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Dynamic state reconciliation and model-based fault detection for chemical processes

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Abstract:

In this paper, we present a method for the fault detection based on the residual generation. The main idea is to reconstruct the outputs of the system from the measurements using the extended Kalman filter. The estimations are compared to the values of the reference model and so, deviations are interpreted as possible faults. The reference model is simulated by the dynamic hybrid simulator, *ProDHyS*. The use of this method is illustrated through an application in the field of chemical process.

Keywords: Fault Detection, Extended Kalman Filter, Dynamic Hybrid Simulation, Object Differential Petri Nets

1 Introduction

With the evolution of the computer power, dynamic simulation has become an efficient study tool in process design and analysis. Indeed, it is a great point of interest, for instance, for the studies of the system behaviour faced with disturbances around a set point (sensitivity to the parameters) or for the initialization of a steady-state simulation (i.e. distillation column). However, the operation states –such as batch production mode, material physical state changes or also abrupt evolutions- make the use of purely discrete or purely continuous models difficult. In this context, the taking into account of these phenomena induces discontinuities of the model and so requires the use of *Hybrid Dynamic Systems (HDS)*. Thanks to their large application field, these systems are a great point of interest for researchers and industrials^[1].

In order to model them, two dynamic schemes have to be described: on the one hand, the continuous dynamic, which are generally represented by a *Differential and Algebraic Equations (DAE)* set, and on the other hand, the discrete one, which are represented by a sets and transitions set. Several formalisms have been defined to combine the continuous and discrete elements. In the literature, these formalisms are generally classified as:

- approaches, which extend models of the continuous field, such as unified models^[2], bond-graphs with switches^[3];
- approaches, which extend models of the discrete field, such as hybrid Petri nets^[4], batch Petri nets^[5], time Petri nets^[6], timed automata^[7];
- and finally mixed approaches, in which discrete and continuous models are exploited in the same structure (the hybrid aspects are taken into account in the interface between the

two parts): hybrid automata^[8], hybrid statecharts^[9], mixed Petri nets^[10], differential predicate-transition Petri nets^[11].

At the same time, several softwares have been developed for the simulation of hybrid systems, such as *gPROMS*^[12], *Omsim*^[13], *BaSIP*^[14], *Shift*^[15], *Chi*^[16]. In these softwares, the hybrid aspect is described via an imperative language.

The considered systems are batch and semi-continuous processes, which are the prevalent mode of production for low volume of high added value products. Such systems are composed of interconnected and shared resources, in which a continuous treatment is carried out. For this reason, they are generally considered as hybrid systems, in which discrete aspects mix with continuous ones.

In this context, the research works performed, for several years within the PSE research department (LGC), on process modelling and simulation, have led to the development of *PrODHyS*^{[17]-[20]}. The adopted hybrid formalism is based on a mixed approach and the object concepts: the *Object Differential Petri nets (ODPN)*.

Otherwise, numerous research works in the field of the Hybrid Dynamic Systems deal with modelling, stability and controllability^[21]. These last years, many works are dedicated to the observability. While the theory of the state observability is well defined in the field of the continuous and discrete systems, some efforts must be made for the field of the hybrid dynamic systems.

Moreover, the state observability is a point of interests for the fault detection and diagnosis studies^[22]. As a matter of fact, the decisions are based on a great number of information. Then, the residual generation with data reconciliation consists in the estimation of the state, or generally of the system outputs and in the use of the estimation mistakes for the residual generation. Clark was one of the first researchers to study this concept^{[22]-[25]}. Next, this approach has been widely exploited and particularly gives rise to the switching state generator^{[26]-[28]}. Whereas the conception of observers for the linear systems seems to be mastered, for the non-linear systems, there is not satisfactory overall solution.

Thus, the first suggested answers consisted in the linearizing of the problem (for example around a steady point), in order to apply the Kalman-Luenberger estimators^{[29]-[32]}. Nevertheless, these methods are not generic. Indeed, let us consider the case where the residual generator is based on a model, which is linearized around a steady point. When the system state deviates appreciably from this steady point, great drifts can be noticed, because of the nonlinear behaviour of the system^[33]. The main drawback of these methods is that they apply only under very restrictive conditions^[34]. Consequently, these methods are not generally used for the non-linear problems^{[35]-[37]}.

Thus, some more adapted methods have been developed. Among them, let us quote some well-known observers:

- In practice, the extended Kalman filter and its derived methods are widely exploited^{[38]-[40]}.
- Gauthier *et al.* defined a high gain observer^[41]. This observer works either for autonomous systems or for nonlinear systems that are observable for any input.
- Also let us quote the non-linear adaptive observer, used when the state and the parameters of the system are unknown. This algorithm estimates both the state and the parameters of the system^[34].
- There are also implicit observers (differential-algebraic equations)^[42].

Kalman filter variants have found widespread applications due to their simplicity and ability to handle reasonable uncertainties and nonlinearities^[43]. The extended Kalman filter doesn't use a lot of CPU times and provides good results for systems with a moderate non linearity^{[44][45]}. Consequently, in this paper, the proposed approach uses an extended Kalman filter for fault detection.

The contributions of this paper are fivefold:

- Since the developed methodology (called *SimAEM*) is based on a hybrid dynamic simulation model, it allows a general and rigorous representation of the monitored process. Indeed, the reference model is built owing to the Object Differential Petri nets formalism. This formalism allows on the one hand an effective description of the synchronization, parallelism and sequencing constraints and on the other hand, a precise and reliable representation of the continuous dynamics thanks to the algebraic differential equations.
- Moreover, the extended Kalman filter has been used and developed for the hybrid dynamic systems. It rests on the dynamic simulation of these systems: during the same simulation, several models are instantiated. Then, the state vector and the covariance matrix have been judiciously initialized for each model change. Thus, the monitoring system is powerful during the transient states.
- In a general way, the use of the object concepts generates a high level description, supports the modularity of the models, allows the creation of generic, extensible and reusable entities (particularly with the specialization and composition mechanisms). So, a whole of fundamental elements models has been developed and allows the creation of more complex models. Thus, this approach is evolutionary owing to the creation of new entities according to the needs.
- The monitoring system is robust with noises and process uncertainties, by the use of the extended Kalman filter, which masks these disturbances and thus avoids false alarms.
- Lastly, the methodology *SimAEM* has been implemented within the dynamic simulation platform *PrODHyS*. This simulator provides software components allowing the integration of the methodology *SimAEM* and its exploitation within the monitoring system. The monitoring module has been demonstrated by the simulation of a monitored process.

This framework is organized as follows. The first part of this communication presents the platform *PrODHyS* and describes the main fundamental concepts of the *ODPN* formalism. Next, the proposed detection approach is presented. This exploits the extended Kalman Filter to a hybrid dynamic system. The main idea is to reconstruct the outputs of the system from the measurement, using observers or Kalman filters and using the residuals for fault detection^{[46]-[51]}. The purpose is to detect the presence of a fault and to locate the occurrence time. The estimations are compared to the nominal parameter values and so, deviations are interpreted as faults. In section 4, a didactic example and its modelling are described. This is a process of addition-evaporation. Then, our detection approach is implemented, and for this, some adjustments are made. Next, the performance of our approach is illustrated through the simulation of a process, during which a fault is introduced at an unknown moment. Finally, Section 7 summarises the contributions and achievements of the paper and some future research works are suggested.

2 PrODHyS environment

Nowadays, object technology is a concrete and efficient answer to extensibility, reutilisability and software quality needs. That is why, *PrODHyS* is based on object concepts and so offers extensible and reusable software components allowing a rigorous and systematic modelling of processes.

