Computers and Chemical Engineering 172 (2023) 108128

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/cace

Review

Sensor data fusion in electrochemical applications: An overview and its application to electrochlorination monitoring

E.A. Ross [a,b], R.M. Wagterveld [a], J.D. Stigter [b], M.J.J. Mayer [c], K.J. Keesman [a,b,*]

[a] Wetsus, European Centre of Excellence for Sustainable Water Technology, Oostergoweg 9, 8911 MA, Leeuwarden, The Netherlands
[b] Mathematical and Statistical Methods - Biometris, Wageningen University and Research, PO Box 16, 6700 AA, Wageningen, The Netherlands
[c] EasyMeasure B.V., Breestraat 22, 3811 BJ, Amersfoort, The Netherlands

ARTICLE INFO

Keywords:
Sensor data fusion
Electrochlorination
Monitoring
Observer
Machine learning
Soft sensor
Chlorate

ABSTRACT

Sensor Data Fusion (SDF) is a widely used means of monitoring electrochemical processes. The application of SDF contributes to solving challenges in process efficiency, control and reliability.

Due to recent, stringent regulations, there is a need to monitor the formation of by-products in electrochlorination, such as chlorate. For this development, the knowledge of SDF produced in neighboring fields of research, such as on batteries or fuel cells, can be of great value.

This paper presents an overview of the application of SDF algorithms to monitor electrochemical processes, and discusses how to best apply SDF to monitor by-product concentrations in the context of electrochlorination. Both first-principles and data-driven approaches are discussed.

Successful application of SDF to electrochlorination monitoring will improve the safety of drinking water supply. In addition, this overview can inspire and improve the application of SDF in the monitoring of other electrochemical systems.

1. Introduction

Electrochemistry is fundamental to several critical technologies, such as battery technology and some metal production processes. Its main strength is its ability to drive chemical reactions that are not spontaneous, and to do so using relatively simple means. Key challenges are that this effect is largely indiscriminate, and that local, complex physics are at the core of the technique. To meet the current challenges in greenhouse gas emissions as well as to increase cost-effectiveness, product quality and production reliability, it is increasingly desirable to monitor such electrochemical processes in real-time (Waag et al., 2014; Lin et al., 2019).

A much-used method of monitoring is that of sensor data fusion (SDF) (Hall and Llinas, 1997; Khaleghi et al., 2013). Such techniques combine data from multiple sensors, as well as related information, to achieve a more specific inference than would be possible with a single sensor (Hall and Llinas, 2001). This has proven especially useful in applications that rely on electrochemical processes, as the variables of interest, such as cell conditions, often cannot be measured directly. For example, SDF has been used to estimating the State of Charge (SOC) in batteries since the 1970s (Karunathilaka et al., 1983). Besides batteries the application of SDF in electrochemistry has been actively researched in the fields of fuel cell technology and the production of aluminum, among others.

Electrochemical processes are also used in the water technology sector (Gupta et al., 2012; de Moura et al., 2014). Here, there is a clear drive to monitor processes more closely as well, with SDF again being a promising means (Mohd Ali et al., 2015). Specific benefits may be to minimize costly sample analysis, and to enhance process control.

One prospective application is the monitoring of by-product formation during electrochlorination, which is an on-site means of producing a chlorine-based disinfectant electrochemically. This has become especially pressing since recent regulations regarding oxychloride concentrations in drinking water strictly limit the chlorate output of electrochlorinators in the European Union (World Health Organization, 2017; Snyder, 2016; Cotruvo and Fawell, 2016; The European Parliament and the Council of the European Union, 2020; The European Commission, 2015). Since there is no chlorate sensor commercially available, the current solution is to frequently analyze samples (Ross et al., 2022). A monitoring system based on SDF could potentially provide chlorate estimates in real-time without frequent sample analysis, which would both reduce cost and benefit safety and compliance.

To monitor electrochlorination through SDF is a new application for a well-developed technology. Therefore, it is worthwhile gain an

* Corresponding author at: Mathematical and Statistical Methods - Biometris, Wageningen University and Research, PO Box 16, 6700 AA, Wageningen, The Netherlands.
E-mail address: karel.keesman@wur.nl (K.J. Keesman).

https://doi.org/10.1016/j.compchemeng.2022.108128
Received 12 August 2022; Received in revised form 28 November 2022; Accepted 23 December 2022
Available online 13 January 2023

Abbreviations

AEKF	Adaptive Extended Kalman Filter
AUKF	Adaptive Unscented Kalman Filter
AKF	Adaptive Kalman Filter
ANN	Artificial Neural Network
ARMA	Autoregressive Moving Average
BMS	Battery Management System
CKF	Cubature Kalman Filter
CNN	Convolutional Neural Network
DNN	Deep Neural Network
DT	Decision Tree
ECM	Equivalent Circuit Model
EKF	Extended Kalman Filter
ESO	Extended State Observer
GPR	Gaussian Process Regression
KF	Kalman Filter
KNN	K Nearest Neighbors
LSTM NN	Long-Short Term Memory Neural Network
ML	Machine Learning
PEMFC	Proton Exchange Membrane Fuel Cell
PID	Proportional, Integral, Derivative
PF	Particle Filter
PSO	Particle Swarm Optimization
RF	Random Forest
RLS	Recursive Least Squares
RNN	Recurrent Neural Network
RUL	Remaining Useful Life
SDF	Sensor Data Fusion
SMO	Sliding Mode Observer
SOC	State of Charge
SOE	State of Energy
SOFC	Solid Oxide Fuel Cell
SOH	State of Health
SOP	State of Power
SPKF	Sigma Point Kalman Filter
SVM	Support Vector Machine
SVR	Support Vector Regression
UKF	Unscented Kalman Filter

overview of the adjacent applications where SDF has been researched and applied, to learn how this technique can best be applied to the monitoring of by-product formation in electrochlorination. In this work will first explain why an uncorrected model is insufficient in the case of electrochlorination, followed by a brief introduction to the various SDF methods. We will subsequently detail the method of gathering relevant sources that apply SDF to electrochemical processes and present the found works. We will finally discuss the implication of the found works to by-product monitoring of the electrochlorination process, followed by a conclusion.

2. Monitoring of electrochlorination

To properly understand the need for Sensor Data Fusion, it is necessary to gain an understanding of the problem, and why, precisely, a model of the process in question cannot suffice. In this section the process of electrochlorination will be described, with the goal of assessing the possibility of modeling the formation of chlorate without employing sensors to correct the model.

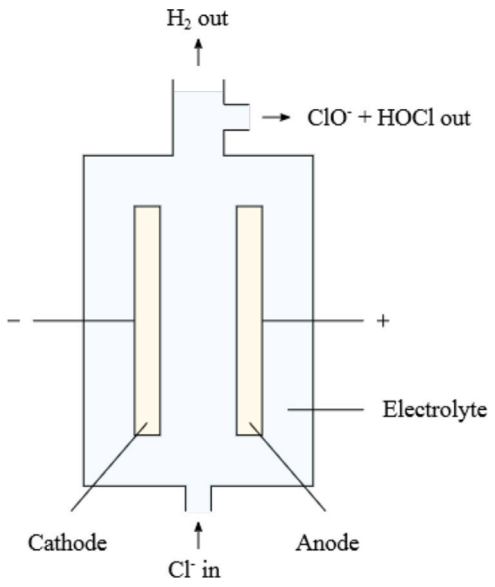

Fig. 1. Electrochlorinator diagram.

