Review

Review and classification of recent observers applied in chemical process systems

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ABSTRACT

Observers are computational algorithms designed to estimate unmeasured state variables due to the lack of appropriate estimating devices or to replace high-priced sensors in a plant. It is always important to estimate those states prior to developing state feedback laws for control and to prevent process disruptions, process shutdowns and even process failures. The diversity of state estimation techniques resulting from intrinsic differences in chemical process systems makes it difficult to select the proper technique from a theoretical or practical point of view for design and implementation in specific applications. Hence, in this paper, we review the applications of recent observers to chemical process systems and classify them into six classes, which differentiate them with respect to their features and assists in the design of observers. Furthermore, we provide guidelines in designing and choosing the observers for particular applications, and we discuss the future directions for these observers.

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Nomenclature

A, B, C, E, F, G	state space matrices
sign	component wise for vector argument of $z = col(z_1, \ldots, z_n)$
x_1	measured component concentration
$\hat{x}$	estimated state vector
$\dot{x}, \dot{z}$	dynamic of state vector
Z	process vector
R_V	measurement noise covariance vector
u_1, u_2	vector partition correspond to auxiliary variables
d	discrete
L, K	observer gain
$\dot{\hat{x}}$	estimated state vector with linear innovative term of discontinuous function
U_1, U_2	external transfer vector
$\mathcal{O}$	observability matrix
P_{k-1}	covariance at time $k-1$
F_{k-1}	nonlinear state transition function
ξ	auxiliary variable
$\hat{D}(s)$	estimated disturbance
A_1, A_2	unique solution of process vector
$D_1(s), D_2(s)$	lumped disturbances in loop including external disturbances

1. Introduction

The implementation of state feedback laws in a controlled plant is often based on the assumptions that all states are available for online measurement; however, in practice, some of them may not be measurable due to a lack of appropriate estimating devices or the high price of sensors (Dochain et al., 2009; Jana, 2010; Soroush, 1997; Wang et al., 1997). As a consequence, measuring the missing states or variables is expensive and time consuming due to the significant technical standard requirements and the high cost of installation of these devices (Gonzalez et al., 2001; Hulhoven et al., 2006). For these reasons, devices called observers have been developed to reconstruct the state vector in order to estimate the missing variables and, at the same time, to reduce the usage of high-priced sensors (Dochain et al., 2009).

Luenberger (Luenberger, 1964, 1966, 1967, 1971) and Kalman (Welch and Bishop, 1995) introduced the basic concepts of state observers and Kalman Filter (KF)-based observers in the 1960s. However, over the years, research in the design of observers has become popular but challenging due to the requirements of high accuracy, low cost and good prediction performances. In fact, many observers today are simply modifications and extended versions of the classical Luenberger observer and Kalman filter. In recent years, various types of observers have been developed to accurately estimate state variables in linear and nonlinear chemical processes (Aguirre and Pereira, 1998; Bastin and Dochain, 1990; del-Muro-Cuellar et al., 2007; Gonzalez et al., 1998; Huang et al., 2010; Lombardi et al., 1999; Pedret et al., 2009). They have been widely used both theoretically and practically through simulations and real plant testing (Bejarano and Fridman, 2010; Busawon and Kabore, 2001; Farza et al., 2011; Lee, 2011; Lin et al., 2003; Oya and Hagino, 2002).

Researchers have also developed observers for systems to tackle problems such as disturbances, mismatches and faults. For this purpose, different types of observers were developed with closely similar formulations designed to overcome the drawbacks of each other. For example, to estimate disturbances, the disturbance observer (DOB) was introduced (Chen et al., 2009; Kim et al., 2011), and later, the modified disturbance observer (MDOB) was developed to target large disturbances and mismatches (Yang et al., 2011). After that, the fractional-order disturbance observer (FO-DOB) and Bode-ideal-cut-off observer (BICO-DOB) (Olivier et al., 2012) were developed to include methodology for tuning and optimizing the estimation performance. Another example is the asymptotic observer, which was first developed based on available measurements of the temperature of a mixture and a subset of the concentrations (Dochain et al., 1992) and later extended on the basis of the energy balance almost similar to the thermodynamic properties of the mixtures (Dochain et al., 2009; Hoang et al., 2012, 2013).

Due to the variety of methodologies in observer design for chemical process systems, combining and classifying them into several different groups would be highly useful to serve as guidelines to select and then design the appropriate observers for a specific chemical application. Previous surveys have only included the study of one or two types of observers. For example, the reviews by Spurgeon (2008) and Hidayat et al. (2011) focused respectively on single observer types such as the sliding mode observers and observers for linear distributed parameter systems. Another survey from Radke and Zhiqiang reviewed the design advantages of a particular type of disturbance observers for practitioners (Radke and Zhiqiang, 2006), whereas Ruhm solely explained the concepts of open and closed loop observers (Ruhm, 2008). Dochain has presented the available results of state and parameter estimation approaches for chemical and biochemical processes, specifically the extended Luenberger (ELO), Kalman (EKO), asymptotic and interval observers (Dochain, 2003). Kravaris and coworkers provided an overview of recent developments regarding the design of nonlinear Luenberger observers, with special emphasis on the exact error linearization techniques, and discussed general issues including observer discretization, sampled data observers and the use of delayed measurements (Kravaris et al., 2012). In addition, Prakash and coworkers reviewed recently developed Bayesian estimators (Prakash et al., 2011), and Daum focused only on the extended nonlinear filters on the basis of the classical KF (Daum, 2005). Chen has also reviewed Bayesian filtering from KF to particle filter, emphasizing the stochastic filtering theory based on Bayesian perspectives (Chen, 2003). However, all of these reviews are specific in nature and do not consider the whole spectrum of the different classes of observers available.