2.1 Software architecture

This environment provides a library of classes dedicated to the dynamic hybrid simulation of processes. The primal contribution of these works consisted in determining and designing the

foundation buildings classes. Currently, this library is made up of more than one thousand classes distributed into three functional layers and nine modules (Figure 1):

- The internal layer corresponds to the simulation kernel of the platform. It provides the basic elements allowing the simulation of any dynamic systems. Today, this layer includes:
 - the module *Disco*^{[18],[52]}, which constitutes the numerical kernel of the systems and allows an object representation of the continuous mathematical models; it provides a set of solvers and integrators (DAE, NLAE);
 - the module *Hybrid*^[19] which contains the set of classes used for the description of the ODPN formalism as well as the hybrid simulation kernel.
- The second layer includes a set of classes allowing the modelling of processes. The "modelling" layer rests on the "simulation" layer and provides a set of general and autonomous entities which can be exploited by any user who wishes to build its own simulation system or prototype. This layer includes:
 - the module *ATOM*^[17] which constitutes the thermodynamic data base of the system; it is based on an object representation of the material and allows the computing of thermodynamic properties.
 - the module *Odysseo*^[53] which gathers the elementary and generic entities allowing the modelling of a process. It is divided into three sub-modules:
 - the sub-module *Process* which gathers a set of often abstract classes, corresponding to a very general description of the process;
 - the sub-module *Reaction* which allows the modelling of chemical reactions;
 - the sub-module *Device* which gathers the "concrete" elementary devices.
 - the module *CompositeDevice* which gathers devices resulting from the composition and the specialisation of the elementary devices defined in the module *Odysseo*.
- The higher layer corresponds to a set of classes dedicated to the process supervision. This "supervision" layer rests on the "simulation" and "modelling" layers and provides a set of entities allowing the realization of monitoring studies. Then, this layer includes:
 - the module *Scheduling*^[54], which couples the simulation module with stochastic optimization methods;
 - the module *PrODHySAEM*^[20] (**P**rocess **O**bject **D**ynamic **H**ybrid **S**imulator for **A**bnormal **E**vent **M**anagement), which contains a set of classes, in charge of the management of the monitoring studies of the processes.

The interest to separate the "simulation" and the "modelling" layers is to build platforms dedicated to various field of applications (mechanical, electronic, etc.) only by developing the suitable engineering "modelling" layer.

2.2 ODPN formalism

A detailed description of this formalism can be found in [19][20]. The PrODHyS components allow a modular and hierarchical modelling of different processes. In consequence, the object concepts and the Petri nets have been exploited in a combined approach in the ODPN formalism. It consists in making interact these features according to two manners (Figure2). Firstly it aims at "introducing the objects into Petri nets". The subjacent philosophy is to model a subsystem by a single Petri net, which handles individualised tokens carrying information. The second approach is based on "the introduction of Petri nets into objects" to describe the internal behaviour of the object (cf. class t). The marking of the Petri net indicates the current state of the object.

The ODPN formalism makes collaborate, within the same structure, DAE systems to describe the continuous evolution of the system with a high level Petri net used to specify the legal sequences of commutation between this set of DAE systems. Moreover, the integration of the DAE system of a differential place can require several tokens of the same type and/or of different types. In this case, the consistency must be assured by the modelling or validated by the simulation. Thus, the Petri net can be seen as DAE monitor. It allows the dynamic creation of a unique simulation model, whose size and structure change between two events (no fixed size of state vector). Besides the resolution of the DAE system (integration based on the Gear method) and of the discrete models (Petri net player specific to this class), the kernel manages other functionalities, such as the exact calculation of the commutation times, the state failing, the checking of the consistency of the new models generated after the commutation, the initialisation of the state variables and their derivatives^[19]...

2.3 Process modelling with *ProDHyS*

To carry out the simulation of such a system, it is necessary to model the command part (the supervisor) and the operative part (the process) at the same time. The model is a priori specific to the recipe and the considered process topology. So, it is completely dissociated from the model of devices, since this model must be reusable whatever the studied context (concept of component).

Moreover, the material model is dissociated from the device which contains the material. These different models are merged just at the time of the instantiation of the simulation model, according to the present state of the process. As a result, a hierarchical organization of models is introduced: the command level contains the recipe to execute, whereas the process level simulates the process behaviour^{[19][20]}. At this level, two kinds of entity are distinguished:

- The active entities: they are devices, whose Petri net has one or several command places, such as the valves, the pumps, the energy feeds, etc.
- The passive entities: they are entities, whose Petri net doesn't have command place (so without direct connection with the recipe Petri net) such as storage tanks, reactors or material.

The evolution of the different models is conditioned by two distinct kinds of event. On the one hand, we have "extern" events, which entail the controlled commutations. These are the signals exchanged between the command level and the process level. So they correspond either with commands send from the recipe Petri net in order to manage the active entities, or with the occurrence of a state event (detection of a threshold) or a temporal event. These events are defined by the user and clearly appear in the recipe Petri net. In this way, all the Petri nets of the command level manage all the Petri nets of the process level and can be compared to the GRAFCET in a DCS of the command level. On the other hand, we have the "intrinsic" events, whose occurrence depends only on the spontaneous process evolution. For example, these autonomous commutations correspond with the state change of a passive entity or with the change from the liquid to the vapour state when the boiling temperature is reached. These commutations don't appear on the recipe Petri net (so the user doesn't specify them) and are dealt with exclusively in the model of the concerned entity (device or material).

3 Supervision module

In chemical plants faults may cause process performance degradation (for example lower product quality) or fatal accidents (for instance the runaway scenario). Fault monitoring could prevent from these undesirable consequences. Several fault diagnosis approaches have been mainly proposed for steady-state processes operating. Nevertheless, application of these techniques to batch processes remains a challenging task, because of their hybrid and

nonlinear dynamics^[55]. Among model-based approaches, observer-based schemes have been used in numerous application fields.

3.1 Architecture

For this purpose, the simulation model of *PrODHyS* is used as a reference model to implement the functions of detection and diagnosis. The simplified principle of this system is shown on the Figure 3. A description of this methodology can be found in [20],[56].

In order to obtain an observer of the physical system, a real-time simulation is done in parallel. So, a complete state of the system will be available at any time. Thus, it is based on the comparison between the predicted behaviour obtained thanks to the simulation of the reference model (values of state variables) and the real observed behaviour (measurements from the process correlated thanks to the Extended Kalman Filter). Detection is realized by comparison with fixed thresholds. For a consistent execution of this task, the measurements must be filtered in order to eliminate the noise. The filter used here is the Extended Kalman Filter.

3.2 Implementation of the Extended Kalman Filter

In a model-based approach, one of the first problems is to differentiate the deviations due to a failure, from those related to the inherent disturbances of the process. For the inherent disturbances, we distinguish the measurement noises, the variations of the operating conditions and the parametric uncertainties. Thus, the failures, which we want to detect, are: the structural variations, which are generated by the wear of the devices, the failures of the actuators, and the failures of the sensors.

In order to mask the inherent disturbances and to avoid the false alarms, we have used an extended Kalman filter. A description of this filter can be found in [20]. Figure 4 illustrates the steps of the estimation of the system state. There are two main steps:

- the prediction, which corresponds to the “a priori” estimation
- and the correction, which corresponds to the “a posteriori” estimation.

Thus, the state vector is initially evaluated from the estimate of the previous step. Then, it is corrected by the measurements in the correction step. Both steps compose of an iterative of this filter (Figure 5).

