3^B(t)$ of material
 454 belonging to S-Lot 'A' and to S-Lot 'B', and the overall mass $m_3(t)$, in Tank 3 are shown in
 455 Fig. 9, that however lacks of information about the cohorts that have been generated during
 456 the filling phase with $q_{32}(t)$. For this reason, Fig. 10 is reported, in which mass content of
 457 Tank 3 is represented in three different time instants. Each cohort is characterized by a
 458 different colour, related to the relative composition in terms of S-Lot 'A' and 'B'. The
 459 influence of product quantisation in Tank 3 on the outflow $q_{03}(t)$ can be seen in Fig. 8,
 460 where indices $\gamma_{OUT,2}^A(t)$ and $\gamma_{OUT,2}^B(t)$ are plotted over time. Results obtained setting a

461 threshold δ_2 equal to 0.02, are reported in Figs. 11 and 12. Note that the generated cohorts
462 are in this case smaller and more homogeneous. A movie of this simulation example was
463 recorded in MPEG files S1 and S2, for thresholds δ_1 and δ_2 , respectively.

464

465

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

467

468 In order to clarify the concepts and the procedures introduced in previous sections, a case
469 study, consisting in seven interconnected tanks depicted in Fig. 13, is now presented. In this
470 example, all compartments behave as FIFO buffers, with the exception of Tank 6, where an
471 agitator ensures a uniform mixing of processed products. At time $t = 0$ s, Tanks 1 to 4 were
472 filled with homogeneous raw material. In more detail, 100 kg of S-lot 'A' and 200 kg of 'B'
473 was stored into Tank 1, Tank 2 was filled with 50 kg of S-lot 'C' and 200 kg of 'D', Tank 3
474 with 200 kg of S-lot 'E', and finally 300 kg of S-lot 'F' and 100 kg of 'G' were stored in
475 Tank 4. Valves opening at time $t_1 = 60$ s allowed product flows $q_{51}(t) = 0.32 \text{ kg s}^{-1}$ and
476 $q_{52}(t) = 0.2 \text{ kg s}^{-1}$ from Tanks 1 and 2 to Tank 5. At time $t_2=120$ s, flows $q_{63}(t)=0.18 \text{ kg s}^{-1}$
477 and $q_{64}(t)=0.28 \text{ kg s}^{-1}$ started from Tanks 3 and 4 to Tank 6, where the incoming products
478 were continuously mixed. Then, at time $t_3=300$ s the product in Tanks 5 and 6 started flowing
479 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
480 evolution of the flows between storage units and processing stations over time. Adopting a
481 quantisation level δ equal to 0.05, six cohorts of final product, characterised by different
482 percentages of S-Lots 'A' to 'G', are generated. The simulation movie of the working plant is
483 reported in MPEG file S3. The manner in which the S-lots spread into the plant and mixed to
484 produce the six cohorts of final product in Tank 7 is demonstrated in Fig. 15 where the
485 composition of each cohort is directly reported in the node. Note that this dispersion graph
486 can be directly used to measure (and possibly to optimise) the performance of the traceability
487 system as proposed in (Dabbene & Gay, 2011). As already remarked, the level of detail of
488 the traceability, and therefore the number of generated cohorts, depends on the choice of the
489 threshold δ . Simulations were performed at different values of δ ranging from 10^{-3} to 10^{-1} .
490 Figure 16 (left) shows how the number of generated cohorts considerably increased for
491 decreasing values of threshold δ . As expected, at increasing number of cohorts, it correspond
492 to smaller average cohort sizes (Fig. 16, right) and more homogeneous compositions. Figure

493 16 shows also the masses of the largest and smallest cohort generated in each simulation of
494 the set. These figures show that there exists a clear trade-off between the quantisation level δ
495 and the number of different lots generated. This trade-off should be taken in due
496 consideration by the supply chain manager in designing and optimising the traceability
497 system.

