

DIPLOMA THESIS

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2023

University of Pannonia
Department of Process Engineering
M. Sc. in Chemical Engineering

DIPLOMA THESIS

Industrial application-focused
stochastic state estimation algorithms

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2023

Diplomamunka feladat vegyészmérnök mesterszak	
Szakirány:	folyamatmérnöki
Diplomamunka címe:	Ipari környezetben alkalmazható sztochasztikus állapotbecslő algoritmusok fejlesztése
Diplomamunka kidolgozásának helye:	Folyamatmérnöki Intézeti Tanszék
Témavezető neve, beosztása:	Dr. Abonyi János
Feladat részletezése (speciális követelmények, határidők): A vegy- és rokonipari rendszerek egyre komplexebbé válásával napjainkban a folyamatmérnökség nagy kihívásai közé tartozik ezen rendszerek modellezése, monitorozása. A rendelkezésre álló információk (pl. mérési adatok, szakértői tudás) gyakran hiányosak, illetve bizonytalanok. Az adattudományi eszközök alkalmazása lehetővé teszi ezen források integrálását, illetve belőlük folyamatszabályozásban, -monitorozásban, -tervezésben használható információk kinyerését. A szakdolgozat témája a fenti célkitűzéshez igazodó sztochasztikus modelleken alapuló állapotbecslő algoritmusok továbbfejlesztése, és ipari alkalmazási lehetőségeinek vizsgálata. A hallgató feladata az állapotbecslő, ezen belül az „importance sampling” és „particle filter” algoritmusok irodalmi áttekintése, implementálása MATLAB környezetben, valamint alkalmazáscentrikus továbbfejlesztése fenntarthatósággal kapcsolatos esetpéldákon keresztül. A cél olyan módszerek kifejlesztése, melyek lehetőséget adnak bizonytalan információkból kiinduló állapot-, illetve paraméterbecslésre, valamint egyéb (pl. hibadiagnosztikai) alkalmazásokra. A hallgató feladatai a következők: • Vonatkozó szakirodalom áttekintése, az alkalmazni kívánt algoritmusok megismerése • Alkalmazáscentrikus módszertan fejlesztése • Az algoritmusok implementálása MATLAB környezetben Az algoritmusok, a kidolgozott módszertan és az eredmények bemutatása fenntarthatósággal kapcsolatos esettanulmányokon keresztül.	
Dátum:	
Témavezető aláírása	Intézeti tanszékvezető aláírása

Thesis Work for Chemical Engineer MSc	
Specialization:	process engineering
Title of thesis:	Industrial application-focused stochastic state estimation algorithms
Department:	Department of Process Engineering
Supervisor name, position:	Dr. János Abonyi
Project description (special requirements, deadline): Nowadays, modelling and monitoring of complex process system are amongst great challenges of process engineering. Available information about the system (e.g. measurement data, expert knowledge) is often incomplete, and even uncertain. Application of data science tools make it possible to integrate these different information sources, thus gaining useful information that can serve process control, monitoring or design. The thesis aims to investigating stochastic state estimation algorithms, and exploring their possible applications in industrial systems. The task of the student is reviewing the importance sampling (IS) and particle filtering (PF) state estimation algorithms, implementing them in MATLAB environment, and applying them for case studies related to sustainability. The goal is to develop methodologies allow state and parameter estimation based on uncertain initial knowledge, as well as other applications (e.g. fault diagnostics). The tasks are the following: • Literature review to get to know the algorithms wanted to be applied • Development of application-focused methodology • Implementing the algorithms in MATLAB environment The algorithms, the methodology and the results have to be presented through case studies related to sustainability.	
Date:	
Signature of supervisor	Signature of head of department

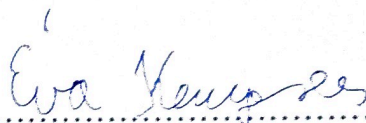
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Abstract

Most of the industrial systems are quite complex, and often described by nonlinear model equations. Besides, the model parameters are often not or not exactly known, and the only information can be gained about behaviour of the system is noisy and incomplete measurement or uncertain experience-based data. In these cases, sampling-based techniques with probabilistic background are promising choices to handle uncertainty and nonlinearity, thereby, estimate the unknown parameters or the unmeasured states thus helping modeling, monitoring and even fault diagnostics tasks.

This work aims to study two variants of these algorithms: the particle filter (PF) algorithm for dynamic systems, and the importance sampling (IS) which is its counterpart for stationer ones. Two case studies are introduced in the two part of the thesis concentrating on processes related to sustainability: the applicability of PF was tested on a wastewater treatment system for state estimation and fault diagnostics, and the IS was used to integrate uncertain expert knowledge to the model of an existing waste separation system thus estimating its parameters.

The contributions of the work are the following: 1) A methodology is introduced how PF can be applied in engineering system for state estimation and its parameters tuned to reach the best performance. 2) Fault diagnostic performance of the PF was also investigated on bias and impact sensor faults. 3) A parameter estimation technique using IS is proposed by integrating uncertain expert knowledge to the system model. 4) The expert knowledge was also validated according to the results.

Results verify, that sampling-based techniques seem to be a promising solution for a wide range of process engineering problems.

Keywords: State estimation, Particle filtering, Fault detection, Wastewater treatment process, Parameter estimation, Waste separation system

Absztrakt

Az ipari rendszerek többsége komplex, sok esetben nemlineáris modellekkel írható le. A modellegyenletek paraméterei gyakran nem, vagy nem pontosan ismertek, így csak zajos, hiányos mérési adatok, illetve tapasztalatalapú szakértői tudás áll rendelkezésre a rendszer viselkedéséről. Ilyen esetekben ígéretes megoldást nyújtanak a valószínűség-számítási háttérű mintavételezés-alapú technikák, melyek egyaránt képesek kezelni a rendszer nemlinearitását és a bizonytalanságokat. Ily módon felhasználhatók ismeretlen paraméterek vagy nem mért állapotváltozók becslésére, segítve a modellezési, monitorozási, hibadiagnosztikai feladatokat.

A jelen tanulmány célja ezen algoritmusok két fő fajtájának vizsgálata: a dinamikus rendszereket feltáró "részecszeszűrő" (PF) algoritmus, és ennek stationer rendszerekre kifejlesztett változata, a fontosság szerinti mintavételezés technikája (IS). A dolgozatban két fenntarthatósággal kapcsolatos folyamatmérnöki esettanulmány kerül bemutatásra: a PF alkalmazhatósága egy szennyvíztisztító rendszer modelljén kerül tesztelésre, állapotbecslési és hibadiagnosztikai célokkal, míg az IS algoritmussal egy létező magyarországi hulladékválogató paraméterbecslési feladata kerül megoldásra bizonytalan szakértői tudásra alapozva.

A munka főbb eredményei a következők: 1) A PF tesztelése mérnöki területen fellépő állapotbecslési feladaton, hatékonyságának növelése a bemutatott hangolási és szenzorhelyezési módszerekkel. 2) A hibadetektálási algoritmus-sal hatékonyan sikerült detektálni időben állandósult és pillanatszerű szenzorhibákat munkapontváltások mellett is. 3) Egy IS-alapú paraméterbecslési technika, mely képes kezelni a bizonytalan szakértői tudást. 4) A paraméterbecslési eredményeket tovább sikerült finomítani a szakértői vélemények súlyozásával, az inkorrekt vélemények eliminálásával.

Az eredmények megerősítik, hogy ezen mintavételezési technikák ígéretesek széleskörű folyamatmérnöki feladatok megoldására.

Keywords: állapotbecslés, részecszeszűrő (PF), hibadetektálás, szennyvíztisztító technológia, paraméterbecslés, hulladékválogató rendszer

Content

1	Introduction	1
2	State estimation-based fault diagnostics	4
2.1	Formalization of the state estimation problem	4
2.2	Details of the particle filter (PF) algorithm	6
2.2.1	Particle filter-based state estimation	6
2.2.1.1	Description of the PF algorithm	7
2.2.1.2	Resampling-based improvement of the PF algorithm	8
2.2.2	A new variant of PF: the intelligent particle filter (IPF)	9
2.2.3	Incorporation of the PF method in fault diagnostics	10
2.3	Experiments on a wastewater treatment reactor-cascade	12
2.3.1	Introduction of the wastewater treatment process	12
2.3.2	Dynamic analysis of the system	14
2.3.3	Implementation of the particle filter	17
2.3.3.1	Method of sensor placement	18
2.3.3.2	Sensitivity analysis of the PF	19
2.3.3.3	PF and IPF comparison	20
2.3.4	Application of PF in fault diagnostics	23
2.3.4.1	Analysis of fault-signal ratio	24
2.3.4.2	Tuning of the sliding window	29
2.4	List of symbols	32
3	An expert knowledge-based technique for parameter estimation	34
3.1	Formalization of the parameter estimation problem	34
3.2	The proposed method for integration of expert knowledge to the system model	37
3.2.1	Representation of uncertain expert knowledge	39
3.2.2	Parameter estimation by importance sampling (IS)	40
3.2.2.1	Importance sampling based on the expert knowledge	41
3.2.3	Application of the proposed method for the validation of experts knowledge	43

3.2.4	Eliminating the incorrect expert judgments	44
3.3	Applications to a waste separation system	45
3.3.1	Introduction to the waste separation technology	45
3.3.2	Available expert knowledge	46
3.3.3	Parameter estimation by importance sampling	47
3.3.3.1	Formalization of the system model	47
3.3.3.2	Identifying the estimable parameters	49
3.3.4	Results of the parameter estimation	51
3.3.5	Evaluation of the expert judgments	55
3.3.6	Elimination of the incorrect expert knowledge	57
3.4	List of symbols	60
4	Conclusions	62
	Appendices	64
	Bibliography	66
	Acknowledgement	70

1 Introduction

This thesis aims to explore the possible applications of two stochastic sampling-based technique, namely, particle filter (PF) and importance sampling (IS) in the field of process engineering.

In our rapidly developing world, changes come one after another. Globalization made our problems more complex, many different aspects have to be considered to make the best decisions as fast as possible. Engineering systems also tend to be characterized by volatility, uncertainty, complexity and ambiguity, the so-called VUCA [1]. This necessitates flexible and robust systems such as techniques that can produce a stable solution besides a turbulent environment in process engineering tasks.

The modeling, monitoring and fault diagnostics of complex process systems is extremely challenging for engineers. In practice, not every state variable of the system is measured and the ones that are available are often in the form of a noisy data. However, knowing their values is desired, e.g. in modeling, process control or fault diagnostics. Experts usually have some intuition about the unknown variables or parameters which can be utilized (e.g. an expert-knowledge-based parameter estimation of algae growth is described in [2]), however, they are often not able to provide exact information. In such cases, the uncertainty can be handled using a probabilistic approach, similarly to fuzzy models (e.g. expert knowledge has been shown to be implemented in decision making using fuzzy logic illustrated by an example of choosing the most suitable solar panel system [3]). Applying state estimation algorithms seems a promising solution for the problem of incomplete and noisy measurements and experience-based expert knowledge can be also integrated to fill the gap of the missing information.

State observers can estimate unmeasured state variables based on measured ones. The simplest and most widely used state observer is the Kalman filter (KF). However, it is only usable if the system can be described with a linear state space model, and the model and measurement noise follow a Gaussian distribution. In other cases, the extended Kalman filter (EKF) is promising. This method is based on the local linearization of nonlinear model equations. However, if the nonlinearity of the model is high, it does not work well as a state observer [4].

Complex process systems are usually nonlinear and environmental noise

is not Gaussian. In this case, particle filtering is suggested to solve state estimation problems [5]. While KF and EKF are based on the covariance matrix of the estimation error and solve an optimization problem, a particle filter (PF) has a probabilistic approach as it is a kind of Monte Carlo (MC) simulation. As this method not only yields the estimated states but their probability density, the PF technique and its counterpart for stationer systems called importance sampling (IS) can be quite well applied for state estimation, fault detection and even parameter estimation purposes [6].

Although particle filter algorithms are widely used in robotics and electronics [7, 8], their utilization in chemical processes is far less. The method has been used for single continuous stirred tank reactors (CSTRs) a couple of times [9, 10], mainly for the purposes of process control [11, 12], but rarely applied in fault diagnostics. On the other hand, a probabilistic approach (e.g. MC simulation) is widely used to handle input or parameter uncertainty (e.g. the performance of a solar collector was predicted under uncertain operating conditions in [13], the prediction of the cooling load of an HVAC system refined in addition to uncertain inputs in [14], or the product yield of a polymerization process with several possible reaction paths estimated in addition to uncertain kinetic parameters [15]), and expert knowledge was also sometimes implemented to estimate parameters (e.g. in the case of a groundwater model [16]) however, examples using importance sampling (IS) to integrate expert knowledge into industrial systems are rarely documented in the industrial field.

The aim of the first part of this thesis is to test the applicability of PF in complex process systems for state monitoring and fault diagnostics purposes on a benchmark wastewater treatment process that represents the aforementioned issues quite well. The performance of a recently developed version of the algorithm called intelligent particle filter (IPF) is tested [17], as well. Besides, a case study is also conducted based on an existing Hungarian waste separation system in the second part of the thesis. One contribution of this part is a methodology that utilizes expert knowledge for the modeling of an industrial system. A method is given to illustrate how subjective and uncertain information from experts can serve as a basis for estimating these values. A technique is also provided that shows how results can be used to evaluate the reliability of expert knowledge.

The contributions of this work follows the points below:

- A dynamic analysis of the wastewater treatment technology benchmark is proposed and PF state estimation algorithm is implemented.
- A method is suggested for determining optimal sensor placement and the tuning of the algorithm.
- The performances of the general PF and IPF are compared.
- The estimation results are used for the purposes of fault detection of bias and impact sensor faults.
- An industrial example is shown how expert knowledge can be implemented to the modelling and analysis of the system.
- An IS-based parameter estimation technique is given involving experience-based expert knowledge.
- Expert judgments are evaluated according to the results, and incorrect ones are eliminated from the estimation.

As for the roadmap of the thesis, Section 2 contains the case studies on the dynamic wastewater treatment process dealing with PF, and Section 3 introduces the IS-based technique used for the parameter estimation of an existing waste separation system according to uncertain data from experts.

The author seeks to use the conventional symbols of process engineering and the related literature, however, because of the different nature of the case studies and applied methods, some symbols may have a different meaning in the two main part of the thesis. To avoid misunderstanding and make it easier to follow the study, a *List of symbols* section is found at the end of both main topic which contains the symbols with their exact meaning in that part of the thesis in detail.

2 State estimation-based fault diagnostics

This part of the thesis offers an insight into the topic of state estimation with a particle filter algorithm and its practical applications in process systems by considering the fault diagnostics of a wastewater treatment cascade reactor benchmark in particular.

The general form of the state estimation problem is outlined in Section 2.1, together with the fault diagnostic concept based on it. The general PF algorithm is introduced in Section 2.2 with its improved version called intelligent particle filter and principles of the fault detection method. Section 2.3 contains the simulation experiments on the wastewater treatment process with cascade reactors. The details of the system model with model equations are introduced in Section 2.3.1, and a dynamic analysis is provided in Section 2.3.2. The PF is implemented in Section 2.3.3. A method is suggested for optimal sensor placement according to the state estimation performance in Section 2.3.3.1. An extensive sensitivity analysis is also proposed to determine the best settings of PF and increase the efficiency in Section 2.3.3.2. Since intelligent particle filters (IPFs) in the field of process engineering are a research gap in the literature, one was also implemented in this cascade reactor system and its performance compared to general PF in Section 2.3.3.3. A PF-based fault detection method was also implemented and evaluated in Section 2.3.4 [6]. This method was tested to determine whether it is applicable in dynamic systems or not. Bias as well as impact sensor faults were examined and a tuning method proposed.

2.1 Formalization of the state estimation problem

In complex process systems, not every state variable is measured because they are immeasurable or the minimum number of sensors is applied to reduce costs. Furthermore, measured data is usually noisy because every measurement has an element of uncertainty. However, the exact values of the state variables must be known, e.g. in process control. State observers are able to solve these outlined problems.

The algorithms they use can estimate the unmeasured states according to the measured ones. For the systems where model equations are nonlinear, the application of a particle filter state observer is suggested. In contrast to the more commonly used Kalman filter, the PF does not require the model

equations to be linear nor supposes Gaussian model and measurement noises. Preliminarily, only the initial state and state space model of the process system are needed.

Since PF estimates states according to the model of the system, besides measurement noise, the uncertainty of the model is also a factor that has to be considered. PF can handle these uncertainties, as these two types of noises are incorporated in the applied state space model:

$$\mathbf{x}_k = f(\mathbf{x}_{k-1}, \mathbf{u}_{k-1}) + \mathbf{v}_k \quad (2.1)$$

$$\mathbf{y}_k = h(\mathbf{x}_k, \mathbf{u}_k) + \mathbf{w}_k \quad (2.2)$$

where $\mathbf{x}_k$ denotes the state vector, $\mathbf{y}_k$ stands for the measurement vector, $\mathbf{u}_k$ represents the input vector, $\mathbf{v}_k$ and $\mathbf{w}_k$ are the model and measurement noises, respectively, at time k , $f()$ refers to the state transfer function and $h()$ represents the measurement function.

Since PF estimates the unmeasured states according to the measured data, it is essential to determine which state variable is most suitable to measure because the accuracy of the estimation depends on it. Otherwise, the parameters of the particle filter algorithm itself have to be tuned. These questions have to be answered before using the PF to achieve the best estimation performance.

In process systems, different faults can occur. One of the most common are sensor faults which is a key issue in PF-based state estimation. This means that the information gained from the process is incorrect. As the operation of the observer is based on the measured data, the estimations of the state variables will also be faulty. However, for the same reason, this is not perceptible without implementing a fault diagnostics algorithm.

The probabilistic approach of the PF allows the faults to be perceived. PF not only yields the most probable values but the probability density of the states too. With a carefully chosen fault decision function, incorrect operation of the sensor can be detected in time from this additional information collected. Therefore, it is possible to repair or replace the faulty sensor and accurately continue the state estimation.

The aforementioned concept is shown in Figure 1:

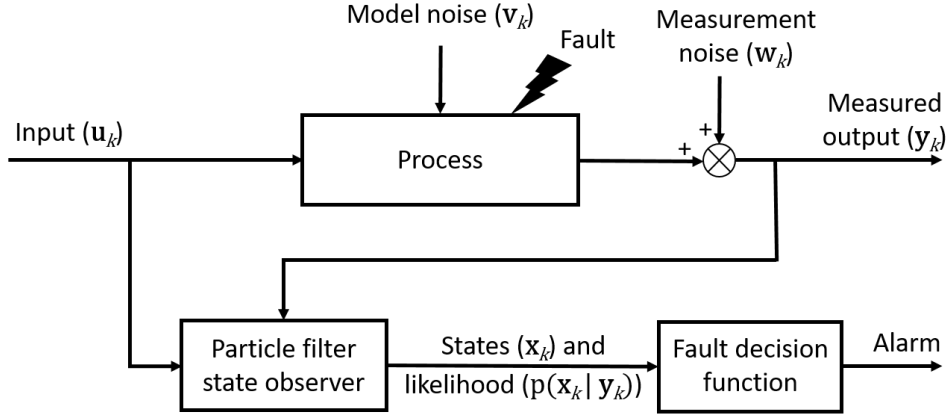


Figure 1: **Particle filter state observer-based fault detection scheme of a process.** The particle filter state observer computes the unmeasured states in light of the measured sensor data and the inputs of the process. According to the fault decision function, the faults can be detected and alarms generated. Faults can be technological faults, parameter uncertainties or sensor faults.

2.2 Details of the particle filter (PF) algorithm

In this section, the methodological background of this research is introduced. The PF and IPF algorithms are described in detail, moreover, the applied fault detection technique is explained.