Therefore, this review paper intends to provide a comprehensive survey considering the unique features of different types of recent observers in chemical process systems (Dochain, 2003; Kravaris et al., 2012) by categorizing them into different classes, a level of organization not currently available in the literature. Six classes are proposed, namely, Luenberger-based observers, finite-dimensional system observers, Bayesian estimators, disturbance and fault detection observers, artificial intelligence (AI)-based observers and hybrid observers. In brief, the main contribution of this review is to provide the list of recent observers that have been applied in chemical process systems and to classify them into six classes with emphasis on their positive highlights based on their estimation performances in specific chemical process systems. Recent observers refer to the observers developed since the year 2000, as most observers before that would be referred to as the classical types (Elicabe et al., 1995; Gonzalez et al., 1998; Lee and Ricker, 1994; Oliveira et al., 1996; Soroush, 1997; Wang et al., 1997). All of these observers can be either linear or nonlinear and have served as specific estimators to several unit operations. However, this review does not include some methodologies such as the recursive error method (Lee et al., 2000) and the partial least square method (Roffel et al., 2003), which have also been considered as estimators.

This paper is organized as follows. The introduction is in Section 1, followed by the classification of observers and their applications in chemical process systems in Section 2. Section 3 discusses the observer design methodology. Section 4 focuses on the current and future trends of observers, while Section 5 concludes the review.

2. Classifications and applications

The formulations of observer design methodologies in research publications have normally been written and explained with merely theoretical emphasis, which makes it difficult for practitioners and researchers, especially newcomers to this area, to choose (potentially) appropriate observers for their systems. In addition, selecting the most suitable observer for any specific system is an important but difficult task for installed systems due to the diversity of the many available methods, observer types, application range and nature of chemical process systems. So far, this research area has been very active and attracts attention from many researchers (Aguilar-Garnica et al., 2011; López-Negrete and Biegler, 2012; Mesbah et al., 2011; Nagy Kiss et al., 2011; Olivier et al., 2012). Based on our extensive review of the recent observers applied to chemical process systems, we can clearly differentiate them into six major classes. These classes are the Luenberger-based observers, finite-dimensional system observers, Bayesian estimators, disturbances and fault detection observers, artificial intelligence-based observers and hybrid observers. The attributes, advantages, limitations and guidelines for practitioners according to each class are given in Table 1, while Table 2 sorts these recent observers into their respective classes. In addition, the selection of the recent observers according to those classes is depicted in Fig. 1 to guide and help researchers in their selection.

The category of Luenberger-based observers is the first class that groups together all of the observers designed based on the Luenberger observer methodology, or, in other words, it involves the extended versions of the classical Luenberger observer itself (Alonso et al., 2004; Dochain, 2003; Fissore et al., 2007; Tronci et al., 2005; Vries et al., 2010). The extended Luenberger observer (ELO), sliding mode observer (SMO), adaptive state observer (ASO), generic and backstepping observers are examples of observers falling into this class. This type of observer is suitable for less complex linear systems with relatively simpler computational methods (Bejarano et al., 2007b).

The second category is the finite-dimensional system observers, which include, among others, the reduced-order, low-order, high-gain, asymptotic and exponential observers. These finite-dimensional system observers are designed for chemical process systems whose dynamics are described by ordinary differential equations (ODEs) (Bitzer and Zeitz, 2002) and are quite straightforward to implement. They suit systems with less kinetic information, but the accuracy of the convergence rate is uncertain. For example, for the case of asymptotic and exponential observers, the convergence rate can only be shown if the process operating conditions are such that the dilution rate is bounded (Dochain et al., 1992; Dochain, 2000; Hadj-Sadok and Gouze, 2001; Hoang et al., 2013). It is worth noting that asymptotic/exponential and interval observers can also be extended to infinite dimensional systems (i.e., distributed parameter systems) such as for tubular reactors and plug flow reactors (Dochain, 2000; Aguilar-Garnica et al., 2011).

Bayesian estimators, in the third category, provide an approach based on the probability distribution estimation of state variables by utilizing the available data of the system (Chen et al., 2004). It assumes that all variables are stochastic in nature, and thus, the distribution of state variables is achievable based on the measured variables. Examples of the Bayesian type of estimators are the extended Kalman filter (EKF), particle filter (PF) and moving horizon estimator (MHE). These are based on probability distribution and are therefore consistent and versatile estimators, which are highly appropriate for fast estimation (Abdel-Jabbar et al., 2005; Fan and Alpay, 2004; Patwardhan and Shah, 2005). However, the computational complexity involved in using this approach makes them infeasible for high-dimensional systems.

The fourth class is the disturbance and fault detection observers. Although they can be of different classes, both are included in one category because they are mostly applied to estimate irregularities in the system, either through disturbances or faults (Olivier et al., 2012). Fault detection observers can also be applied to estimate parameters for fault diagnosis of chemical process systems. Examples of disturbance and fault detection observers are the disturbance observer (DOB), the modified disturbance observer (MDOB), the unknown input observer (UIO) and the nonlinear unknown input observer (NUIO). These are highly specific types of observers and focus only on disturbances or fault detection related variables during the estimation process (Chen et al., 2009; Rocha-Cózatl and Wouwer, 2011; Sotomayor and Odloak, 2005; Yang et al., 2011). They are mostly suitable for estimating disturbances and faults, which provide early warning to operators prior to causing disruption to the process units (Sotomayor and Odloak, 2005; Zarei and Poshtan, 2010).