498

499 **5. Conclusions and future directions**

500

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

518 Two representative cases of product containers, namely UM and the FIFO compartments
519 were analysed. It is however important to notice that the approach introduced in the paper can
520 be extended to the more general case of storage compartments that do not show either UM or
521 FIFO behaviour. Fundamental in this case is the availability of an accurate description of the
522 dynamics governing the way the material delivered to the compartment is stored within its
523 volume, and of the laws by which such material is combined into the output flow. The
524 problem of experimentally determining such laws has been the subject of growing interest in

525 the literature. See, for instance, the recent works of Ganesan, Rosentrater, and
526 Muthukumarappan (2008), González-Montellano, Ramírez, Gallego, and Ayuga (2011),
527 Mellmann et al. (2011), Sielamowicz and Czech (2010), and Sielamowicz, Czech, and
528 Kowalewski (2011), which applied finite/discrete elements techniques to describe tank
529 filling/emptying dynamics. Indeed, once the laws governing the storing and mixing
530 phenomena taking place in the tanks are adequately modelled, these mathematical models can
531 be directly integrated in the framework discussed so far, since compartmental models are
532 well-suited to cope with such situations. Specific cases are currently under study, and will be
533 the subject of further works.

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

544

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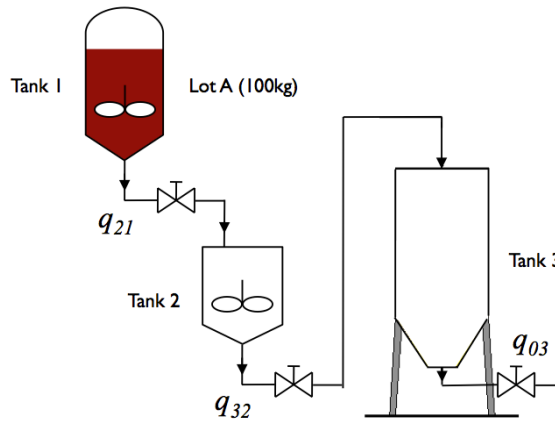


Fig. 1. Scheme of the plant in examples 1 and 2

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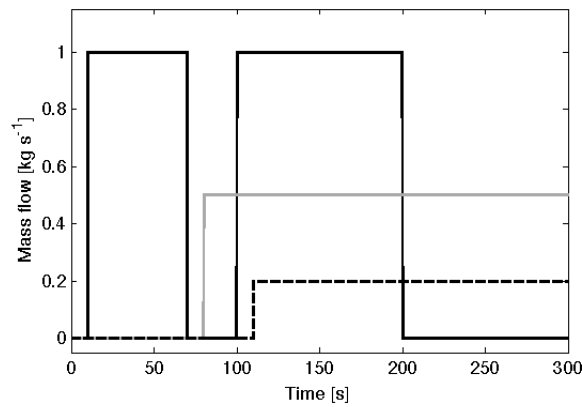


Fig. 2. Mass flow q_{21} (black solid) from Tank 1 to Tank 2, q_{32} (grey solid) from Tank 2 to Tank 3, and q_{03} (black dashed) from Tank 3 out of the system

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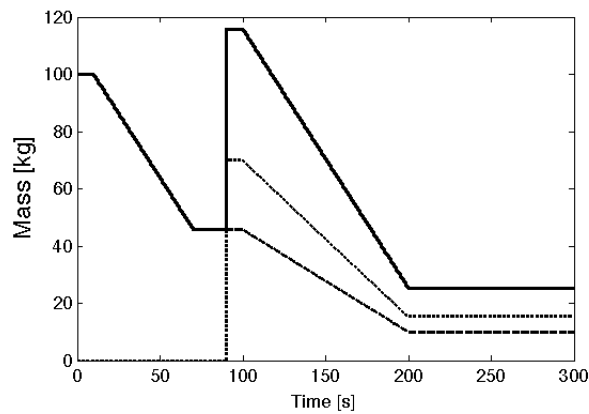


Fig. 3. Mass of product belonging to S-lot A (black dashed), S-lot B (black dotted), and overall mass amount in Tank 1 (black solid).