This filter is described by the class *kalmanFilter* (Figure 5). Its initialization is carried out by the call of the method *initialize*. The class *kalmanFilter* has two attributes *_systemDynamic* and *_measurementDynamic* of type *dynamicModel*. The first attribute represents the dynamic of the system and the second represents the dynamic of the observations. Then, the dynamic models are not explicitly included in the computation of the filter, since they are defined by the class *dynamicModel*. Thus, the procedure applies to any type of system: the linear physical system or not and the linear dynamics of the observations or not.

The execution of the filter is made through the call of the method *perform* (Figure 6). This method gathers the two steps of the Kalman filter:

- The methods *predictStateVector* and *predictCovarianceMatrix* manage the prediction step,
- and for the correction step, these are the methods *calculateKalmanGain*, *updateStateVector* and *updateCovarianceMatrix*.

3.3 Simulation in parallel

According to the suggested architecture (Figure 3), our approach requires the on-line simulation in parallel of a reference process and of the extended Kalman filter. A main recipe is generated and groups together these both recipes. In order to distinguish the places and the transitions of these Petri nets, a prefix is added to their names:

- “M-“ for the recipe of the reference model,
- “K-“ for the recipe used by the Kalman filter.

Figure 7 represents the general concept. When the transition TR_{BEGIN} is fired, each place $BEGIN$ of the Petri nets is marked. When the horizon time of the simulation is passed, the place END is marked.

4 Application

A didactic example, shown on Figure 8, has been chosen in order to illustrate the proposed approach. This is the process of addition-evaporation. This is generally used to change solvents. The operation conditions are listed in the Table 1. The values of the minimum and maximum hold-ups are respectively 200 and 800 moles. Before each addition of solvent, the reactor is cooled up to the temperature of 300.15K. The pressure is supposed to be constant during this operation. The goal of this process is to have a molar composition of methanol in the reactor at 0.95.

4.1 Process recipe description

The operating of the substitution of the solvent A for the solvent B follows the following recipe:

1. The initial holdup is higher than the minimum holdup (U_{min}). The first step consists of the concentration of the solvent A. Figure 9 a) represents this step. The mixture is heated until its boiling point of and its vaporization is partial. This stage takes place, until the minimum holdup (U_{min}) is reached.
2. The reactor is then filled by a continuous feed (Figure 9 b)). A quantity of the substitution solvent (solvent B) is thus added to the mixture.
3. Then, two evolutions are possible (Figure 9 c)):
 - If the wanted quality of the product B is reached, the operating sequence is finished.
 - Otherwise, the feed is closed when the maximum holdup is reached (U_{max}). The operating sequence continues with a new evaporation step (step4).
4. The mixture is then evaporated (Figure 9 d)). The mixture is heated until its boiling point of and its vaporization is partial.
5. Next, two evolutions are possible (Figure 9 e)):
 - If the wanted quality of the product B is reached, the operating sequence is finished.
 - Otherwise, the evaporation in the reactor continues until the minimum holdup is reached. Then, the cooling of the mixture takes place.
6. The cooling is maintained until the specified temperature is reached. Figure 9 f) represents this step. The next operating sequence is a new addition stage (step 2).

Its recipe describes a succession of evaporations and additions of the new solvent, until the wanted final quality of the substitution solvent is reached.

4.2 Mathematical model

The mathematical model of this system at the thermodynamic equilibrium and in its maximal state (i.e., liquid/vapour) is as follows.

$$\frac{dU_l}{dt} - F_B + V = 0 \quad (1)$$

$$\frac{d(U_l \cdot x_i)}{dt} - F_B x_{Bi} + V y_i = 0 \quad (i=1, n_c) \quad (2)$$

$$\frac{d(U_l h)}{dt} - F_B h_B + V H - Q = 0 \quad (3)$$

$$h_l - \frac{U_l V_{ml}}{S_c} = 0 \quad (4)$$

$$y_i - K_i \cdot x_i = 0 \quad \text{for } i=1, n_c \quad (5)$$

$$\sum_{i=1}^{n_c} (x_i - y_i) = 0 \quad (6)$$

$$K_i - mK_i(T, P, x, y) = 0 \quad \text{for } i=1, n_c \quad (7)$$

$$h - mh(T, P, x) = 0 \quad (8)$$

$$H - mH(T, P, y) = 0 \quad (9)$$

$$V_{ml} - mV_{ml}(T, P, x) = 0 \quad (10)$$

$$V_{mv} - mV_{mv}(T, P, y) = 0 \quad (11)$$

The outlet vapour being open on the outside, the pressure P is supposed to be constant and the vapour holdup U_v is neglected in front of U_l . Equations (1), (2) and (3) represent the material and energy balances respectively. Equation (4) determines the liquid height h_l according to the tank area S_c , the molar volume of the liquid phase V_{ml} and the liquid holdup U_l . Equations (5) and (6) represent the liquid/vapour equilibrium. Finally, equations (7), (8), (9), (10) and (11) are the models used for the liquid/vapour equilibrium constants K_i , the liquid enthalpy h , the vapour enthalpy H , the liquid molar volume V_{ml} and the vapour molar volume V_{mv} within the tank.

4.3 Recipe Petri net

The recipe of this process is described by the Petri net of the Figure 10. Initially, the tank contains the two solvents and the liquid holdup is contained between the minimum and maximum values. The material and energy feeds are closed and the detectors are in position off.

- The marking of the place *Begin* allows the beginning of the operation. Then, the transition t_1 is fired. The marking of the place *mHeat* conveys the order sent by the recipe to the energy system, and the marking of the place *Evaporation* means that the first step takes place. Next, two evolutions are possible:
 - o The composition of the new solvent reaches the target value. This information is transmitted to the recipe by the marking of the place *mOn* of the composition detector. In this case, the transition t_5 is fired and allows the marking of the place *End*.
 - o The minimum holdup is reached. This information is transmitted to the recipe by the marking of the place *mOn* of the low holdup detector. Then, the transition t_2 is fired and allows the marking of the place *Cooling*.
- The cooling is maintained until a preliminary specified temperature is reached. This event is transmitted to the recipe by the temperature sensor (transition t_3).
- The next step consists in the adding of the new solvent. This is represented by the marking of the place *Filling*. Then, two evolutions are possible:
 - o The composition of the new solvent reaches the target value. This event is detected by the composition detector (transition t_6).
 - o The maximum holdup is reached. This information is transmitted to the recipe by the marking of the place *mOn* of the high holdup detector. The operation continues with a new evaporation step (transition t_4).

5 Adjustments of the filter

To perform a monitoring of a process, some off-line adjustments must be made. As a matter of fact, the values of the covariance matrices of the model and measurement disturbances have to be determined.

5.1 Measurements noises

The system observations are obtained by the use of specific sensors. So, the measurement mistakes are relatively well-known by the manufacturer or by experimentation. Thus, it is easy to define an estimate of the measurement covariance matrix.

5.2 Model disturbances

Before activating the extended Kalman filter, it is important to estimate the sensitivity of the filter to the model parameters. Thus, these works are based on a sampling scheme for the measurement perturbations and the model noise. This allows the estimation of the statistics of the model uncertainties. Then, we made numerous simulations during which uncertainties are generated. These uncertainties are obtained by disturbing at random one of the input parameters or one of the modelled physical processes. Therefore, a sampling of possible trajectories of the model is established. This method is based on the following hypothesis: the sampling average corresponds to the best estimate of the system state (our model is supposed to be unbiased), and the dispersion around this average corresponds to a measurement of the mistake of this estimate^{[57],[58]}. Thus, we estimate a wide uncertainty on the modelled physical processes, in order to be certain that the obtained dispersion includes the real behaviour of the system. Then, if the behaviour of the system goes beyond this distribution, its behaviour is abnormal. So, the detection thresholds are determined according to the model disturbances.

