

Review

State Estimators in Soft Sensing and Sensor Fusion for Sustainable Manufacturing

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Abstract: State estimators, including observers and Bayesian filters, are a class of model-based algorithms for estimating variables in a dynamical system given the sensor measurements of related system states. They can be used to derive fast and accurate estimates of system variables that cannot be measured directly ('soft sensing') or for which only noisy, intermittent, delayed, indirect, or unreliable measurements are available, perhaps from multiple sources ('sensor fusion'). In this paper, we introduce the concepts and main methods of state estimation and review recent applications in improving the sustainability of manufacturing processes across sectors including industrial robotics, material synthesis and processing, semiconductor, and additive manufacturing. It is shown that state estimation algorithms can play a key role in manufacturing systems for accurately monitoring and controlling processes to improve efficiencies, lower environmental impact, enhance product quality, improve the feasibility of processing more sustainable raw materials, and ensure safer working environments for humans. We discuss current and emerging trends in using state estimation as a framework for combining physical knowledge with other sources of data for monitoring and controlling distributed manufacturing systems.

Keywords: state observer; Kalman filter; particle filter; sustainable manufacturing; soft sensor; digital twin



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1. Introduction

Sustainable manufacturing is currently a very significant principle that industries must adopt due to many factors driven by environmental issues, including more stringent legislation, higher energy costs, and consumer preference for environmentally benign products and services [1]. Manufacturing processes have a direct impact on the consumption of natural resources and their resultant emissions [2]. The emergence of Industry 4.0 provides significant opportunities for the development of intelligent manufacturing environments that have greater production flexibility and resource efficiency [3]. The deployment of sensors, Internet of Things (IoT), and Cyber-Physical Systems (CPS) within manufacturing is predicted to contribute to addressing some of the global challenges with respect to resource and energy efficiency [4]. Greater sensorisation of manufacturing processes is a central pillar of the Industry 4.0 concept and is critical to improving resource efficiency and sustainability. The ability to monitor key process variables in real-time enables a tight

control of processes to avoid defects; eliminates waste of raw materials and energy in producing scrap; prevents harmful environmental emissions; and facilitates processing of more sustainable but difficult to process raw materials such as recyclates. However, it is not always feasible to physically measure critical variables in real-time due to, e.g., a lack of an available sensor technology, lack of sensor accessibility, high cost, poor accuracy, high latency, etc. In this case, concepts such as soft sensing and data and sensor fusion may provide a solution, enabling the variable(s) of interest to be inferred from available information in a connected cyber-physical system. Often, this may be achieved by using purely data-based approaches via Machine Learning; however, this will often require a large amount of historical training data, high computational resources for model training, and typically results in models that do not generalise well to different systems/raw materials and which may exhibit poor long-term robustness. An alternative in some situations is to use an observer-based state estimation method, whereby the future value of the system states is predicted based on the current value according to some model of the system. Then, in the next time step, the estimate is updated with measurement data available from the system—which may be indirectly related to the variables of interest and/or of limited reliability. This ‘predict-correct’ structure, as illustrated in Figure 1, exploits an often approximate, physical model of the system to derive an algorithm which provides sufficiently accurate and fast estimates with limited need for training data and with good robustness to variations in the process over time.

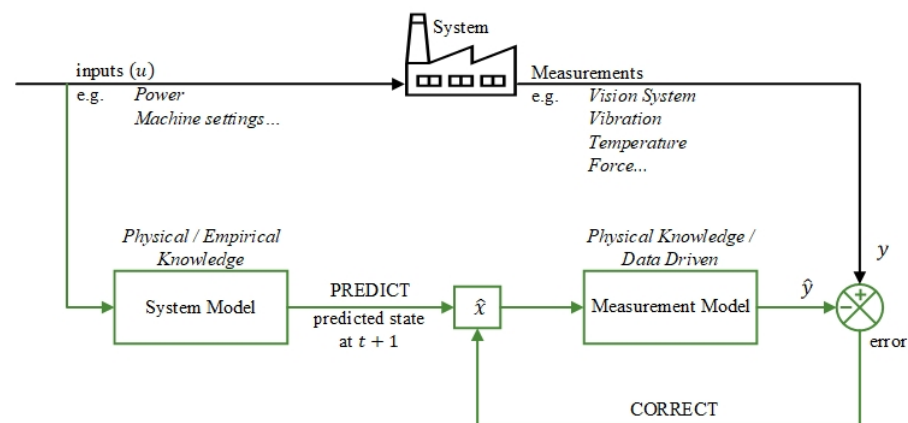


Figure 1. Predict-correct structure of state estimators.

State estimators can be deterministic (‘observers’) or stochastic (Bayesian filters such as the Kalman filter and its extensions). In the stochastic case, uncertainties in models and measurements are explicitly handled to derive an optimal estimate of the variable(s) of interest together with a measure of the uncertainty in the estimate. These state estimation methods have been applied to navigation problems since the late 1960s, with the Kalman filter famously considered a key factor in the success of the Apollo 11 moon landing [5]. The Kalman filter is the optimal state reconstructor for linear systems subject to white noise; however, this optimality is lost with nonlinear systems and/or systems with non-Gaussian noise distributions [6]. In recent decades, increasing computational power has facilitated more sophisticated algorithms, which deal better with nonlinear systems and more complex uncertainty distributions, that are fundamental to recent developments in self-driving cars for example [7]. The concepts are less well known in some aspects of the manufacturing community; however, we show in this review that several studies indicate the potential of various state estimation methods in manufacturing processes, moving from automation of a defined task (Industry 3.0) to a wider systems-level approach (Industry 4.0). As manufacturing enterprises are currently undergoing a period of considerable disruption, driven on the one hand by an urgent need to enhance sustainability and, on the other hand, enabled by progress in sensorisation, connectivity, and computation, state estimation concepts can in future play a greater role in driving improvements in the

flexibility and quality of manufacturing processes as well as reducing energy consumption and waste generation.