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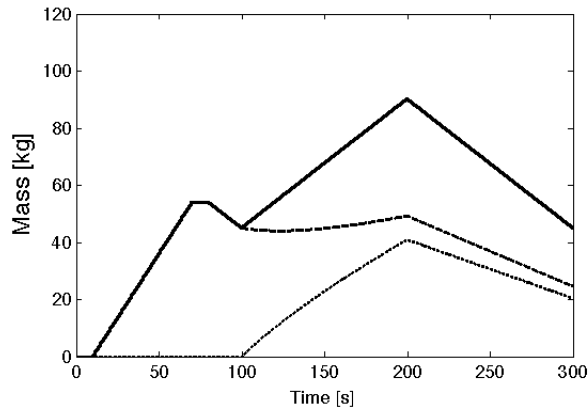


Fig. 4. Mass of product belonging to S-lot A (black dashed), S-lot B (black dotted), and overall mass amount in Tank 2 (black solid).

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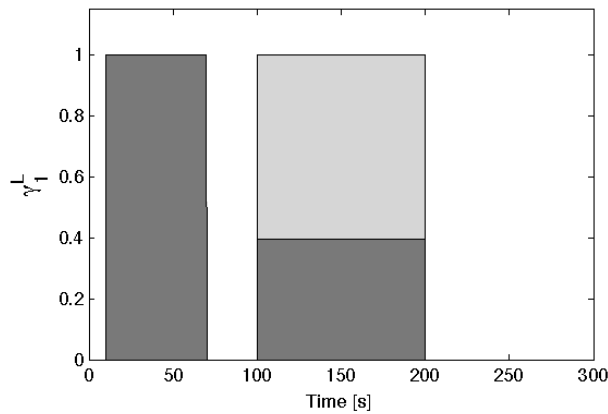


Fig. 5. Relative fractions $\gamma_1^A(t)$ (dark grey) and $\gamma_1^B(t)$ (light grey) of q_{21} flow constituted by mass belonging to lot of product A and B respectively. The sum of $\gamma_1^A(t)$ and $\gamma_1^B(t)$ is always equal to 1.

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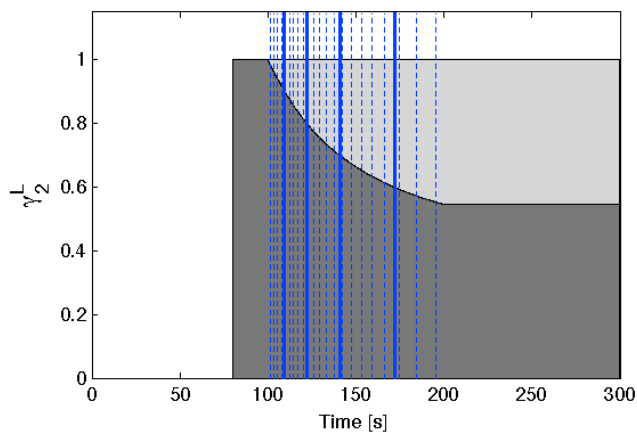


Fig. 6. Relative fractions $\gamma_2^A(t)$ (dark grey) and $\gamma_2^B(t)$ (light grey) of flow q_{02} constituted of mass belonging to S-lot A and B respectively. The sum of $\gamma_2^A(t)$ and $\gamma_2^B(t)$ is always equal to 1. Time instants in which a new cohort is generated inside Tank 3 are represented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

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```
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  $d(\gamma_{IN,i}(t), \gamma_{IN,i}(t_j)) > \delta$  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.

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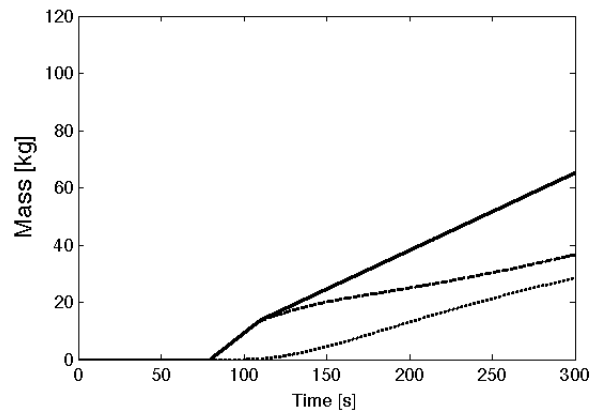


Fig. 8. Mass of product belonging to S-lot A (black dashed), S-lot B (black dotted), and overall mass amount in Tank 3 (black solid).