2.2.1 Particle filter-based state estimation

A particle filter (PF) is a kind of Monte Carlo simulation in which a set of particles represents the different states of the system.

The particles are distributed according to the system and measurement noises in the state space. The coordinates of the particles are the state variables, and every particle has a weight that represents the probability of the particle. At every time step, the PF computes the probability of each particle according to the given new measurement data, thereby calculating the estimated states.

The algorithm of the general particle filter consists of three parts: the prediction step, the correction step and the resampling step. The method is described in more detail in this chapter of the study. An intelligent particle filter (IPF) is an improved version of the general particle filter that uses a genetic algorithm in the resampling step to achieve a higher level of efficiency. This subject is covered below as well.

2.2.1.1 Description of the PF algorithm

In order to use a particle filter, the state-space model of the process (Equations 2.1 and 2.2), the initial states and the measurement data of at least one state variable must be known.

The initial state is defined by a set of randomly drawn particles from the state space around the real initial state. This set of particles is defined by their localization at the state space and their weights as $\{\mathbf{x}_0^i, \omega_0^i\}_{i=1}^{N_s}$, where N_s denotes the number of particles. Similarly, the set of particles at time k is represented by $\{\mathbf{x}_k^i, \omega_k^i\}_{i=1}^{N_s}$. The initial weights of the particles are equal.

The posterior probability density function, the so-called posterior pdf, is sought at every time step during the estimation. The prior pdf is given at every k . It is represented by the initial set of particles at time $k = 1$. If $k > 1$, the prior pdf at k equals the estimation result of the last time step, that is the posterior pdf at $k - 1$. The prior pdf can be approximated to a sampled density:

$$p(\mathbf{x}_k | \mathbf{y}_{1:k}) \approx \sum_{i=1}^{N_s} \omega_k^i \delta(\mathbf{x}_k - \mathbf{x}_k^i) \equiv \{\mathbf{x}_k^i, \omega_k^i\}_{i=1}^{N_s} \quad (2.3)$$

where $\mathbf{x}_k$ refers to the estimated state vector, ω_k^i represents the normalized weights of the particles and $\mathbf{y}_{1:k}$ stands for the measured data points from the first to the k th time step. In order to determine the posterior pdf, the task is to estimate these weights at every time step.

The first step of the particle filter algorithm is the prediction step. Every particle progresses forward by one time step, thus the following pdf is calculated:

$$p(\mathbf{x}_{k+1} | \mathbf{y}_{1:k}) = \{\mathbf{x}_{k+1}^i, \omega_k^i\}_{i=1}^{N_s} \quad (2.4)$$

The new $\mathbf{x}_{k+1}^i$ state vectors can be determined using the state transfer function and the ω_k^i weights remain the same in this step of the algorithm.

The second step of the algorithm is the correction step. The new ω_{k+1}^i weights are estimated from the previous ones (ω_k^i) recursively according to the new measurement data and normalized as:

$$\omega_{k+1}^i = \frac{\omega_k^i \cdot p(\mathbf{y}_{k+1} | \mathbf{x}_{k+1}^i)}{\sum_{i=1}^{N_s} \omega_k^i \cdot p(\mathbf{y}_{k+1} | \mathbf{x}_{k+1}^i)} \quad (2.5)$$

Since $\mathbf{x}_{k+1}^i$ remains the same in this step of the algorithm, the posterior pdf

is defined as:

$$p(\mathbf{x}_{k+1} \mid \mathbf{y}_{1:k+1}) = \{\mathbf{x}_{k+1}^i, \omega_{k+1}^i\}_{i=1}^{N_s} \quad (2.6)$$

The prediction and correction steps are repeated iteratively. Although these two steps provide the core of the algorithm, different problems can occur during the estimation, so additional steps are required. These improved algorithms will be introduced in the following parts of the chapter.

The derivations of the equations above are available in [4] and [18]. The prior pdf was used as an importance function and a Markov process assumed.

2.2.1.2 Resampling-based improvement of the PF algorithm

Using only the prediction and correction steps iteratively, a degeneracy problem is faced after a few time steps. One or a few particles will have large weights and all the others will be negligibly small. This phenomenon leads to less accurate estimation results with an unnecessarily high computational effort. To avoid this problem, a resampling step in the algorithm must be used.

The set of particles can be evaluated in terms of degeneracy with the effective sample size:

$$N_{eff} = \frac{1}{\sum_{i=1}^{N_s} (\omega_k^i)^2} \quad (2.7)$$

If N_{eff} is below an N_t threshold after the correction step, resampling takes place. In other cases, the current particle set is good enough to continue the estimation with the prediction step. N_t is conveniently chosen as half the value of N_s . While more than half of the particles are effective, the estimation is sufficiently robust.

Resampling means that a new particle set is produced. The new particles are chosen from the old ones. Every $\mathbf{x}_k^i$ is drawn with the probability of ω_k^i normalized weight, so the probability density of the particle set remains the same as before. The weights of the new particles are identical.

Four main resampling methods exist: multinomial, stratified, systematic and residual resampling. Systematic resampling was used in the present research, which is shown as the most favorable in [19]. A detailed description of this method is given in Appendix A.

2.2.2 A new variant of PF: the intelligent particle filter (IPF)

Besides the degeneracy problem, sample impoverishment is another inconvenience of general particle filters. Therefore, the variance in the particle states is relatively small, so many particles will be located in almost the same place. This phenomenon can mislead the estimation and reduce the level of accuracy. A good solution to the problem is to apply an intelligent particle filter (IPF).

This algorithm implements a genetic algorithm between the correction and resampling steps in order to increase the diversity and broaden the range of particles. A description of the algorithm is given in Algorithm 1.

Algorithm 1 Genetic algorithm-based part of intelligent particle filter [17]

- 1) Calculate N_{eff} from the normalized particle weights after the correction step.
- 2) Set the particles in descending order according to their weights.
- 3) Choose the weight that belongs to the N_{eff} th particle and classify the particles into the "large weight" group if $\omega_k^i > \omega_k^{N_{eff}}$ and "small weight" group in all other cases. $\mathbf{x}_{kH}^l$ denotes large-weight particles and $\mathbf{x}_{kL}^j$ the small-weight ones.
- 4) Crossover step: modify the small-weight particles and make them more efficient by an arithmetic crossover:

$$x_{kC}^j = \alpha x_{kL}^j + (1 - \alpha)x_{kH}^l \quad (2.8)$$

where $\mathbf{x}_{kC}^j$ refers to the new particle that $\mathbf{x}_{kL}^j$ is replaced by and $\alpha \in [0, 1]$. For every small-weight particle, a large-weight one is randomly selected.

- 5) Mutation step: further modify the small-weight particles and broaden their range:

$$\mathbf{x}_{kM}^j = \begin{cases} 2\mathbf{x}_{kH}^l - \mathbf{x}_{kC}^j & \text{if } r_L \leq p_M \\ \mathbf{x}_{kC}^j & \text{if } r_L > p_M \end{cases} \quad (2.9)$$

where $r_L \in [0, 1]$ is drawn from the uniform distribution and p_M denotes the mutation probability.

- 6) Reevaluate the ω_k^i particle weights.
-

As can be seen in Algorithm 1, the genetic algorithm in the PF consists of two main steps: crossover and mutation. During the crossover step, the small-weight particles are modified into larger ones. The α parameter determines how strong the effect of small-weight particles is during the modification.

On the other hand, the mutation step extends the range of the particles and further increases the level of diversity. It has a p_M parameter that defines the probability of modification.

The two parameters of Algorithm 1 (α and p_M) have to be tuned before using the method, depending on the system to be estimated.

In this work, the performance of the PF and IPF are compared. It is shown that by using an IPF, the accuracy of the estimation is somewhat increased. The metric was used to evaluate the performances of the two methods is the one proposed in [17]:

$$e_{av} = \frac{1}{N_r \cdot T} \sum_{r=1}^{N_r} \sum_{k=1}^T e_{rk} \quad (2.10)$$

where N_r denotes the number of simulations, T refers to the time steps in one simulation and e_{rk} stands for the absolute value of the difference between the estimated and real states. e_{av} was calculated for each state variable and made the conclusions made in this manner.

2.2.3 Incorporation of the PF method in fault diagnostics

One of the main application areas of particle filtering is fault diagnostics, which forms the subject of this part of the study.

The main steps of this case study are summarized in Figure 2. After the dynamic analysis of the benchmark system, the PF is implemented. Now the measured state variable must be chosen, and the PF algorithm appropriately tuned. After these preliminary steps, the method can be tested for fault detection problems.

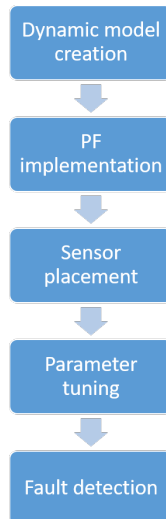


Figure 2: **Outline of the main steps of the experiment.** The study introduces the work from the creation of the dynamic model through the implementation of the PF to its application in fault detection.

Traditional fault detection techniques are based on forming residuals. These methods calculate the difference between the estimated and measured states as well as detect faults according to this value. However, these methods require multiple sensors (e.g. simplified observer scheme (SOS)) or even multiple state observers (e.g. generalized observer scheme (GOS)), leading to increases in computational and instrumentation costs [20].

Knowing the probability distribution of the states, i.e. the weights of the particles at every time step, enables faults to be detected. Some practical examples can be seen in a three-tank and a helicopter system in [17] and [21], respectively. However, very few papers in the literature have dealt with the chemical engineering application in operational units.

In the present work, the method proposed in [6] was applied, which is based on the sum of the log-likelihood of particle weights which decreases if a fault occurs.

First of all, the measurement function has to be evaluated for each particle, i.e. the likelihood of the measurement, assuming that the state represented by the particle is the real state. The next step is to determine its average in terms of particles:

$$L_k = \frac{1}{N_s} \sum_{i=1}^{N_s} p(\mathbf{y}_k | \mathbf{x}_k^i) \quad (2.11)$$

The model parameters are assumed to be constant.

The normalized decision function is defined as:

$$d_k = \frac{1}{M} \sum_{j=k-M+1}^k \ln(L_j) \quad (2.12)$$

where M denotes the so-called sliding window and k stands for the time at that moment.

If $-d_k$ is higher than a threshold h , a fault is detected and an alarm generated. In this work, the method introduced in [17] is used to determine h , which selects the $-d_k$ that belongs to the 98% confidence interval of the fault-free operation as a threshold.

A log-likelihood-based method is also used for chemical engineering examples in [22]. However, this work only examines the processes and the fault detection technique in steady-state cases using general PF. In this thesis, the method was tested simultaneously with the dynamic behavior of the bench-

mark system by applying the IPF state estimation algorithm and proposed an analysis in the cases of impact and bias additive sensor faults.

2.3 Experiments on a wastewater treatment reactor-cascade

In this section, some ideas about the technology that was chosen to implement the aforementioned experiments are given. Results are also presented.

Firstly, the dynamic analysis of the system is presented and the test ranges determined. Afterwards the implementation of PF and its sensitivity analysis are conducted. Some ideas are also given about the optimal location of sensors according to the state estimation performance. The estimation efficiency is increased by implementing an IPF and its performance is also compared with that of the PF in this section. At the end of this section, the results of PF-based fault detection experiments are shown and a method given for tuning the sliding window parameter.

The above-mentioned experiments were executed on the dynamic model of an organic-carbon-removal wastewater treatment process in which nonlinear behavior excludes the use of the Kalman filter.

2.3.1 Introduction of the wastewater treatment process

In this case study, the behavior of the standard reactor cascade (SRC) model of an organic-carbon-removal wastewater treatment technology was examined. Since the reactions that take place in the reactors can be modeled by Monod growth kinetics, the process accurately represents the nonlinear behavior of complex systems [23].

The task of this process is to remove the carbon content of sewage using microorganisms. The system consists of two bioreactors in series and a settling unit, as is seen in Figure 3. In the reactors, biological organic carbon removal from the wastewater takes place. The feed flows into Reactor I with the recycled stream. The effluent of this unit forms the influent of Reactor II. The purified wastewater flows into the settling unit, which separates the light and heavy phases. A part of the heavy phase is recycled to enhance efficiency. The reactors are assumed to be well stirred and aerated, moreover, their volumes are equal.

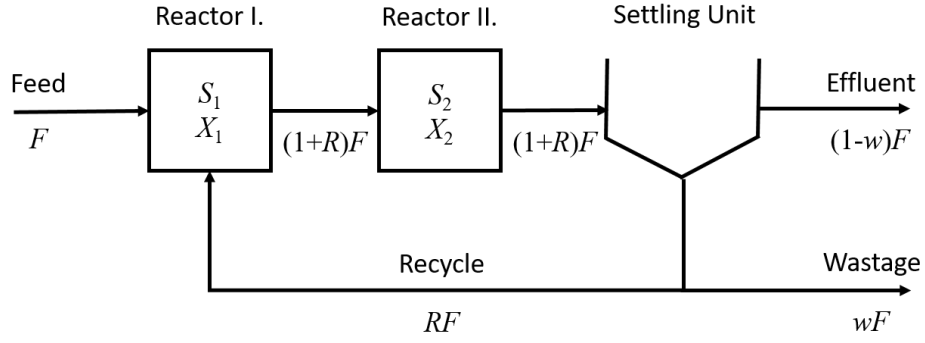


Figure 3: **Block diagram of the standard reactor cascade (SRC) of the wastewater treatment process.** The figure contains the names of the flows above the arrows and the flowrates below the arrows. F refers to the flowrate, R denotes the recycle ratio, S_i and X_i represent the concentrations of the substrate and microorganisms (i stands for the number of the reactors), and w is the waste fraction.

Four state variables can be determined during the process, namely the concentrations of the substrate and microorganisms in both reactors. However, measuring all these concentrations is expensive. This problem can be avoided by using a state observer. In this case, it is sufficient to install only one sensor and estimate the other three concentrations, thereby reducing investment costs. As the wastewater treatment process is nonlinear, a particle filter is suggested as a state observer.

Although this wastewater treatment process was thoroughly analyzed under steady-state conditions, a dynamic analysis was not carried out [23]. As the temporal behavior of the system is examined in the present work, firstly its dynamic behavior needed to be analyzed and its physical constraints determined.

Since the biochemical reactions in the process can be described by Monod growth kinetics, the four model equations of the system can be defined as:

$$V \frac{dS_1}{dt} = F(S_0 - S_1) + RF(S_2 - S_1) - V \frac{\mu_m S_1 X_1}{K_s + S_1} \cdot \frac{1}{\beta} \quad (2.13)$$

$$V \frac{dX_1}{dt} = -FX_1 + RF(CX_2 - X_1) + V \frac{\mu_m S_1 X_1}{K_s + S_1} - V k_d X_1 \quad (2.14)$$

$$V \frac{dS_2}{dt} = F(1 + R)(S_1 - S_2) - V \frac{\mu_m S_2 X_2}{K_s + S_2} \cdot \frac{1}{\beta} \quad (2.15)$$

$$V \frac{dX_2}{dt} = F(1 + R)(X_1 - X_2) + V \frac{\mu_m S_2 X_2}{K_s + S_2} - V k_d X_2 \quad (2.16)$$

where bottom indexes refer to the parameters of the first (1) and second (2) reactors, V denotes the reactor volume, and S and X stand for the concentrations of the substrate and microorganisms. The input variables of the system are the feed concentration S_0 , flowrate F and recycle ratio R . The other parameters of Equations 2.13-2.16 along with their names and values can be seen in Table 1:

Table 1: **Constant parameters of the model equations.** The parameter values was taken from [23]. The reactor volume used is from [24].

Label	Name	Value
μ_m	maximum specific growth rate (day ⁻¹)	1
β	yield factor (mg MLSS/mg COD)	0.5
K_s	Monod constant (mg COD/L)	100
C	concentration factor (-)	1.5
k_d	death coefficient (day ⁻¹)	0.028
w	waste fraction (-)	0.1
V	reactor volume (m ³)	125

C denotes the so-called concentration factor that refers to the performance of the settling unit. Its minimum value is $C = 1$, which means that the unit functions as a recycling unit. For the experiments, an intermediate value for C was chosen which determines the maximum value of R as follows:

$$R_{max} = \frac{1 - wC}{C - 1} \quad (2.17)$$

where w denotes the waste fraction, which is an empirical constant. $R_{max} = 1.7$ in the present case.

2.3.2 Dynamic analysis of the system

The system has three input variables: S_0 , R and F . The reason why S_0 changes is the fluctuation in the composition of the sewage over time. R and F are manipulated variables that the operators in the plant can handle to achieve the required level of performance. However, these variables have physical constraints to preserve the stability of the washout solution and avoid process failures [23].

The maximum value of F can be calculated from the critical residence time that is a function of R and S_0 , as introduced in [23]. The detailed equations can be found in Appendix B.

F_{max} determines the boundary of the washout phenomenon. The values of F_{max} belongs to the R and S_0 values that were examined are shown in Table 2.

Table 2: **Maximum values of F given different R and S_0 values.** The same feed concentration $S_0 = 4000$ mg COD/L was used as in [23]. Another two values above and below this were chosen. Regarding R , the same values were used as in [23].

	$R = 0.5$	$R = 1$	$R = 1.5$
$S_0(\text{mg COD/L}) = 3000$	267	438	916
$S_0(\text{mg COD/L}) = 4000$	270	442	923
$S_0(\text{mg COD/L}) = 5000$	271	444	928

As can be seen in Table 2, F_{max} depends very little on S_0 . However, R has a great effect on it which must be considered when choosing the setpoints.

After examining the constraints, the dynamic model and simulation of the system were created in MATLAB. Equations 2.13-2.16 were discretized and solved. As a first step, validation of the model was necessary. With parameters $C = 1.5$ and $R = 1.5$, the system achieved 90% carbon removal when the residence time was about 0.1545 days, which is in line with the results in the literature [23]. The setpoint changes and results are shown in Figure 4.

It can be concluded that the system is underdamped and yields a first-order response following the changes to R , F and S_0 . The time constants of the process are a few days long as wastewater treatment is a slow process. They are higher in the periods when F is close to the value of F_{max} . Another interesting observation is that changes to S_0 cause sudden, impulse-like responses in S_1 and S_2 , but the stationery values of S_2 stay almost unchanged. This can be explained by the fact that S_0 directly affects the substrate concentrations, however, once the microorganism concentration adapts to this change, the process can achieve nearly the same level of performance as before.

Regarding the dynamic experiments above, the model and the set of input variables are suitable for further investigations.