This paper provides an accessible introduction to the key concepts and methods of state estimation with a comprehensive review of the application of such methods to improving the sustainability of manufacturing processes and systems across a range of industrial sectors including the following: material processing, machining, additive manufacturing, semiconductor manufacturing, and industrial robotics. Current trends in combining state estimation concepts with Machine Learning and/or physics-based computational models are highlighted. We discuss the future potential for state estimators to be incorporated into ‘digital twin’ approaches for improving the sustainability of manufacturing processes.

2. State Estimation Methods

2.1. State Observers

Originating in control theory, a state space model is a specific model structure whereby a dynamic system is described by inputs u , outputs y , and state variables x related by first order differential equations (continuous case) or difference equations (discrete case). State variables are variables of the system for which values evolve over time depending on the current value of the variables and any external input to the system. For example, in modelling a d.c. motor, motor position and speed are suitable state variables to capture the system’s dynamics in response to changes in input voltage. The complete state space model comprises the ‘state equation’ (or ‘system model’), which describes the evolution of the values of the state variables, and a ‘measurement equation’ (or ‘measurement model’), which describes the relationship between the state variables and measurements (outputs) of the system over time. Equation (1) illustrates the general form of a state space model for a discrete linear system. We focus here on the discrete case due to the dominance of digital systems in manufacturing. In simple terms, the values of the state variables at the next time step are predicted by the state equation from the current values of the variables and the current value of any input to the system. The relationship between the actual measurements of the system and the state variables is described by the measurement equation.

$$\begin{aligned}x(k+1) &= Ax(k) + Bu(k) \\y(k) &= Cx(k) + Du(k)\end{aligned}\tag{1}$$

Observability of a system relates to the ability to reconstruct the values of all the state variables from the measurements and the input in a finite time. Obviously, this requires that the unmeasured states are not independent from the measurements, which can be checked by the construction of an observability matrix derived from system A and C matrices. Provided a system is indeed observable, an observer can be constructed as in Figure 2, which depicts the discrete time Luenberger observer [8]. The values of the state variables at the next time step are predicted from the current values and the input via the state equation, and the measured values are then predicted from the estimated values of the state variables. In the next time step, the predicted and measured values are compared and the error is fed back to correct the estimates of the state variables.

$$\hat{x}(k+1) = Ax(k) + Bu(k) + L(y(k) - \hat{y}(k))\tag{2}$$

Provided that the measurement equation is accurate (which is usually the case, as typically the measurements are a subset of entire state variables), the estimates converge to the true values. The gain feedback matrix L requires careful design such that convergence can be ensured to occur more rapidly than the dynamics of the plant (i.e., faster than the values of the variables are themselves changing) but without introducing excessive noise into the estimates. The Luenberger observer is a full-order observer, i.e., it estimates the values of all the state variables and not only the unmeasured ones. Reduced-order observers, in contrast, use system measurements to estimate only the ‘hidden’ states. They are more complicated to design but can result in better performance [9].

The estimator equation for the Luenberger observer is given by (2).

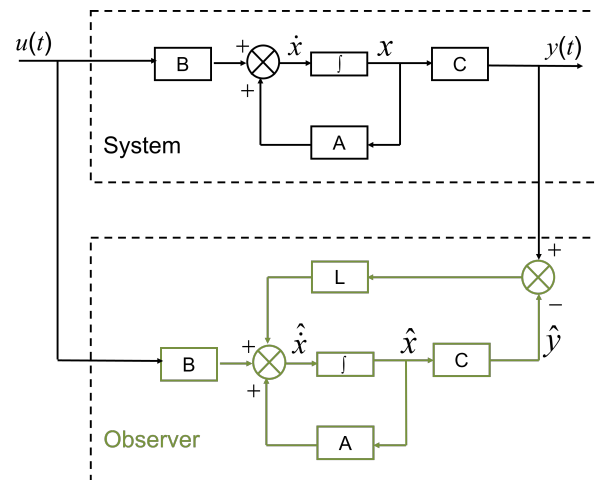


Figure 2. The Luenberger observer.

Luenberger observers are, however, usually unable to estimate plant states in the presence of unknown disturbance signals or model uncertainties. The sliding mode observer (SMO) has emerged as one of the most popular approaches in recent years to deal with such issues. A sliding mode observer feeds back the output estimation error via a nonlinear switching term rather than via a simple gain matrix. Essentially there is a suite of feedback control laws and a decision rule. The decision rule, termed the switching function, has as its input some measure of the current system behaviour and produces as an output, the particular feedback law which should be used at that instant in time. Provided a bound on the magnitude of the disturbances is known, the ability to generate a sliding motion on the error between the measured plant output and the output of the observer ensures that an SMO can force the output estimation error to converge to zero in finite time, while the observer states converge asymptotically to the system states. Consider 3 as an uncertain linear system, where ζ is an unknown but a bounded function representing the disturbance.

$$\begin{aligned}\dot{x}(t) &= Ax(t) + Bu(t) + D\zeta(t, y, u) \\ y(t) &= Cx(t)\end{aligned}\quad (3)$$

An observer can be defined as in (4), where $e = z - x$, G_1 , and G_n are gain matrices and v is the discontinuous ‘injection’ term, which is designed to force the trajectories of the state estimation error onto the sliding surface. The behaviour of the system varies on either side of the sliding surface. Details of designing the sliding motion and surface can be found in [10].

$$\dot{z}(t) = Az(t) + Bu(t) - G_1 Ce(t) + G_n v \quad (4)$$

An advantage of the SMO is that the applied observer injection signal (equivalent signal) can be used for the identification of the mismatch between the actual system and the observer model. This equivalent signal has been used in many applications such as fault detection and condition monitoring [11].