In practice, we made a set of simulations in parallel by adding a noise to the process or to a parameter, uniformly distributed between $-\sigma$ and σ (where σ is the typical range). Thus, it is possible to deduce the characteristics (average and typical range) of the dispersion of the system distribution function. Table 2 summarizes the applied uncertainties.

For example, Figure 11 represents the results obtained by modifying the initial value of the reactor liquid holdup. The curves represent the time evolution of the balanced typical ranges of the following state variables: the reactor liquid holdup (U_l), the molar liquid composition of the product B (x_B) and the temperature (T). Notice that these typical ranges are normalized in order to compare them between themselves. The system states are also illustrated on Figure 11. Notice that the evolution changes of the typical ranges are linked to the change of the system state. For example, at $t = 258$ min, we note a first peak of the typical range of the temperature. This corresponds to the change from the state *Evaporation* to the state *Filling*. Besides, the two following peaks (for the liquid holdup and the molar liquid composition of the product B) point out the change from the state *Filling* to the state *Cooling* and at $t = 390$ min, the third peak underlines the stopping of the system cooling.

Consequently, the model is more sensitive to the input parameter uncertainties during the transient modes. Thus, during these modes, the use of the extended Kalman filter is importance.

This study is reproduced for all the uncertainties exposed in Table 2. Then, a value of the modelling uncertainties is estimated (Table3).

5.3 Initialization of the extended Kalman filter

We point out that our works are based on dynamic simulation. Thus, during a simulation, there are several models of the system. So, for each model change, it is necessary to initialize judiciously the state vector and the covariance matrix.

5.3.1 Initialization of the state vector

Since our variables are continuous, the state vector of the new model is initialized with the value of the previous state (Figure 12).

5.3.2 Initialization of the covariance matrix

The covariance matrix of the modelling uncertainties of the new model could be initialized with the value of the previous model. This would mean that we have as much confidence in the new model as in the old one. However, the model disturbances are one of the most important causes in the divergence of the Kalman filter. This divergence is due to the fact that the filter has a too much confidence in the model. This is the case when the model noise is low. As a matter of fact, the terms of the covariance matrix representing the model disturbances and those of the gain matrix decrease. Thus the filter doesn't take into account the observations. Thus, it is necessary to adjust intelligently the covariance matrices, in order to solve this problem. One of the mainly used solutions is to increase the uncertainty of the model. For this, we suggest that, for each model change, the covariance matrix of the new model is initialized by the initial value of the covariance matrix of (Figure 12), i.e. the value of Table 3.

6 Results

The simulations of the reference model are first presented. Then, the results of the detection are exposed.

6.1 Simulation of the reference model

The simulation of the reference process is made. The dynamics are illustrated on Figure 13: they represent respectively the time evolutions of the liquid compositions.

The final molar methanol composition in the tank is equal to 0.95 (Figure 13) and was obtained during the adding of the new solvent. The total operation requires four additions and four evaporations.

6.2 State reconciliation

Figure 14 shows that the estimated state fits the reality. Moreover, in the model changes, the initialization of the extended Kalman filter allows its convergence. Thus, the state is well estimated during the transient modes.

6.3 Detection

This process is a system based on thermal phenomena. A fault on the tank thermal system is a risk for the success of this operation. That is why, it is important to detect it as soon as possible.

We remind that the thresholds for the detection correspond to the model uncertainties obtained by the adjustment of the Extended Kalman filter (Table 3). A fault on the heating energy feed of the reactor takes place at $t = 20$ min. This energy feed provides a heat quantity lower than the nominal one. Figure 15 shows the detection step. It illustrates the residuals evolution linked to the liquid composition of water and methanol. From $t = 80$ min, the both residuals go beyond the area of the nominal performance. The diagnosis is launched at $t = 95$ min.

7 Conclusion

In this paper, the feasibility of using the Extended Kalman Filter as a tool for fault detection is described. The method developed in this study rests on a hybrid dynamic simulator PrODHyS. This simulator is based on an object oriented approach. It brings many advantages in terms of software quality (extensibility, reutilisability, flexibility), but especially in terms of modelling thanks to a hierarchical and modular description which is both abstracted and close to reality. Then, PrODHyS provides software components intended to model and simulate more specifically the industrial processes. The implementation of a formalism on high level of abstraction associated with powerful numerical methods of integration led to the construction of a robust hybrid dynamic simulator. In this communication, the potentialities of PrODHyS are illustrated through the modelling and the simulation of a process. The works in progress aim at integrating this simulation model within a model based diagnosis system. Different diagnosis approaches mixing model-based and data classification techniques will be studied and compared.

Appendix A. Nomenclature

F_i	Liquid flow rate (mol/min)
h_i	Liquid enthalpy (J/mol)
H_i	Vapour enthalpy (J/mol)
K_i	Equilibrium constant
n_c	Constituent number
P	Pressure (Pa)
Q_i	Energy quantity (W)
S_c	Area (m ²)
T	Temperature (K)
U_l	Liquid holdup (mol)
U_v	Vapour holdup (mol)
V_i	Vapour flow rate (mol/min)
V_{ml}	Liquid molar volume (m ³ /mol)
V_{mv}	Vapour molar volume (m ³ /mol)
x_i	Liquid composition
y_i	Vapour composition

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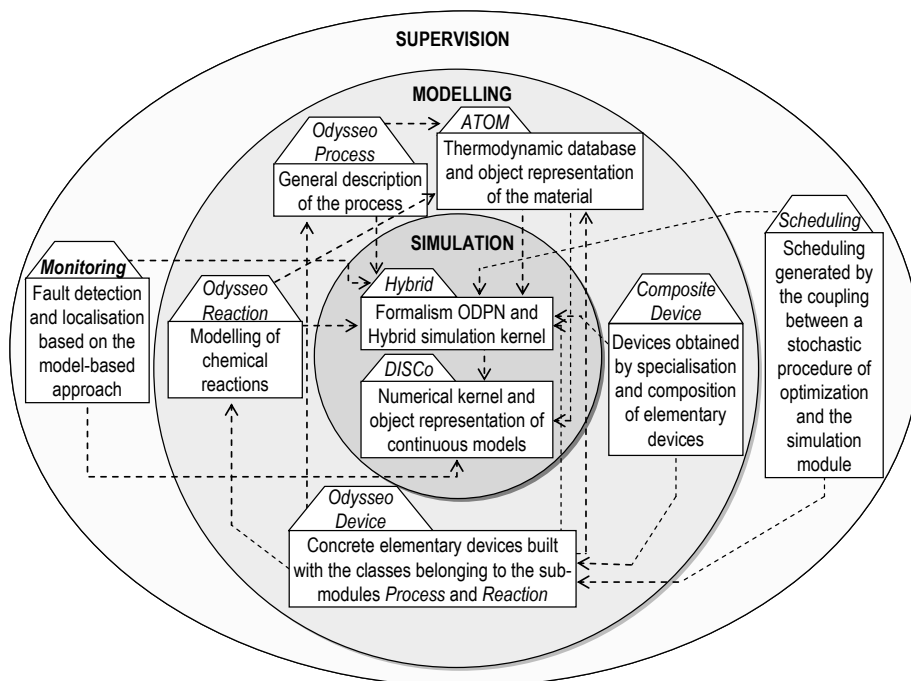


Figure 1. Software architecture of PrODHyS[20]