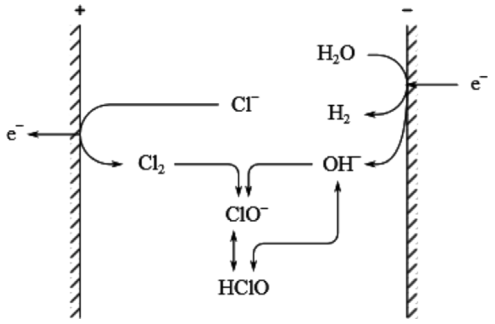

Fig. 2. Electrochlorination process, simplified.

An electrochlorinator is, in essence, a flow cell, consisting of a bath with a set of electrodes, as illustrated in Fig. 1. An overview of the chemical species evolution without parasitic reactions is given in Fig. 2.

The feed consists of a sodium chloride solution of approximately 30 g/l, sea water or wastewater (Black & Veatch Corporation, 2009). The water is typically softened and strained if necessary. At the cathode, water is electrolyzed into hydrogen gas and hydroxide.

$$2\,H_2O + 2\,e^- \longrightarrow 2\,OH^- + H_2 \quad (1)$$

The hydrogen forms bubbles, as it rapidly saturates the water when formed. The gas moves upwards due to the difference in density compared to water, and pulls the solution through the electrode gap. The hydroxide is rejected from the cathode surface, through both diffusion and migration induced by the electrical potential.

At the same time, chloride is attracted to the anode by both migration and a diffusion gradient, as it is consumed at the electrode surface. At the electrode surface the chloride is oxidized into chlorine.

$$2\,Cl^- \longrightarrow Cl_2 + 2\,e^- \quad (2)$$

Typically this forms chlorine bubbles, due to an over saturation at the electrode surface, which then diffuse to the bulk of the fluid. Since the process in question is intended for industrial production, it is usually controlled such that the current density and electrode potential are relatively high.

The chlorine gas quickly reacts with the hydroxide to form hypochlorite.

$$Cl_2 + 2\,OH^- \longrightarrow Cl^- + ClO^- + H_2O \quad (3)$$

The hypochlorite, in turn, forms an equilibrium with hypochlorous acid, as it reacts with hydroxide. This effect would, if no other reactions occur, stabilize the fluid at about pH 10, depending on temperature (Czarnetzki, 1989; Agency for Toxic Substances and Disease Registry (ATSDR), 2010).

$$ClO^- + H^+ \leftrightarrow HOCl \tag{4}$$

The above reactions are desired, and the process conditions and electrode material are chosen with the production of free chlorine in mind. The electrochemical formation of chlorate is considered parasitic, and is thought to occur through several possible paths. The most commonly assumed mechanism is that of direct hypochlorite oxidation, and to a lesser degree, the oxidation of hypochlorous acid, at the anode (Czarnetzki, 1989). These reactions are called the Foerster reactions. Naturally, the reactants have to move to the electrode from the bulk.

$$6\,ClO^- + 3\,H_2O \longrightarrow 2\,ClO_3^- + 4\,Cl^- + 6\,H^+ + \frac{3}{2}\,O_2 + 6\,e^- \tag{5}$$

$$6\,HClO + 3\,H_2O \longrightarrow 2\,ClO_3^- + 4\,Cl^- + 12\,H^+ + \frac{3}{2}\,O_2 + 6\,e^- \tag{6}$$

Another pathway is the oxidation of hypochlorite to chlorate via chlorite (Tasaka and Tojo, 1985).

$$ClO^- + 2\,OH^- \longrightarrow ClO_2^- + H_2O + 2\,e^- \tag{7}$$

$$ClO_2^- + 2\,OH^- \longrightarrow ClO_3^- + H_2O + 2\,e^- \tag{8}$$

Direct oxidation of chlorine is also thought to be possible (Tasaka and Tojo, 1985).

$$Cl^- + 3\,H_2O \longrightarrow ClO_3^- + 6\,H^+ + 6\,e^- \tag{9}$$

Finally, chlorate may be formed via electrochemically generated hydroxide radicals, or its strongly oxidative derivatives such as ozone and peroxide (Siddiqui, 1996). Although Reaction (5) is criticized for its complexity (Cornell et al., 2003), the direct oxidation of hypochlorite was found to be the most prominent pathway of electrochemical chlorate formation on Pt/Ti electrodes (Jung et al., 2010).

Another anodic reaction that is considered to be parasitic is the formation of oxygen, by the electrolysis of water.

$$2\,H_2O \longrightarrow O_2 + 4\,H^+ + 4\,e^- \tag{10}$$

The electrode materials are chosen such that the chlorine evolution is preferred over oxygen formation, but the formation of oxygen will not be wholly prevented (Czarnetzki, 1989).

The actual process is still more complex. Oxychlorides may each decompose, perchlorate may be formed, and additional equilibria exist between oxychlorides and their protonated variants. In addition, impurities such as bromine may react as well.

The rates of the reactions are usually expressed as current densities, that is, the current that is utilized for that reaction, per unit of electrode surface area. The current density may be limited by electrode kinetics, by mass transport, or both. In case the current density for a particular species evolution is only determined by a mass transport limitation, the following equation may be used. We assume that the reaction has only one reactant.

$$i = nFk(c_b - c_s) \tag{11}$$

Here, i is the current density for the reaction rate of interest. Furthermore, n is the number of electrons involved with the reaction, F is Faraday's constant, k is the mass transport coefficient and c_b and c_s are the reactant concentrations in the bulk and at the electrode surface, respectively.

In case the current density is only determined by the electrode kinetics, i may be found using the Butler–Volmer equation, shown below in extended form.

$$i = i_{o,ref}\left(\frac{c_s}{c_{ref}}\right)^{\gamma}\left[\exp\left(\frac{\alpha_a F\eta_s}{RT}\right) - \exp\left(-\frac{\alpha_c F\eta_s}{RT}\right)\right] \tag{12}$$

Here, $i_{o,ref}$ is the reference exchange current density at reactant concentration c_{ref}, γ the activity coefficient, α_a and α_c are, respectively, the anodic and cathodic charge transfer coefficients, η_s is the surface overpotential, R is the universal gas constant and T is the temperature. The Butler–Volmer equation is semi-empirical, which means that part of its parameters are determined experimentally per implementation, under standard and steady-state conditions. To find the actual current density Eq. (11) and Eq. (12) may be equated to one another and solved numerically.

A critical aspect is that the final current density depends on the species activity at the electrode. Due to the high overpotential, the mass transfer is expected to be limiting, at least in part (Fuller and Harb, 2018). The mass transfer, in turn, depends highly on the degree of mixing that occurs due to bubble formation. Although empirical approximations of mass transfer coefficients exist (Mohanta and Fahidy, 1977; Sedahmed and Nirdosh, 2007), this problem remains difficult to solve accurately, even with Computational Fluid Dynamics modeling, due to the multiphase and multidimensional nature of the problem. The amount of bubble formation and its dynamics also depends on temperature, as well as the electrode reactions themselves. This means that with the current technology it is infeasible to accurately determine the bubble formation, and by extension the electrochemical reaction rates, in real-time.