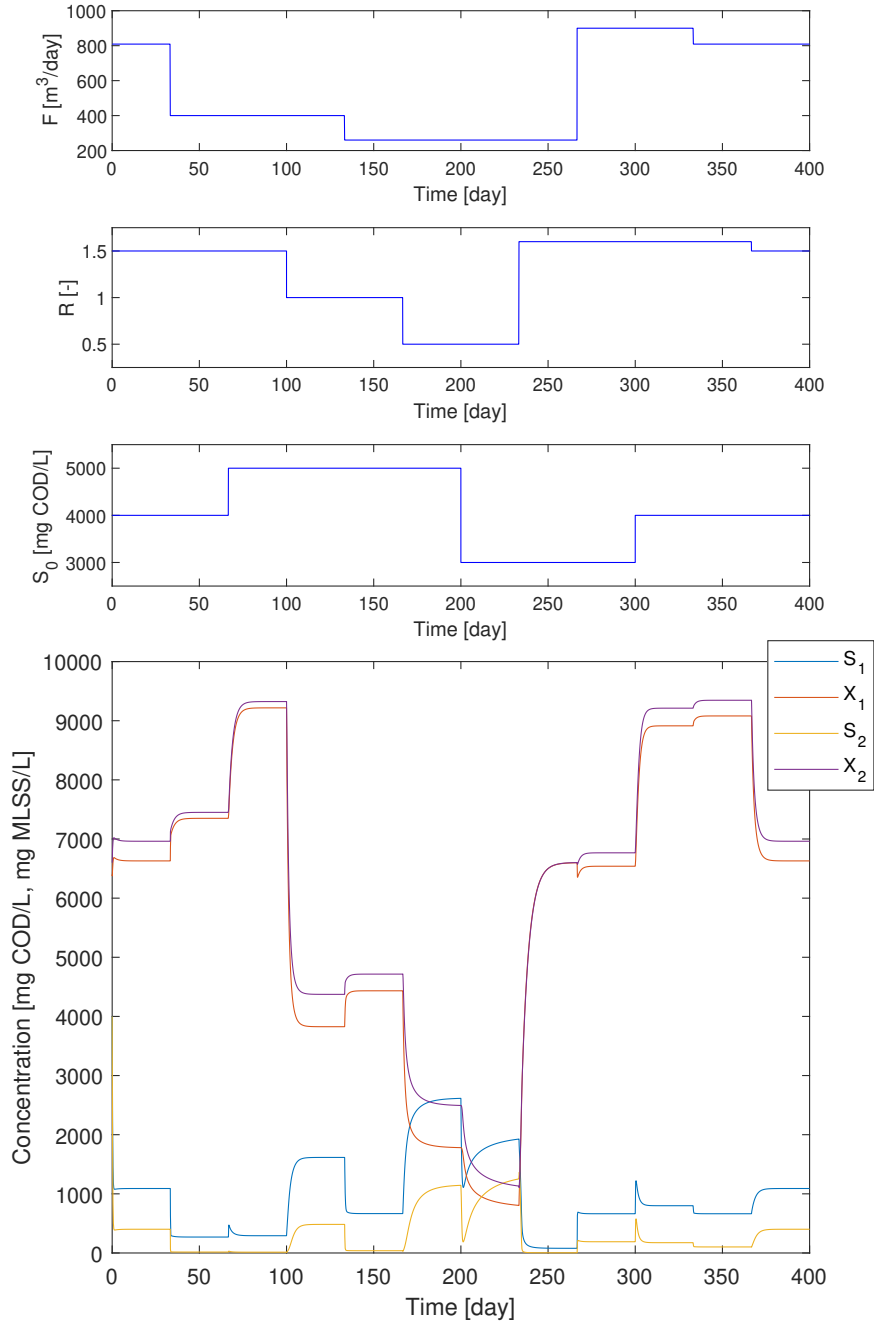


Figure 4: **The input and state variables over time.** According to Table 2, $F \leq F_{max}$ in every period of time. Equations 2.13-2.16 were discretized and solved iteratively with a sampling time of $dt = 0.01$ days to acquire the model outputs. The initial state vector was $\mathbf{x}_0 = [S_{1,0} \ X_{1,0} \ S_{2,0} \ X_{2,0}] = [4000 \ 6400 \ 4000 \ 6600]$.

2.3.3 Implementation of the particle filter

After analyzing the dynamic behavior of the system, particle filter state observer was implemented to see if the state estimation task was feasible. A MATLAB implementation based on [4] was used and modified according to current research goals.

First of all, since the program had to be validated, it was tested to see if the estimated states followed the real states. State S_2 was measured first, as it is the most important of the four, being the one to be controlled. 50 particles were used for the estimation.

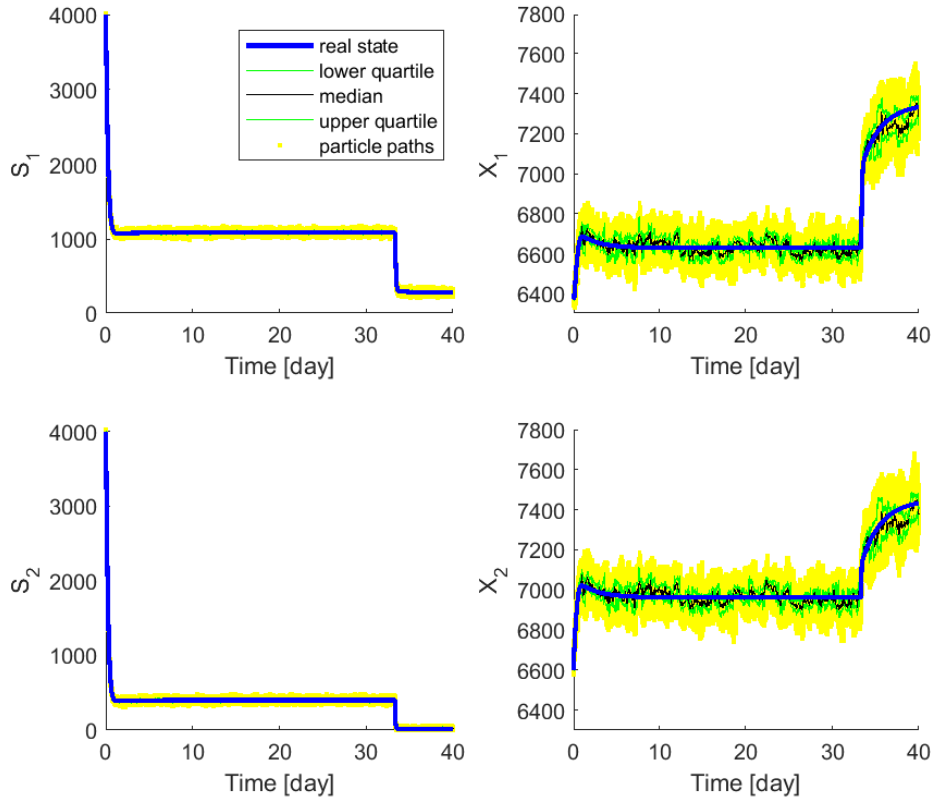


Figure 5: **Comparison of the estimated and real states.** The concentrations of the substrate are shown in mg COD/L and of the microorganisms in mg MLSS/L. Deviations of $\sigma_v = 10$ and $\sigma_w = 25$ were used for noises.

The particle paths and the median of the particle states are in line with the real state represented by blue lines as can be seen in Figure 5. Although only the first 40 days were illustrated due to visibility, conclusions are the same throughout the entire time period.

Regarding the performed experiments, this MATLAB implementation of the PF works well and is suitable for further examinations.

2.3.3.1 Method of sensor placement

The next emerging issue is to determine which state variable is the most suitable to measure. Despite the fact that an explicit cost function is not available, the different configurations are comparable according to the estimation errors. Therefore, PF is used, the basic performance of which is satisfactory as introduced before. The placement of the sensor is determined by these measures, before the PF is fine-tuned in Section 2.3.3.2.

Online COD and suspended solids sensors are also used in wastewater treatment, like in [25], of different accuracies, namely: 5% for the former and about 2% for the latter. These values were used to define the standard deviations of the measurement noise in the simulation. Different measuring ranges in the two cases were also considered, so $\sigma_w = 25$ was used for the COD and $\sigma_w = 140$ for the suspended solids sensors.

Regarding the above-mentioned issues, the estimation performance was examined in all four cases by using 50 particles as well. For the evaluation, Equation 2.10 was used to calculate the estimation error.

Table 3: **Error of the estimated states (e_{av}) at different sensor locations.** The error values were calculated as an average of $N_r = 10$ simulations over the first 40 days (with a sampling time of $dt = 0.01$ days corresponds to $T = 4000$ time steps). $N_S = 50$.

Measured state	$e_{av}(S_1)$	$e_{av}(X_1)$	$e_{av}(S_2)$	$e_{av}(X_2)$
S_1	7.17	25.45	4.99	26.44
X_1	4.43	17.37	4.23	17.36
S_2	5.67	25.58	6.80	26.49
X_2	4.42	16.52	4.31	17.62

According to Table 3, the cases when the concentration of microorganisms was measured produced much lower estimation errors because they are more sensitive to changes in the input variables, as seen in Figure 4. Therefore, if the measured state is chosen from them, PF can provide a more accurate estimation. Another reason is that the measurement noises are relatively lower in these cases. The estimation performances are almost the same when comparing X_1 and X_2 as measured states. However, since the accuracy of S_2 is

the most crucial state in terms of the process control, X_1 is measured in this wastewater treatment model.

Another interesting observation is that by considering the rows in Table 3 separately, the same types of concentrations are almost identical. Moreover, any variation is always for the benefits the unmeasured state, e.g. when measuring S_1 , the estimation of S_2 is more accurate than the that of S_1 .

It is important to note that the results described above pertain to the actual process model with the current parameters. For example, the value of the measurement noise has a significant impact on them. However, besides the given parameters and state-space model, the optimal sensor location can be determined by the aforementioned method.

2.3.3.2 Sensitivity analysis of the PF

As the previous example illustrated, some assumptions and parameters of the process significantly affect the effectiveness of state estimation. On the other hand, the parameters of the particle filter itself are also worth tuning. In Monte Carlo simulations, one main disadvantage is definitely high simulation time. The number of particles (N_s) has a great effect on it; however, reducing N_s can decrease the accuracy of the estimation. Therefore, the aim of this section is to determine its optimal value for the present system.

Regarding the results of the last section, X_1 was chosen as a measured state and executed the estimation using four different values of N_s . The results are depicted in Figure 6.

During the evaluation, estimation errors were considered against the simulation time. The estimation errors decrease exponentially and become nearly constant beyond a determined value of N_s . On the contrary, the simulation time increases linearly as the number of particles rises. According to the curves of Figure 6, the optimal N_s is about 30. Below this value, estimation errors increase rapidly, while above it, they remain nearly constant. For further investigations, this value will be used.

In the presented case study, the simulation time is not a crucial factor as the time constant of the system is a few days. However, for the state estimation of more complex systems with a shorter time constant, hundreds of particles may be needed and the simulation time can be a constraint, since it should always be lower than the sampling time of the system.

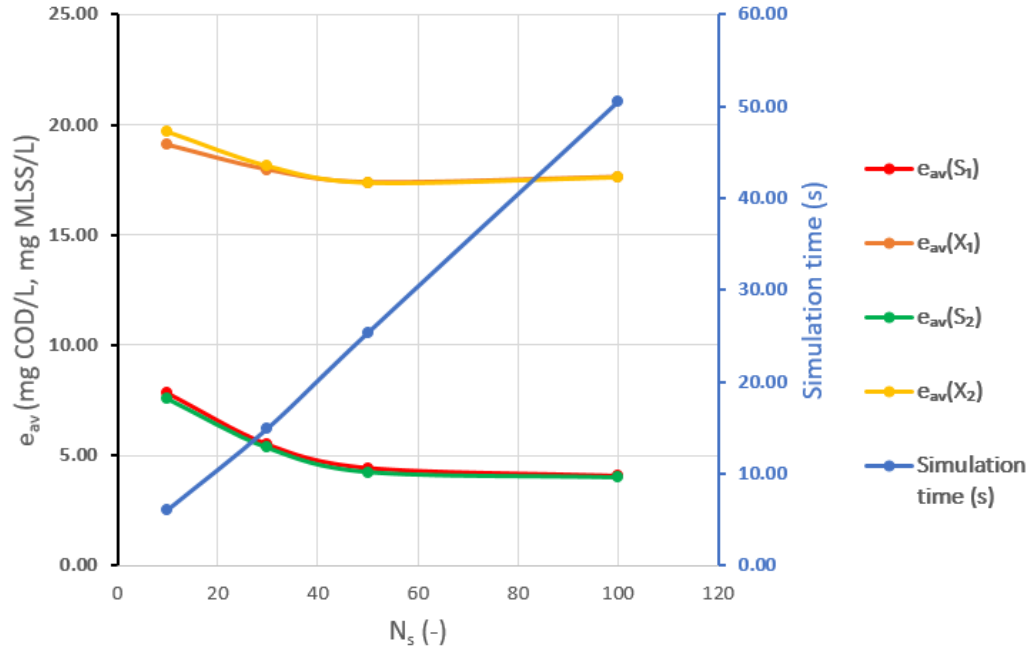


Figure 6: **The average estimation (absolute) errors (e_{av}) and the simulation time for different numbers of particles (N_s).** $N_s = 10, 30, 50$ and 100 were simulated. The presented simulation times refer to the duration of one simulation ($T = 4000$). The number of simulations is $N_r = 10$.

According to these principles, the N_s parameter of the PF can be tuned in a similar manner, even for other processes.

2.3.3.3 PF and IPF comparison

The simulation time and estimation errors are conflicting factors, as was seen in Section 2.3.3.2. The question arises whether estimation accuracy could be increased without significant growth in the simulation time. A good opportunity in this regard is to test IPF in the present environment, which improves the level of efficiency by handling phenomenon of sample impoverishment of general PF. IPF has not yet been applied in biochemical systems nor reactors. Its performance is tested in this section, besides setpoint changes.

The MATLAB program was coded according to the algorithm shown in [17]. In order to be used, firstly, the two parameters (α, p_M) of the algorithm had to be tuned. This task was executed in a similar manner to the above-mentioned issues: by keeping in mind the average error, the optimal set of the parameters was determined. With this method, $\alpha = 0.2$ and $p_M = 0$ were derived. Therefore, for the purpose of increasing the accuracy of the

estimation, the particles only need to be better distributed in the same interval and it is not necessary to broaden it. From this result, it can be concluded that sample impoverishment is not a severe problem in this system. However, the level of efficiency could also be increased in this case by distributing the particles better.

The tuned parameters were used to test the performance of the IPF compared to that of the PF.

The results are shown in Table 4. It can be seen that the IPF performs better in all states but particularly in X_1 and X_2 . Although the IPF contains one more calculation step, the simulation times are almost identical because of the number of resamplings in the two cases. Investigating this issue, the average number of resamplings was 170 in the case of the PF and 158 in the case of the IPF ($N_r = 10$). Therefore, if the IPF is used, resampling is needed less frequently.

Table 4: **Comparison of the PF and IPF with regard to the average error (e_{av}) and simulation time.** $N_r = 10$, $N_S = 30$, $T = 4000$.

	PF	IPF
$e_{av}(S_1)$	5.50	5.09
$e_{av}(X_1)$	17.96	15.55
$e_{av}(S_2)$	5.34	4.88
$e_{av}(X_2)$	18.12	15.72
Simulation time (s)	14.89	14.26

Regarding the results of this section, it is recommended to use IPF instead of general PF to enhance the estimation accuracy.

As Figures 7 and 8 present, the aforementioned conclusions also have pertinence in the case of different N_s values. Furthermore, it can be concluded that $N_s = 30$ is still the optimal value of the number of particles, even if IPF is applied.

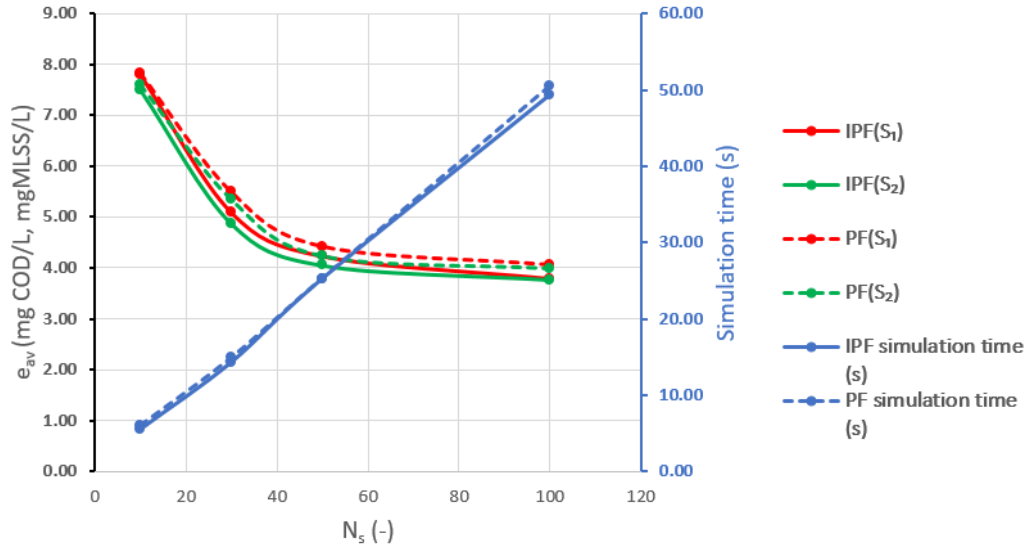


Figure 7: **Comparison of PF and IPF: The estimation errors (e_{av}) of the substrate concentrations and the simulation time regarding the different numbers of particles.** The curves belonging to PF are represented by dashed lines and those belonging to IPF by continuous ones. the red and green colors refer to the S_1 and S_2 state variables, respectively. The other parameters are the same as before ($N_S = 10, 30, 50, 100$; $T = 4000$; $N_r = 10$).

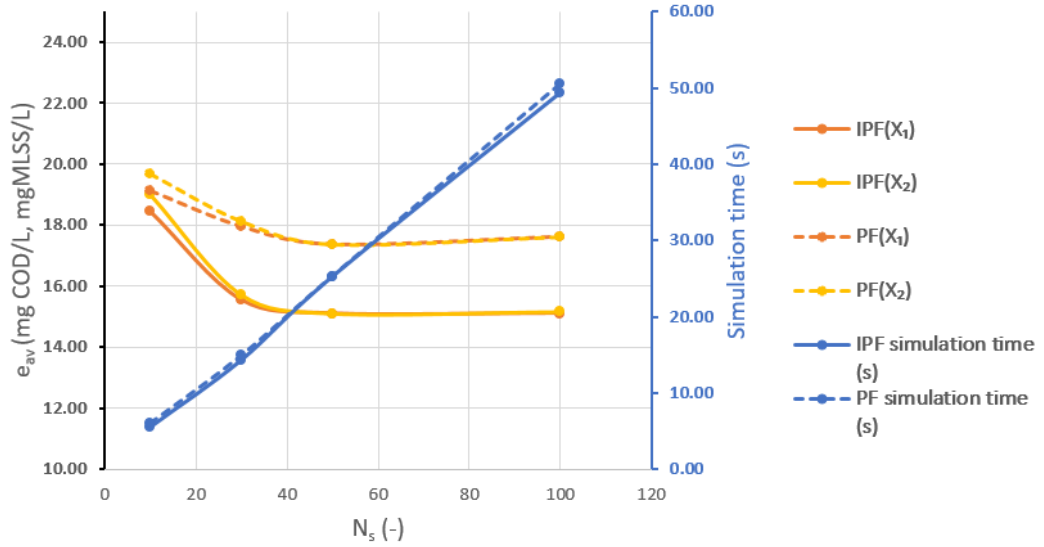


Figure 8: **Comparison of PF and IPF: The estimation errors (e_{av}) of the concentrations of microorganisms and the simulation time regarding the different numbers of particles.** The curves belonging to PF are represented by dashed lines and those belonging to IPF by continuous lines. The orange and yellow colors refer to the X_1 and X_2 state variables, respectively. The other parameters are the same as before ($N_S = 10, 30, 50, 100$; $T = 4000$; $N_r = 10$).

To check if the IPF's performance is better than the PF's even besides more setpoint changes, a longer part of the simulation was even used to compare the two algorithms in the case of the optimal $N_s = 30$. It contained three setpoint changes so that the dynamic behavior could be examined more profoundly. The conclusions were the same as above, namely the estimation error and number of resamplings were also lower in the case of IPF.

With this method, differences in the performances of the two algorithms can be investigated and the optimal value of the N_s parameter determined.

2.3.4 Application of PF in fault diagnostics

With the carefully chosen and tuned MATLAB implementation of the particle filter, different fault detection problems can be solved. As state estimation with particle filters is based on the information gained from the process, it is essential to have fault-free measurement data. If the sensor is faulty, the estimation will be inaccurate, and it is not observable according to the estimation results. However, the particle filter is able to indicate the faults by following the method described in Section 2.2.3.