The fifth class is the artificial intelligence (AI)-based observers. AI is the science of making the program perform intelligence-based tasks, which include methods such as fuzzy logic, artificial neural networks (ANN), expert systems and genetic algorithms. These types of observers have been widely utilized as estimators in recent times. For example, the work by Hussain and coworkers utilized a hybrid neural network (HNN) to predict porosity in a food drying process (Hussain et al., 2002), and the research by Aziz and coworkers applied ANN to estimate the heat released from a polymerization reactor (Aziz et al., 2000). Other applications of AI-based observers can also be found in many papers (Barton and Himmelblau, 1997; Islamoglu, 2003; Khazraee and Jahanmiri, 2010; Kordon et al., 1996; Kuroda and Kim, 2002; Liu, 2007; Ng and Hussain, 2004; Turkdogan-Aydınol and Yetilmezsoy, 2010; Wang et al., 2006, Wei et al., 2007). However, this review paper covers only recent types of AI-based observers coupled with conventional (model-based) types, as purely AI observers are not recent in nature. Examples of these recent types are the fuzzy Kalman filter (FKF) and the EKF-neural network observers (Porru et al., 2000; Prakash and Senthil, 2008). These AI-based observers overcome the limitations of single-based observers and are suitable for systems with incomplete model structure and information. The formulation of AI-based observer may be difficult and time consuming compared to the other hybrid observers in some systems (Senthil et al., 2006). In addition, the AI elements must first be adapted for online implementation (Himmelblau, 2008; Lashkarbolooki et al., 2012; Rivera et al., 2010).

The sixth class is the hybrid observers, which are combinations of more than one observer to obtain improved estimation in certain systems. An example of this is the extended Luenberger observer (ELO) combined with the asymptotic observer (AO) (Hulhoven et al., 2006). ELO provides good convergence factors, while AO estimates parameters without any kinetics data. Therefore, the combination results in an improved hybrid observer that contains both features. Hybrid observers are good at overcoming the limitations of the single observer, but choosing the appropriate combination may be tedious and time consuming (Aguilar-Lopez and Maya-Yescas, 2005; Bogaerts and Wouwer, 2004; Goffaux et al., 2009). Normally this class of observer is suitable for conditions where the single-based observer is not accurate enough for the process systems, for instance, to compensate for offsets in estimation resulting from the use of the single observer (Hulhoven et al., 2006).

Table 1
Observers' overall evaluation according to classes.

No.	Class of observers	Example of observer equation	Attributes	Advantages	Limitations	Guidelines for practicing engineers
1	Luenberger-based observers	For sliding mode observer: $\dot{\hat{x}} = A\hat{x} + Bu + Lsign(y - C\hat{x})$	Extension of classical Luenberger observer	Simple computational methods	Design is always based on the perfect knowledge of system parameters	For less complex linear systems, this type of observer is sufficient for crucial parameter estimation
2	Finite-dimensional system observers	For exponential observer: $\frac{d\xi}{dt} = F\xi + Gx_1 - LU_1 + U_2$	Knowledge of process system kinetics is not necessary	Easy implementation and simple formulation	Convergence factor depends strongly on the operating condition	Suitable for systems with less kinetics information
3	Bayesian estimators	For extended Kalman filter: $P_{k\|k-1} = F_{k-1}P_{k-1\|k-1}F_{k-1}^T + R_v$	Based on probability distribution and mathematical inference of the system	Fast estimation based on prediction-correction method and versatile estimators	The complexity of their computational method is sometimes infeasible for high dimensional systems	For fast estimation results based on probability theory, Bayesian estimators may be applied
4	Disturbance and fault detection observers	For disturbance estimation: $\tilde{D}(s) = \tilde{D}_1(s) + \tilde{D}_2(s) + \cdots + \tilde{D}_n(s)$	Focus on estimating disturbances and detecting faults within the system	Good at estimating disturbances and predicting faults before they can affect the unit operations of the plant	May ignore other uncertainties during the estimation process	If the objective is to estimate disturbances and parameters to predict faults, then these type of observers are the most appropriate
5	AI-based observers	According to AI-elements, example using fuzzy logic where the IF-THEN rule is: $IF\ e\ is\ negative\ small\ AND\ \Delta e\ is\ zero$ $THEN\ \hat{x}_{estimated} = x_{actual}$	Combination of observers with AI elements	Overcome limitations of single observer and suitable for systems with incomplete model structure	May be difficult and time consuming For online implementation, the AI elements must first be adapted to the system	For highly nonlinear systems with an incomplete or unknown model
6	Hybrid observers	For combination of extended Luenberger and asymptotic observer: $\frac{dZ(t)}{dt} = D(t)Z(t) + A_1u_1(t) + A_2u_2(t)$	Combination of two or more observers	Overcome the limitations of a single observer	Choosing appropriate combination may be tedious	This is suitable for systems where a single type of observer is not accurate enough

The detailed applications of the various observers under these six classes are listed in Table 3. The table does not need any further elucidation because it is comprehensive and self-explanatory in nature, covering the objectives, the positive highlights, applications in various unit operations and the relevant references involved for each of the observer types.

3. Methodology for observer design

Observers were first designed based on linear formulation; these original observers were known as linear observers and used to estimate states and unknown variables in a linear process in the eventual presence of disturbances or noise (Bara et al., 2001; Bejarano and Fridman, 2010; Bejarano et al., 2007a,b; Bodizs et al., 2011; Busawon and Kabore, 2001; El Assoudi et al., 2002; Fissore, 2008; Jafarov, 2011; Lee, 2011; Oya and Hagino, 2002; Vries et al., 2010). Later, because most processes exhibit highly nonlinear behavior, researchers formulated nonlinear observers (Besancon, 2007; Bitzer and Zeitz, 2002; Boulkroune et al., 2009; Busawon and Leon-Morales, 2000; de Assis and Filho, 2000; Di Ciccio et al., 2011; Dong and Yang, 2011; Farza et al., 1997, 2011; Floquet et al., 2004; Hashimoto et al., 2000; Kalsi et al., 2009; Kazantzis and Kravaris, 2001; Kazantzis et al., 2000; Ko and Wang, 2007; Kravaris et al., 2007; Maria et al., 2000; Schaum et al., 2008).

Most researchers developed observers based on the mathematical model of the systems and used the first principles model prior to developing the observer's equation (Dochain et al., 2009).

Table 2
Recent observers categorized under different classes.