However, it may be feasible to employ a model that compromises on accuracy, which is then corrected through additional sensor data and a sensor data fusion (SDF) algorithm. This approach is frequently used in the monitoring of other electrochemical systems. This paper aims to give an overview of the available knowledge, in support of a broader application of SDF in the monitoring of electrochemical systems.

3. Approaches to monitoring

3.1. The state–space context

To understand why the choices in the various fields of application correlate or differ, it is necessary to gain an understanding of sensor data fusion, which is a broad set of techniques in itself. The available SDF methods and the differences between them can be better understood when placed in a state–space framework, as defined in mathematical systems theory. The equations may be nonlinear, and it is possible to construct a state–space model based on empirical relations. In its most generic and extensive form, the state–space representation for finite-dimensional systems is given by:

$$\frac{d}{dt}x = f(t, x, u, w; \theta) \tag{13}$$

$$y = g(t, x, u, v; \theta) \tag{14}$$

Here, x is a vector which contains the current states of the system and potentially the dynamic process variables used to describe the system, and y is the vector containing the outputs of the system. The variable t is time, vector u represents the control inputs and vector θ contains the model parameters that are assumed to be constant. The stochastic vectors w and v represent system noise and measurement noise, respectively.

3.2. Model-based sensor data fusion

A commonly-used class of SDF algorithms is that of state observers. In classical observer theory, the output vector y is used to represent the sensor outputs, while the state vector x represents the internal states that drive the modeled process. This includes the states that are to be monitored, either directly or indirectly. The input u is generally assumed to be known. A model of a real system, described in Eqs. (13) and (14) by only the determinate terms, can then be corrected in real time using sensor data (Luenberger, 1964; Dochain, 2003):

$$\frac{d}{dt}\hat{x} = f(t, \hat{x}, u, \theta) + L(y - \hat{y}) \tag{15}$$

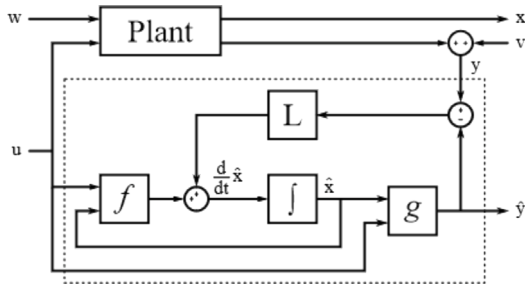

Fig. 3. Diagram of a Luenberger observer (dashed box) connected to a plant.

$$\hat{y} = g\,(t, \hat{x}, u, \theta) \tag{16}$$

Here the "hat" indicates estimates, and y is the sensor data as measured. L represents a gain matrix, used to map and scale the prediction error $(y - \hat{y})$ to the corrections on $\hat{x}$. The resulting algorithm is called a Luenberger observer, shown graphically in Fig. 3.

This approach may be expanded upon by considering uncertainties, as expressed in terms of known or assumed covariance matrices of the system noise (w) and sensor noise (v). Applying such considerations to a linear system has lead to the well-known Kalman Filter (KF), which, given the uncertainties in w and v, aims to optimally balance the model output with the sensor data (Kalman, 1960; Kalman and Bucy, 1961). If both w and v are Gaussian, the basic KF leads to the exact Bayesian filtering distribution, sharing the connection between Kalman and Bayesian filtering. One well-known variant of the basic Kalman filter is the Extended Kalman Filter (EKF) for non-linear systems (Eq. (15)–(16)).

The Kalman filter updates a state estimate covariance matrix based on the predetermined system and noise covariance matrices, the innovation (that is, the difference between y and $\hat{y}$) and the system's dynamics (Keesman, 2011). Through this state estimate covariance matrix, the previous performance affects the next estimation. The state estimate covariance matrix may also be determined by calculating predictions for multiple sample points, from which the state estimate covariance matrix may be determined, such as in the Unscented Kalman Filter (UKF). While the KF, EKF and UKF assume and describe Gaussian probabilities through mean and (co)variances, Monte Carlo methods such as the Particle Filter (PF) describe the state probabilities using the sample distribution itself (Gordon et al., 1993; McAfee et al., 2022).

Alternatively, rather than using a covariance matrix or particle distribution to encode previous error statistics, the estimation may be based on a moving window of previous inputs and measurements. These Moving Horizon Estimators (MHE) may be based on a state–space model, or on data-driven models, such as a Neural Net. In the former case, the goal is to optimize the estimated states $\hat{x}$ by minimizing the innovation, given the recorded previous inputs (Hu et al., 2018).

Methods that use multiple sample points or optimization routines are more computationally demanding than an EKF. Though the availability of computational power has steadily increased (Sui et al., 2021), this is still noted as a significant downside in recent works (Chang et al., 2022; Shi et al., 2022a; Wu et al., 2022a).

3.3. Observability and detectability

A critical problem in SDF is the question of whether there is sufficient information available to accurately determine the state that is estimated. In the case of observers, the model structure can be analyzed to answer this question. The model structure should preferably be such that, by observing the difference between estimated model output data $\hat{y}$ and real sensor data y, the estimated state vector $\hat{x}$ can be corrected, and converges to the real, but unknown, state x. For linear, time-invariant systems Kalman devised a test that can prove whether this is the case (Kalman, 1963), but for non-linear systems the observability problem becomes more difficult (Stigter et al., 2017).

In certain cases it is possible to construct a stable observer, where $\hat{x} \to x$, in spite of a lack of full observability (Zhang et al., 2021b; Ross et al., 2022). In this case, the system needs to be detectable, that is, the states that are not observable must always be stable. The consequence is that the error dynamics of the non-observable, but stable states are determined by the dynamics of the system (Kwakernaak and Sivan, 1972).

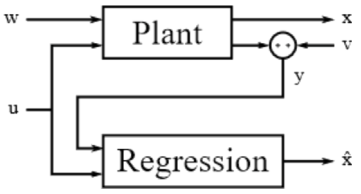

Fig. 4. Diagram of a regressor connected to a plant.

3.4. Data-driven sensor data fusion

Instead of developing a model based on first-principles, one can estimate an unknown variable using a model based solely on data, via regression or classification analysis. Machine Learning methods fall in this category. As in observer-based SDF, both inputs u and outputs y can be used. In the case of the estimation of a continuous variable, the key difference with observers is that the sensor data is not used to correct state-equations, but is rather used as an input for a regressor (in this case, the variables that are used as input are named independent variables, or features). Note that both the input signal u and sensor data y can be subjected to noise (see Fig. 4).

A machine learning algorithm is fit by optimizing a generic model's parameters such that the error between x and $\hat{x}$ is minimized. Once fit, the model can be applied to new data, under the assumption that the data is sufficiently similar to that used in the fitting process. The different machine learning algorithms used in the context of the monitoring of electrochemical systems are categorized in Ng et al. (2020), Shu et al. (2021), Rauf et al. (2022), Oji et al. (2021), Sui et al. (2021), Vanem et al. (2021), Li et al. (2019), Zheng et al. (2013).