Fault occurrence is evaluated according to the $-d_k$ value which is the negative sum of logarithms of the particle weights. If a faulty measurement occurs, the sum of the particle weights decreases, so $-d_k$ increases. With a carefully chosen threshold, the fault can be detected.

First of all, the fault-free operation was tested, and the threshold belonging to its 98% confidence interval determined. The distribution of $-d_k$ values along with the threshold are shown in Figure 9.

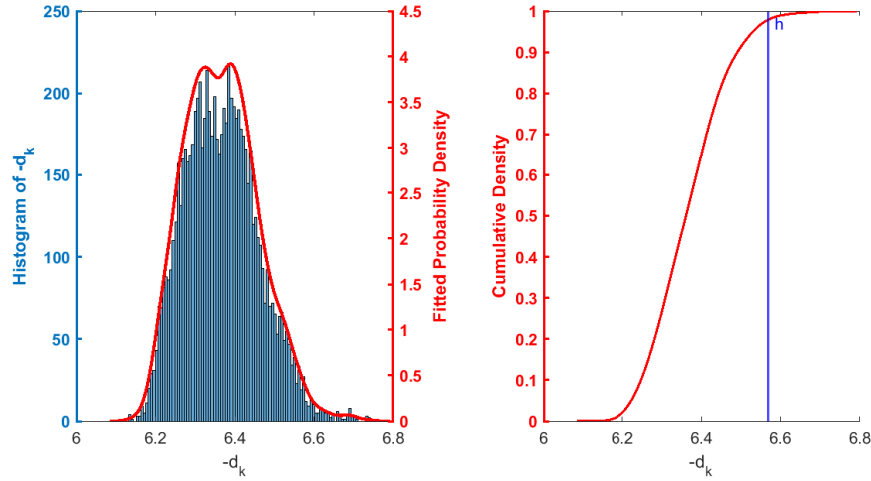


Figure 9: **Fault-free operation: the histogram, empirical probability density function (pdf) and cumulative distribution function (cdf) of $-d_k$.** Threshold h is denoted by a vertical line. The sliding window is $M = 50$. $T = 8000$.

2.3.4.1 Analysis of fault-signal ratio

A sensor fault can be modeled by an additive constant in the measurement function:

$$\mathbf{y}_k = h(\mathbf{x}_k, \mathbf{u}_k) + \mathbf{w}_k + \mathbf{f} \quad (2.18)$$

where $\mathbf{f}$ represents the fault. One of the main factors in fault detection is the fault-to-signal ratio. Therefore, the lowest value of $\mathbf{f}$ that can already be detected must be determined.

Four different values of $\mathbf{f}$ were examined: 5, 10, 15 and 20% of the value of measured state X_1 at the first stationary state. The fault occurred on the 25th day and lasted until the 55th day, as is shown in Figure 10. Furthermore, two setpoint changes were modeled around the 33rd and 66th days, one within the faulty time interval and the other after the fault had been rectified.

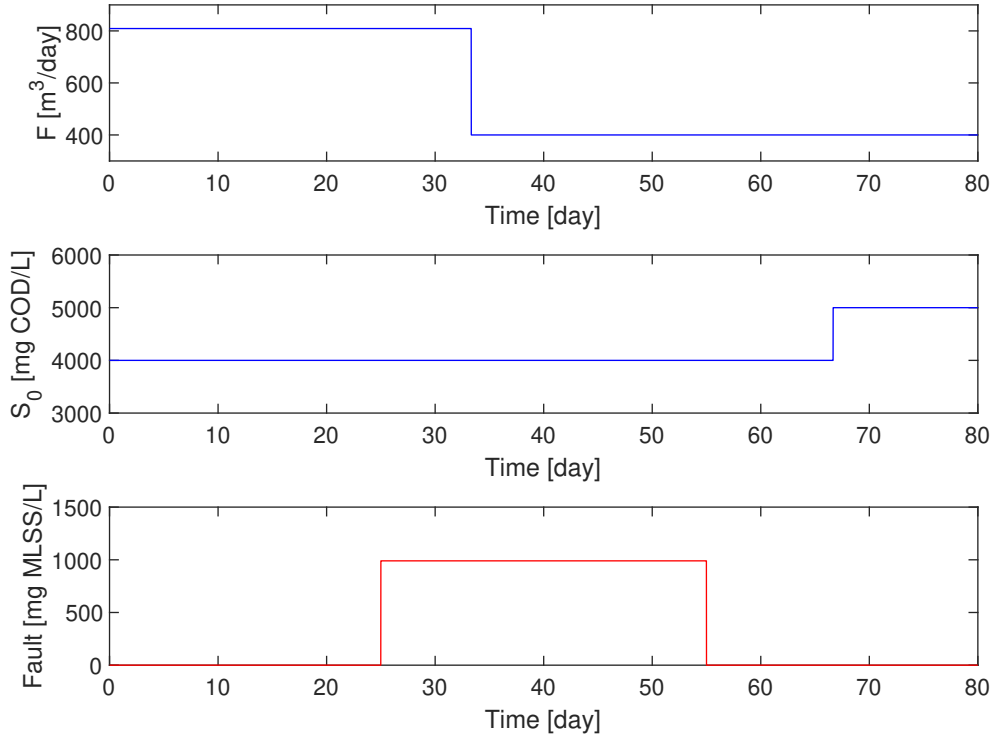


Figure 10: **Operation with a fault: setpoint changes and the fault.** The fault refers to the case of a 15% fault which is 990 mg MLSS/L. $T = 8000$.

The results are illustrated in Figure 11. It can be seen that $-d_k$ is quasi-constant during fault-free operations, so setpoint changes do not have an effect on it and the dynamic behavior of the process does not influence the efficiency of fault detection. Otherwise, the moment of fault occurrence is detected in all cases. However, $-d_k$ is once again quickly below the threshold in terms of the 5% and 10% faults. In the case of the 15% and 20% faults, this is above the threshold for almost the whole duration of the fault.

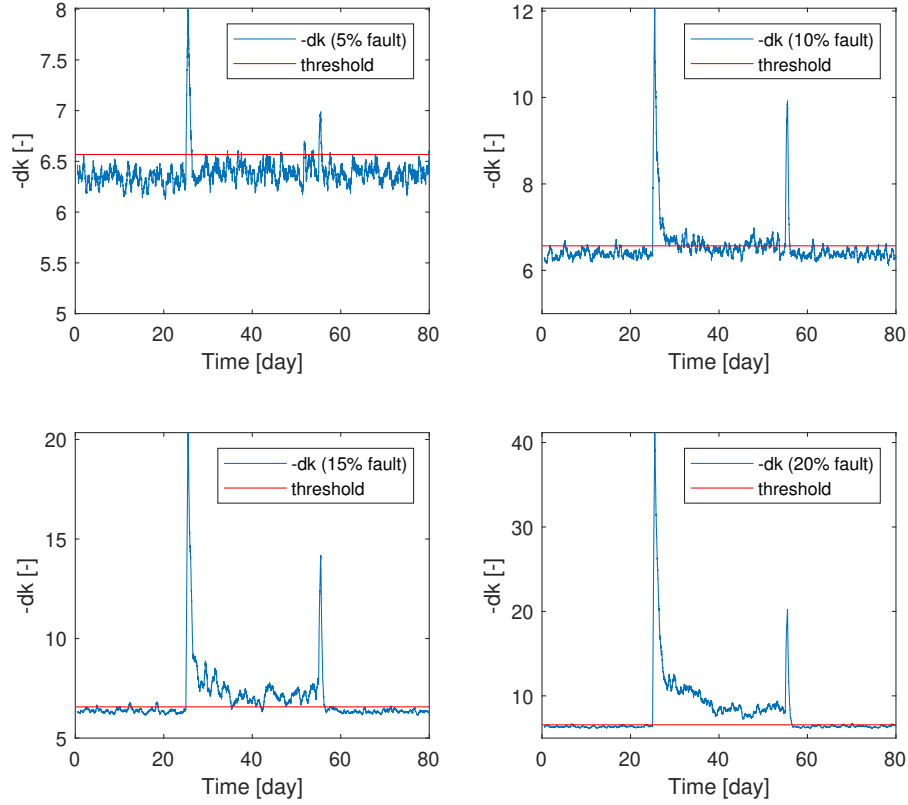


Figure 11: **Operation with a fault: results according to different fault amplitudes.** One of the setpoint changes occurs within the fault duration and one once it has been resolved, as is seen in Figure 10. The threshold is $h = 6.57$, calculated by the 98% confidence interval of the fault-free operation. Sliding window is $M = 50$. $T = 8000$.

The aforementioned difference between the small and large fault amplitudes is explained by Figures 12 and 13. These results show that in the case of minor faults, the estimated state is in line with the measured values after the fault occurs. However, in the case of the 20% fault, a residual error is recorded not only between the estimated and real states but even between the estimated and measured states.

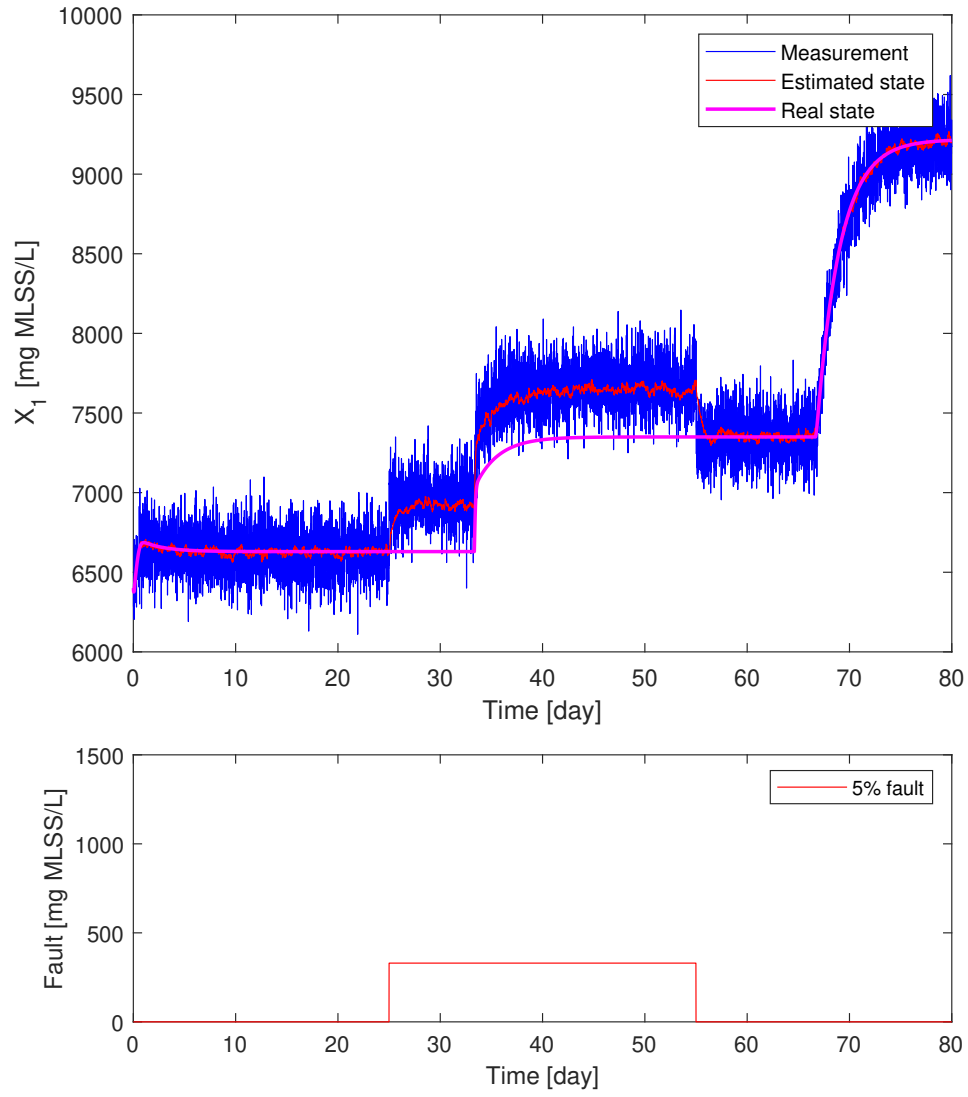


Figure 12: **Real, measured and estimated values of the state variable X_1 by the 5% fault.** The value of the 5% fault is 330 mg MLSS/L. $T = 8000$.

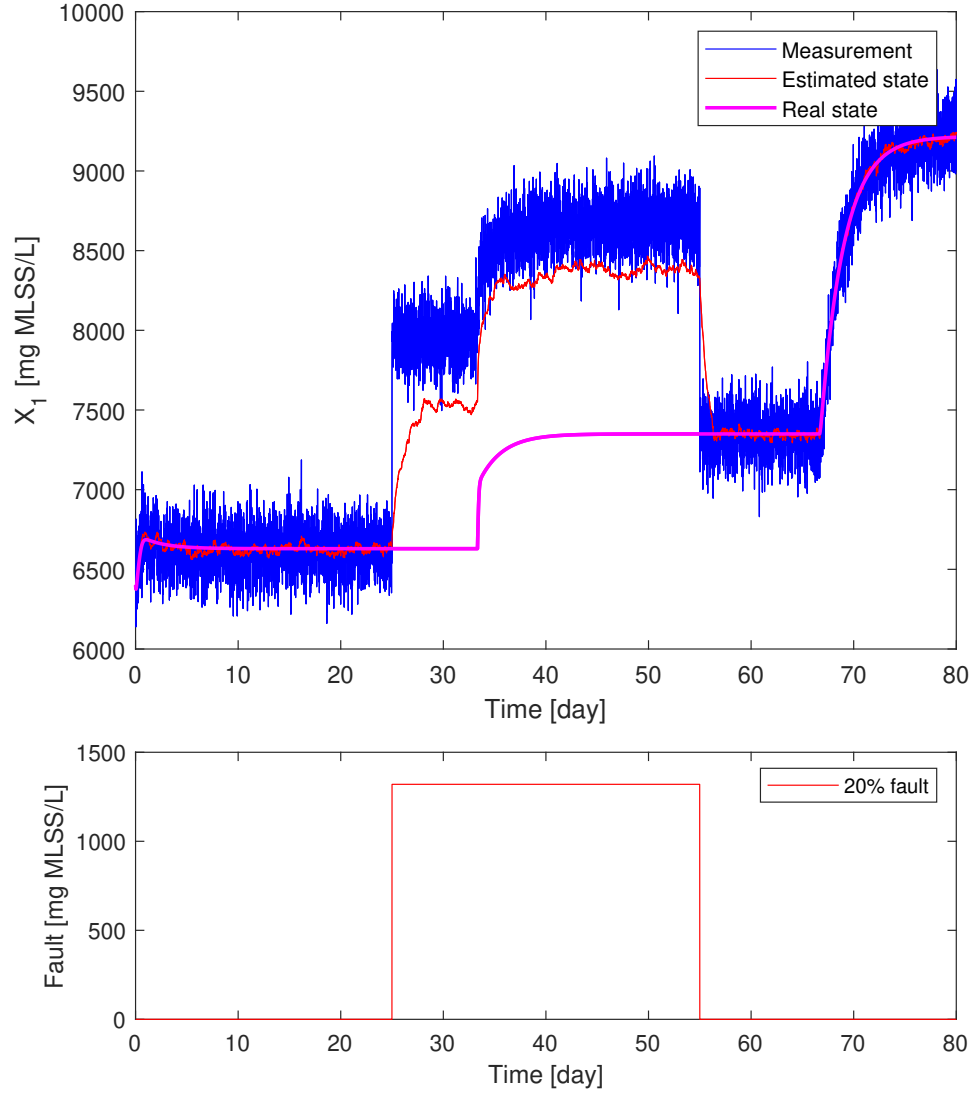


Figure 13: **Real, measured and estimated values of the state variable X_1 by the 20% fault.** The value of the 20% fault is 1320 mg MLSS/L. $T = 8000$.

On the one hand, the reason for this phenomenon is that during the resampling step, the PF chooses new particles from the set of the prior particles. If the change is very significant, resampling cannot follow it. On the other hand, the particles try to converge with the real state as the state space model is deterministic.

For the aforementioned reasons, $-d_k$ does not return to below the threshold while the fault lasts.

Once the fault has ceased, $-d_k$ returns to its initial value in all the cases in Figure 11, moreover, the rectification of the fault is indicated by a spike.

It was noticed that in the case of minor faults, only the beginning and the end of the faulty time interval could be detected. However, considering the number of resamplings, information could be gained about the existence of the fault. As is shown in Table 5, since the average number of resamplings per day is higher while the fault lasts, the duration of the fault can be unambiguously determined by following the tendency of $-d_k$ and the number of resamplings.

Table 5: **Average number of resamplings per day by different values of the faults.** $T = 8000$.

Fault	Before the fault	Faulty time interval	After the fault
5%	3.64	5.70	4.56
10%	3.84	10.73	4.68
15%	3.64	18.93	5.04
20%	3.80	27.43	5.64

The effect of the setpoint changes is insignificant. In the case of the fault-free interval (setpoint change in S_0), the setpoint change is not perceptible in Figure 11. The setpoint change in F while the fault occurs is also negligible. For further investigations, the case of the 15% fault was chosen as it is the lowest that gives an alarm throughout the entire duration of the fault according to $-d_k$.

2.3.4.2 Tuning of the sliding window

In the fault decision function (Equation 2.12), the M sliding window parameter functions as a smoothing parameter. The effect of this parameter on the noisiness of the $-d_k$ signal is shown in Figure 14. If M is small, the fluctuations in $-d_k$ are large, while if M is larger, $-d_k$ is more filtered.

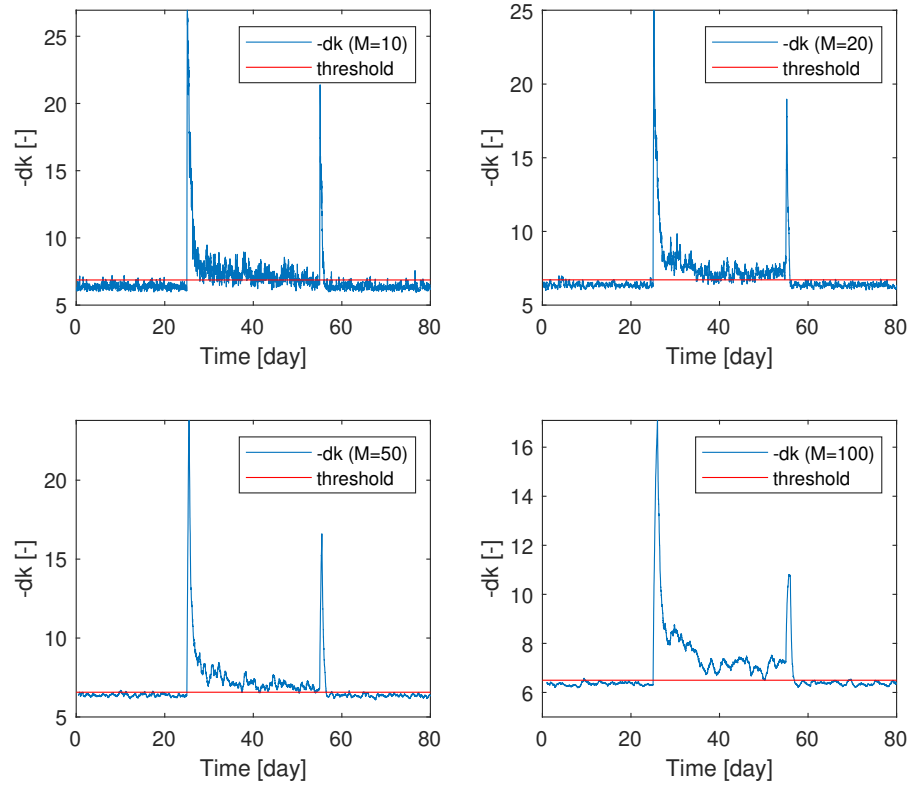


Figure 14: **Sensitivity analysis by the sliding window (M): bias faults.** Bias sensor faults are defined in the same way as above. $M = 10, 20, 50$ and 100 time steps. The 15% fault was used, that is 990 mg MLSS/L. $T = 8000$.