Sliding mode observers have also been developed for uncertain nonlinear systems; for details on designing an SMO for second and high order systems, see [12–14].

Although sliding mode is currently one of the most popular approaches, many different methods of nonlinear observer design have been proposed. The interested reader is referred to recent reference [15], which provides an overview of the general designs available in the literature.

2.2. Kalman Filter and Extensions

The Kalman filter (KF) is essentially a stochastic observer, that is, it explicitly models the uncertainty in the state equation and in the measurements and utilises Bayesian inference to determine the optimum estimate of the states (in the sense that the uncertainty is minimised) [16]. Compared to the linear discrete state observer, the Kalman filter state and measurement equations (Equation (5)) contain noise terms. $w(k)$ represents the uncertainty in the model ('process noise') while $e(k)$ represents the measurement noise associated with sensor readings. All noise terms are assumed to be normally distributed.

$$\begin{aligned}x(k+1) &= Ax(k) + Bu(k) + Gw(k) \\y(k) &= Cx(k) + Du(k) + e(k)\end{aligned}\quad (5)$$

Bayes law (Equation (6)) determines a posterior probability distribution $p(x | y)$ from the product of a prior distribution $p(x)$ and the 'likelihood' distribution $p(y | x)$, which arises from measurements. In the context of the Kalman filter, the likelihood is the probability distribution for the observed measurements y at sample k as a function of the state variables x at sample k through the measurement equation.

$$p(x | y) \propto p(x)p(y | x) \quad (6)$$

The concept is illustrated with a simple one-dimensional example in Figure 3. The previous estimate of the state variables, $\hat{x}_{k-1|k-1}$ (i.e., the estimate of x at sample $k-1$ given all the information up to and including sample $k-1$), and its covariance $P_{k-1|k-1}$ is propagated through state Equation (5) to produce $\hat{x}_{k|k-1}$ (i.e., the estimate of x at sample k given all the information up to and including sample $k-1$). This step is sometimes referred to as the 'time update'. Estimate $\hat{x}_{k|k-1}$ has a larger covariance $P_{k|k-1}$ as more uncertainty is introduced due to the process noise term $w(k)$ in the state equation. This estimate is the prior distribution at sample k . The new measurement data y at sample k yields the likelihood function $p(y_k|x_k)$. The optimal (minimum variance) estimate of x at sample k $\hat{x}_{k|k}$ is then determined by combining the prior and the likelihood in the 'measurement update' step.

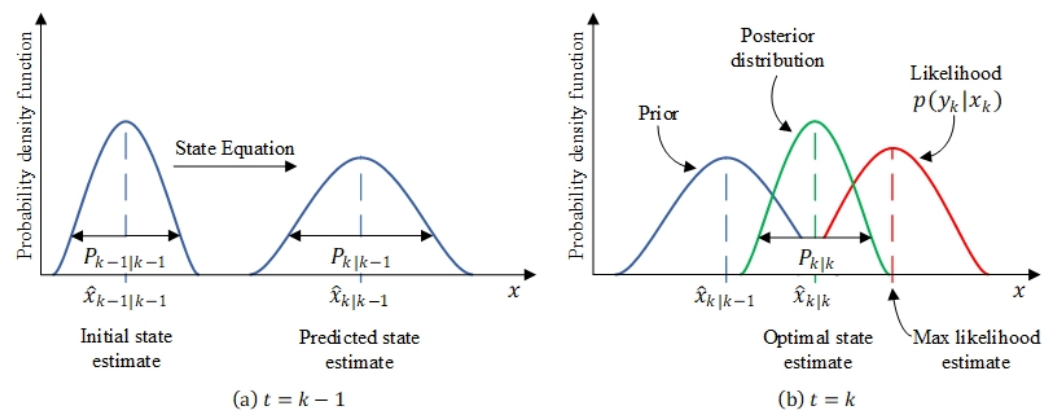


Figure 3. One-dimensional illustration of the operation of the Kalman filter.

The Kalman estimation equation can be written in terms of the Kalman gain matrix K :

$$\hat{x}(k|k) = \hat{x}(k|k-1) + K(y(k) - \hat{y}(k)) \quad (7)$$

where $\hat{y}(k)$ is the predicted measurement vector (obtained by substituting $\hat{x}(k|k-1)$ into the measurement equation (Equation (5))). The Kalman gain matrix K is designed to minimise posterior error covariance $P(k|k)$. If the process noise $w(k)$ is low, the predicted measurement is trusted more than the actual measurements. However, if the measurement noise $e(k)$ is low, then the predicted measurement will be more heavily corrected. The

Kalman estimator equation (Equation (7)) has a similar ‘predict-correct’ structure relative to the Luenberger observer estimation equation (Equation (2)). However, the KF has functions beyond the observation of unmeasured states as it also allows for the optimal fusion of multiple sources of measurement data according to their uncertainty.

The Kalman Filter applies to linear systems with an assumption that model uncertainty and sensor noise can be described by a Gaussian distribution. A challenge in the practical implementation is that the covariance matrices of the process and measurement noises must be provided a priori, and this is a difficult task, particularly for the process noise which is usually difficult to quantify [17]. To fulfill the requirement of achieving the filter optimality, an adaptive Kalman filter (AKF) can be utilised for tuning noise covariance matrices [6]. Adaptive filters are based on dynamically adjusting the parameters of the supposedly optimum filter based on the estimates of the unknown parameters. Another solution to circumvent the system noise matrix specification is to parameterise the gain and include its elements in the estimation process [18].

The Kalman Filter has been extended to non-linear systems under two main approaches. The first, the Extended Kalman Filter (EKF), involves the linearisation of non-linear system equations using a Taylor series expansion and then applying the usual KF recursions [19]. The classic EKF involves retaining only the first order terms of the Taylor series expansion; however, if the system behaviour is significantly nonlinear over the sample period or the noise is high, then better performance may be achieved by including the second derivative term in the Taylor series expansion. A drawback is that the determination of the first and second-order derivative terms can be computationally intensive [20].