The data used as input to the machine learning algorithm is often processed prior to use (Zhang et al., 2022b; Li et al., 2019). For instance, in the case of a many-cell system, dimensionality reduction may be applied, via Principle Component Analysis (PCA) or similar algorithms (Zheng et al., 2013; Zhang et al., 2022b). Such feature engineering techniques can improve the model's accuracy in spite of using the same data, since the data provided to the machine learning algorithm is richer in information (Ang and Paw, 2021).

3.5. Hybrid models

First-principles and data-driven models each have their benefits and drawbacks (Sansana et al., 2021). First-principles models require detailed knowledge of the system, both in the form of mechanisms and parameters. They are more laborious to formulate than data-driven models, but once formulated they are relatively broadly applicable. Data-driven models require little to no *a priori* knowledge, but do require significantly more data to create. They are only applicable to the circumstances in which the data was gathered.

By combining first-principles and data-driven (sub)models, these benefits and drawbacks may be balanced (von Stosch et al., 2014). This can lead to a higher accuracy, better calibration and extrapolation

properties, and improved interpretability, with similar resources spent in terms of engineering effort and data acquisition.

In electrochemical applications, one of the early techniques was to tailor machine learning algorithms to physical mechanisms or constraints (Richard et al., 2009; Ahmed et al., 2010; Xu et al., 2022a; He et al., 2022a). Such an approach was shown to improve prediction accuracy, both in interpolation and extrapolation, and was more interpretable (von Stosch et al., 2014). First-principles models are also frequently used as a means of feature engineering (Li et al., 2019). In the monitoring of battery systems observers and regressors are frequently used concurrently. In this case, an observer monitors the State of Charge in the short term, which is then used as an input to a machine learning algorithm that determines the State of Health in the long term (Jiang and Song, 2022; Adaikkappan and Sathiyamoorthy, 2021).

3.6. Adaptive models

Model parameters (θ) can also be identified in real time, instead of being set in advance. This is especially relevant to electrochemical applications, as electrochemical cells may degrade over time. If so, the model used for an SDF algorithm may no longer be accurate, and requires updating.

In adaptive models a selected set of parameters is considered to be time-varying, rather than constant. In case of classical observer theory these parameters become part of the, now augmented, state vector (x). Consequently, the selected model parameters are included in an observability analysis and in the correction loop, much like the process states (Goodwin and Payne, 1977). Alternatively, Reinforcement Learning techniques may be applied to adapt model parameters in real-time (Natella and Vasca, 2021).

4. Search methodology

The search for relevant works was done using the Web of Science database, and was done in three stages. First, the adjacent fields were identified. This was done by searching with a combination of a term related to electrochemistry and a term related to sensor data fusion. The exact search term used is as follows:

```
(Electrochemi* OR Electrode OR Anode OR Cathode) AND (''Sensor fusion'' OR ''Data fusion'' OR Observer OR ''Machine learning'' OR Kalman)
```

The title, abstract and keywords were searched, and medical and non-chemical subjects were excluded.

In the next phase, a search was performed to identify any existing review papers. This was done per field of application using the following search line, replacing the term "application" as appropriate:

```
(Application) AND (''Sensor fusion'' OR ''Data fusion'' OR Observer OR ''Machine learning'' OR Kalman) AND (Review OR Overview)
```

Finally, the individual fields of application were researched. This was done using the following term:

```
(Application) AND (''Sensor fusion'' OR ''Data fusion'' OR Observer OR ''Machine learning'' OR Kalman)
```

This was done for time periods after the latest relevant review paper. Only works from Q1 and Q2 journals have been included in the results.

5. Results and discussion

The results of the search are listed in Appendix A, along with a brief description of each of the found fields of application. Fig. 5 gives an overview of the results, specifically of what goals and approaches are relevant to the fields of application. In this section we will detail how the works are related to the monitoring of by-product formation in electrochlorination, and what lessons may be taken from them.

5.1. Applicability of SDF methods to electrochlorination monitoring

Currently, little work has been published regarding the application of SDF to electrochlorination (Ross et al., 2022). However, the works found in adjacent fields of application can help finding a better approach to SDF for electrochlorination.

In terms of objective, the need to determine a chemical matrix is also present in fuel cell technology (Liu et al., 2020b), aluminum smelting (Shi et al., 2022b; Zhang et al., 2017, 2018) and flow batteries (Nolte et al., 2021). Frequently, this is not the final goal. Instead, estimating concentrations or partial pressures is in service of estimating the SOH, or for controlling the process.

As shown in Fig. 5, the type of model that is applied varies greatly. From the found works it is clear that estimators based on first-principles are preferred in case they are used to inform control algorithms, as observers are readily integrated with control theory (Liu et al., 2020b; Shi et al., 2022b). These use voltage and current signals along with a simplified electrochemical model or Equivalent Circuit Model (ECM) (Waag et al., 2014; Fleischer et al., 2014; Ng et al., 2020).

The arguments in favor of using a data-driven solution to estimate concentrations regard the process' complexity. It is argued that, in contrast to first-principles models, machine learning methods are able to capture the complexity of electrochemical processes, and that a lack of knowledge regarding the process would preclude the development of an accurate first-principles model (Zhang et al., 2018). Nonetheless, first-principles models have been used successfully, at least in case the concentrations to estimate strongly affect the sensor signals.

In case the objective is to monitor by-product concentrations, the by-products may not affect the sensor readings significantly, which complicates the application of SDF. This is especially true in the absence of ion-selective sensors or distinct signals such as a usable electromagnetic absorption peak, as is the case with chlorate (Monteiro et al., 2021; Ross et al., 2022). Since by-products are typically small in amount relative to the main product or components, these species influence sensors that measure bulk properties only weakly. Although sensor data fusion has been used for the estimation of by-product concentrations (Mohd Ali et al., 2015; Chairez et al., 2007), to the authors' knowledge there is no research in which the by-product stems from an electrochemical process. The closest example is that of impurity detection in copper production (Wikström et al., 1998a,b).

Whether the sensor signals can be sufficient to accurately estimate by-product concentrations remains to be researched. In the absence of a signal that has a direct correlation with the by-product concentration, four approaches are currently foreseen. The first is to still attempt to use the sensors measuring bulk properties, such as electrical conductivity or potentials, using a first-principles model. In this case it is crucial that the system noise w and sensor noise v have a very low bias. While variance is important in terms of uncertainty, the downside of a high variance can be mitigated over time by observing a large number of measurements. This is not possible with an unknown bias. Ensuring a very low bias is especially difficult in the case of electrochemical systems, as electrodes deteriorate over time, and sensors may drift (Nolte et al., 2021).

Similarly, a data-driven model may be used that employs the same sensors and inputs. The fundamental difficulties are the same, as deterioration of the electrodes and sensor drift would strongly affect the accuracy of the estimate of the by-product concentration.