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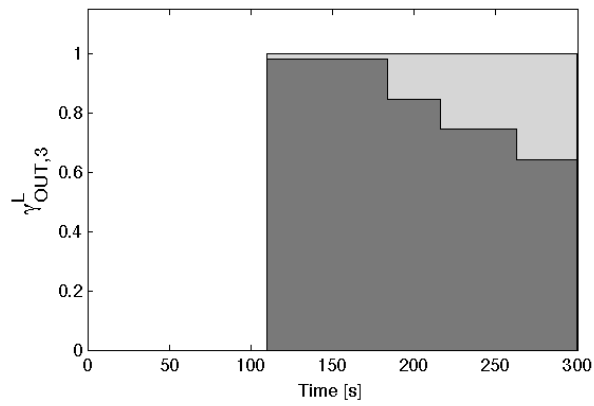


Fig. 9. Relative fractions $\gamma_{OUT,3}^A(t)$ (dark grey) and $\gamma_{OUT,3}^B(t)$ (light grey) of flow q_{03} constituted of mass belonging to S-lot A and B respectively, in the case of quantisation level δ equal to 0.1

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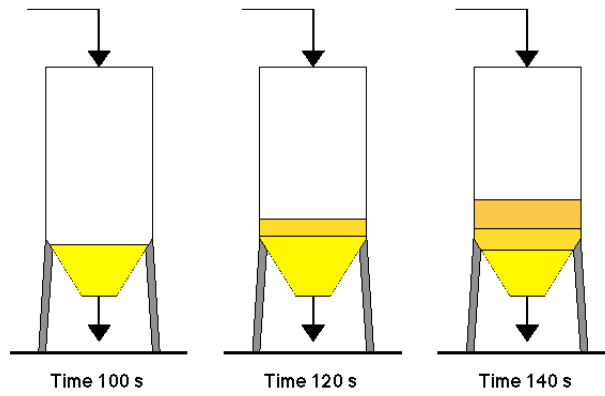


Fig. 10. Tank 3 content at $t=100, 120$ and 140 seconds, in the case of quantisation level δ equal to 0.1. Different cohorts are represented with colour hues proportional to the % of product belonging to S-Lot A and S-Lob B.

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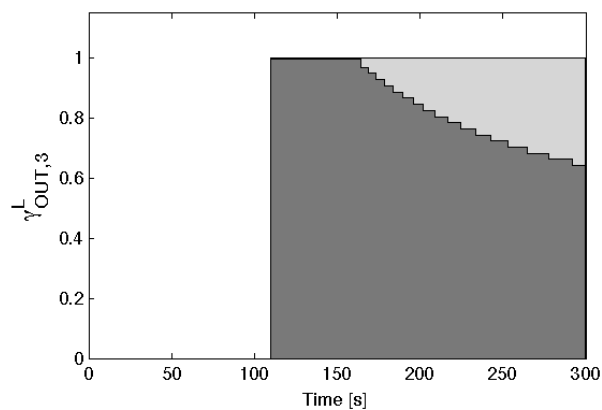


Fig. 11. Relative fractions $\gamma_{OUT,3}^A(t)$ (dark grey) and $\gamma_{OUT,3}^B(t)$ (light grey) of flow q_{03} constituted of mass belonging to S-lot A and B respectively, in the case of quantisation level δ equal to 0.02.