Class					
Luenberger-based observers	Finite-dimensional system observers	Bayesian estimators	Disturbance and fault detection observers	Artificial intelligence-based observers	Hybrid observers
Specific observer 1. Extended Luenberger observer (ELO) 2. Sliding mode observer (SMO) 3. Adaptive state observer (ASO) 4. High-gain observer 5. Zeitz nonlinear observer 6. Discrete-time nonlinear recursive observer (DNRO) 7. Geometric observer 8. Backstepping observer	1. Reduced-order observer 2. Low-order observer 3. High gain observer 4. Asymptotic observer (AO) 5. Exponential observer 6. Integral observer 7. Interval observer	1. Particle filter (PF) 2. Extended Kalman filter (EKF) 3. Unscented Kalman filter (UKF) 4. Ensemble Kalman filter (EnKF) 5. Steady state Kalman filter (SSKF) 6. Adaptive fading Kalman filtering (AFKF) 7. Moving horizon estimator (MHE) 8. Generic observer 9. Specific observer	1. Disturbance observer (DOB) 2. Modified disturbance observer (MDOB) 3. Fractional- order disturbance observer 4. Bode-ideal cut-off observer 5. Unknown input observer (UIO) 6. Nonlinear unknown input observer 7. Extended unknown input observer 8. Modified proportional observer	1. Fuzzy Kalman filter 2. Augmented fuzzy Kalman filter 3. Differential neural network observer 4. EKF with neural network model	1. Extended Luenberger-asymptotic observer 2. Proportional-integral observer 3. Proportional-SMO 4. Continuous-discrete observer 5. Continuous-discrete-interval observer 6. Continuous-discrete-EKF 7. High-gain-continuous-discrete

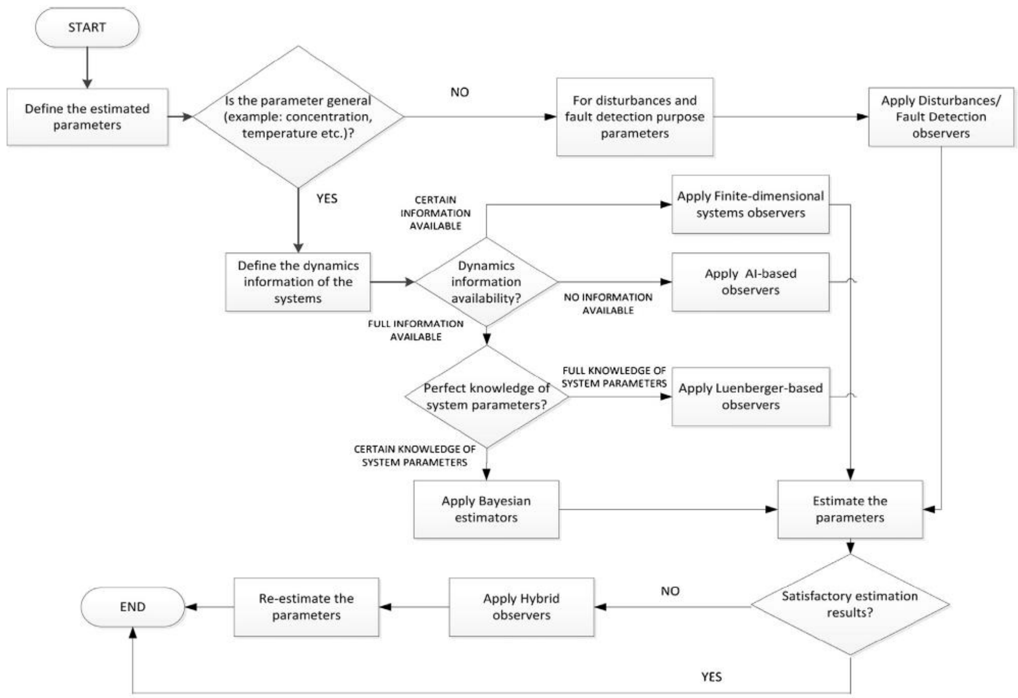

Fig. 1. General guideline for selecting recent observers according to their classification.

Therefore, most observer designs are model-based approaches (Damour et al., 2010a, 2010b; Dochain et al., 2009; Salehi and Shahrokhi, 2008) with the exception of the AI-based observers (Bahar and Ozgen, 2010; Lahiri and Ghanta, 2008; Mohebbi et al., 2011; Rezende et al., 2008; Wei et al., 2010). The gain of the observer and its estimation error dynamics are also significant in designing the model-based observers, as shown in several references (Aguilar-Lopez and Martinez-Guerra, 2007; De Battista et al., 2011; Hulhoven et al., 2008; Porru et al., 2000). However, the success of observer designs is evaluated based on their capabilities in estimating the difficult-to-measure states with satisfactory convergence rates (Bitzer and Zeitz, 2002; Ciccio et al., 2011; Hashimoto et al., 2000; Kravaris et al., 2007; Lafont et al., 2011; Morel et al., 2006) and with approximately zero estimation errors (Benaskeur and Desbiens, 2002; Bogaerts and Wouwer, 2004; Kazantzis et al., 2000; Liu, 2011).

The first important step before designing the observer is to consider the detectability or observability condition of the system because observers have to be designed for a detectable or observable system. Observability is the condition in which all initial states are observable and a system is said to be observable if, for any initial condition vectors, its internals states can be inferred by knowledge of its (external) outputs (Evangelisti, 2011; Moreno and Dochain, 2008; Soroush, 1997). Detectability is a weaker condition than observability, where the non-observable states can still decay to zero asymptotically (Evangelisti, 2011; Moreno and Dochain, 2008). Both concepts will influence the feasibility conditions of the observers (Dochain et al., 1992; Hoang et al., 2013; Moreno and Dochain, 2008). The concept of observability is central in reconstructing unmeasurable state variables. This explains the need of observers to estimate unknown states prior to developing control laws and the fact that not all states are available directly through on-line measurements (Ogata, 1995). Extensive discussions on observability and detectability can be found in various references (Astolfi and Praly, 2006; Evangelisti, 2011; Hermann and Krener, 1977; Moreno and Dochain, 2008; Soroush, 1997; Zuazua, 2007).