Another solution is to develop a model that is detectable, rather than observable (Zhang et al., 2021b; Ross et al., 2022). This implies that a part of the state equations are corrected, and that the state equations that determines the by-product formation remain uncorrected. In the case of the monitoring of by-product formation in an electrochemical process, the uncorrected state equations would include the submodel of the electrode kinetics of the by-product formation. Although semi-empirical models exist, it is not yet known whether

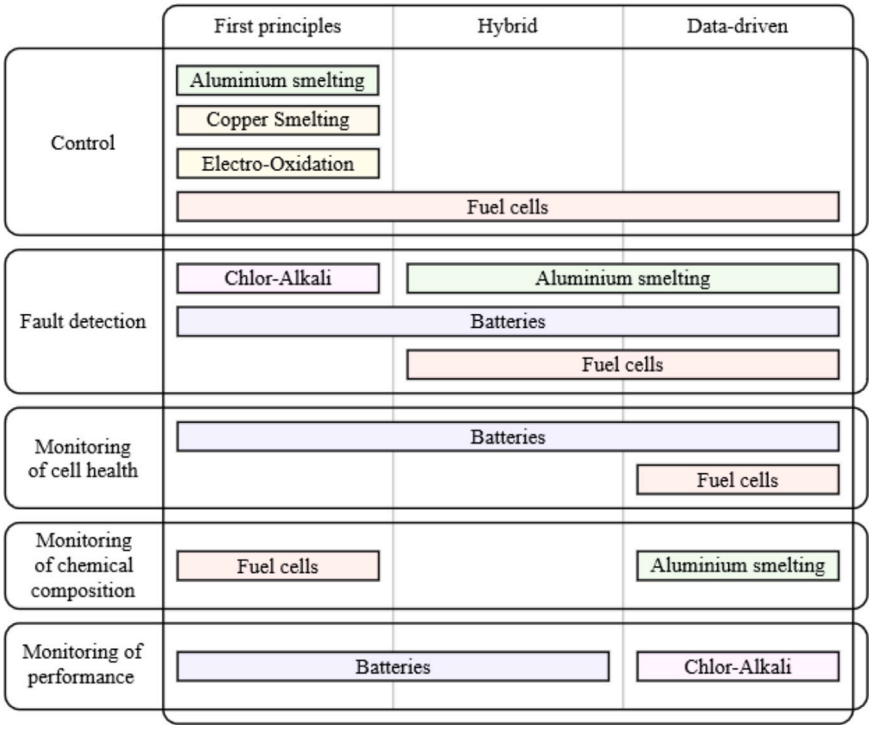

Fig. 5. The electrochemical process monitoring fields categorized by SDF goals and approaches.

these are sufficiently robust for the electrochlorination case, and bubble formation complicates the calculation, as mentioned previously.

Finally, a combination of the previously mentioned approaches may be employed, in the form of a hybrid approach (von Stosch et al., 2014; Sansana et al., 2021; Karniadakis et al., 2021). Although hybrid architectures have not been extensively used to estimate the chemical composition of a fluid, they are expected to offer benefits in terms of accuracy and data requirements. This is because, although it is difficult to model the electrochemical processes accurately, high-level aspects such as changes in temperature and the mixing of fluids can be described well using first-principles models. To model these aspects through a first-principles model means there are determined robustly and in a manner that is broadly applicable, which eases the task set for the data-driven model.

5.2. Additional considerations

In addition to the general architecture of estimation algorithms, a number of additional considerations will inform or limit the design of the SDF algorithm.

The SDF estimation is dependent on what inputs u and sensor data y with their uncertainties is available. The prevalent sources of information in the found works were the potentials and currents over the electrodes. These can be determined affordably and in real-time, and often need to be known regardless, to control the process, for example. Another aspect is whether sensors can feasibly be added. In aluminum smelting the environment is corrosive, with high temperatures and with a strong magnetic field, which complicates the placement of additional sensors (Viumdal and Mylvaganam, 2010; Yue et al., 2017). In battery systems surface temperature measurements are often used, though not per-cell, due to the quantity of cells in a battery (Vennam et al., 2022; Elsergany et al., 2022; Pang et al., 2021; Raijmakers et al., 2019). Electrochlorination lends itself well to the placement of additional sensors. There is a bulk product flow with relatively high concentrations, and it is sufficiently benign for most commercial, industrial sensors. For instance, in Ross et al. (2022), a UV-a absorption sensor was used in conjunction with temperature and pH probes to monitor the free chlorine concentration, which is a major component of the chemical matrix.

In case a data-driven model is used, obtaining the data becomes a consideration. While the use of data can be powerful, the data is specific to a system or set of systems, as well as the conditions present during the data gathering campaign. To reduce the need to gather data for new situations, such as a new cell, transfer learning has become an important topic (Wang et al., 2022a; Deng et al., 2022). Using such techniques data-driven models can be made applicable to a situation different from that on which the data is based, through limited additional data regarding the new situation. Furthermore, hybrid methods can reduce the demands regarding data, as a portion of the process is modeled using first-principles, and should theoretically not require data to represent, other than for sensor calibration and model parameters (von Stosch et al., 2014). This is especially relevant in electrochemical applications, as the electrochemical processes are affected by a large number of chemical and physical parameters.

In the case of by-product monitoring, each data entry represents a sample of the fluid, that needs to be taken and analyzed. As such, the cost per data entry is not trivial and datasets may be limited in size. This may limit the use of highly complex machine learning models. In addition, as the process depends on variables such as feed chemistry and electrode quality, the problem of a high dimensionality strongly applies.

A method of increasing the amount of available data is to collect the data of a large number of product instances, and train models at a central server, leading to so-called cloud-connected products (Shu et al., 2021; Wang et al., 2021b; Wassiliadis et al., 2021). Transfer learning methods can aid with bridging the gap between the different product instances (Vanem et al., 2021).

A current line of research is to update the models in real-time, using incremental, self-learning or autoregressive models (Shu et al., 2021; Sui et al., 2021). In this case the algorithm's model parameters are updated based on the error of the estimations. Such a strategy is valuable in the face of slowly changing conditions, such as changes in feed quality, electrode degradation or sensor drift. Unfortunately, in contrast to SOH estimation, for instance, the estimates are expected

to be verified infrequently in the case of the estimation by-product concentrations due to the cost of sample analysis. Consequently, the estimation algorithm cannot be updated frequently on the basis of the estimation error.

5.3. General discussion

Electrochemical models based on first-principles generally assume that the chemical composition and reactions are fully known. For electrochlorination this will not be the case. While the source water is treated and there are specifications that the used sodium chloride salts should meet, the chemical composition of the feed water will still vary highly between locations. Within one location, the feed might gradually change over time, as well. Varying chemical composition of feed material can be seen in the fuel cell- and smelting applications too. Adaptive models, such as applied when accounting for cell degradation in batteries, seem to be a suitable solution to this problem (Nolte et al., 2021). In addition, research is done on how to improve classical observers with neural networks, to account for such complex chemistry (Porru et al., 2000).

In the literature, the gap between theoretical or laboratory work and operating the algorithms in practice, is seen as one of the main issues persisting today (Shu et al., 2021; Sui et al., 2021; Vanem et al., 2021; Wang et al., 2021b; Wassiliadis et al., 2021; Peng et al., 2021; Wang et al., 2021h). There are different reasons that are noted. First, modeling simplifications such as ignoring non-linearities and hysteresis raise concerns (Wang et al., 2021b). Frequently temperature changes are left out of scope, even when it is known that these will affect the estimates (Nolte et al., 2021; Wang et al., 2021b; Yang et al., 2021b; Wang et al., 2021h). This is often done in the absence of temperature sensor data (Wei et al., 2021). Second, the laboratory conditions often fail to represent practical conditions, especially when the goal is to determine the RUL, or to detect faults (Shu et al., 2021; Sui et al., 2021; Wang et al., 2021h). This is because temperature changes, vibrations and dynamic operating conditions may all affect the degradation of the electrochemical systems in question. Finally, the quality of the available data that is available when the algorithm is implemented in practice may not be as accurate as assumed (McCarthy et al., 2021; Vanem et al., 2021; Yang et al., 2021b).