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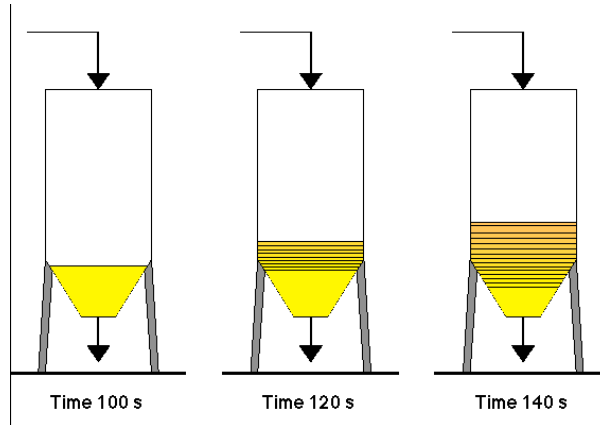


Fig. 12. Tank 3 content at $t=100$, 120 and 140 seconds, in the case of quantisation level δ equal to 0.02. Different cohorts are represented with colour hues proportional to the % of product belonging to S-Lot A and S-Lob B.

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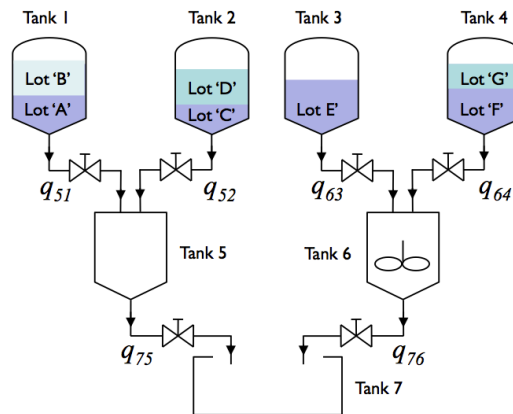


Fig. 13. Scheme of the plant in the case study at time $t = 0$

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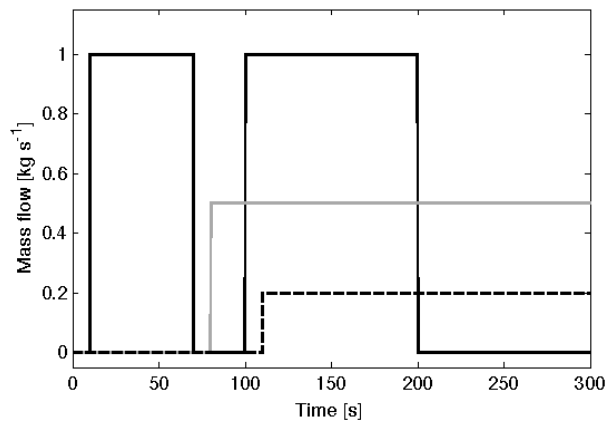


Fig. 14. Mass flows $q_{51}(t)$ (black solid) from Tank 1 to 5, $q_{52}(t)$ (grey dashed) from Tank 2 to 5, $q_{63}(t)$ (grey dotted) from Tank 3 to 6, $q_{64}(t)$ (black dashed) from Tank 4 to 6, $q_{75}(t)$ (grey solid) from Tank 5 to 7, and $q_{76}(t)$ (black dotted) from Tank 6 to 7.

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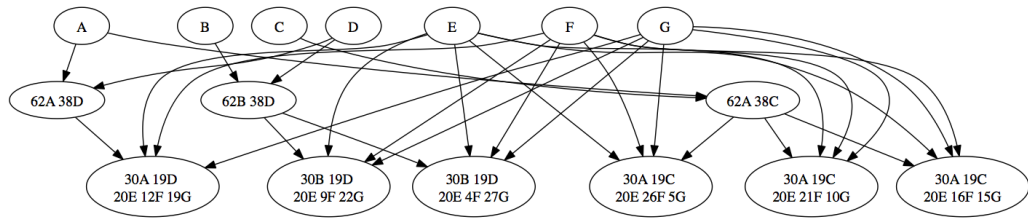


Fig. 15. Graph of the composition of the six cohorts. The label of each node in the graph reports the composition of the cohort, where the numbers express the percentage of the different S-lots (A to G).