To determine the optimal value of M , impact faults were also considered. The results are shown in Figure 15. It can be concluded that the larger M is, the less acute the spikes are and the intensity of the fault signal decreases.

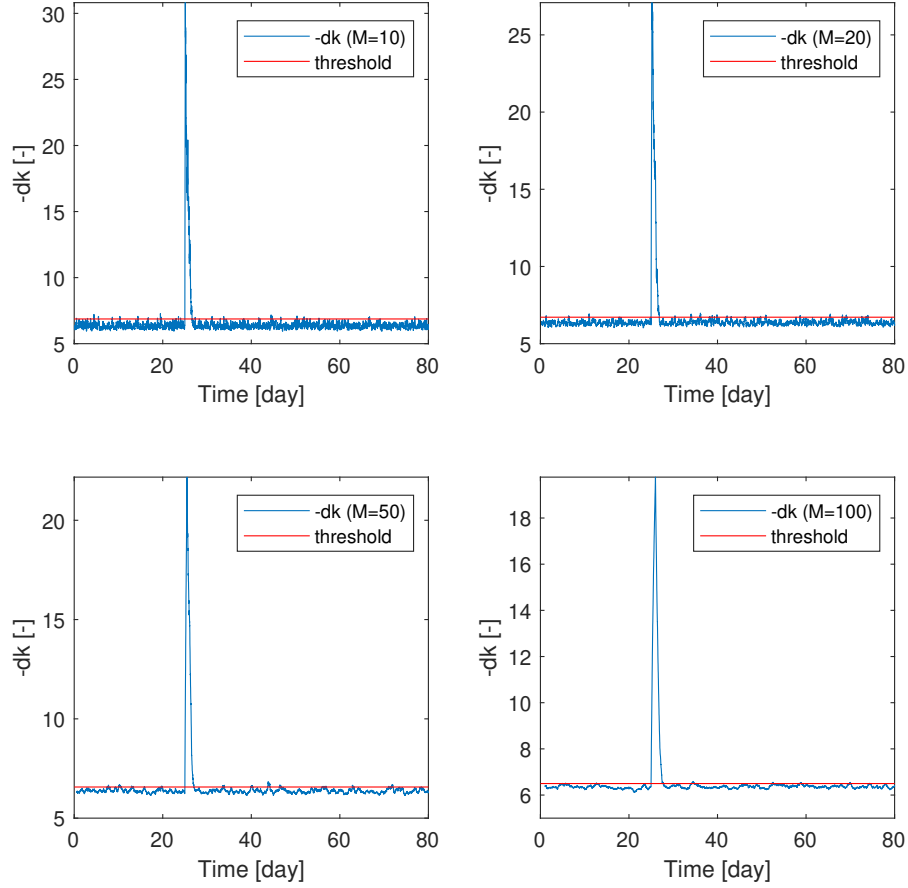


Figure 15: **Sensitivity analysis by the sliding window (M): impact faults.** The fault occurs from the 25th to the 26th day. $M = 10, 20, 50$ and 100 time steps. The 15% fault was used, that is 990 mg MLSS/L. $T = 8000$.

According to these aspects, if the aim is to rapidly detect impact faults and sudden changes, a smaller M is suggested. However, if the duration of the bias fault is wanted to be indicated, a larger M is preferred. In the present case, $M = 50$ is optimal to detect both bias and impact faults.

Besides the conclusions already made, the aforementioned experiments also point out that the implementation of IPF instead of general PF does not require changes to be made to the fault detection method. It can also be applied as in the case of general PF and is able to detect both bias and impact faults with highly efficient.

The threshold values used above, calculated by the 98% confidence interval, are summarized in Table 6. As the M sliding window functions as a smoothing parameter, the larger M is, the narrower the distribution of $-d_k$ that results.

Therefore, h decreases as M increases.

Table 6: **Summary of h threshold values.**

M	h
10	6.87
20	6.71
50	6.57
100	6.50

In this chapter, a PF-based fault detection technique was introduced. Based on the given method, it is feasible to determine the h threshold of alarm generation as well as tune the value of the M sliding window according to how the system responds to bias and impact sensor faults. To detect the existence of bias faults more accurately, the number of resamplings should also be considered.

2.4 List of symbols

The following symbols are used in Section 2:

$\mathbf{x}_k$	estimated state vector at time k
$\mathbf{y}_k$	measurement vector at time k
$\mathbf{u}_k$	input vector at time k
$\mathbf{v}_k$	model noise at time k
$\mathbf{w}_k$	measurement noise at time k
$f()$	state transfer function
$h()$	measurement function
N_S	number of particles
$\mathbf{x}_0^i$	initial state vector of the i th particle
ω_0^i	initial weight of the i th particle
$\mathbf{x}_k^i$	estimated state vector of the i th particle at time k
ω_k^i	weight of the i th particle at time k
$\mathbf{y}_{1:k}$	measurement data points from time 1 to time k
$\delta()$	Dirac delta function
N_{eff}	effective sample size
N_t	threshold of N_{eff}
$\mathbf{x}_{kH}^l$	large-weight particles before crossover step at time k
$\mathbf{x}_{kL}^j$	small-weight particles before crossover step at time k

$\mathbf{x}_{kC}^j$	new particles after crossover step at time k
$\mathbf{x}_{kM}^j$	new particles after mutation step at time k
α	parameter of the IPF's crossover step
p_M	parameter of the IPF's mutation step
N_r	number of simulations
T	number of time steps
e_{uk}	absolute error at time k in the u th simulation
e_{av}	average absolute error
L_k	average likelihood of the measurement by particles at time k
M	sliding window
d_k	normalized fault decision function at time k
h	fault threshold
F	flowrate
R	recycle ratio
S_i	substrate concentration in the i th reactor
X_i	concentration of microorganisms in i th reactor
S_0	substrate concentration of the feed entering the first reactor
w	waste factor
t	time
V	reactor volume
μ_m	maximum specific growth rate
β	yield factor
K_S	Monod constant
C	concentration factor
k_d	death coefficient
n	volume ratio of the two reactors
b_{SRC}	parameter for calculating critical residence time
τ_{min}^*	dimensionless critical residence time
$S_{i,0}$	initial substrate concentration in the i th reactor
$X_{i,0}$	initial concentration of microorganisms in the i th reactor
σ_v	deviation of the model noise
σ_w	deviation of the measurement noise
$\mathbf{f}$	fault
$\#$	count of occurrences

3 An expert knowledge-based technique for parameter estimation

This part of the thesis provides a technique for parameter estimation besides uncertain and/or incomplete information about the process involving expert knowledge. It is shown that importance sampling (IS) technique is applicable for solving this kind of problems, and the expert judgments can be also evaluated according to the results.

The experiments were made on an existing Hungarian waste separation system, which model and expert-based data were available. In Section 3.2, the methodological background of the research is introduced, containing some ideas about the representation possibilities of uncertain expert knowledge in Section 3.2.1, describing the proposed parameter estimation technique based on IS in Section 3.2.2, introducing the application of the results for the validation of expert judgments in 3.2.3, and providing a method for the elimination of incorrect expert assessments in Section 3.2.4. The experimental results are provided in Section 3.3. The investigated waste separation system is introduced in Section 3.3.1, the available expert knowledge about the system in Section 3.3.2, the experiments and results of parameter estimation are presented in detail in Section 3.3.3 and 3.3.4, the evaluation of the expert judgments in Section 3.3.5, and the investigations on the outer iteration circle to eliminate incorrect expert judgments thus refining the parameter estimation results are introduced in Section 3.3.6.

3.1 Formalization of the parameter estimation problem

The behavior of complex systems is difficult to predict. On the one hand, a lot of variables can be defined in these systems that depend on each other. On the other hand, the number of connections between variables is also high. This aggregation of variables and connections is difficult to see through without using a system model. Although a model cannot describe reality entirely, the aim is to approximate the real system as much as possible. If a valid model is available, it can also be used for the development and optimization of the system.

Models often appear in a mathematical form, where the outputs ($\mathbf{y}$) of the system are functions of the inputs ($\mathbf{u}$) and the parameters (Θ):

$$\mathbf{y} = f(\mathbf{u}, \Theta) \quad (3.1)$$

However, the parameters and input of the model are often not known or uncertain, especially when the technology is in the design phase. For example, the composition of the feed, the effect of a new catalyst on the reaction rate in a reactor, the heat transfer coefficient of a new structural material or coating, or the separation efficiency of a distillation column. These parameters are often estimated using the available measurement data of the model output. However, measurement data are not always available as was declared before. In this case, another source of information is needed. For example, the experience-based knowledge of experts can be used.

As expert knowledge is subjective, the assessments of more experts can be aggregated and represented by a probability distribution [26]. If the model structure of the complex system ($f()$) is known, the available uncertain expert knowledge can be integrated. Thereby, the unknown parameters or inputs of the system can be estimated, thus refining the model, and outputs can also be calculated. In the this part of the paper, the uncertain variables and parameters of the model needed to be estimated are gathered in a vector $\mathbf{x}$:

$$\mathbf{x} = [\mathbf{u}^T, \Theta^T, \mathbf{y}^T]^T \quad (3.2)$$

and one elements of $\mathbf{x}$ is denoted by x_i in this part of the thesis.

In the this section, a case study about a waste separation system is introduced, where the inputs ($\mathbf{u}$) were known from measurements, however, about the parameters (Θ) and outputs ($\mathbf{y}$) of the technology the operators had only some uncertain intuitions, which they gave in the form of intervals. Transforming this information into a mathematical form, uniform distributions are gained, similarly to the example of estimating the numerical meaning of linguistic variables in [27].

The gained probability distributions make it possible to estimate the parameters and outputs of the system if the model structure is known. The results can be evaluated by a Monte Carlo (MC) simulation of the expert-based probability distributions of the parameters and the system model, and the results can be compared to those suggested by the experts. Thus, the consistency of the expert knowledge about the parameters and outputs can be examined. Based on the probability distributions of expert-based outputs, the parameters

can be further refined by the importance sampling (IS) technique. Executing these two steps iteratively, the imprecise information of the parameters and outputs can be brought to a consensus, and the calculations converge to a result in the form of probability distributions as seen in Figure 16.

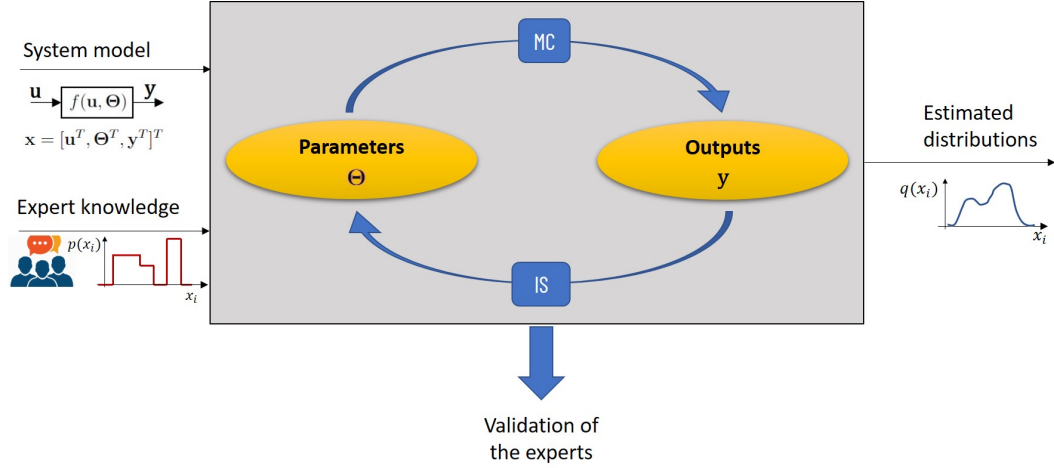


Figure 16: **Parameter estimation and evaluation of expert knowledge based on the integration of expert-based information into the system model.** The expert knowledge is available in the form of probability distributions of the parameters and outputs. Outputs are estimated by Monte Carlo (MC) simulation based on the system model and the sampled probability distributions of parameters, and parameters are deduced and refined according to the expert-based outputs by importance sampling (IS), iteratively. Expert knowledge can be also evaluated according to the results. $\mathbf{u}$, Θ and $\mathbf{y}$ are represent the input, parameter and output vector of the system, respectively. The ones of them needed to be estimated gathered to vector $\mathbf{x}$, and its elements are marked by x_i .

Comparing the estimated probability distributions to the original ones provided by experts, the judgments of the experts can be characterized by the goodness values thus evaluated. With this method, incorrect judgments can be identified and even eliminated from the estimation by using an outer iteration circle.

The above-mentioned experiments are executed and the results are introduced through the case study of an operating Hungarian waste separation technology. This system satisfies the conditions above, namely, the parameters are not known, measurements are rarely available in this type of processes, and the knowledge of experts has a distribution because of subjectivity. Moreover, experts cannot give their assessments of the parameters and outputs as exact values, only as intervals. With these features, the system is applicable

to achieve the above-mentioned research goals.

Regarding the roadmap of this part of the thesis, in Section 3.2, the methodological background of the study is introduced, containing some ideas about the representation possibilities of uncertain expert knowledge in Section 3.2.1, describing the proposed parameter estimation technique based on IS in Section 3.2.2, introducing the application of the results for the validation of expert judgments in 3.2.3, and providing a method for the elimination of incorrect expert assessments in Section 3.2.4. The experimental results are provided in Section 3.3. The investigated waste separation system is introduced in Section 3.3.1, the available expert knowledge about the system in Section 3.3.2, the experiments and results of parameter estimation are presented in detail in Section 3.3.3 and 3.3.4, the evaluation of the expert judgments in Section 3.3.5, and the investigations on the outer iteration circle in Section 3.3.6.

3.2 The proposed method for integration of expert knowledge to the system model

In this section, the methodological background of the paper is introduced. Initial uncertain expert knowledge about the parameters and outputs is transformed into probability distributions. MC simulation is used to handle this knowledge, and IS is used to estimate the most likely probability distributions of the parameters and outputs based on the available information. To evaluate experts, the distributions created from the intervals provided by them are weighted compared to the estimated distributions; thus, goodness values are generated. Figure 17 outlines the method in which elements are introduced in detail in this section.

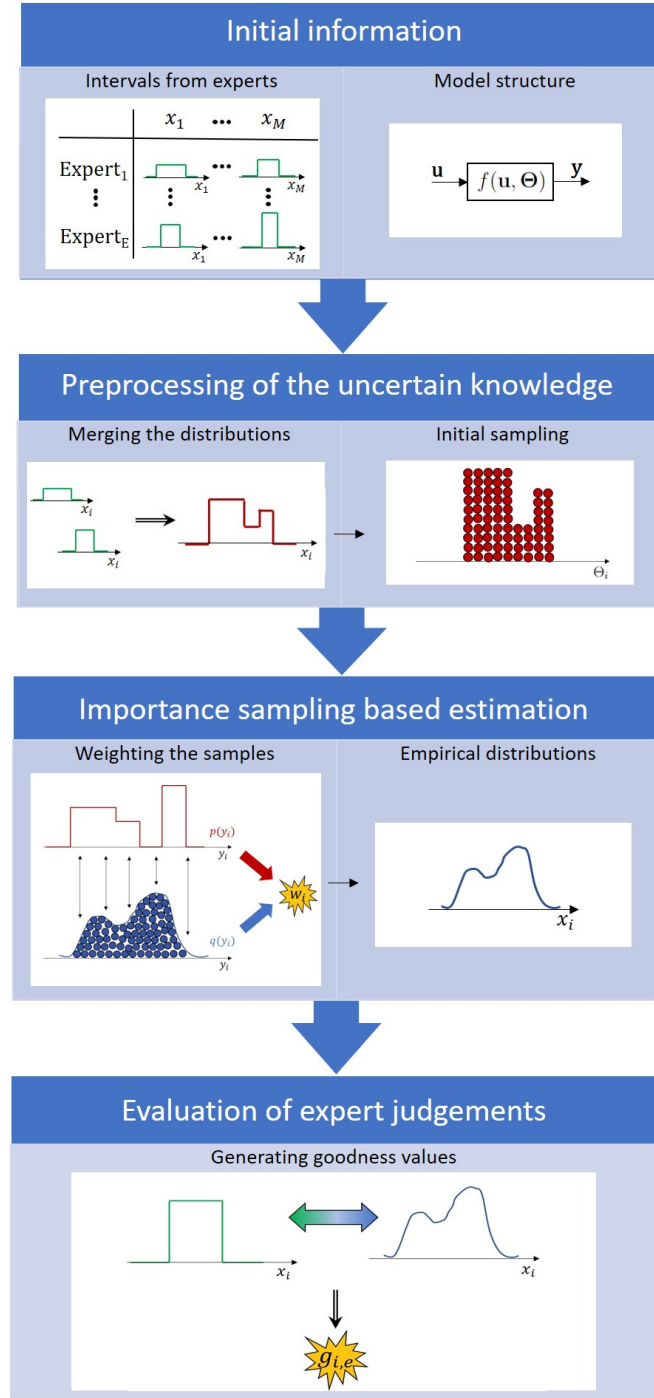


Figure 17: **The steps of the procedure used in Section 3.2 to integrate expert knowledge into the system model.** The initial information from the experts is represented by uniform distributions, which are aggregated for each estimable x_i variable. Sample elements are drawn from the aggregated distributions of the parameters and are weighted (w_i) according to those of the outputs (y_i). Thereby, empirical distributions are generated and compared to the original expert-based distributions, thus creating goodness values ($g_{i,e}$) of expert judgments.

3.2.1 Representation of uncertain expert knowledge

Expert knowledge is a set of subjective assessments of several professionals who created their judgments independently from each other. If they can give their judgment about the unknown variable as an exact value, the uncertainty of the assessment can be modeled well with normal distribution. However, sometimes experts are not able to give an exact estimation for the unknown values, but they provide an interval by minimum $x_{i,min}$ and maximum $x_{i,max}$ bounds, e.g., in the case of the e th expert:

$$x_i \in [x_{i,min}^e, x_{i,max}^e] \quad (3.3)$$

This information is usually handled in the form of uniform distribution if there is no reason to assume that the experts consider some elements of the given interval more likely than others:

$$p_e(x_i) = \begin{cases} \frac{1}{x_{i,max}^e - x_{i,min}^e} & \text{for } x_{i,min}^e \leq x_i \leq x_{i,max}^e \\ 0 & \text{for } x_i < x_{i,min}^e \text{ or } x_i > x_{i,max}^e \end{cases} \quad (3.4)$$

where $p_e(x_i)$ represents the opinion of the e th expert about x_i .

If more expert assessments are available, the individual distributions should be aggregated for every x_i as seen in the second row of Figure 17 by forming the mean of them. Thereby, all expert judgments were handled with the same weights:

$$p(x_i) = \frac{\sum_{e=1}^E p_e(x_i)}{E} \quad (3.6)$$

where E denotes the number of experts.

If some variables or parameters of the system are available as a probability distribution instead of an exact number, a sample that represents them has to be generated. Monte Carlo simulation is a good solution for the problem. According to the technique, samples are drawn from the probability distributions of uncertain inputs ($p(u_i)$) and parameters ($p(\Theta_i)$):

$$p(x_i) \approx \{x_i^j\}_{j=1}^N \quad (3.7)$$

where x_i^j is the j th sample element from $p(x_i)$, and N is the number of the samples.