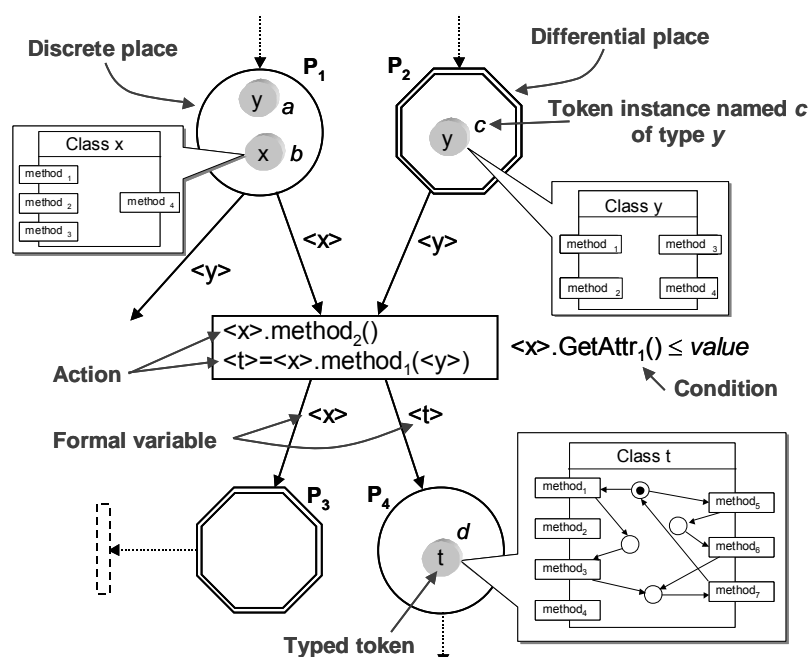


Figure 2. Elements of ODPN formalism

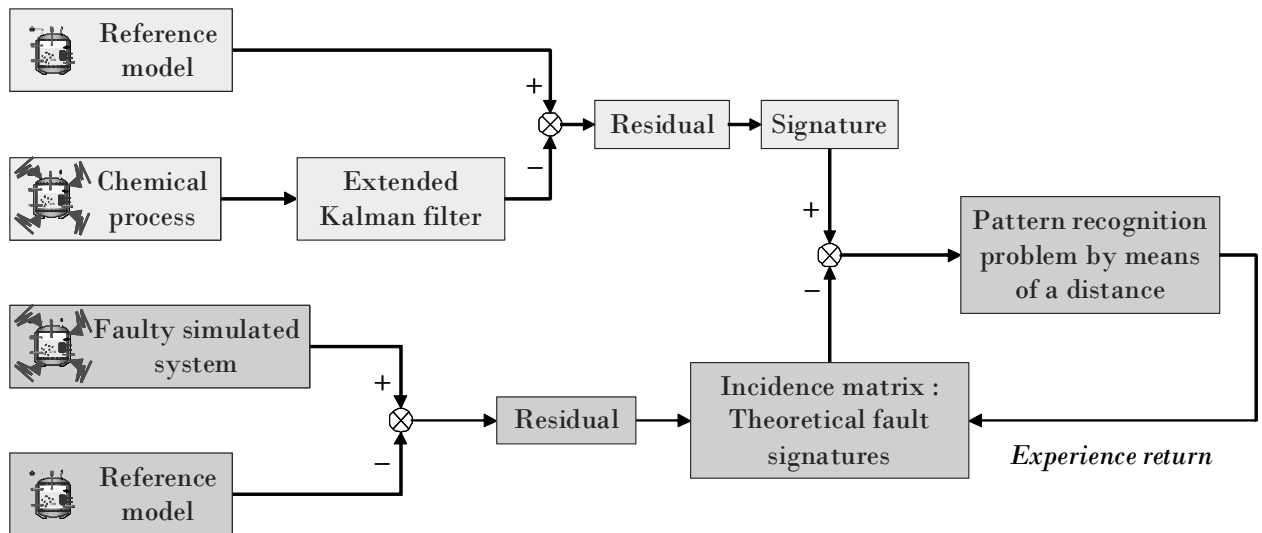


Figure 3. Supervision Architecture

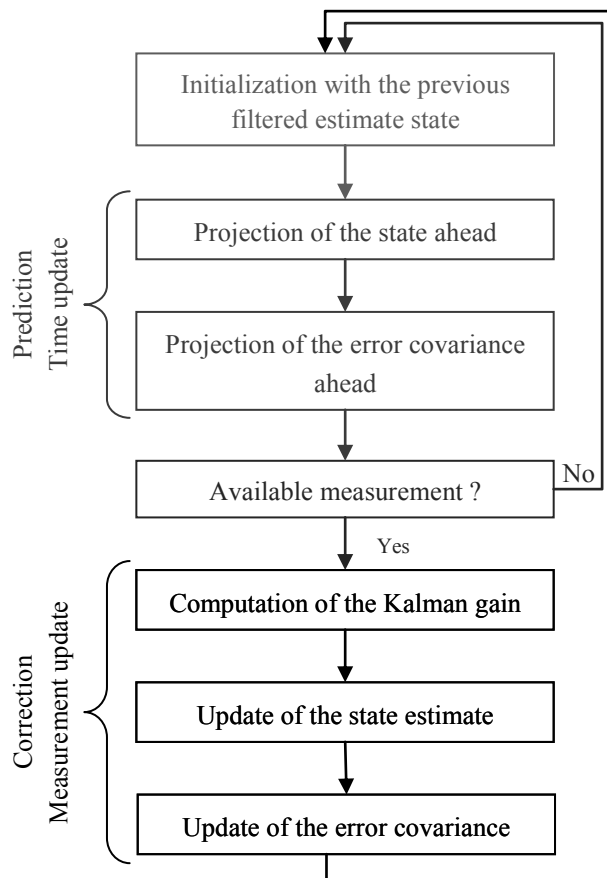


Figure 4. Extended Kalman filter algorithm

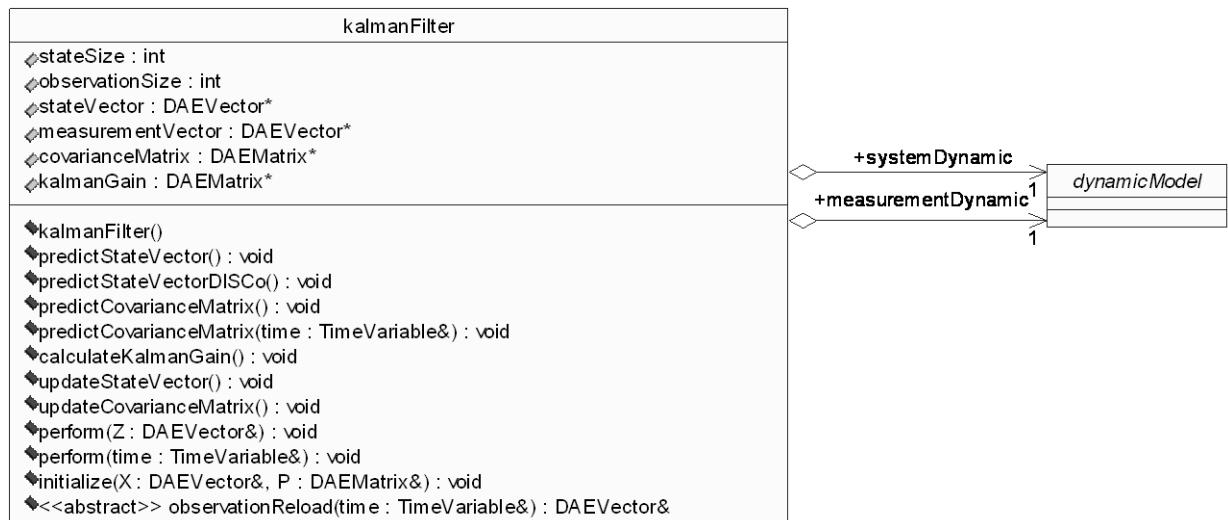


Figure 5. Class diagram of the extended Kalman filter

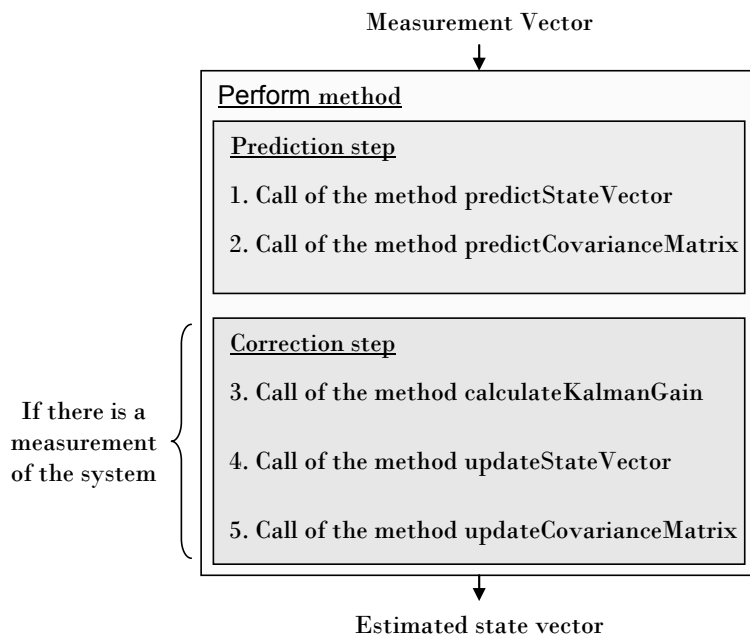


Figure 6. Architecture of the method “perform”