When designing a monitoring algorithm for use in practice, the computational resources available need to be considered (Shu et al., 2021; Wassiliadis et al., 2021; Yang et al., 2021b; Zhou et al., 2022), though the amount of computational power available is expected to increase (Sui et al., 2021). In addition, power-constrained applications such as mobile devices, the power to run the algorithms is a significant concern (McCarthy et al., 2021). To find a good balance between accuracy and efficiency, prudent model and feature selection is required (Shu et al., 2021; Wang et al., 2021b). Analyzing the sensitivity of the model to its inputs and parameters can help here (Wang et al., 2021b), and feature reduction may reduce complexity without significantly reducing accuracy (Shu et al., 2021). For self-learning data-driven methods, it is necessary to consider the amount of training time required to update the model as well (Shu et al., 2021). This aspect of training data is an on-going research item in the field of design of experiments, as found in statistical and system identification literature.

6. Conclusions

The monitoring of chlorate formation in electrochlorination has become important due to new and stringent regulations. Due to the complexity of the electrochemical process it is not possible monitor chlorate formation with a model that simply simulates, and is not corrected by sensor data. This trait is shared with a number of other electrochemical processes, where the challenge is to monitoring the process. Sensor Data Fusion has been used as solution, in different forms. It was found that especially the battery and fuel cell applications are well-researched, though there are a number of fields that receive a smaller amount of attention as well. The differences in applied methods can be traced back to the distinct properties of the processes in question, as well as the demands of the products they are part of.

When designing algorithms for electrochlorination by-product monitoring main challenge is that the by-product concentrations to be estimated are low relative to the bulk product, which means they have only a small influence on the sensor readings. Four potential solutions are foreseen. One approach is to reconstruct the chlorate concentration from the small influence that the chlorate in the solution has on 'bulk' sensor readings, such as the electrical conductivity, through a first-principles model. A purely data-driven approach is also possible, by simply attempting to correlate sensor readings and process conditions with the chlorate concentration. A detectable first-principles model may devised, and finally, a hybrid solution may be possible, that can better balance data requirements, robustness and accuracy. Research specific to electrochlorination is required to determine whether these approaches are feasible.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgments

This work was performed in the cooperation framework of Wetsus, European Centre of Excellence for Sustainable Water Technology (https://www.wetsus.eu). Wetsus is co-funded by the Dutch Ministry of Economic Affairs and Climate Policy, the Northern Netherlands Provinces and the Province of Fryslân. The authors would like to thank the participants of the research theme "Sensoring" for the fruitful discussions and financial support.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.compchemeng.2022.108128.

References

Adaikkappan, M., Sathiyamoorthy, N., 2021. Modeling, state of charge estimation, and charging of lithium-ion battery in electric vehicle: A review. Int. J. Energy Res. 2141–2165.

Agency for Toxic Substances and Disease Registry (ATSDR), 2010. Toxicological Profile for Chlorine. Technical Report, U.S. Department of Health and Human Services.

Ahmed, N., Atiya, A., El Gayar, N., El-Shishiny, H., 2010. An empirical comparison of machine learning models for time series forecasting. Econometric Rev. 29 (5), 594–621.

Ang, E.Y.M., Paw, Y.C., 2021. Efficient linear predictive model with short term features for lithium-ion batteries state of health estimation. J. Energy Storage 44 (B), 103409.

Black & Veatch Corporation, 2009. White's Handbook of Chlorination and Alternative Disinfectants, fifth ed. John Wiley and Sons, Inc.

Chairez, I., Poznyak, A., Poznyak, T., 2007. Reconstruction of dynamics of aqueous phenols and their products formation in ozonation using differential neural network observers. Ind. Eng. Chem. Res. 46, 5855–5866.

Chang, Y., Zou, J., Fan, S., Peng, C., Fang, H., 2022. Remaining useful life prediction of degraded system with the capability of uncertainty management. Mech. Syst. Signal Process. 177, 109166.

Cornell, A., Haåkansson, B., Lindbergh, G., 2003. Ruthenium-based dimensionally stable anode in chlorate electrolysis. J. Electrochem. Soc. 150 (1), D6–D12.

Cotruvo, J., Fawell, J.K., 2016. Chlorine Dioxide, Chlorite and Chlorate in Drinking-water. Background Document WHO/FWC/WSH/16.49, World Health Organization.

Czarnetzki, L., 1989. Aspects of electrochemical production of hypochlorite and chlorate (Ph.D. thesis). Technische Universiteit Eindhoven.

de Moura, D.C., de Araújo, C.K.C., Zanta, C.L., Salazar, R., Martínez-Huitle, C.A., 2014. Active chlorine species electrogenerated on Ti/Ru0.3Ti0.7O2 surface: Electrochemical behavior, concentration determination and their application. J. Electroanal. Soc. 731, 145–152.

Deng, Z., Lin, X., Cai, J., Hu, X., 2022. Battery health estimation with degradation pattern recognition and transfer learning. J. Power Sources 525, 231027.

Dochain, D., 2003. State and parameter estimation in chemical and biochemical processes: A tutorial. J. Process Control 13, 801–818.

Elsergany, A.M., Hussein, A.A., Wadi, A., Abdel-Hafez, M.F., 2022. An adaptive auto-tuned polynomial-based extended Kalman filter for sensorless surface temperature estimation of Li-ion battery cells. IEEE Access 10, 14038–14048.

Fleischer, C., Waag, W., Heyn, H.M., Sauer, D.U., 2014. On-line adaptive battery impedance parameter and state estimation considering physical principles in reduced order equivalent circuit battery models part 2. Parameter and state estimation. J. Power Sources 262, 457–482.

Fuller, T.F., Harb, J.N., 2018. Electrochemical Engineering. John Wiley and Sons, Inc.

Goodwin, G.C., Payne, R.L., 1977. Dynamic System Identification: Experiment Design and Data Analysis. Academic Press.

Gordon, N.J., Salmond, D., Smith, A.F.M., 1993. Novel approach to nonlinear/non-Gaussian Bayesian state estimation. IEE Proc. F 140, 107–113, (6).

Gupta, V.K., Ali, I., Saleh, T.A., Nayak, A., Agarwal, S., 2012. Chemical treatment technologies for waste-water recycling—an overview. RSC Adv. 2, 6380–6388.

Hall, D.L., Llinas, J., 1997. An introduction to multisensor data fusion. Proc. IEEE 85 (1), 6–23.

Hall, D., Llinas, J., 2001. Handbook of Multisensor Data Fusion, first ed. CRC Press LLC.

He, Q., Stinis, P., Tartakovsky, A.M., 2022a. Physics-constrained deep neural network method for estimating parameters in a redox flow battery. J. Power Sources 528, 231147.