An alternative approach is to use a nonlinear transformation, and the Unscented Kalman Filter (UKF) [21], which utilises the unscented transform, has emerged as a popular alternative to the EKF. The unscented transform involves generating sigma points from the distribution of the model input parameters. In the case of UKF, these points are the mean of the state estimates and symmetric deviations around the mean which are computed from the covariance matrix. These sigma points are then propagated through the nonlinear model and the mean and covariance of the model output (predicted state estimates or predicted measurements) are estimated by applying weights to the sigma points after the nonlinear mapping, as illustrated in Figure 4. UKF has the advantage of not requiring the formation of derivative terms as needed for the EKF, and it may result in better performance depending on the form of the nonlinearity in the system. It should be noted that the optimality of the Kalman filter is lost with EKF, UKF, or any higher-order filter.

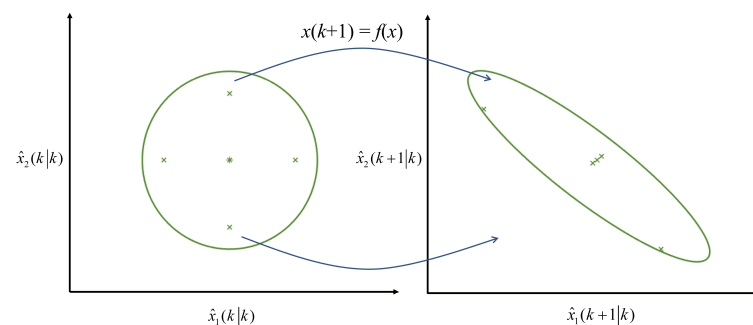


Figure 4. Two-dimensional illustration of the unscented transform to estimate the mean and covariance of state estimates in the UKF ‘time update’. Sigma points are generated from the noise distribution following the last measurement update $P_{k|k}$ and propagated through the nonlinear state equation $f(x)$. The mean and covariance of the state estimates $\hat{x}_{k+1|k}$ are estimated by a weighted sum of the sigma points following the nonlinear transformation.

The Kalman Filter and EKF and UKF extensions have limitations in very high dimensional nonlinear systems (i.e., having a large number n of state variables), since it is necessary to calculate the $n \times n$ covariance matrix at each recursion, requiring a large amount of time, high-capacity storage, and high-speed processors [22]. The ensemble

Kalman filter (EnKF), originally developed in modelling geophysical systems, instead estimates the full covariance matrix using a sample of evolved states (the ‘ensemble’) [23]. EnKF is a Monte Carlo-based application of KF, propagating only the mean of an ensemble of $N < n$ state estimations through KF recursions. The resulting mean and covariance matrices are then estimated from the evolved samples. This method has reduced computational complexity and can be applied to nonlinear state-space models and non-Gaussian noise. For linear Gaussian systems, if $N \rightarrow \infty$, EnKF converges to the KF results [24].

2.3. Particle Filter

The particle filter was developed to deal with systems having multi-modal probability distributions, i.e., as opposed to the estimates having a normal (Gaussian) probability distribution, and there may be a distribution with more than one peak [25–27]. In navigation problems, where the technique emerged, this would arise where there may be more than one likely map location for a target vehicle based on the information available. In this scenario, a numerical approximation of the distribution which can be propagated through the prediction and correction recursions is needed. This can be performed by representing the probability distribution of the state estimates as a set of samples or ‘particles’ via Monte Carlo methods (repeated random sampling). Figure 5 illustrates the principles of the particle filter in five general stages, which can be described as follows:

1. Weighted particles from last measurement update (usually sampled from a uniform distribution on initialization).
2. Bootstrap resampling: Take N samples with replacement from the set, where the probability of selection is proportional to the weighting. All new samples have equal weighting so that the distribution is represented by particle density rather than weight.
3. Each particle is propagated through the state equation adding noise generated by sampling from the distribution for the process noise $w(k)$ to provide time updates (prediction at $t = k + 1$).
4. Measurement update: The predicted measurements given by the particles are compared to the true measurements to update the weights.
5. The states are estimated by, e.g., a maximum a posteriori (MAP) estimate of the approximated posterior distribution.

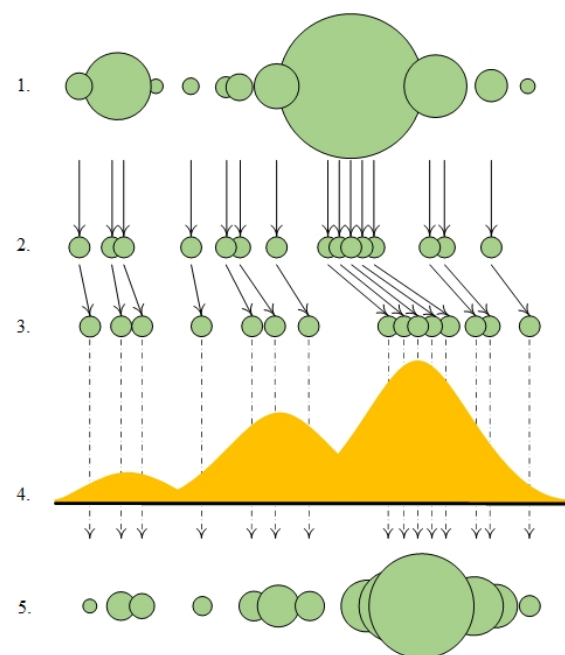


Figure 5. Schematic illustrating the basic principles of a particle filter.