Thus, the original continuous probability distribution is represented by a discrete sample as seen in Figure 18.

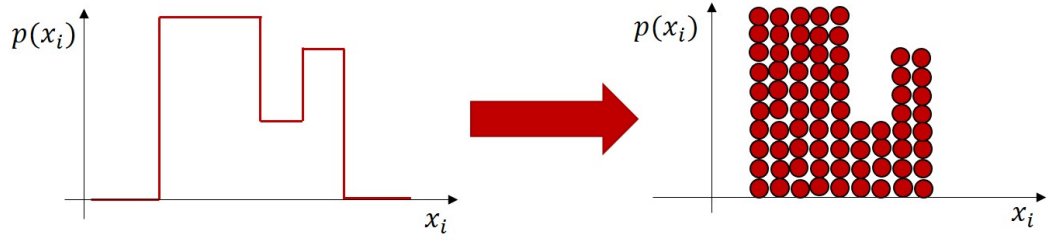


Figure 18: **The outline of MC simulation.** Samples are drawn from the continuous distribution to represent it. The variable that the distribution belongs to is denoted by x_i .

Then, the output of the model can be calculated for every sample element according to Equation 3.1. If the sample size is large enough, the resulting probability distributions of the outputs will consequently be the same for every run of the simulation.

In this study, the input of the system is available from measurements; however, the uncertain information about the parameters and outputs provided by the experts in the form of data ranges is treated by the technique described above. Expert judgments were handled as uniform distributions, and, as more expert evaluations were available, the distributions were aggregated. Then, the distributions of the parameters were sampled and a Monte Carlo simulation was executed to calculate the estimated outputs, and the aggregated distributions of outputs are used to validate the results that will be described in the next section.

3.2.2 Parameter estimation by importance sampling (IS)

If the assessments on the parameters and the results were gained from two independent groups of experts, these pieces of information may not harmonize with each other. In the following, a technique is introduced on how these elements of knowledge can be made consistent.

According to the estimated outputs ($q(y_i)$) in Section 3.2.1, the system model can be validated by involving some measurement data and comparing them with the estimated values. However, if the measurement data are not available, asking for some information from experts is again a favorable possibility [28].

Similarly to the case of parameters, experts sometimes can provide only intervals of the outputs that can be modeled by uniform distributions. Therefore, aggregated distributions of them ($p(y_i)$) also provide the basis for model validation.

Using these pieces of information, the parameters of the model can be estimated by an iterative technique: the sample elements of the output obtained by the MC simulation are weighted (w_i) by IS, thus new empirical probability distributions of the parameters are generated, and new samples are drawn from them. Then the output is calculated again for every sample element. These steps are repeated until the results converge. An outline of the procedure can be seen in Figure 19.

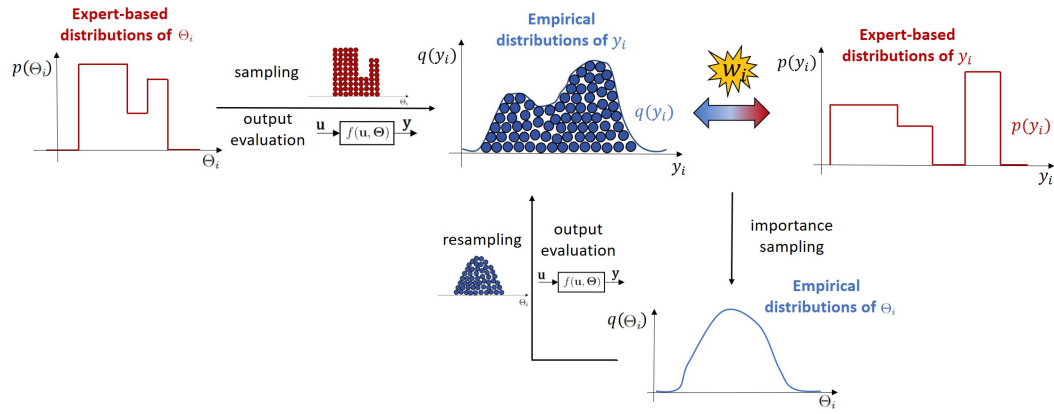


Figure 19: **The schematic figure of the parameter estimation technique using expert knowledge.** It is assumed that the input vector ($\mathbf{u}$) of the system is known. Θ and $\mathbf{y}$ denote the parameter and output vector of the system with the elements of Θ_i and y_i , respectively. w_i refers to the weights generated by importance sampling. The expert-based distributions are represented by red color and the empirical distributions by blue.

3.2.2.1 Importance sampling based on the expert knowledge

The importance sampling (IS) technique is suitable for giving weights to the sample elements by comparing the resulting distribution of outputs with expert-based ones in every iteration step. Therefore, new empirical distributions of the parameters can be generated and an iterative circle created.

As presented in Section 3.2.1, the estimated outputs are available as sample densities from the MC simulation. Empirical probability density functions (pdf) fitted to these will serve as the so-called importance functions or proposal distributions, denoted $q(y_i)$ in Figure 19 where y_i is an element of the

output vector ($\mathbf{y}$). The expert-based distributions used for the comparison are indicated by $p(y_i)$ as seen in Figure 19.

The interoperability between $p(y_i)$ and $q(y_i)$ can be described as:

$$E_p[y_i] = \int y_i p(y_i) dy_i = \int y_i \frac{p(y_i)}{q(y_i)} q(y_i) dy_i = E_q[y_i \cdot \frac{p(y_i)}{q(y_i)}]. \quad (3.8)$$

where $E_p[]$ and $E_q[]$ denote the expected values of the argument that is distributed according to $p()$ and $q()$, respectively.

Therefore, with respect to discrete distributions:

$$E_p[y_i] \approx \frac{1}{N} \sum_{j=1}^N y_{i,p}^j = \frac{1}{N} \sum_{j=1}^N y_{i,q}^j \cdot \frac{p(y_{i,q}^j)}{q(y_{i,q}^j)} = \frac{1}{N} \sum_{j=1}^N y_{i,q}^j w_i^j \quad (3.9)$$

where $y_{i,p}^j$ and $y_{i,q}^j$ are the j th element sampled from $p(y_i)$ and $q(y_i)$, respectively, w_i^j denotes to the so-called importance weight of $y_{i,q}^j$, and N to the sample size.

Equations 3.8 and 3.9 clarify that the sample elements can be weighted by calculating w_i^j . The original sample elements have equal weights. They obtain new normalized weights according to the $p(y_i)$ distribution provided by the experts as

$$w_i^j = \frac{p(y_i^j)}{q(y_i^j)}, \quad (3.10)$$

where y_i^j is the i th output belonging to the j th sample element, and w_i^j denotes to the weight of this element according to y_i^j .

After the sample elements were weighted by importance sampling, new probability distributions of the parameters come up. New sample elements can be drawn from these empirical distributions applying resampling step of the PF algorithm which principles are described in Appendix A. Thereby, an iterative circle can be generated.

In the present work, more parameters are needed to estimate, thus all of them are resampled and assigned to the sample elements independently. Then the results are calculated again for each sample element and the iteration seen in Figure 19 is executed until the empirical distributions converge.

3.2.3 Application of the proposed method for the validation of experts knowledge

Based on the results, expert knowledge can be evaluated. The estimated empirical distributions ($q(x_i)$) of the parameters and the output can be compared with the originals of the experts ($p_e(x_i)$).

One of the most simple techniques to compare two probability distributions is the measure of Jaccard index, which will be used as goodness values of expert judgments. As the original method is able to represent the similarity of two datasets, a generalization of the technique is needed here to apply.

Firstly, the two density functions to compare should be discretized by a Δx_i value, and the density functions should be evaluated at those points. Then, the Jaccard index of the two resulting datasets can be calculated [29]. Thereby, the goodness values of the expert judgments:

$$g_{i,e} = J(\mathbf{p}_e, \mathbf{q}) = \frac{\sum_{k=1}^K \min(p_{e,k}, q_k)}{\sum_{k=1}^K \max(p_{e,k}, q_k)} \quad (3.11)$$

where $g_{i,e}$ marks the goodness value belonging to the judgment of the e th expert about x_i , $\mathbf{p}_e$ and $\mathbf{q}$ represent the two datasets gained from $p_e(x_i)$ and $q(x_i)$, K refers to the size and $p_{e,k}$ and q_k denote to the elements of them, respectively.

The scheme of the method can be seen in Figure 20.

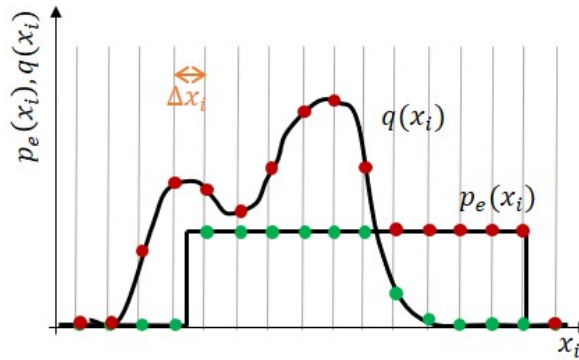


Figure 20: **Comparison of two probability distribution by calculating the Jaccard index.** The $p_e(x_i)$ and $q(x_i)$ distributions are discretized by Δx_i and probability density functions are evaluated at that points. The elements two datasets are compared pairwise: the maximum and minimum values are denoted to red and green color, respectively. Then, Equation 3.11 is used to calculated Jaccard index, which is the ratio of the areas under the red and green curves, actually.

Applying the technique to compare the resulting empirical probability densities with the original ones based on experts, expert assessments can be characterized by the goodness values calculated ($g_{i,e}$), thus being evaluated.

3.2.4 Eliminating the incorrect expert judgments

The goodness values resulting in Section 3.2.3 are also applicable to give weights to the initial uniform distributions of the experts ($p_e(x_i)$) and to generate an outer iteration circle to further refine the estimation. Weights can be created by normalizing the goodness values for each x_i :

$$\tilde{g}_{i,e} = \frac{g_{i,e}}{\sum_{e=1}^E g_{i,e}} \quad (3.12)$$

where $\tilde{g}_{i,e}$ refers to the normalized goodness value of the judgment of the e th expert about x_i .

Using these weights, new aggregated distributions can be created from the initial ones as follows:

$$p(x_i) = \sum_{e=1}^E \tilde{g}_{i,e} p_e(x_i) \quad (3.13)$$

Thus, feedback is obtained from the estimated distributions as seen in Figure 21.

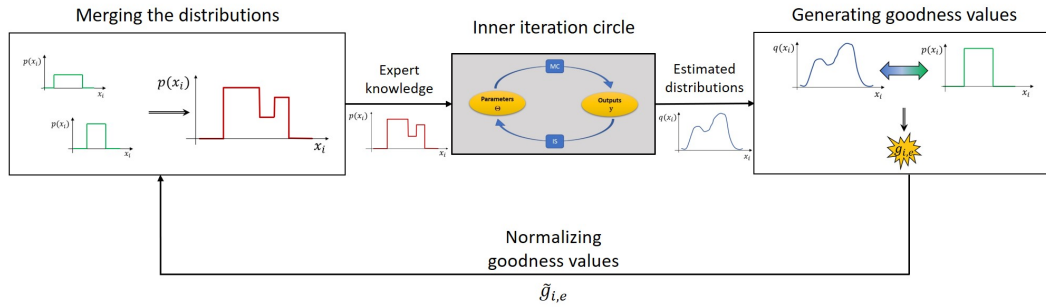


Figure 21: **Outline of the outer iteration circle.** The initial distributions from experts are merged again in every iteration according to the normalized goodness values ($\tilde{g}_{i,e}$) gained by comparing these distributions to the estimated ones resulted in the inner circle.

Weighting the initial distributions according to their correctness gives the possibility of eliminating the incorrect expert judgments, thus refining the estimation. In this study, the convergence in the outer circle is also investigated.

3.3 Applications to a waste separation system

Nowadays there is a great emphasis on waste management in our society. As the population and consumption grow, the amount of municipal waste also increases and must be handled in some way. The main area to focus on is waste recycling.

To be able to recycle waste, it should first be efficiently separated by different types of materials, and contaminants must be removed. For this aim, many types of industrial waste equipment can be used based on the composition of the waste, thus building the waste sorting technology. As the quality of municipal waste is not constant due to changing material regulations, technologies also have to adapt to these changes. This flexibility requires knowing the model of the system and its parameters as much as possible.

Due to the importance of the issue, my investigations were conducted on an operating waste separation system in Hungary. This gives the opportunity to gather information from experts who have worked with the technology for a long time. The system, the handling of expert knowledge and the output estimation of the system were thoroughly described in [30]. In the present part of the thesis, the parameter estimation and the evaluation of expert knowledge are investigated.

In the following, the technology is described in detail in Section 3.3.1. Section 3.3.2 contains a short description of the available expert-based data, Sections 3.3.3 and 3.3.4 the principles and results of parameter estimation, respectively. Section 3.3.5 introduces how the results can be used for the evaluation of expert knowledge. Section 3.3.6 presents the results applying an outer iteration circle to eliminate incorrect expert knowledge from the estimation.

3.3.1 Introduction to the waste separation technology

The technological scheme of the waste processing plant that was chosen to examine can be seen in Figure 22 [30]. It operates with seven units. The pre-shredder has one input and one output, as it changes only the size distribution of the waste. Therefore, the compositions of its input and output are the same. All other units can be considered as flow splitters: They have one input and two outputs in all cases. Magnetic and eddy-current separators remove iron and aluminum from the waste, respectively. The drum screen extracts nonrecyclable components (RDF: refuse-derived fuel) from the waste, those

that go for burning to produce electricity. The air separator splits the rest of the waste according to its shape into 2D and 3D components. Finally, optical separators working in the near-infrared (NIR) spectra sort the waste by material quality.

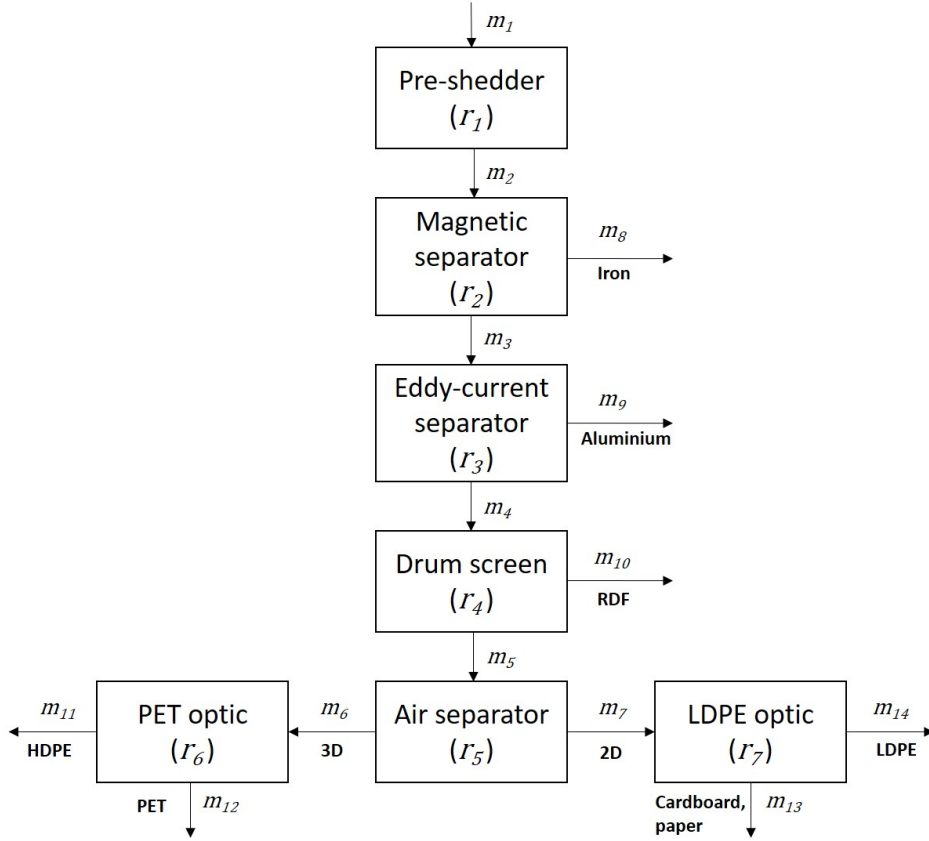


Figure 22: **Block diagram of the waste processing technology.** m_i ($i = 1, \dots, 14$) represents the technological mass flows, and r_j ($j = 1, \dots, 7$) represents the set of the separation efficiencies of the j th unit on components. The titles of the arrows indicate in which component the related flow is rich. RDF: refuse-derived fuel, PET: polyethylene terephthalate, LDPE: low-density polyethylene, HDPE: high-density polyethylene.

3.3.2 Available expert knowledge

Expert knowledge was surveyed by asking them about the separation efficiencies and some yields of the system. As introduced in [30], they provided their assessment about all of the r_j ($j = 1, \dots, 7$) values for all components, and the yields of the PET, LDPE, iron and aluminum components for the out-flows they accumulate. Knowing the feed of the system from measurements, the information about the yields depends only on the leaving component mass

flows.

Separation efficiencies and yields were asked from two independent groups of experts with two and three members, respectively [30]. As revealed in Section 3.2.1, they were unable to provide exact values, but intervals that were handled as uniform aggregated distributions.

3.3.3 Parameter estimation by importance sampling

MC simulation has already been used for the chosen waste separation technology to represent the expert-based distributions of separation efficiencies by discrete sample and estimate the outflows. It was shown that if the sample size is large enough, the resulting distributions of the outflows are the same for all runs of the simulation. These distributions were also compared with experts' intervals about the outflows where they were available, thus validating the model [30].

Using importance sampling (IS), feedback is gained: sample elements can be weighted on the basis of the available distributions about the outflows, and separation efficiencies resampled according to these weights. Therefore, the parameter estimation of the system can be executed by the iterative circle introduced earlier in Figure 16. In the present case, the separation efficiencies serve as parameters (Θ), and the yields form the outputs ($\mathbf{y}$) of the system.

For applying the method, first the structure of the system model is defined in Section 3.3.3.1. Then, the estimable parameters are identified in Section 3.3.3.2.

3.3.3.1 Formalization of the system model

The model of the introduced waste separation system model has an input ($u = m_1$), whose mass and composition are known from measurements. Component mass flows that come in and out of units are used as state variables. The parameters of the model are the separation efficiencies ($\Theta = [r_1, r_2, \dots, r_7]^T$) which are specified by the components. They always give the ratio of the outflow marked with a smaller number and the inflow of the unit for a chosen component.

The steady-state state-space model of the system can be set for component c as

$$0 = \mathbf{m}^c(\mathbf{A}^c - \mathbf{I}) + \mathbf{B}^c u^c \quad (3.14)$$

where $\mathbf{m}^c$ denotes to a 14-element vector that contains the component mass flows of component c . $\mathbf{A}^c$ refers to the state transition matrix of component c with a size 14×14 , which non-zero elements represent the connections between the flows. $\mathbf{I}$ refers to the unit matrix with the same size as $\mathbf{A}^c$. $\mathbf{B}^c$ denotes to the input vector $([1, 0, \dots, 0]^T)$, and $u^c = m_1^c$ to the input of the system in the case of component c .

The matrix $\mathbf{A}^c$ defines the connections between the flows containing the separation efficiencies belonging to the component c . The structure of it is as follows.

$$\mathbf{A}^c = \begin{bmatrix} 0 & r_1^c & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & r_2^c & 0 & 0 & 0 & 0 & 1 - r_2^c & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & r_3^c & 0 & 0 & 0 & 0 & 1 - r_3^c & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & r_4^c & 0 & 0 & 0 & 0 & 1 - r_4^c & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & r_5^c & 1 - r_5^c & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & r_6^c & 1 - r_6^c & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & r_7^c & 1 - r_7^c \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

As for the outputs, they can be defined as:

$$\mathbf{y}^c = \mathbf{C}^c \mathbf{m}^c \quad (3.15)$$

where the output matrix is marked by $\mathbf{C}^c$, and the output vector of the system by $\mathbf{y}^c$ for component c .