Hu, X., Cao, D., Egardt, B., 2018. Condition monitoring in advanced battery management systems: Moving horizon estimation using a reduced electrochemical model. IEEE/ASME Trans. Mechatronics 23 (1), 167–178.

Jiang, S., Song, Z., 2022. A review on the state of health estimation methods of lead-acid batteries. J. Power Sources 517, 230710.

Jung, Y.J., Baek, K.W., Oh, B.S., Kang, J.-W., 2010. An investigation of the formation of chlorate and perchlorate during electrolysis using Pt/Ti electrodes: The effects of pH and reactive oxygen species and the results of kinetic studies. Water Res. 44 (18), 5345–5355.

Kalman, R.E., 1960. A new approach to linear filtering and prediction problems. J. Basic Eng. 82 (1), 35–45.

Kalman, R.E., 1963. Mathematical description of linear dynamical systems. J. Soc. Ind. Appl. Math. Ser. A Control 1 (2), 152–192.

Kalman, R., Bucy, R., 1961. New results in linear filtering and prediction theory. J. Basic Eng. 83, 95–108.

Karniadakis, G., Kevrekidis, Y., Lu, L., Perdikaris, P., Wang, S., Yang, L., 2021. Physics-informed machine learning. Nat. Rev. Phys. 3, 422–440.

Karunathilaka, S., Hampson, N., Hughes, M., Marshall, W., Leek, R., Sinclair, T., 1983. The prediction of the state-of-charge of some commercial primary cells. J. Appl. Electrochem. 13 (5), 577–586.

Keesman, K.J., 2011. System Identification. Springer.

Khaleghi, B., Khamis, A., Karray, F.O., Razavi, S.N., 2013. Multisensor data fusion: A review of the state-of-the-art. Inf. Fusion 14 (1), 28–44.

Kwakernaak, H., Sivan, R., 1972. Linear Optimal Control Systems. John Wiley and Sons, New York.

Li, Y., Liu, K., Foley, A.M., Zülke, A., Berecibar, M., Nanini-Maury, E., Van Mierlo, J., Hoster, H.E., 2019. Data-driven health estimation and lifetime prediction of lithium-ion batteries: A review. Renew. Sustain. Energy Rev. 113, 109254.

Lin, R.-H., Xi, X.-N., Wang, P.-N., Wu, B.-D., Tian, S.-M., 2019. Review on hydrogen fuel cell condition monitoring and prediction methods. Int. J. Hydrogen Energy 44 (11), 5488–5498, The 6th International Conference on Energy, Engineering and Environmental Engineering.

Liu, Z., Chen, J., Liu, H., Yan, C., Hou, Y., He, Q., Zhang, J., Hissel, D., 2020b. Anode purge management for hydrogen utilization and stack durability improvement of PEM fuel cell systems. Appl. Energy 275, 115110.

Luenberger, D.G., 1964. Observing the state of a linear system. IEEE Trans. Mil. Electron. 8 (2), 74–80.

McAfee, M., Kariminejad, M., Weinert, A., Huq, S., Stigter, J.D., Tormey, D., 2022. State estimators in soft sensing and sensor fusion for sustainable manufacturing. Sustainability 14 (6), 3635.

McCarthy, K., Gullapalli, H., Ryan, K.M., Kennedy, T., 2021. Review—use of impedance spectroscopy for the estimation of Li-ion battery state of charge, state of health and internal temperature. J. Electrochem. Soc. 168, 080517.

Mohanta, S., Fahidy, T., 1977. The effect of anodic bubble formation on cathodic mass transfer under natural convection conditions. J. Appl. Electrochem. 7, 235–238.

Mohd Ali, J., Ha Hoang, N., Hussain, M.A., Dochain, D., 2015. Review and classification of recent observers applied in chemical process systems. Comput. Chem. Eng. 76, 27–41.

Monteiro, M.K.S., Moratalla, Á., Sáez, C., Dos Santos, E.V., Rodrigo, M.A., 2021. Production of chlorine dioxide using hydrogen peroxide and chlorates. Catalysts 11 (12), 1478.

Natella, D., Vasca, F., 2021. Battery state of health estimation via reinforcement learning. In: 2021 European Control Conference. ECC, Institute of Electrical and Electronics Engineers Inc., pp. 1657–1662.

Ng, M.-F., Zhao, J., Yan, Q., Conduit, G.J., Seh, Z.W., 2020. Predicting the state of charge and health of batteries using data-driven machine learning. Nat. Mach. Intell. 2, 161–170.

Nolte, O., Volodin, I.A., Stolze, C., Hager, M.D., Schubert, U.S., 2021. Trust is good, control is better: A review on monitoring and characterization techniques for flow battery electrolytes. Mater. Horiz. 8, 1866–1925.

Oji, T., Zhou, Y., Ci, S., Kang, F., Chen, X., Liu, X., 2021. Data-driven methods for battery SOH estimation: Survey and a critical analysis. IEEE Access 9, 126903–126916.

Pang, H., Guo, L., Wu, L., Jin, J., Zhang, F., Liu, K., 2021. A novel extended Kalman filter-based battery internal and surface temperature estimation based on an improved electro-thermal model. J. Energy Storage 41, 102854.

Peng, J., Huang, J., Wu, X.-l., Xu, Y.-w., Chen, H., Li, X., 2021. Solid oxide fuel cell (SOFC) performance evaluation, fault diagnosis and health control: A review. J. Power Sources 505, 230058.

Porru, G., Aragonese, C., Baratti, R., Servida, A., 2000. Monitoring of a CO oxidation reactor through a grey model-based EKF observer. Italy Chem. Eng. Sci. 237, 331–338.

Raijmakers, L., Danilov, D., Eichel, R.-A., Notten, P., 2019. A review on various temperature-indication methods for Li-ion batteries. Appl. Energy 240, 918–945.

Rauf, H., Khalid, M., Arshad, N., 2022. Machine learning in state of health and remaining useful life estimation: Theoretical and technological development in battery degradation modelling. Renew. Sustain. Energy Rev. 156, 111903.

Richard, C., Bermudez, J., Honeine, P., 2009. Online prediction of time series data with kernels. IEEE Trans. Signal Process. 57 (3), 1058–1067.

Ross, E., Wagterveld, M., Mayer, M., Stigter, H., Højris, B., Li, Y., Keesman, K., 2022. Sensor data fusion as an alternative for monitoring chlorate in electrochlorination applications. Sustainability 14 (10), 6119.

Sansana, J., Joswiak, M.N., Castillo, I., Wang, Z., Rendall, R., Chiang, L.H., Reis, M.S., 2021. Recent trends on hybrid modeling for Industry 4.0. Comput. Chem. Eng. 151, 107365.

Sedahmed, G.H., Nirdosh, I., 2007. Intensification of rate of diffusion controlled reactions in a parallel plate electrochemical reactor stirred by a curtain of electrochemically generated gas bubbles. Chem. Eng. Technol. 30 (10), 1406–1411.

Shi, N., Chen, Z., Niu, M., He, Z., Wang, Y., Cui, J., 2022a. State-of-charge estimation for the lithium-ion battery based on adaptive extended Kalman filter using improved parameter identification. J. Energy Storage 45, 103518.