Particle filter methods are very flexible, easy to implement, and present an attractive approach to approximate the posterior distributions when the model is nonlinear and when the sources of noise are not Gaussian. The main constraint of particle filter methods is that they are computationally demanding; however, they have been used in practical applications in systems with up to four state variables [28]. They are used in self-driving cars for Simultaneous Localisation and Mapping (SLAM) tasks and also have applications in image processing, econometrics, and in industrial fault detection and diagnostics applications. For more in-depth readings on the theory and implementations of the particle filter, the reader is referred to the following excellent resources by Gustafsson [28–30]. Table 1 summarises the advantages and limitations of the main types of state estimator.

Table 1. Comparison of different state estimators.

State Estimator	Advantages	Limitations
Luenberger observer	<ol style="list-style-type: none"> 1. Simple to design and implement 2. Suitable for well-defined linear systems 	<ol style="list-style-type: none"> 1. Poor estimation in the presence of model uncertainties
Reduced-Order observer	<ol style="list-style-type: none"> 1. Better Performance 2. Lower computational cost 	<ol style="list-style-type: none"> 1. Complicated to design
Sliding Mode Observer	<ol style="list-style-type: none"> 1. Suitable for linear and nonlinear systems 2. High robustness 3. Fault detection capabilities 	<ol style="list-style-type: none"> 1. Chattering of the estimator 2. Complexity of the design
Kalman Filter	<ol style="list-style-type: none"> 1. Suitable for noisy systems 2. Allows fusion of different measurement sources 	<ol style="list-style-type: none"> 1. Suitable for linear system 2. Not Suitable for non-Gaussian noise 3. Not suitable for high order systems
Adaptive Kalman Filter	<ol style="list-style-type: none"> 1. Suitable for noisy systems 2. Allows fusion of different measurement sources 3. Suitable for unknown noise covariance 	<ol style="list-style-type: none"> 1. Suitable for linear system 2. Not suitable for non-Gaussian noise 3. Not suitable for high order systems
Extended Kalman Filter	<ol style="list-style-type: none"> 1. Suitable for noisy systems 2. Allows fusion of different measurement sources 3. Suitable for nonlinear systems 	<ol style="list-style-type: none"> 1. High computational time 2. Not suitable for high order systems
Unscented Kalman Filter	<ol style="list-style-type: none"> 1. Suitable for noisy systems 2. Allows fusion of different measurement sources 3. Suitable for nonlinear systems 4. Lower computational cost 	<ol style="list-style-type: none"> 1. Not suitable for high order systems
Ensemble Kalman Filter	<ol style="list-style-type: none"> 1. Suitable for noisy systems 2. Allows fusion of different measurement sources 3. Suitable for nonlinear systems 4. Low computational cost 5. Suitable for high order systems 	<ol style="list-style-type: none"> 1. Not suitable for non-Gaussian noise
Particle Filter	<ol style="list-style-type: none"> 1. Suitable for multimodal probability distributions 2. Suitable for nonlinear systems 	<ol style="list-style-type: none"> 1. High computational time and cost

3. Application of State Estimators in Improving Manufacturing Sustainability

3.1. Industrial Robotics

As the global manufacturing industry enters its fourth revolution, innovations such as robotics, combined with artificial intelligence (AI) and IoT, are considered a cornerstone of competitive manufacturing, which aims to combine high productivity, quality, and adaptability at minimal cost [31]. Industrial robots were first used commercially on assembly lines in the early 1960s. Essentially, these devices were primitive in that they were

sensorless, featured limited programmability, mostly featuring hydraulic and pneumatic arms, and were primarily used for heavy lifting. Throughout the late 1960s and early 1970s, industrial robotics gradually shifted toward handling and precision work as the need for the automation of manpower-intensive tasks in manufacturing increased. Eventually, smaller electric robots with advanced controls, microprocessors, miniaturized motors, gyros, and servos were realised, which were ideal for lighter assembly tasks, e.g., bolt and nut tightening. As a natural progression, the capabilities of robots expanded further to include tasks such as material transferring, painting, and arc welding, replacing humans in certain dangerous and hazardous scenarios, by the late 1970s [32].

Advancements in sensors and machine vision, coupled with a substantial reduction in the costs of computer hardware, have resulted in a steep advancement in industrial robotic capabilities. Through the application of high precision sensors, e.g., force sensors, vision and lasers, etc, combined with suitable observers and estimators and high computational power, enhanced high fidelity perception of the robot workspace as well as the surrounding environment became possible. Features attainable through such accurate reliable perception include enhanced safety through collision detection and the implementation of effective human–robot collaboration, which ultimately paves the way forward towards more sustainable manufacturing.

Traditionally, industrial robots operate within a safety fence without any human interaction. Cobots are relatively small manipulators that are specially designed to operate safely in close proximity or even in direct contact with humans, sharing workspace. This effectively results in bringing together the best of each partner, robot and human, by combining coordination, dexterity and cognitive capabilities of humans with the robots' accuracy, agility, and the ability to produce repetitive work [33]. They utilise advanced technology, including force-limited joints and computer vision to detect the presence of humans in their environment. Cobots are often much smaller and lighter than traditional industrial robots, are easily moveable, and trainable to perform specific tasks. Robots' external perception relies on sensing technology; thus, capturing accurate sensor information is vital for ensuring robotic security and improving human–machine interaction performance. Amongst other sectors, the manufacturing industry has benefited significantly by using mobile robots to increase efficiencies and reduce costs while operating autonomously alongside humans [34]. However, to allow the mobile robot to navigate its environment, self-localization is critical in autonomous mobile robots. SLAM algorithms serve exactly this purpose and are the most widely used strategy for self localization in an unknown environment through continuously constructing and/or updating the map of the environment while keeping track of the robot in the environment [35]. SLAM comprises the simultaneous (i) estimation of the state of a robot equipped with onboard sensors and (ii) the construction of a map (grid of obstacles) of the environment as perceived by onboard robot sensors. While the robot state is normally described by its pose (position and orientation), the map is a representation of aspects of interest (e.g., position of landmarks and obstacles) describing the environment in which the robot is able to operate.