Once the system dynamics fulfill the observability or detectability conditions, observers can then be designed to estimate the state variables. In this respect, the choice of a suitable observer according to the six classes provided in Section 2 is therefore of great importance. Prior to that, the desired estimated states (i.e. the exact values of the observed states) and initial conditions must be defined clearly (Farza et al., 2011). After that, tests are run to compare the estimates with the actual values to determine the performance of the proposed observer (Aamo et al., 2005; De Battista et al., 2011; Hajatipour and Farrokhi, 2010; Jana et al., 2006; Nagy Kiss et al., 2011; Salehi and Shahrokhi, 2008). The test not only is important for the design of the single observer but also determines whether a hybrid observer is further needed to estimate the parameter (Goffaux et al., 2009; Hulhoven et al., 2006; Sheibat-Othman et al., 2008). If there are huge discrepancies between the actual and estimated values, a hybrid observer should be developed to improve the estimates. Furthermore, if systems are complex and models are difficult to obtain from the first principles, hybrid AI-based observers would possibly be a suitable choice (Chairez et al., 2007; Porru et al., 2000; Prakash and Senthil, 2008).

The design guideline for these observers based on the six classes is depicted in Fig. 2 with detailed explanation in the following subsections.

Table 3
Application of recent observers in chemical process systems under different classes.

Observer	Objective/estimate(s)	System	Positive highlight(s)	Ref.
Class 1: Luenberger-based observers				
ELO	Crystal mass	Crystallization unit	Good estimation without perfect initial condition	Damour et al. (2010a,b)
ELO	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
ELO	Process kinetics, influent concentrations	Fixed bed reactor	Easy to implement, simple structures	Mendez-Acosta et al. (2008)
SMO	Substrate concentration, specific growth rate	Fermentation process	Smooth estimates	Pico et al. (2009)
SMO	Specific growth rate	Fed-batch bioreactor	Accurate and error free estimation	De Battista et al., 2011
SMO	Substrate concentration	Bioreactor	Proven stability factor	Gonzalez et al. (2001)
SMO	Biomass and substrate concentration	Bioreactor	Proven stability factor	Hajatipour and Farrokhi (2010)
DNRO	Reactor parameters	CSTR	Stable estimator	Huang et al. (2010)
ASO	Growth rate, kinetic coefficient	Bioreactor	Guaranteed convergence factor	Zhang and Guay (2002)
ASO	Liquid, vapor flow rate, reboiler coefficient	Debutanizer	Precise estimates under mismatch condition	Jana et al. (2009)
ASO	Radical concentration	Polymerization process	Estimates without information of initiator	Sheibat-Othman et al. (2008)
ASO	Distribution coefficients	Distillation column	Guaranteed convergence factor	Jana et al. (2006)
ASO	Compositions, partially known parameters	Batch distillation column	Good convergence factor	Murlidhar and Jana (2007)
Backstepping	Concentrate and tailing grade	Solid-solid separation unit	Guaranteed convergence, zero estimation error	Benaskeur and Desbiens (2002)
Zeitz nonlinear observer	Nitrogen oxide (NO_x) inlet concentration, outlet reactant conversion	Loop reactor	Fast, reliable estimates	Fissore et al. (2007)
Geometric	Product compositions	Distillation column	Overcomes ill-conditioning of the observability matrix	Tronci et al. (2005)
Geometric	Compositions, solid mass fraction, production rate	Copolymerization reactor	Accurate estimation	López and Alvarez (2004)
Class 2: Finite-dimensional system observers				
Reduced-order	Down hole pressure	Gas-lift well	Stable estimates	Aamo et al. (2005)
Reduced-order	Reactor concentration	CSTR	Good concentration estimates	Salehi and Shahrokhi (2008)
Reduced-order	Substrate concentration	Bioreactor	Robust estimation	Kazantzis et al. (2005)
Low-order	Steady state profiles	30-tray distillation column	Robust against noise	Singh and Hahn (2005c)
High-gain	Reaction heat	CSTR	Robust against noise and disturbances	Aguilar et al. (2002)
High-gain	Reactor concentration and temperature	CSTR	Precise estimates	Biagiola and Figueroa (2004b)
Exponential	Reactor concentration	Tubular reactor[a]	Good estimation without process kinetics	Dochain (2000)
Exponential	Top tray compositions	Batch distillation column	Good convergence properties	Jana (2010)
Exponential	Microorganisms concentration	Bioreactor	Guaranteed convergence	El Assoudi et al. (2002)
AO	Concentrations, enthalpy	CSTR	Good estimation, not sensitive to noise	Dochain et al. (2009)
AO	Reactor concentration	Tubular reactor[a]	Good estimation without process kinetics	Dochain (2000)
AO	Growth rate	Activated sludge process	Precise estimation without process kinetics	Hadj-Sadok and Gouze (2001)
Interval	Organic concentration, growth rates	Activated sludge process	Converge toward bounded interval	Hadj-Sadok and Gouze (2001)
Interval	Reactant concentration	Plug flow reactor[a]	Robust estimation	Aguilar-Garnica et al., 2011
Interval	Residual parameters	Separator (grinding process)	Good convergence factor	Meseguer et al. (2010)
Integral	Heat of reaction	CSTR	Robust estimation	Aguilar-Lopez (2003)
Class 3: Bayesian estimators				
SSKF	Time-delay	Stirred tank heater	Consistent estimates even with noise	Patwardhan and Shah (2005)
SSKF	Product compositions	Batch distillation column	Stable estimation	Venkateswarlu and Avantika (2001)
EKF	Interface temperature	Freeze-drying process	Good estimation without perfect initial condition	Velardi et al. (2009)
EKF	Component's concentration	Batch distillation column	Simple observer design yet accurate estimation	Yildiz et al. (2005)
EKF	Product compositions	Batch distillation column	Precise estimate even with noise	Venkateswarlu and Avantika (2001)
EKF	Outlet reactor concentration	CSTR	Accurate concentration estimation	Himmelblau (2008)
EKF	Liquid compositions	Reactive distillation column	Robust against modeling error	Olanrewaju and Al-Arfaj (2006)
EKF	Top tray compositions and flow rates	Distillation column	Guaranteed convergence factor	Jana et al. (2006)
EKF	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
UKF	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
UKF	Particle size distribution	Semi-batch reactor	Good estimation without accurate model	Mangold et al. (2009)