Shi, J., Yao, Y., Bao, J., Skyllas-Kazacos, M., Welch, B.J., Jassim, A., Mahmoud, M., 2022b. Advanced model-based estimation and control of alumina concentration in an aluminum reduction cell. JOM 74 (2), 706–717.

Shu, X., Shen, S., Shen, J., Zhang, Y., Li, G., Chen, Z., Liu, Y., 2021. State of health prediction of lithium-ion batteries based on machine learning: Advances and perspectives. iScience 24 (11), 103265.

Siddiqui, M.S., 1996. Chlorine-ozone interactions: Formation of chlorate. Water Res. 30 (9), 2160–2170.

Snyder, S., 2016. Perchlorate in Drinking-water. Background Document WHO/FWC/WSH/16.46, World Health Organization.

Stigter, H., Joubert, D., Molenaar, J., 2017. Observability of complex systems: Finding the gap. Sci. Rep. 7, 16566.

Sui, X., He, S., Vilsen, S.B., Meng, J., Teodorescu, R., Stroe, D.I., 2021. A review of non-probabilistic machine learning-based state of health estimation techniques for lithium-ion battery. Appl. Energy 300, 117346.

Tasaka, A., Tojo, T., 1985. Anodic oxidation mechanism of hypochlorite ion on platinum electrode in alkaline solution. J. Electrochem. Soc. 132, 1855–1859.

The European Commission, 2015. Commission recommendation (EU) 2015/682 of 29 April 2015 on the monitoring of the presence of Perchlorate in food.

The European Parliament and the Council of the European Union, 2020. Directive (EU) 2020/2184 of the European Parliament and of the Council of 16 December 2020 on the quality of water intended for human consumption (recast).

Vanem, E., Salucci, C.B., Bakdi, A., Alnes, O.A., 2021. Data-driven state of health modelling-a review of state of the art and reflections on applications for maritime battery systems. J. Energy Storage 43, 103158.

Vennam, G., Sahoo, A., Ahmed, S., 2022. A survey on lithium-ion battery internal and external degradation modeling and state of health estimation. J. Energy Storage 52, 104720.

Viumdal, H., Mylvaganam, S., 2010. Beyond the dip stick: Level measurements in aluminum electrolysis. JOM 62 (11), 18–25.

von Stosch, M., Oliveira, R., Peres, J., Feyo de Azevedo, S., 2014. Hybrid semi-parametric modeling in process systems engineering: Past, present and future. Comput. Chem. Eng. 60, 86–101.

Waag, W., Fleischer, C., Sauer, D.U., 2014. Critical review of the methods for monitoring of lithium-ion batteries in electric and hybrid vehicles. J. Power Sources 258, 321–339.

Wang, Y.-X., Chen, Z., Zhang, W., 2022a. Lithium-ion battery state-of-charge estimation for small target sample sets using the improved GRU-based transfer learning. Energy 244 (B), 123178.

Wang, Z., Feng, G., Zhen, D., Gu, F., Ball, A., 2021b. A review on online state of charge and state of health estimation for lithium-ion batteries in electric vehicles. Energy Rep. 7, 5141–5161.

Wang, J., Yang, B., Zeng, C., Chen, Y., Guo, Z., Li, D., Ye, H., Shao, R., Shu, H., Yu, T., 2021h. Recent advances and summarization of fault diagnosis techniques for proton exchange membrane fuel cell systems: A critical overview. J. Power Sources 500, 229932.

Wassiliadis, N., Schneider, J., Frank, A., Wildfeuer, L., Lin, X., Jossen, A., Lienkamp, M., 2021. Review of fast charging strategies for lithium-ion battery systems and their applicability for battery electric vehicles. J. Energy Storage 44 (B), 103306.

Wei, Z., Zhao, J., He, H., Ding, G., Cui, H., Liu, L., 2021. Future smart battery and management: Advanced sensing from external to embedded multi-dimensional measurement. J. Power Sources 489, 229462.

Wikström, C., Albano, C., Eriksson, L., Fridén, H., Johansson, E., Nordahl, Å., Rännar, S., Sandberg, M., Kettaneh-Wold, N., Wold, S., 1998a. Multivariate process and quality monitoring applied to an electrolysis process: Part I. Process supervision with multivariate control charts. Chemometr. Intell. Lab. Syst. 42 (1–2), 221–231.

Wikström, C., Albano, C., Eriksson, L., Fridén, H., Johansson, E., Nordahl, Å., Rännar, S., Sandberg, M., Kettaneh-Wold, N., Wold, S., 1998b. Multivariate process and quality monitoring applied to an electrolysis process: Part II. Multivariate time-series analysis of lagged latent variables. Chemometr. Intell. Lab. Syst. 42 (1–2), 233–240.

World Health Organization, 2017. Guidelines for Drinking-Water Quality: Fourth Edition Incorporating First Addendum, fourth ed. + 1st add.

Wu, J., Fang, C., Jin, Z., Zhang, L., Xing, J., 2022a. A multi-scale fractional-order dual unscented Kalman filter based parameter and state of charge joint estimation method of lithium-ion battery. J. Energy Storage 50, 104666.

Xu, Y., Ge, X., Shen, W., Yang, R., 2022a. A soft short-circuit diagnosis method for lithium-ion battery packs in electric vehicles. IEEE Trans. Power Electron. 37 (7), 8572–8581.

Yang, B., Wang, J., Cao, P., Zhu, T., Shu, H., Chen, J., Zhang, J., Zhu, J., 2021b. Classification, summarization and perspectives on state-of-charge estimation of lithium-ion batteries used in electric vehicles: A critical comprehensive survey. J. Energy Storage 39, 102572.

Yue, W., Chen, X., Gui, W., Xie, Y., Zhang, H., 2017. A knowledge reasoning fuzzy-Bayesian network for root cause analysis of abnormal aluminum electrolysis cell condition. Front. Chem. Sci. Eng. 11 (3), 414–428.

Zhang, D., Couto, L.D., Moura, S.J., 2021b. Electrode-level state estimation in lithium-ion batteries via Kalman decomposition. IEEE Control Syst. Lett. 5 (5), 1657–1662.

Zhang, X., Hu, Y., Deng, J., Xu, H., Wen, H., 2022b. Feature engineering and artificial intelligence-supported approaches used for electric powertrain fault diagnosis: A review. IEEE Access 10, 29069–29088.

Zhang, Y., Yang, X., Shardt, Y.A., Cui, J., Tong, C., 2018. A KPI-based probabilistic soft sensor development approach that maximizes the coefficient of determination. Sensors 18 (9), 3058.

Zhang, S., Zhang, T., Yin, Y., Xiao, W., 2017. Alumina concentration detection based on the kernel extreme learning machine. Sensors 17 (9), 2002.

Zheng, Z., Petrone, R., Péra, M., Hissel, D., Becherif, M., Pianese, C., Yousfi Steiner, N., Sorrentino, M., 2013. A review on non-model based diagnosis methodologies for PEM fuel cell stacks and systems. Int. J. Hydrogen Energy 38 (21), 8914–8926.

Zhou, S., Shearing, P.R., Brett, D.J.L., Jervis, R., 2022. Machine learning as an online diagnostic tool for proton exchange membrane fuel cells. Curr. Opin. Electrochem. 31, 100867.