The matrix $\mathbf{C}^c$ selects the outputs of the system from the $\mathbf{m}^c$ states and transforms them to yields:

$$\mathbf{C}^c = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{u^c} \end{bmatrix}$$

It can be seen that the formalized model of the waste separation system is congruent with the generalized one described by Equation 3.1.

3.3.3.2 Identifying the estimable parameters

As seen from the formalization in Section 3.3.3.1, the mass flows of the components of the system can be calculated independently for each component from the relevant separation efficiencies. Therefore, the parameters r_i^c ($i = 1, \dots, 7$) have an effect only on the mass flows of the c component and not on the others. As expert-based information about the output is available only to four outflows out of the seven and only to the component in which that flow is rich, separation efficiencies belonging to the rest of the components are not estimable based on the provided data. The reduced vector $\mathbf{y}$ can be defined as:

$$\mathbf{y} = \left[\frac{m_{12}^{PET}}{u^{PET}}, \frac{m_{14}^{LDPE}}{u^{LDPE}}, \frac{m_8^{Iron}}{u^{Iron}}, \frac{m_9^{Aluminium}}{u^{Aluminium}} \right]^T \quad (3.16)$$

In addition to the above-mentioned, only the parameters of those units affect the outputs, which are before the output location in the row of units as seen in Figure 23.

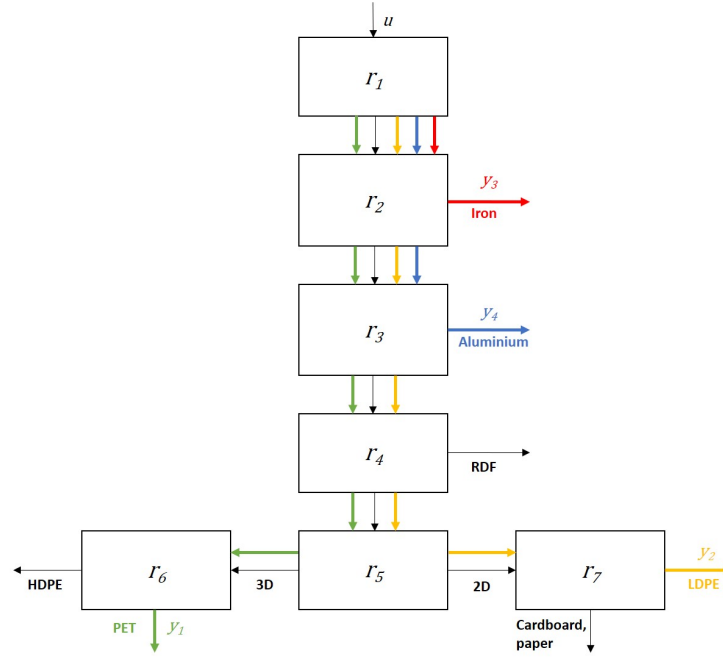


Figure 23: **Effects of the parameters on the outputs.** The four outputs about which expert-based information was obtained are referred to y_i ($i = 1, \dots, 4$). Green, yellow, red and blue colors mark which units have an effect on the different outputs. u denotes to the input, and r_i ($i = 1, \dots, 7$) represents the parameters of the i th unit.

Taking into account the above-mentioned issues, the parameters that can be estimated are summarized in Table 8. The table does not contain the pre-shedder unit as it has only one output, thus its separation efficiencies are surely 100% for all components.

Table 8: **Summary of the estimable parameters.** The components of which expert-based distribution about the output is available are represented by red color. The gray cells represent the estimable parameters, and the white cells the non-estimable ones. Columns specify the unit and rows refer to the component to which the estimable or non-estimable separation efficiency belongs.

	Magnetic separator (r_2^c)	Eddy-current separator (r_3^c)	Drum screen (r_4^c)	Air separator (r_5^c)	PET optic (r_6^c)	LDPE optic (r_7^c)
PET	✓	✓	✓	✓	✓	
LDPE	✓	✓	✓	✓		✓
HDPE						
Hazardous						
Iron	✓					
Aluminium	✓	✓				
RDF						
Cardboard						
Paper						

3.3.4 Results of the parameter estimation

The estimation of the system parameters was carried out using the iterative circle represented in Figure 19 for the parameters marked in Table 8. The simulation stop criteria was defined by the Kolmogorov-Smirnov test of two samples in addition to the 20% confidence interval. As will be seen later, this criterion is strict enough to stop the iteration. $M = 3000$ sample size was used which is large enough to not affect the result [30].

During simulation, all the estimable parameters r_i^c introduced in Table 8 were resampled according to the importance weights generated based on the relevant output simultaneously. The simulation stopped when the distributions of all parameters and outputs converged. For that, 19 iterations were needed in addition to the 20% confidence interval. Figures 24 and 25 show the convergence of outputs, and Figure 26 shows that of the parameter $r_3^{Aluminium}$.

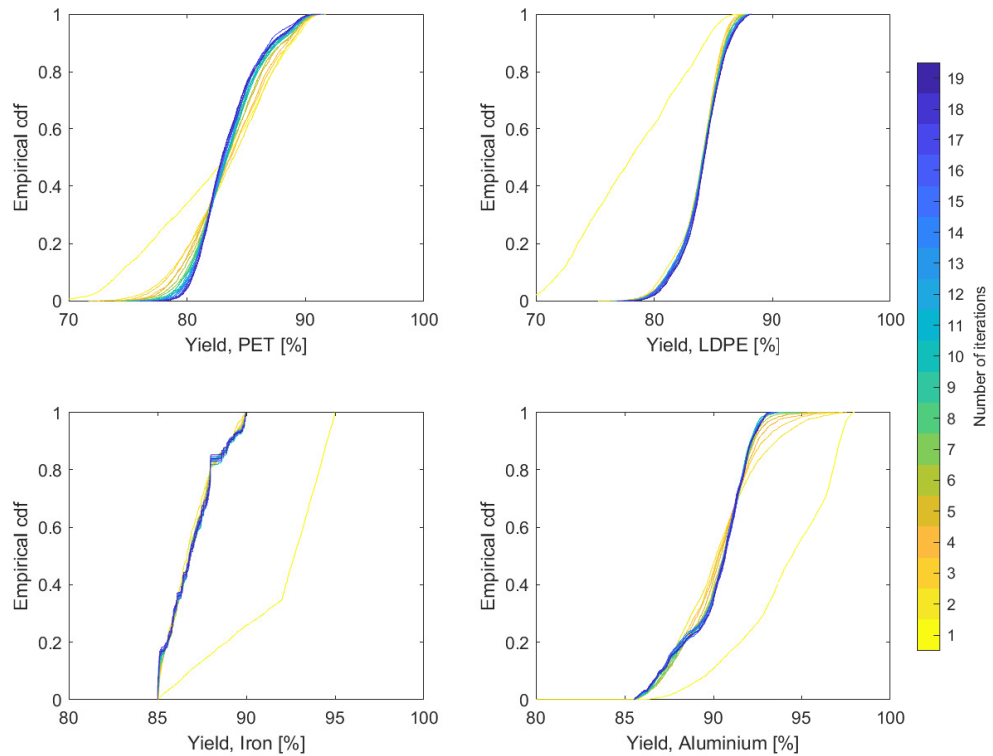


Figure 24: **Empirical cumulative density functions (cdf) of the outputs along the iteration steps.** The lines turn blue from yellow as the iteration is progressing.

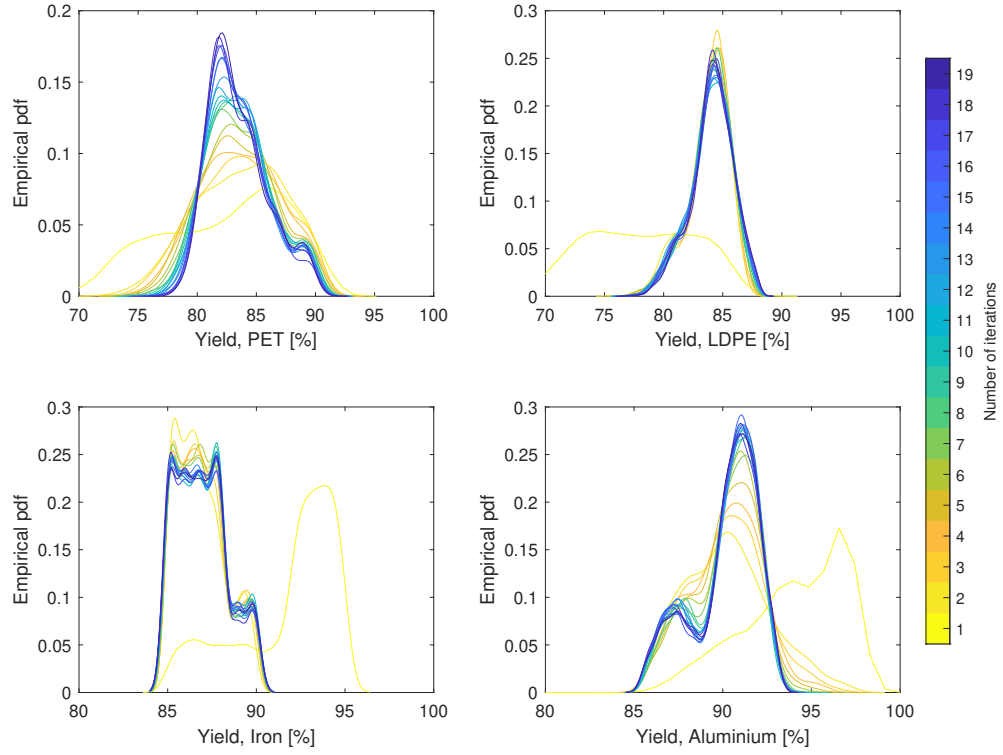


Figure 25: Empirical probability density functions (pdf) of the outputs along the iteration steps. The lines turn blue from yellow as the iteration is progressing.

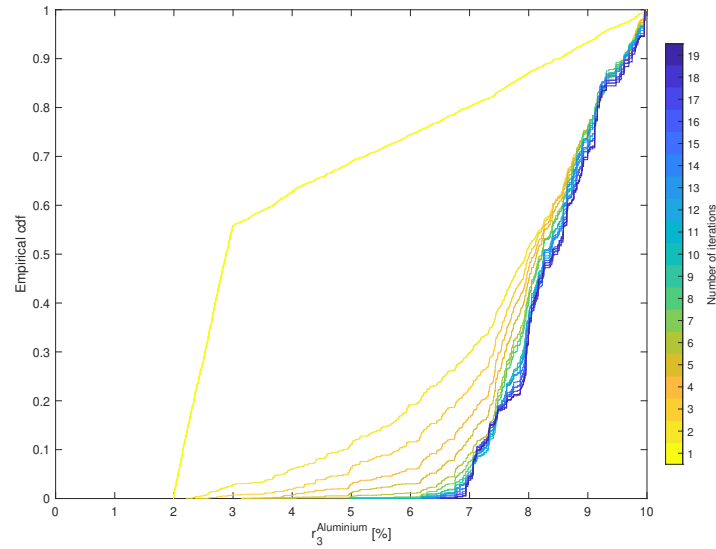


Figure 26: Empirical cumulative density functions (cdf) of the $r_3^{Aluminium}$ parameter along the iteration steps. The lines turn blue from yellow as the iteration is progressing.

As seen in Figures 24, 25, and 26, the convergence is satisfactory, so no more iteration is needed. Convergence of the other parameters provides similar results.

The estimated outputs are shown with the intervals provided by experts in Figure 27.

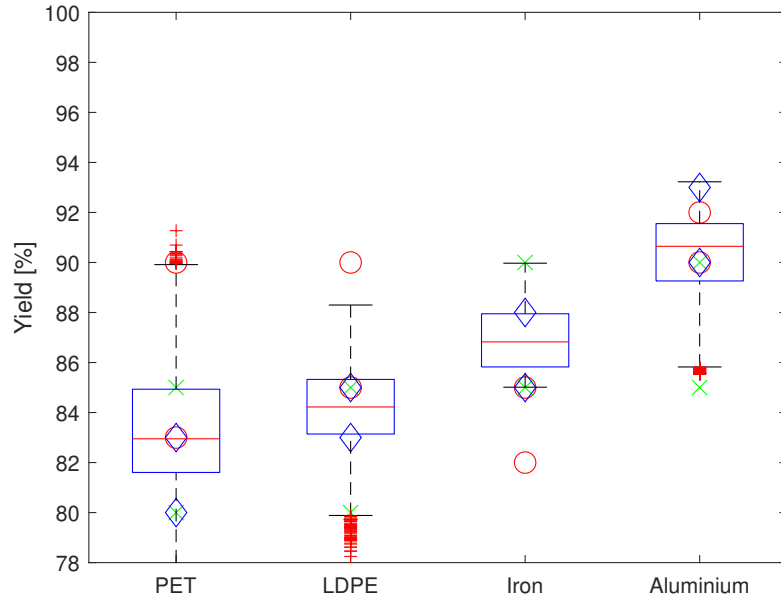


Figure 27: **The estimated and the expert-based outputs.** Formers are represented by boxes with a red line in the median, and latters by markers (red o, green x and blue diamond) at the edges of the provided intervals by the three experts.

Comparing these results with those of [30], it can be concluded that standard deviations are much smaller for iron and aluminum production, and the medians are more likely within the limits of experts. Therefore, the output estimation is more precise with the improved method used in this study. This result induces that the estimated parameter distributions must also be more accurate than those provided by the experts.

The estimation results can be compared to the expert knowledge based, e.g., Figure 28 introduce the case of LDPE. As seen, estimated distributions fall into the intervals covered by expert-based information in all the cases. Otherwise, the estimated output is nearly normal because it depends on the product of five uncertain parameters, so the differences equalize.

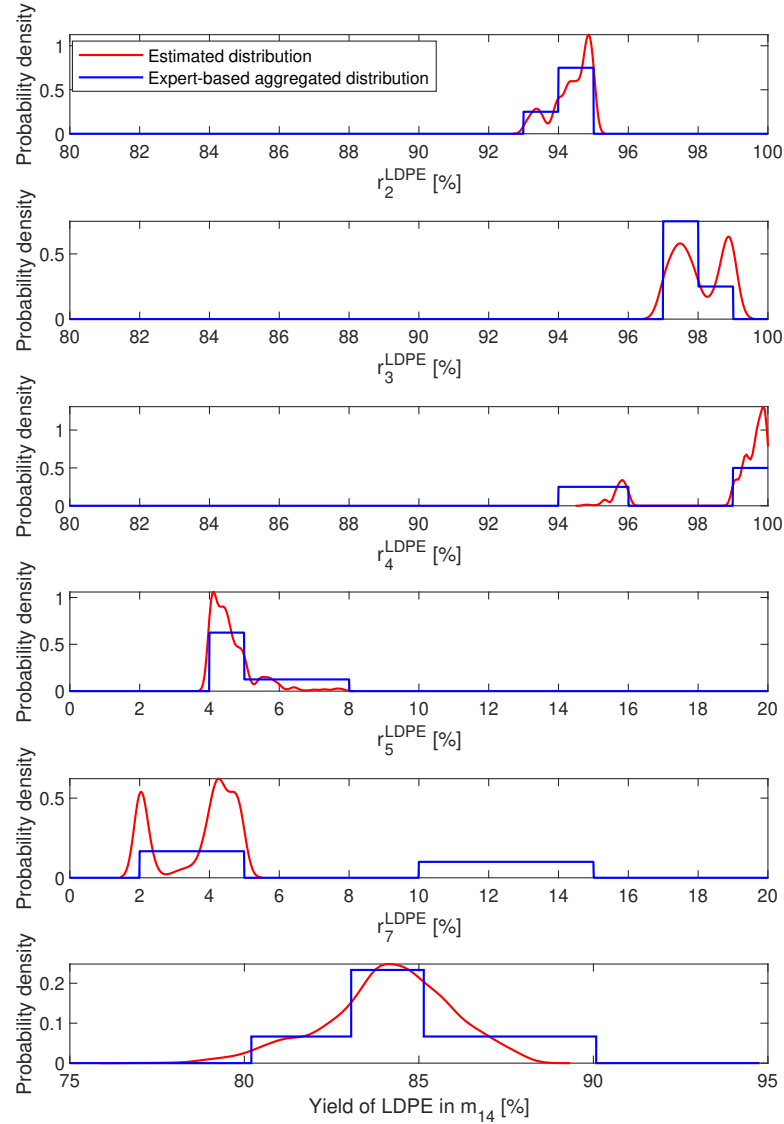


Figure 28: **Estimated and expert-based distributions of the estimable parameters and output belonging to LDPE.**

As also seen in Figure 28, in some cases experts gave disjunct intervals. It can be easily assumed that in these cases one of them is wrong. The estimated distributions usually cover only the preferable one of these intervals, and the other is neglected. Therefore, if the estimated distributions are used for sampling the parameters, some wrong information are eliminated, and thus more exact output estimation can be provided as was declared above.

Individual expert judgments can also be evaluated according to the estima-

tion results. In Section 3.3.5, the method is introduced in detail.

3.3.5 Evaluation of the expert judgments

This section aims to give an evaluation method for the provided expert judgments by comparing the original expert-based distributions before aggregation to the estimated ones.

An example of a graphical comparison of two distributions can be seen in the Q-Q plot of r_2^{LDPE} in the case of Expert 2. in Figure 29. A Q-Q plot depicts the quantiles of two distributions on the axes. If the two distributions to compare are the same, the plot covers the 45-degree line.

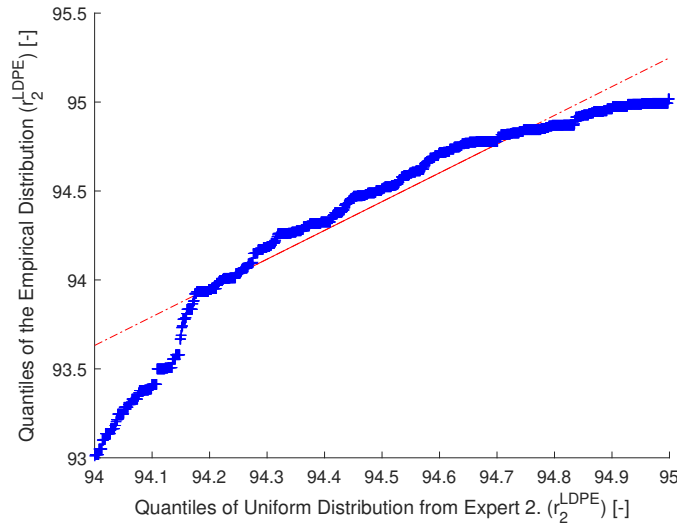


Figure 29: **Q-Q plot for comparing the uniform distribution provided by Expert 2. and the estimated empirical distributions of r_2^{LDPE} .** If the two distribution were the same, the plot would appear linear.

As seen in Figure 29, the plot tends to be linear, so the two distributions are supposed to be close to each other in the case of r_2^{LDPE} . To give a more precise measure, the Jaccard index is calculated, which serves as the goodness values of the expert judgments.

Using the resulting empirical distributions in Section 3.3.4, the goodness values ($g_{i,e}$) of the expert judgments can be calculated according to the method introduced in Section 3.2.3. This measure represents how similar the distribution given by an expert is to the estimated one.

The outputs were assessed by three experts and the parameters by two who were independent of the former. The uniform distributions created from the

intervals they provided were compared to the estimated distributions. The calculated goodness values for the outputs and the parameters can be seen in Figures 30 and 31, respectively.