In [36], the main methods of sensor data fusion for cobot environment perception are classified as 'AI' or 'stochastic'. The latter group encompassing Bayesian filtering and Dempster–Shafer evidence theory, while the former includes fuzzy algorithms, neural networks, and fuzzy-neuro approaches. Kalman filtering has been applied for robot positioning [37–39], while the particle filter is shown to provide accurate positioning together with a consistent mapping of the 3D environment of the robot via simultaneous localisation and mapping [34,40–43]. In their recent review, Ding et al. [36] concluded that stochastic algorithm approaches are accurate and mature while AI approaches currently have limitations in practical cobot applications.

Recently, Li et al. [44] developed an Augmented Reality (AR) teleoperation method to monitor and control a robot in real-time using a Kalman filter. Precise teleoperation can facilitate the use of robots in applications where high precision is required and in environments where human safety is compromised. In this work, a LeapMotion sensor is

used to track the movement of the operator's hands for gesture detection while a Kinect V2 camera measures the corresponding motion velocities in 3D. The authors used a Kalman filtering (KF) algorithm to fuse the position and velocity signals to teleoperate a Baxter robot in real-time. It was shown that, with the application of the KF sensor fusion, the performance index is improved on average by about 33%. It is concluded that the proposed teleoperation strategy has better tracking performance after the application of the KF-based sensor fusion.

It has been demonstrated that both the Kalman filter and particle filter are highly beneficial approaches for sensor fusion in industrial robotics and currently have advantages over AI-based approaches. Sensor fusion via these Bayesian filtering methods results in robotic systems with higher precision, speed, and adaptability and safer robot–human interaction, ultimately leading to more efficient manufacturing processes and reducing the exposure of human workers to hazardous environments.

3.2. Chemical Process Industries

While state observer concepts were initially applied and developed in tasks related to localisation, tracking, and navigation, such as in the field of robotics, the same algorithms were later applied to various other state estimation problems. In particular, state estimation methods have been of considerable interest in process industries since the 1990s. Many industrial chemical processes have a high degree of variability and a large number of process variables requiring measurement and control in real-time. However, online measurement of many variables of interest, such as reactant concentrations, etc., is not possible using physical sensors and as such require sensorless control. A 'soft sensor' measurement can yield lower cost, increased reliability, lower maintenance requirements, and thereby increased sustainability [45].

State estimation concepts in monitoring and controlling industrial chemical processes has been the subject of previous reviews [46–48]. Here, we focus on recent examples of state estimation as a form of sensorless measurement in improving the sustainability of polymerisation as an important source of raw materials for manufacturing industries.

Polymerisation

Polymerisation is a chemical process for the synthesis of polymers, which are long-chained molecules made of repeating monomer units. Although traditionally synthesised from petroleum-based products, much research activity is ongoing to replace such polymers with those derived from more sustainable and ecofriendly plant sources such as polylactide (PLA), which can be synthesised from natural feedstocks including corn starch, rice, potatoes, sugar beet, and seaweed [49]. The process of manufacturing polymers via chemical polymerisation has inherent nonlinear and time-varying dynamics, which are a challenge to control [50]. Various studies have been carried out to model and control the dynamics of the polymerisation processes to improve yield, improve product quality and reproducibility, and enhance safety and sustainability [51].

Salas et al. [52] applied an EKF for the approximation of the nonlinear behaviour in semi-batch polymerisation to track the molecular weight (Mw) trajectories. Molecular weight is critical to the properties of the resulting polymer product but can only be directly measured offline using time-consuming techniques such as gel permeation chromatography (GPC). They used a state-space mathematical model for the free radical polymerisation process and followed the proposed approach by Crowley [53] for the calculation of molecular weight distribution (MWD). They tested the method in an open-loop system to estimate Mw and MWD and good estimation capability was confirmed with offline GPC analysis. They compared the closed-loop control of the polymerisation process using a PID controller with and without EKF state estimation. The result showed that, with the incorporation of the EKF, there was approximately a 50% reduction in the absolute error between the actual and the set point of the Mw trajectory after the initialisation of the experiment.

The experiments confirm that the nonlinear state estimation provides an opportunity of achieving full polymer characterization in real-time.

Zhao et al. [54] proposed a method using data fusion and cubature KF for nonlinear state estimation with delayed measurement. The cubature KF is equivalent to a UKF with specific parameters for generating sigma points. For the delayed measurement, they introduced and compared two data fusion methods, excluding mutual information (EMI) and covariance intersection (CI). These data fusion methods were then combined with cubature KF to incorporate delayed measurements, for example, measurements from offline testing which are only available post-production. They implemented their proposed method in the nonlinear chemical polymerisation process. The results illustrated that the combination of EMI and cubature KF has a higher speed, while CI is more accurate for nonlinear and complex systems. Under classic state estimation approaches, data from delayed, offline measurements cannot be incorporated, although these are usually more accurate. The proposed method offers a potential framework to improve the accuracy of real-time estimation of unmeasured process states by exploiting these delayed measurements.

Luo et al. [55] studied batch-to-batch polymerisation and proposed an adaptive hinging hyperplane (AHH) model for the process, which is a type of piecewise linear model for nonlinear systems. A MIMO (multi-input multi-output) model was developed to predict the process behaviour. They used a KF to reduce the measurement noise, which corrects the AHH predictions of the current batch by applying information gathered from previous batches. A sequential quadratic programming method (SQP) was applied to solve the optimal control of each batch. The method was implemented for the polymerisation of styrene to achieve the desired values for number-average and weight-average chain length. The method resulted in improved accuracy and stability for the estimated process behaviours.