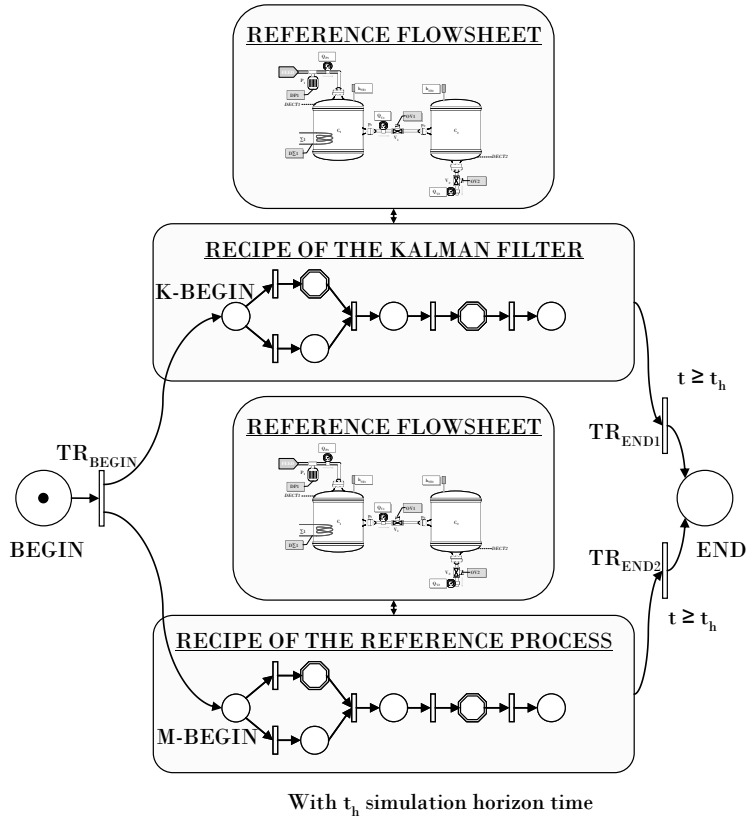


Figure 7. Petri net of the main recipe

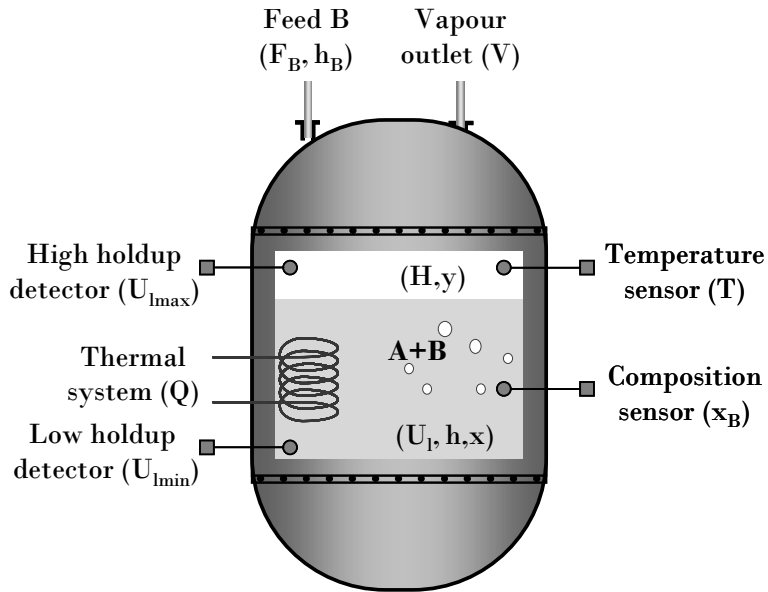


Figure 8. Flowsheet of the example

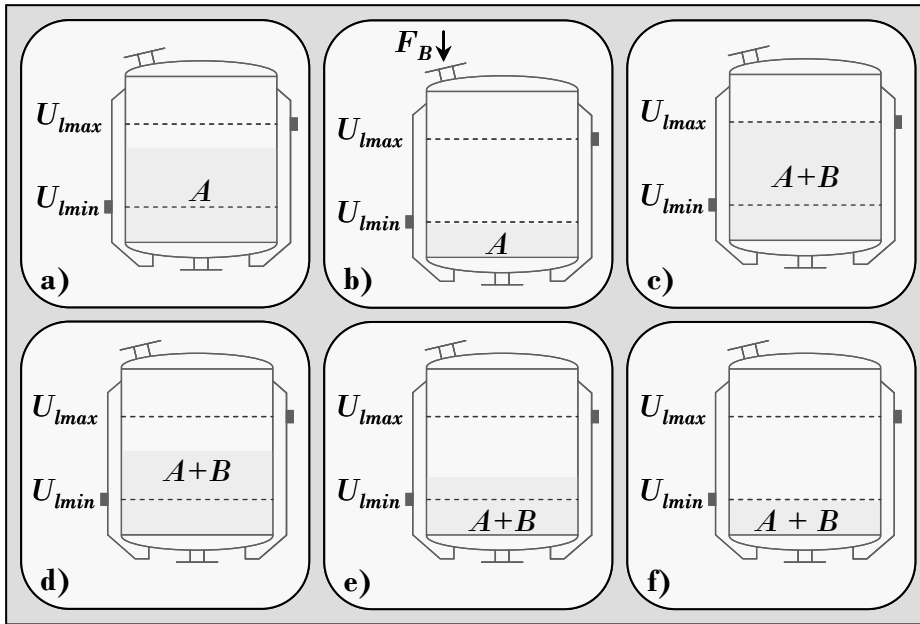


Figure 9. Process recipe

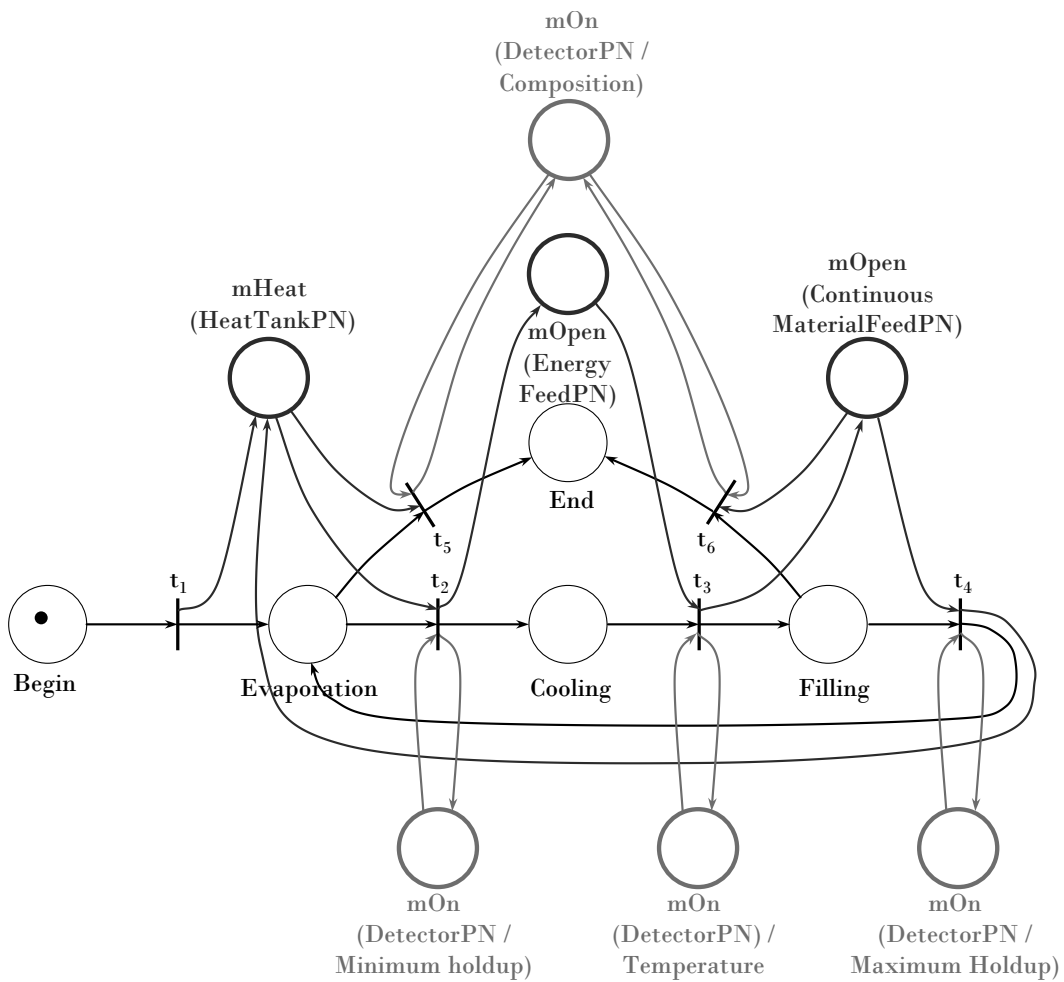


Figure 10. Recipe Petri net

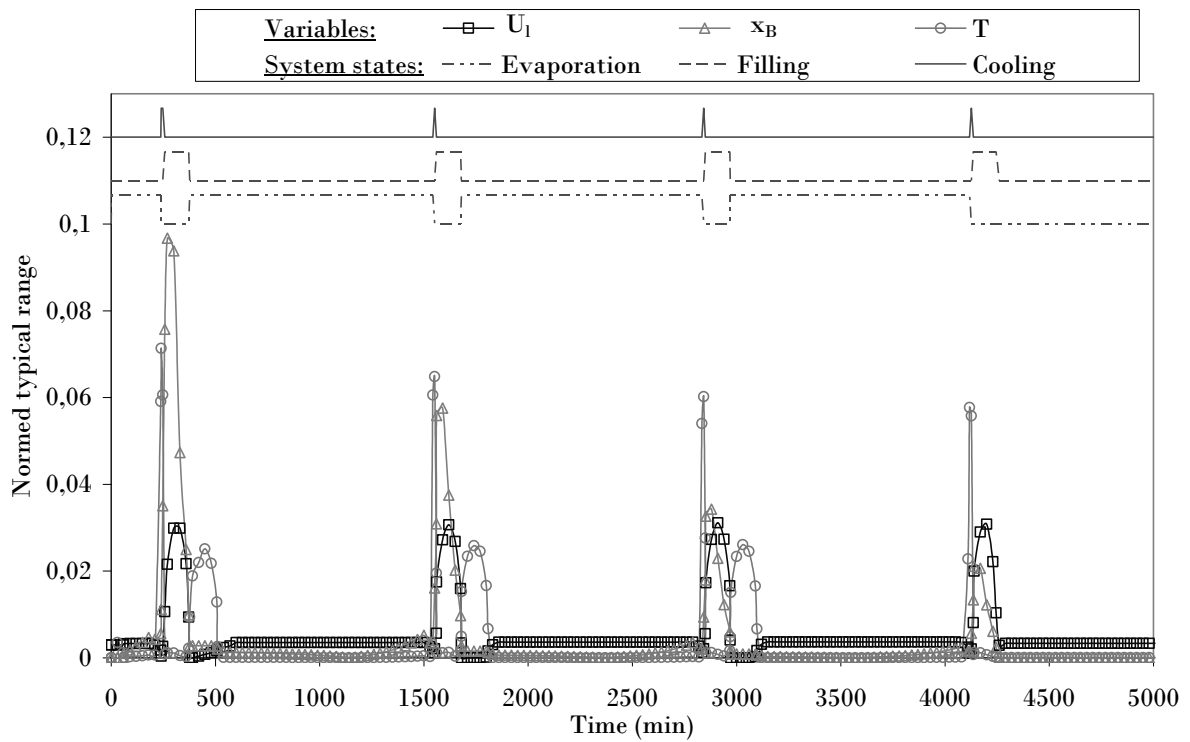


Figure 11. Results of the sampling method

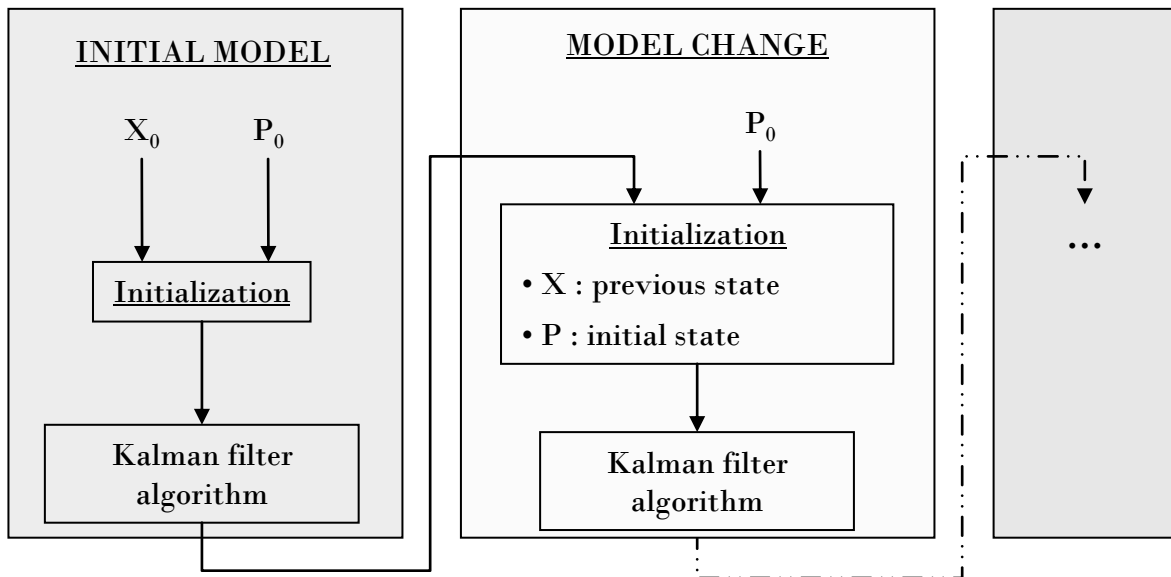


Figure 12. Kalman filter initialization

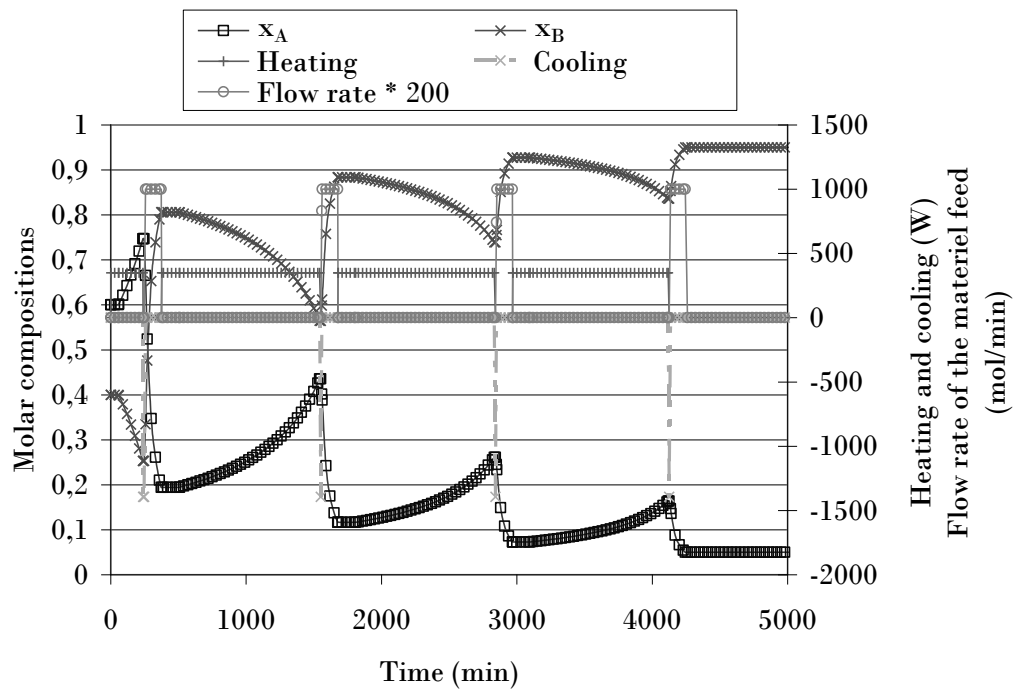


Figure 13. Results of the reference process

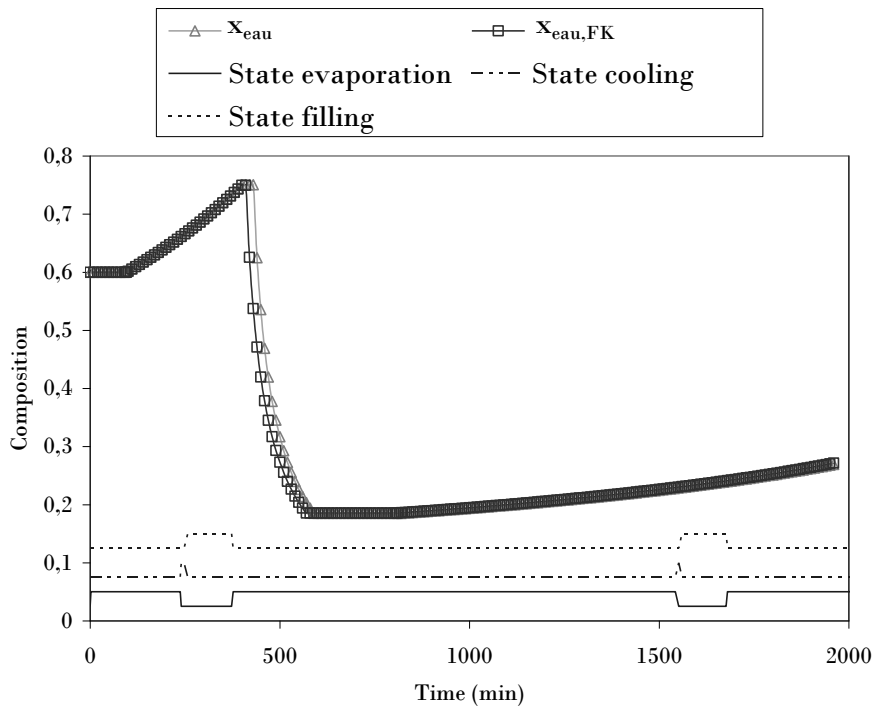


Figure 14. Results of the state reconciliation