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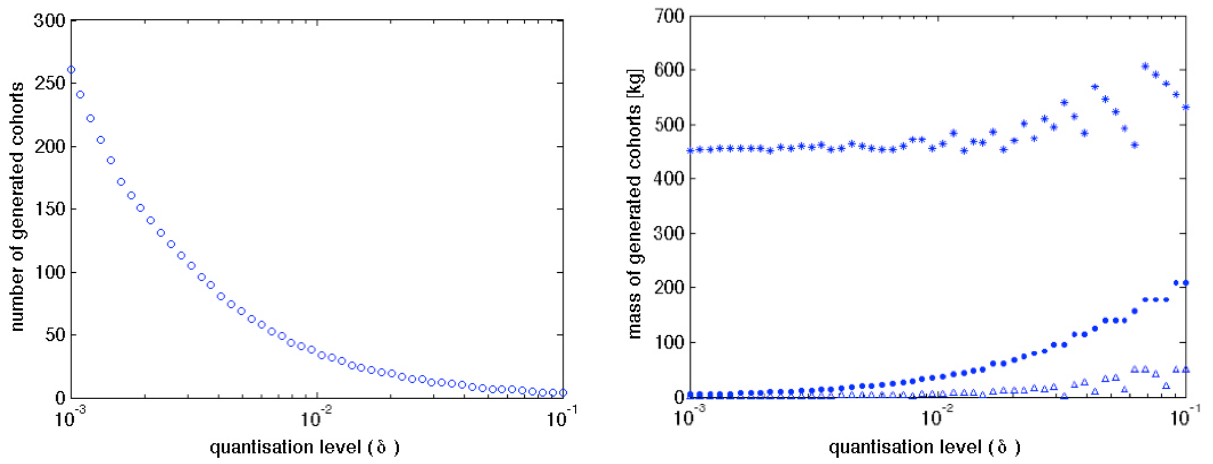


Fig. 16. Number (on the left) and average mass (dotted, on the right) of generated cohorts obtained with different quantisation levels δ ranging from 10^{-3} to 10^{-1} in Example 3. On the right, masses of the biggest (*) and smallest (Δ) cohort are also reported.

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Highlights

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711 ➤ Development of a model for traceability of bulk products, like liquids, powders,
712 crystals, or grains

713 ➤ Based on compartmental models of process in terms of transfer, combination, and
714 storage of mass

715 ➤ 2 representative cases with the uniform-mixing and plug-flow behaviour described

716 ➤ Method is based on formal identification and definition of lots of homogeneous
717 product

718 ➤ Results gives the basis for efficient recall procedures to minimise losses

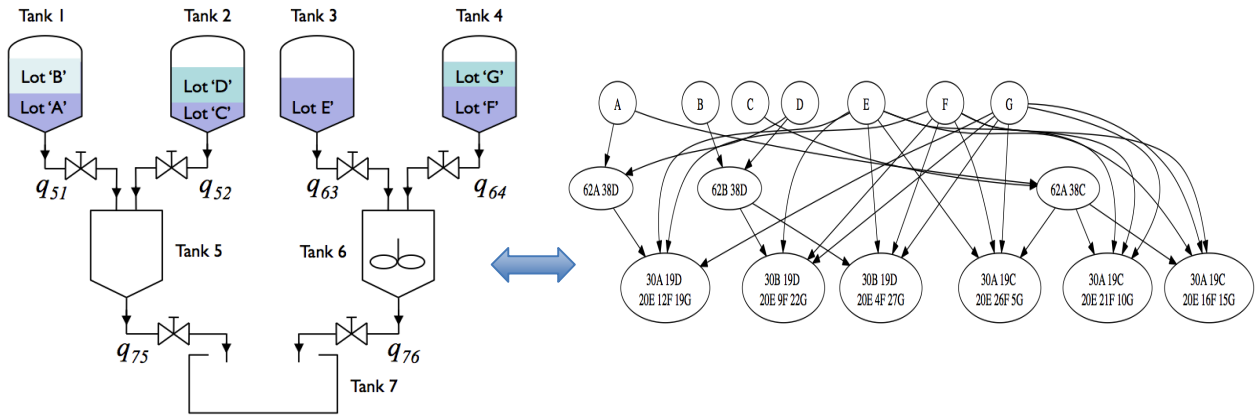
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Graphical abstract



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