Recently, Rangegowda et al. [56], used a new approach, receding-horizon KF (RHKF), to estimate the state of methyl methacrylate polymerisation. RHKF is a combination of moving window-based methods, such as moving horizon estimator (MHE), and Bayesian estimators. It has the advantages of both methods, including simultaneous smoothing and filtering with a relatively low computational cost. The RHKF applies simultaneous state and parameter estimation in a moving window. They also compared partial likelihood and complete likelihood parameter estimations for the measurement update in RHKF. Results in polymerisation illustrated that RHKF based on complete likelihood parameter estimations performed better, and this method required much less computational time and produced accurate state estimations.

3.3. Material Forming Processes

The sustainability of raw material supply is an urgent, global challenge. Economies must adapt to become more climate-change resilient, more resource efficient, and to remain competitive. As a fundamental step in the lifecycle of many products and systems, efficiency in material processing is paramount, as is increasing the capability in processing 'circular' materials derived from waste and products which have reached the end of life. This presents new challenges for producers with raw material properties typically being more variable and making the manufacture of consistent quality products more challenging. In this section, we review the application of state estimation methods in material processing towards zero-defect sustainable manufacturing.

3.3.1. Injection Moulding

Injection moulding involves melting a polymer and injecting it at high pressure into a mould. It is one of the most used industrial processes for the formation of polymer products. Improvements in monitoring and control of the process can reduce energy consumption and waste generation as well as enable the processing of more complex, sustainable raw material streams [57].

Liu et al. [58] used an EKF to improve the part quality in a micro-injection moulding process by controlling the pressure signature. The pressure signature is generated by a pressure transducer as the plastic melt passes through the nozzle. Electromagnetic noise on the pressure signature can lead to short-shot (under-filling the mould) or flashing (overfilling the mould) because of the incorrect control of injection volume. The authors proposed an adaptive EKF based on F-distribution to track the pressure signature around the nozzle. The experimental results on a real microinjection moulding process showed that the adaptive EKF performed well in eliminating the noise and tracking the true pressure signature at both high and low injection speeds. Cao et al. [59] combined KF with iterative learning control to consider the effect of disturbances and random noises from batch-to-batch in repetitive processes such as injection moulding. First, they used a KF to estimate the current batch based on the information from previous batches—they called this estimation a ‘coarse guess’. They then refined it with iterative learning control. They proposed two different types of optimal control and two different types of suboptimal controllers to save memory and computational cost. They developed a linear steady-state model for the air shot phase in injection moulding and compared these four optimal controllers with conventional KF in 100 batches. The result illustrated that, unlike the standard KF, the four optimal and suboptimal controllers (combining conventional KF with iterative learning control) are able to reject the batch-to-batch noises and disturbances in injection moulding.

In the injection moulding process, in order to change from the filling phase (velocity control scheme) to the packing phase (pressure control scheme), a switchover point exists. The switchover point is determined empirically by experiments; however, if applied at the wrong time, the cavity pressure profile is affected, resulting in defects in the injection-moulded parts. Stemmler et al. [60] proposed a cross-phase controller method to eliminate this switch-over point and replaced it with a continuous pressure trajectory. They first derived a model for the filling and packing stages of the process. Then, the model was piece-wise linearised. The proposed model was applied in an EKF to estimate the states in an MPC (Model Predictive Controller) for optimization. Based on EKF predictions, the MPC specifies the controller output corresponding with the reference input. The comparison of the proposed approach to a PID controller in an actual injection moulding process resulted in the superior performance of the cross-phase controller method. Recently, they further developed the work to propose a model-based norm-optimal iterative learning controller to track a desired reference for the cavity pressure (based on PVT-optimisation) to optimise the part’s weight during an injection moulding cycle [61]. They used the piece-wise linearised steady-state model for injection moulding based on their previous work [60]. EKF was applied to track the desired cavity pressure and to estimate the process state. The experimental setup with the embedded pressure sensors resulted in manufacturing injection moulded parts that weighed 50% less than the non-optimised ones. The approach has the potential to achieve significantly higher efficiency in raw material use.

Chen et al. [62] proposed a method to detect the presence of a foreign body in an injection mould and minimised the ‘detected distance’ (i.e., the amount which a detected foreign body is compressed by the mould closure). Such a system can prevent damage to the mould, which results in defective parts, downtime, and costly repair. A state-space model is derived for the toggle mechanism, driven by a servo system (which closes the mould), and an EKF was used to filter the electric current readings of the drive for the toggle mechanism, which was then used to self-adapt the mould protection system to keep the current in a safe range. The system showed a reduction in the detected distance of foreign bodies of 22%. As damaged tools result in the fabrication of poor-quality parts and harm to the entire injection moulding machine, this approach can enhance the lifespan of the equipment as well as reduce scrap.

3.3.2. Other Forming Processes

Extrusion is a continuous process for forming polymer or metal products by forcing the material through a die to achieve a certain geometrical profile of the part. In polymer extrusion, it is essential to find the appropriate operating conditions for each feed material, as incorrect operating conditions can waste large amounts of energy, time, and material. Melt viscosity is one of the most important parameters relating to the product quality, but it is challenging to measure online parameters with physical sensors. Liu et al. [63] implemented a non-linear state observer approach to estimate the melt viscosity. Viscosity and pressure were modelled by a Genetic Algorithm (GA)-based dynamic Gray-box model with NFIR (nonlinear finite impulse response) structure. The viscosity was predicted from the process input parameters, and the predicted viscosity was then used to estimate the barrel pressure. The error between the predicted and measured barrel pressure was used to correct the viscosity estimation. The proposed method was applied to a real extrusion process with six different polymers and resulted in an RMS (root mean square) error of less than 1%. The method is proposed for use in the production of consistent products from recycled polymer feedstock despite having inherently variable viscosity behaviour.