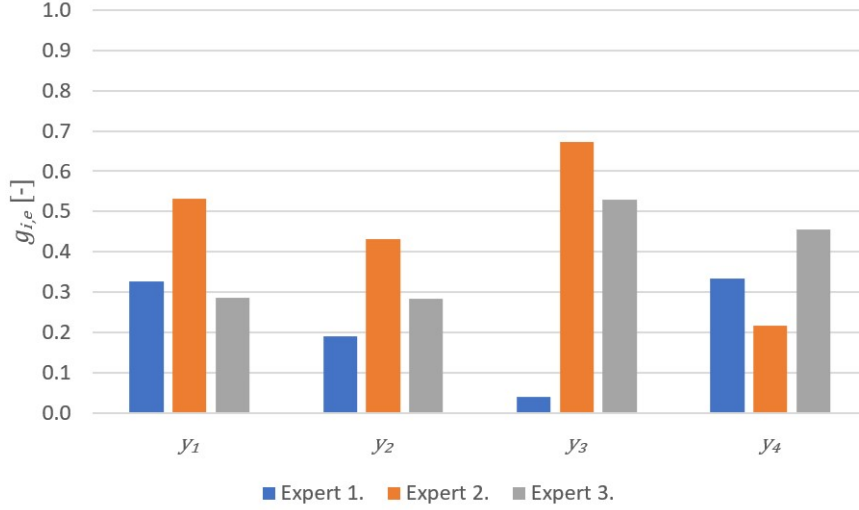


Figure 30: Goodness values belonging to the outputs.

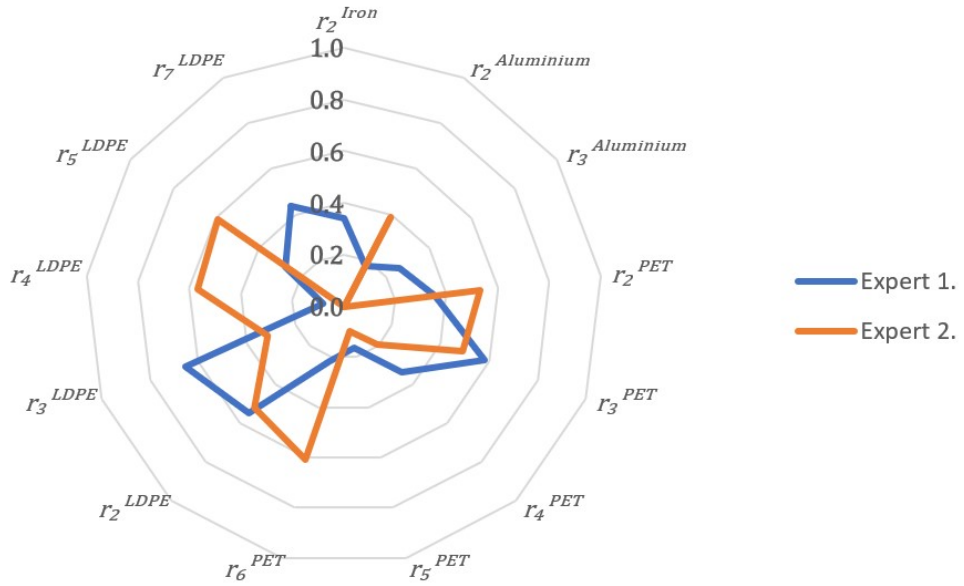


Figure 31: **Goodness values belonging to the estimable parameters.** The labels on the axes mark which parameter the goodness value belongs to.

The goodness values fall into the $[0, 1]$ interval, showing the similarity of the two distributions. If they are the same, the goodness value belonging to them is 1, and if they are completely different, they get 0. As seen in Figures 30 and

31, there are some values around 0, suggesting that there are incorrect expert judgments that would be preferable to be eliminated from the estimate.

3.3.6 Elimination of the incorrect expert knowledge

As was declared in 3.3.5, there are some low-weight expert judgments in the case of the parameters and also the system output. To eliminate them from the estimation, an outer iteration circle is suggested to be generated by weighting the initial distributions according to the technique introduced in detail in Section 3.2.4.

At the beginning of the procedure, during the aggregation of the probability distributions of the experts, the judgments of each expert were considered with equal weights. However, as seen before, some assessments seem to be closer to real values than others. By normalizing the goodness values for each variable, weights can be given to the initial uniform distributions of the experts, and new aggregated distributions can be created as the input of the estimation in the inner circle. Therefore, an outer iteration circle can be generated as introduced in Figure 21.

New aggregated distributions were created for parameters and outputs as well. The convergence of the inner circle outputs in the case of the system outputs ($\mathbf{y}$) is introduced in Figure 32 for the first steps of iteration 20 in the outer circle.

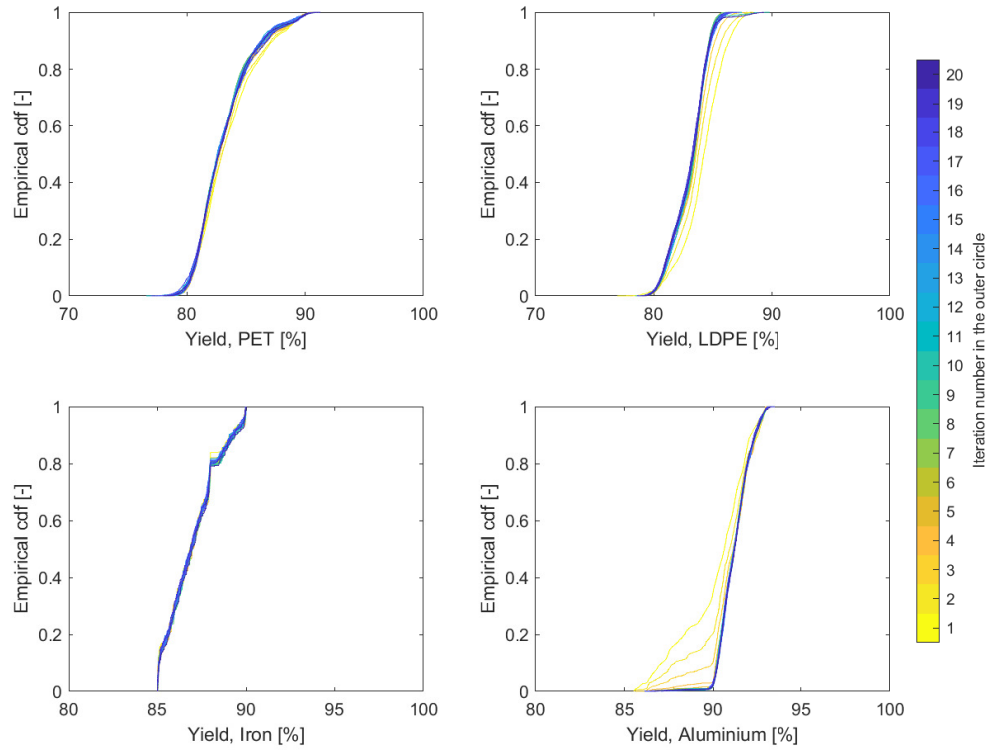


Figure 32: **Convergence of the empirical distributions of the four outputs (y) estimated in the inner circle.** The lines turn blue from yellow as the iteration is progressing in the outer iteration circle.

As seen in Figure 32, the system outputs converge, so the estimation is refined. The convergence of the normalized goodness values belonging to the outputs and the number of iterations in the inner circle along the outer iterations can be seen in Figure 33.

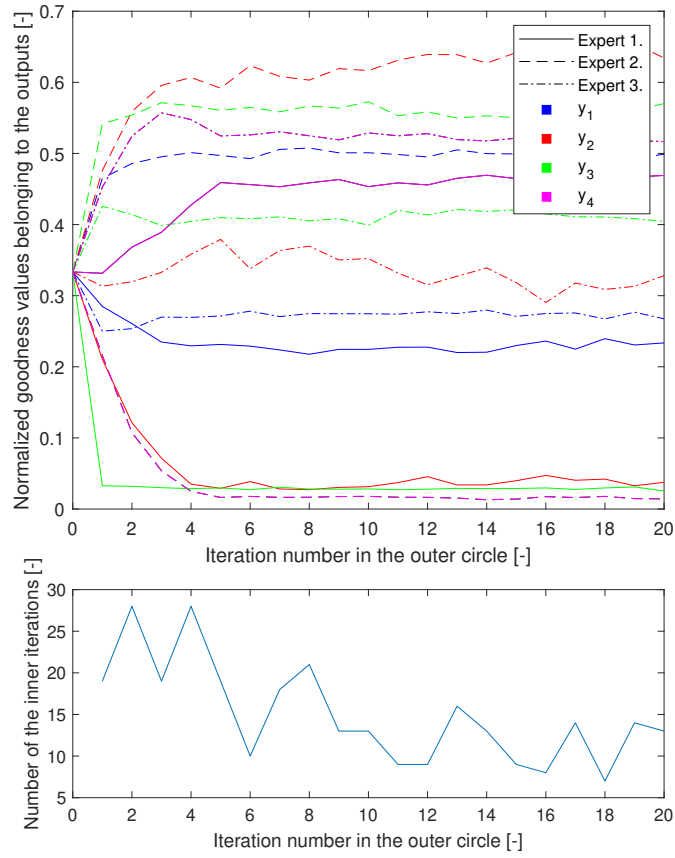


Figure 33: **Normalized goodness values ($\tilde{g}_{i,e}$) belonging to the system outputs (y) and the number of inner iterations along the outer iterations.** The three experts are marked with different line styles and the four outputs with different colors.

As seen in Figure 33, all the lines start from 0.33, since expert judgments were considered with equal weights in the first iteration. However, after a few iterations, all the lines fluctuate around specific values. Some of them are close to zero, which means that incorrect judgments are largely eliminated from the estimation. It is also seen that the number of iterations in the inner circle decreases after the weights are set. This suggests that the aggregated distributions of the parameters and outputs forming the input of the inner circle become more consistent, thus less iteration is needed for the convergence in the inner circle.

As seen from the results, the outer iteration circle helped refine the estimation by decreasing the weights of the less correct expert judgments and increasing the better ones.

3.4 List of symbols

The following symbols are used in Section 3:

$\mathbf{y}$	a vector gathers the outputs
$\mathbf{u}$	a vector gathers the inputs
Θ	parameter vector
$f()$	model structure of the complex system
$\mathbf{x}$	a vector gathers the estimable variables and parameters
M	the size of $\mathbf{x}$
Θ_i	an element of Θ
y_i	an element of $\mathbf{y}$
x_i	an element of $\mathbf{x}$
$x_{i,min}^e$	the lower bound of the interval provided by the e th expert as a judgment about x_i
$x_{i,max}^e$	the upper bound of the interval provided by the e th expert as a judgment about x_i
$p_e(x_i)$	the uniform distribution that the interval provided by the e th expert about x_i was transformed to
$p(x_i)$	the expert-based aggregated distribution of x_i
E	number of the experts
x_i^j	the j th sample element from $p(x_i)$
N	sample size
$q(x_i)$	the empirical probability distribution of x_i
$E_p[]$	expected value of the argument distributed according to $p()$
$E_q[]$	expected value of the argument distributed according to $q()$
$y_{i,p}^j$	the j th sample element drawn from $p(y_i)$
$y_{i,q}^j$	the j th sample element drawn from $q(y_i)$
w_i^j	the weight of the j th sample element according to the y_i output
s_n	the random numbers generated during resampling
$\mathbf{p}_e$	the dataset gained by the discretization of $p_e(x_i)$
$\mathbf{q}$	the dataset gained by the discretization of $q(x_i)$
$p_{e,k}$	an element of $\mathbf{p}_e$
q_k	an element of $\mathbf{q}$
K	the size of $\mathbf{p}_e$ and $\mathbf{q}$
$J()$	Jaccard-index

$g_{i,e}$	the goodness value belonging to the judgment of the e th expert about x_i
$\tilde{g}_{i,e}$	the normalized goodness value of the e th expert judgment about x_i
m_i	the component mass flows of the waste separation system
r_i	the separation efficiencies
$\mathbf{m}^c$	a 14-element vector contains the component mass flows of component c
$\mathbf{A}^c$	the state transition matrix of component c
$\mathbf{I}$	the unit matrix
$\mathbf{B}^c$	the input vector in case of component c
u^c	the input of the system in case of component c
$\mathbf{y}^c$	the output vector of the system in case of component c
$\mathbf{C}^c$	the output matrix in the case of component c

4 Conclusions

This thesis introduced how novel sampling-based algorithms can support engineering practise by handling uncertainty and lack of information about the process. It was shown that these techniques can be applied effectively in various process engineering tasks such as modelling, fault diagnostics, state or parameter estimation.

In engineering practise, a common problem is that poor amount of information is available about the process. For economical reasons, only the most necessary measurements are implemented, and these are also inaccurate thus can provide only noisy data. Uncertainties can be handled well by sampling-based techniques with a probabilistic approach such as the investigated particle filter (PF) and importance sampling (IS) algorithms. Experience-based expert knowledge, which can provide some information about the unmeasured factors, can be also implemented by these type of techniques as was declared.

In the first part of the thesis, the applicability of the PF state estimation algorithm was investigated on a case study of a carbon removal wastewater treatment process. One contribution of the work is a method obtained to determine the optimal sensor placement. Based on the principles declared in this work, the method is usable in all similar cases by applying the actual state-space model and parameters.

Another novelty is a technique for tuning the PF and a proposed sensitivity analysis. To increase the estimation accuracy, a new variant of the PF, the genetic algorithm-based IPF, was implemented and tested under **setpoint changes**. This improved method reduced the estimation errors and even the number of resamplings.

The PF estimation algorithm was also tested for fault detection problems. A PF-based fault detection technique was implemented and evaluated. The effect of the setpoint changes was examined and a tuning method presented for the sliding window by taking into consideration the bias and impact faults, as well. With the applied method, these faults were detected highly efficient.

The second part of the thesis introduced a case study of an operating Hungarian waste separation system. Separation efficiencies by components served as model parameters, and yields as the model outputs. Expert-based information was available about all the parameters and four outputs of the system by **two independent groups of experts**. They could give only intervals instead of

exact values, that were represented by probability distributions.

In this study, a method was provided that applied IS to execute parameter estimation based on the available expert knowledge and investigated the consistency of the expert-based information about the parameters and output in an iteration circle. The estimated distributions of the yields by the IS-based technique were more precise than those of a previous study applying only MC.

It could also be noticed that there were some disjunct expert opinions, which implied that some of them are wrong. For investigating this issue, a technique was also provided for the validation of expert knowledge according to the estimation results. It was introduced that estimated distributions can be further refined by creating an outer iteration circle, where the weights of the expert judgments converge.

One main limitation of the investigated methods is that the model structure of the system has to be known to apply these algorithms. However, in contrast to other algorithms, nonlinearities and complex model equations can be easily handled. As for the expert knowledge-based methodology, it is clear that results will only be satisfactory if **a sufficient number of experts can be found, who are qualified at the required level and experienced enough**. The advantage of the proposed method is that incorrect expert judgments can be eliminated, however, only in the case if most of the judgments are correct, otherwise, the estimation will be wrong.

This thesis introduced one dynamic and one stationer case study related to sustainability; a method was introduced to enhance the monitoring and fault diagnostics of a wastewater treatment system, and the modeling of waste separation systems was also supported by a novel technique thus promoting the appropriate operation of these systems. It was shown that the suggested algorithms were applicable for a wide range of engineering problems in both cases. For the **future**, it would be interesting to explore which other process engineering fields (e.g., **process control, optimisation, input estimation**) can be supported by them. The topic of exploiting **expert knowledge and measurement data** simultaneously is also a possible research direction. A methodology for integrating information from different sources would help us to get the most complete knowledge about the system.

Appendices

Appendix A Systematic Resampling

After the correction step in PF, the sample elements so-called particles with ω_i normalized weights become available. The aim of resampling is to draw new particles from the old ones with the probability equal to their normalized weights. As this weights are normalized, the cumulative sum of the weights is:

$$Q^{(m)} = \sum_{i=1}^m \omega_i \in [0, 1] \quad (\text{A.1})$$

where $1 \leq m \leq N_S$.

During the systematic resampling, the $[0, 1]$ interval is divided into N_S subintervals equidistantly. From every subinterval, a z_j number is chosen. z_1 is randomly drawn from the uniform distribution on $(0, 1]$, and the others are determined by z_1 :

$$z_j = z_1 + \frac{j-1}{N_S}, \quad j = 2, 3, \dots, N_S \quad (\text{A.2})$$

These z_j ($j = 1, 2, \dots, N_S$) values are used to select the new particles from the old ones. $\mathbf{x}_m$ particle is chosen when:

$$Q^{(m-1)} < z_j \leq Q^{(m)} \quad (\text{A.3})$$

Therefore, the particles are selected with a probability equal to their weights. Figure 34 represents the systematic resampling scheme.

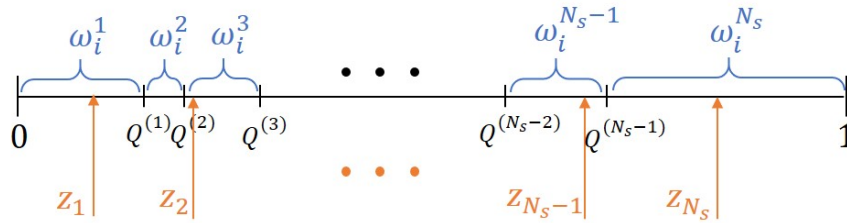


Figure 34: The schematic figure of systematic resampling. The generated $z_j \in (0, 1]$ random numbers are represented by orange arrows and the weights of the sample elements are denoted by blue ω_i^j ($j = 1, \dots, N_S$). If an arrow points to the interval of ω_i^m , $\mathbf{x}_m$ is chosen as new sample element.

The new particles are considered to be of equal weights.

Appendix B Derivation of the Critical Residence Time and F_{max}

The critical residence time can be calculated in the following way:

$$b_{SRC} = (4Cn + (1 - n)^2)R^2 + 2(2Cn + (1 - n)^2)R + (1 - n)^2 \quad (\text{B.1})$$

$$\tau_{min}^* = \frac{1 + \frac{S_0}{K_S}}{2(\frac{S_0}{K_S} - (1 + \frac{S_0}{K_S})\frac{k_d}{\mu_m})} \cdot \frac{(1 + n)(1 + R) - \sqrt{b_{SRC}}}{n} \quad (\text{B.2})$$

where τ_{min}^* refers to the dimensionless critical residence time and n denotes the volume ratio of the two reactors. As the reactor volumes are assumed to be equal, $n = 1$ in the present case, therefore, Equations (B.1) and (B.2) are simplified to the following forms:

$$b_{SRC} = 4CR^2 + 4CR \quad (\text{B.3})$$

$$\tau_{min}^* = \frac{1 + \frac{S_0}{K_S}}{2(\frac{S_0}{K_S} - (1 + \frac{S_0}{K_S})\frac{k_d}{\mu_m})} \cdot (2(1 + R) - \sqrt{b_{SRC}}) \quad (\text{B.4})$$

F_{max} can be calculated from τ_{min}^* :

$$F_{max} = \frac{V\mu_m}{\tau_{min}^*} \quad (\text{B.5})$$

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Acknowledgement

I would like to say thank you, at first, to my parents who let me spending enough time on studying from my childhood, the result of which cumulated in this work.

Secondly, I owe thanks to my friends, who all helped me in different way: some of them by sharing the pleasure of competitions or research with me, others by supporting to make my decisions, and anothers only by listening my working troubles which could be the birth of new ideas.

Finally, I am sincerely grateful to my supervisor, János Abonyi, who always motivated me to do my best, gave an objective eye on my work by answering my every little question, and freedom where creativity could flourish.