Table 3 (*Continued*)

Observer	Objective/estimate(s)	System	Positive highlight(s)	Ref.
UKF	Biomass concentration	Fermentor	Effective estimation despite using the simplified mechanistic model	Wang et al. (2010)
UKF	Uncertain parameters	Hybrid tank system	Effective control and good estimation	Prakash et al. (2010)
EnKF	Solute concentrations	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
EnKF	Unmeasured disturbances	Hybrid tank system	Effective control and good estimation	Prakash et al. (2010)
AFKF	Product compositions	Batch distillation column	Precise estimate despite noisy conditions	Venkateswarlu and Avantika (2001)
AFKF	Temperature	Heat exchanger	Good estimation without coefficient adjustment	Bagui et al. (2004)
PF	Yield parameter	Fermentor	Good estimation based on maximization algorithm theory	Chitralekha et al. (2010)
PF	Conditional density	CSTR	Few assumptions required for estimation	López-Negrete et al. (2011)
PF	Conditional density	Batch Reactor	Few assumptions required for estimation	López-Negrete et al. (2011)
MHE	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
MHE	Molecular weight distribution	Polymerization reactor	Smooth estimates	López-Negrete and Biegler (2012)
MHE	Tray efficiencies	Binary distillation column	Able to handle constraint during estimation	López-Negrete and Biegler (2012)
MHE	Biomass concentration	Animal cell cultures	Accurate estimates	Raïssi et al. (2005)
Generic observer	Carbon and nitrogen concentrations	Sequential batch reactor	Robust against modeling error	Boaventura et al. (2001)
Specific observer	Carbon and nitrogen concentrations	Sequential batch reactor	Robust against modeling error	Boaventura et al. (2001)
Class 4: Disturbances and fault detection observers				
DOB	Disturbances related to time delay	Conveyor (grinding process)	Overcome the effect of internal disturbances	Chen et al. (2009)
FO-DOB	Disturbances due to mismatch	Cyclone (grinding process)	Optimize the estimation even with huge disturbances	Olivier et al. (2012)
BICO-DOB	Disturbances due to mismatch	Cyclone (grinding process)	Optimize the estimation even with huge disturbances	Olivier et al. (2012)
MDOB	Closed-loop system disturbances	Jacketed stirred tank heater	Smooth disturbances estimate	Yang et al. (2011)
Modified proportional	Uncertainties in reactive concentration, reactor and jacket temperature	CSTR	Robust against uncertainties	Aguilar-Lopez and Martinez-Guerra (2005)
UIO	Fault in actuator and sensor	Polymerization reactor	Accurate estimation	Sotomayor and Odloak (2005)
UIO	Fault in input sensor	CSTR	Accurately estimating fault even in the presence of disturbances	Zarei and Poshtan (2010)
QUIO	Faults in concentration, flow rates, light intensity	Bioreactor	Satisfactory estimates	Rocha-Cózatl and Wouwer (2011)
NUIO	Fault in residuals	CSTR	Acting as alternative fault alarm	Zarei and Poshtan (2010)
EUIO	Fault in residuals	CSTR	Acting as alternative fault alarm	Zarei and Poshtan (2010)
Class 5: AI-based observers				
FKF	Reactor temperature and concentration	CSTR	Unbiased estimation	Prakash and Senthil (2008)
ASFKF	Reactor temperature and concentration	CSTR	Satisfactory unbiased estimates	Prakash and Senthil (2008)
DNNO	Anthracene dynamics decomposition and contaminant concentration	Microreactor	Good agreement with the actual value	Poznyak et al. (2007)
DNNO	Formic acid, fumaric acid, maleic acid, oxalic acid	Wastewater treatment plant	Guaranteed small estimation error	Chairez et al. (2007)
EKF-NN	Outlet reactor concentration	Heterogeneous reactor	Further reduction in estimation error compared to EKF	Porru et al. (2000)
Class 6: Hybrid observers				
ELO-AO	Biomass concentration	Bioreactor	Stable rate of convergence	Hulhoven et al. (2006)
Continuous-discrete	Biomass concentration	Batch reactor	Robust against modeling error	Aguilar-Lopez and Martinez-Guerra (2005)
Continuous-discrete-interval	Process kinetics	Bioreactor	Avoids growth of interval sizes during estimation	Goffaux et al. (2009)
Continuous-discrete-EKF	Biomass, substrate concentration	Bioreactor	Accurate estimates, reduced error	Bogaerts and Wouwer (2004)
Proportional-SMO	Polymer molecular weight, monomer concentration, reactor temperature	Polymerization reactor	Robust against noise and uncertain parameters	Aguilar-Lopez and Maya-Yescas (2005)
Proportional-integral	Unknown inputs	Wastewater treatment plant	Stable estimation rate	Nagy Kiss et al. (2011)
High-gain-continuous-discrete	Rate coefficient	Polymerization process	Estimates without information of initiator	Sheibat-Othman et al. (2008)

[a] Finite-dimensional system observers may be extended to the infinite-dimensional systems such as for tubular and plug flow reactor.