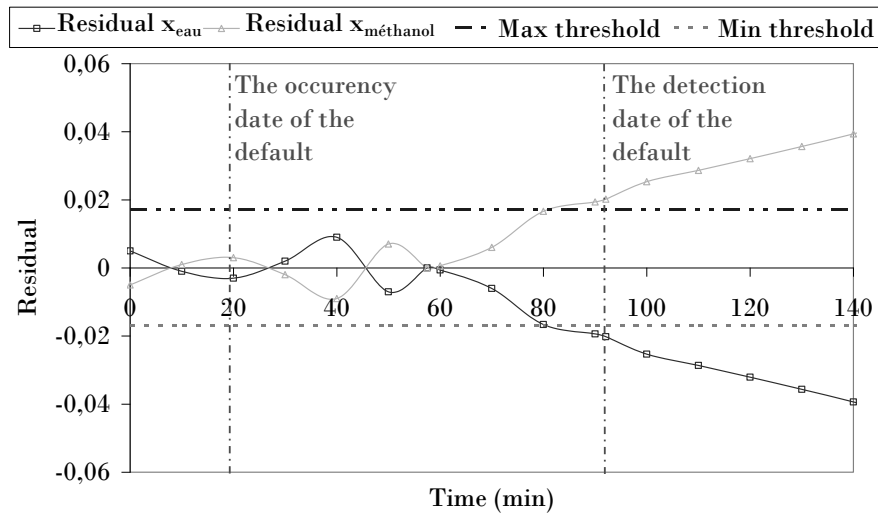


Figure 15. Detection results

Variables	Reactor	Material Feed
T (K)	298.15	298.15
P (atm)	1	1
$x_{A=\text{eau}}$	0.6	0.01
$x_{B=\text{méthanol}}$	0.4	0.99
U_1 (mol)	300	-
Flow rate (mol/min)	-	5

Table 1. Operating conditions

Parameters	Uncertainties
Liquid retention in the reactor	$U_1^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 20)$
Flow rate of the material feed	$F_B^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 0.5)$
Composition in the reactor	$x_A^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 0.05)$
Composition threshold	$x_B^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 0.05)$
Maximum holdup threshold	$U_{1\text{max}}^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 20)$
Minimum holdup threshold	$U_{1\text{min}}^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 20)$
Cooling energy quantity	$Q_{\text{cool}}^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 100)$
Heating energy quantity	$Q_{\text{heat}}^{\text{ref}} + \varepsilon$ avec $\varepsilon \in N(\mathbf{0}, \sigma = 100)$

Table 2. Uncertainties of the parameters and of the initial conditions

T	y_A	y_B	x_A	x_B	U_1
3.5 K	0.01	0.015	0.015	0.015	30 mol

Table 3. Modelling uncertainties