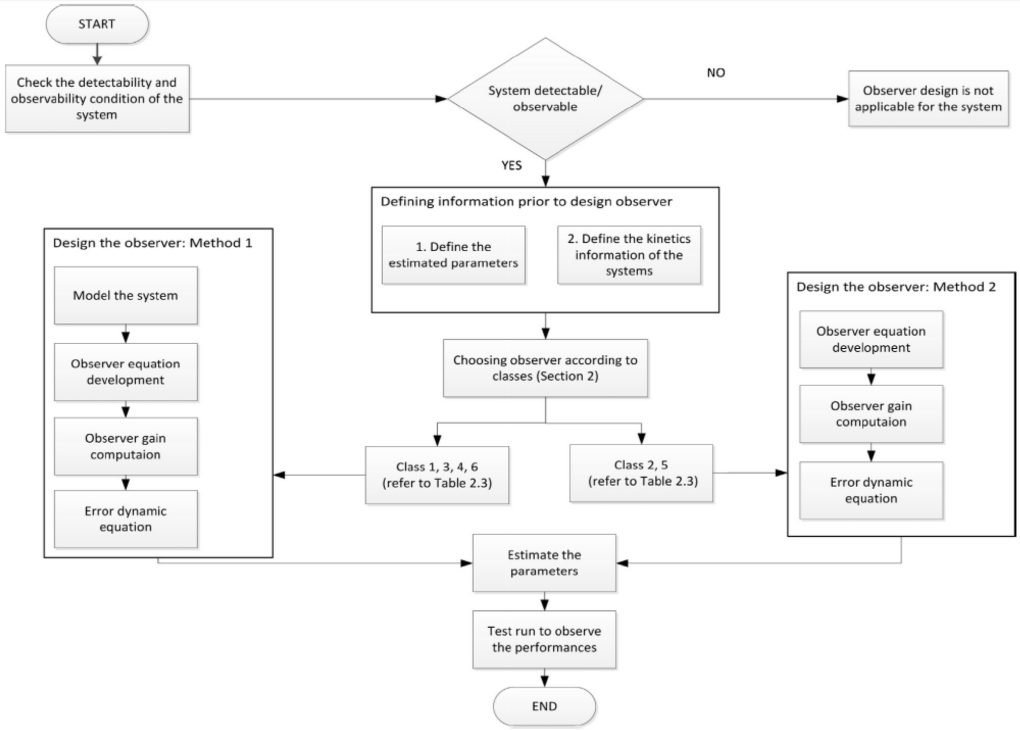

Fig. 2. General methodology for observer design.

3.1. *Observability conditions*

Two types of observability conditions typically applied for observer designs are the observability matrix and the observability Gramian. The observability matrix appears with the alteration of the state space models such as conversion to canonical forms, while the observability Gramian arises when considering the operator properties including system reduction and optimal linear quadratic regulators (Curtain and Zwart, 1995; Singh and Hahn, 2005a). Both the observability matrix and the observability Gramian provide sufficient conditions for the observability of a system; however, the observability matrix is related to the differential properties, while the observability Gramian is based on the integral conditions (Tsakalis, 2013). Furthermore, the type of observability used to detect the observable condition will depend on the formulation of the systems. Brief formulations of both observability conditions are given in Appendices A and B, respectively.

3.2. *Estimated variables*

The estimated variables are the difficult-to-measure parameters intended to be estimated using observers. They are system-dependent and not specific to one parameter for a particular process unit (Liu, 1999) such as reactor concentration in a CSTR (Salehi and Shahrokhi, 2008), production rate and solid mass fraction in a polymerization reactor (López and Alvarez, 2004) or specific growth rate in a bioreactor (De Battista et al., 2011). The estimated parameters are normally the crucial parameters that may potentially lead to uncertainty in the process and can affect product quality (Alanis et al., 2010; Fan and Alpay, 2004; Mesbah et al., 2011; Olivier et al., 2012). The parameters should also be updatable for online implementation and to eliminate bias between simulation and the online estimation implementation (Sandink et al., 2001). Examples of estimated parameters in various chemical process systems are given in Section 2 (we refer the readers to the 'Objective/Estimate(s)' column in Table 3).

3.3. *Kinetics information of the system*

The kinetics information of the system determines the system's nonlinearities based on the mathematical model that represents it (Biagiola and Figueroa, 2004b). This information is required to aid in the selection of the appropriate observers. For a system where this information is complete and system parameters are well known, the Luenberger-based observer is appropriate, while the Bayesian estimator is used for systems in which only certain system parameters are known (Dochain, 2000, 2003). When less kinetic information is available, researchers can apply exponential or asymptotic observers (Dochain, 2000; El Assoudi et al., 2002; Hadj-Sadok and Gouze, 2001; Hoang et al., 2013; Hulhoven et al., 2008). AI-based observers may be suitable for systems with incomplete model information.

3.4. *Observer formulation*

Since most observers are model-based (Boaventura et al., 2001; Chen et al., 2009; de Canete et al., 2012; Prakash et al., 2011; Vicente et al., 2000; Yang et al., 2011), the design steps include modeling of the systems prior to developing the observer equation, computing the gain of the observer and deriving the estimation error model or the error dynamic equation (D'Attellis et al., 1997; Di Ruscio, 2009; Dochain, 2003; Gajic, 2003; Soroush, 1997). Classification of recent observers into six classes as in Section 2 can be helpful in designing the observers, as we can now apply either method 1 or 2 in the design (we refer the readers to Fig. 2). For example, modeling can be simplified if the observers are from the finite dimensional and AI-based classes because those two classes can be designed for systems with incomplete models or less kinetic information (Dochain et al., 1992, 2009; Senthil et al., 2006). If the systems require specific parameter estimation such as disturbances, the focus can be narrowed down to the disturbances and fault detection observer types. Thus, we can directly apply the disturbances and faults detection observers and obtain the best estimation performance. Furthermore, if our systems are simple linear systems with easy-to-formulate models, we can apply the Luenberger-based observers instead of choosing from all other types of observers available (Damour et al., 2010a, 2010b; Mesbah et al., 2011). In addition, we can apply the hybrid observer to overcome the limitations of single observers and to improve the estimation performance (Goffaux et al., 2009; Hulhoven and Bogaerts, 2002; Hulhoven et al., 2006).

3.4.1. Model of the system

The system for observer design is normally based on a mathematical model (Ahn et al., 1999; Bagui et al., 2004; Mohseni et al., 2009), which is typically incorporated into the mass and energy balance of the systems (Bernard and Gouze, 2004; Dochain et al., 2009; James et al., 2002; Salehi and Shahrokhi, 2008) and consequently it may range from the finite-dimensional to the infinite-dimensional case. It can also include several appropriate assumptions, for example, assuming perfect mixing and constant physical parameters to simplify the modeling steps (Biagiola and Figueroa, 2004a).

3.4.2. Observer equation

The observer equation is developed to determine the observer structure for a given system based on dynamic knowledge and incorporated with the observer gain and the error dynamic equation (Bitzer and Zeitz, 2002; Cacace et al., 2010). For a linear model-based observer, the state space representation is normally used to describe the observer equation, and the measurement equation is also involved in the formulation (Fuhrmann, 2008; Patwardhan et al., 2006; Patwardhan and Shah, 2005; Senthil et al., 2006). The number of measured variables will also affect the sensitivity of the estimation (Venkateswarlu and Avantika, 2001).

3.4.3. Observer gain

The design of the observer structure will require an appropriate gain (Dochain, 2003), and it is chosen based on the stability of the error dynamics of the system (Busawon and Kabore, 2001; Yang et al., 2012). The observer gain can be solved using the Butterworth polynomial and the Ackermann formula (Di Ruscio, 2009). Additionally, the Riccati equation is also applied to determine the gain value by observing the error dynamic output (Farza et al., 2011).

3.4.4. Error dynamic equation

The error dynamic equation is needed to ensure the observer structure is bounded to the modeling error (Wang et al., 1997) to increase the robustness of the observer (Jung et al., 2008). It can be represented in terms of the linear time-varying system (Mishkov, 2005; Röbenack and Lynch, 2004) and must be designed in such a way that it is asymptotically or exponentially stable (Biagiola and Figueroa, 2002; Härdin and van Schuppen, 2007; Iyer and Farell, 1996; Röbenack and Lynch, 2004; Zambare et al., 2003). In certain systems, where the dynamic information is limited and it is difficult to develop the error bounds due to large uncertainties (Dochain, 2000), the error dynamic equation can be ignored in the observer design. This can be seen in the development of the asymptotic observer (Dochain et al., 1992, 2009).

3.5. Evaluating the observer

The performance of an observer is usually tested in simulation followed by online implementation (BenAmor et al., 2004; Bogaerts and Wouwer, 2004; Escobar et al., 2011). The test will begin with a nominal or simulator model that is different from the observer model and includes both the process and possibly measurement noise (Di Ruscio, 2009). Normally, some reasonable model errors are introduced to the simulator model to test its performance under plant model mismatches (Aguilar-Lopez and Martinez-Guerra, 2005; Aguilar-Lopez and Maya-Yescas, 2005; Jana et al., 2006; Lin et al., 2003). Poor noise assumptions can lead to bias estimation and divergence and require more assumptions for the design (Biagiola and Figueroa, 2004a).

4. Current and future trends

In previous years, single-based observers (i.e., Luenberger-based and finite-dimensional observers) have commonly been used to estimate the difficult-to-measure parameters in a chemical process system prior to generating the control design and to replace high-priced sensors in the plant. These observers, however, started to face challenges in handling uncertainties in both model and measurements (Dochain, 2003). In addition, many of these observers require accurate knowledge of the process dynamics for the design, which are difficult to obtain, especially in nonlinear chemical processes. AI-based observers have become popular for nonlinear systems due to their reduced dependency on accurate models but also are limited in terms of robustness. Thus, in order to overcome these limitations and challenges, hybrid observers have been introduced (Hulhoven and Bogaerts, 2002; Hulhoven et al., 2006; Poznyak et al., 2007). These hybrid observers also have the advantage of being easy to formulate and implement with the availability of powerful modern computing resources.

Therefore, in general, the trend in the use of observers for chemical process has changed from single-based observer design (Bara et al., 2001; Benaskeur and Desbiens, 2002; Hadj-Sadok and Gouze, 2001; Kazantzis et al., 2000) to hybrid observers design (Goffaux et al., 2009; Hulhoven et al., 2006; Prakash and Senthil, 2008), including AI-based designs, as seen in the trend pattern for the usage of recent observers in chemical process systems shown in Fig. 3. The statistics given in the figure show that although all other classes of observers have always been in use, the trends have been inconsistent and very much dependent on the particular system to be resolved. However, the hybrid observer, which did not exist before 2000, has been consistently increasing in its usage since then. This could be due to many factors but one main reason is the availability of many types of observers (as seen in Section 2) that could be easily combined in the modern software available at present (de Assis and Filho, 2000; de Canete et al., 2012; Escobar et al., 2011; Rivera et al., 2010). Hybrid observers has also becoming popular due to their ability to obtain better estimation performances, handle offsets efficiently and increase the rate of convergence (Aguilar-Lopez and Martinez-Guerra, 2007; Hulhoven and Bogaerts, 2002).

The sliding mode observer hybrid with an asymptotic/exponential observer is an example where a sliding mode observer provides good convergence rate with guaranteed robustness and stability (Hajatipour and Farrokhi, 2010) while the asymptotic/exponential observer supports a process system with minimal kinetic data (Jana et al., 2006), which is beneficial in situations where there is a lack of information or data regarding

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