Amoaoui et al. [64] developed an observer for the liquid composite molding process, which is a method for fabricating large composite parts with complex geometries, such as in the aerospace industry. This process suffers from issues of void formation at the flow front during resin impregnation, which reduces mechanical performance. An observer was developed for monitoring the system pressure (output) and the permeability (unmeasured state), which is inaccessible to physical measurements. They first derived a steady-state model for the process and designed a non-linear state observer using Lyapunov theory and a linear matrix inequalities technique. The performance of the observer was demonstrated by using simulation, which showed that the estimated permeability values converge to the true state values. Application of the method to real-time monitoring of void formation has the potential to reduce the production of scrap parts which do not meet the required specifications.

Remelting is a process to produce homogeneous metal ingots. The ingots should be defect-free with a fully dense and desired grain structure, as defects cannot be removed with heat treatment post-production. Achieving the desired grain structure requires precise control of temperatures in the process. Ahn et al. [65] investigated the temperature distribution in the electrode of the electroslag remelting process. They proposed a reduced-order melting model for the process and estimated the temperature using three different estimators; EKF, UKF, and steady-state nonlinear estimators. The controller with UKF had the best performance as it had less overshoot and responded better to disturbances. Lopez et al. [66] studied the Vacuum Arc Remelting Process, used in aerospace applications. A dynamic model capturing the melting and solidification stages was used and the goal was to track the solidification front. For state estimation, a PF was applied to the system. However, the system is nonlinear and noisy with low signal to noise ratio, meaning a lot of particles were required for high accuracy. They applied the PF with a GPU containing a large number of processors to enable parallelisation. The PF outperformed KF when used with a large number of particles, but with a high computational cost.

To improve resource efficiency and reduce weight, there is a demand for increasingly thin yet high strength steel sheeting. In automotive and aerospace sectors, a reduction in weight has a direct impact on reducing the energy consumption and carbon emissions associated with transport. However, metal forming processes are a challenge to control and model because of strong nonlinearity, complex material behaviour, and high variability due to varying raw material and lubrication properties, tool wear, etc. The mechanical properties of steel sheets are determined by the temperature profile during cooling which affects the resulting microstructure. The precise control of the cooling curve is, therefore, extremely important but is hampered by the difficulty in physically monitoring the temperature distribution. Various studies have been performed to estimate the internal spatial temperature distribution in sheet rolling using state estimation concepts.

Zheng et al. [67] used EKF to estimate the transient temperature distribution in the hot-rolled strip cooling process. They developed a nonlinear high-dimension (14 state variables) state-space model from a thermodynamic model of partial differential equations using a 2D finite volume scheme. The validation of the method with numerical simulation resulted in an accurate temperature estimation with EKF. Speicher et al. [68] used full and reduced EKF to estimate plate temperature in heavy plate rolling based on a few thermocouple measurements. They used a similar approach to discretise a partial differential equation model of thermodynamics using a finite difference method. As the quantification of the process noise is the major practical challenge in implementing an EKF, they propose a systematic method for tuning of the process noise covariance matrix via an analysis of the extended dynamic system. The approach was tested in an industrial rolling mill and shown to successfully estimate the temperature distribution. The reduced and full EKF performed similarly in estimation, however the reduced EKF simplifies the simulation and reduces computational time.

Kloeser et al. [69] examined the spatiotemporal estimation of temperature distribution in the hot sheet metal-forming process. Rather than using a coarse grid finite difference method to derive the state-space model, they instead designed a dynamical Reduced Order Model (ROM) from a high-dimensional thermo-mechanical model by proper orthogonal decomposition (POD). Starting with a refined model of several thousand states, they use POD to project the states onto a reduced order state space model, which preserves the most important dynamics in the system. A disturbance model was added to the EKF to address simplifications and modelling errors. The approach was validated in a simulation of the hole-flanging process by a reduction in the number of states from 17,000 down to 30. The experimental results confirmed the approach in the estimation of spatial-temporal temperature distribution in realtime by using sparse local temperature measurements.

Havinga et al. [70] used a PF with online force measurements to estimate the physical state (sheet thickness, friction, angle after bending, etc.) of the product in a metal forming process based on force measurements. They built a 2D FEM model of the bending process and then applied POD along with Radial Basis Function interpolation to create a fast model. The proposed approach was used in the numerical simulation of the bending process and successfully predicted the state changes based on variations in process forces.

The applications of state estimators in polymer synthesis and material processing and the resulting potential impact on sustainability are summarised in Table 2.

Table 2. State-estimators used to improve material synthesis and forming processes.

Process Industry	Method	Desired Output	Sustainability Impact	Refs
Polymerisation	Cubature KF	Concentrations and molecular weight distribution (MWD)	Inline monitoring of the process and efficiency improvement	[54]
Polymerisation	PID and EKF	Molecular weight (Mw)	Better estimation of process, less waste and higher process quality	[52]
Polymerisation	KF	Number-average and weight-average chain length	Better estimation of process and efficiency improvement	[55]
Polymerisation	Receding-horizon KF	State of methyl methacrylate polymerisation	Less computational time and efficiency improvement	[56]
Micro-injection moulding	EKF	Pressure signature	Improvement in part quality and less material waste	[58]
Injection moulding	KF and iterative learning control	State estimation	Improvement in machine control and part quality and efficiency	[59]
Injection moulding	EKF and MPC	Pressure trajectory	Improvement in part quality and process	[60]

Table 2. Cont.

Process Industry	Method	Desired Output	Sustainability Impact	Refs
Injection moulding	EKF	Cavity pressure	Production of lighter parts and less raw material use	[61]
Injection moulding	EKF	Detected distance	Increase the tool life and efficiency improvement	[62]
Polymer Extrusion	Nonlinear State Observer	Melt viscosity	Part quality enhancement Ability to process recycled materials less waste and rework	[63]
Liquid composite molding	State observer	Pressure and permeability	Part quality and process efficiency enhancement by less waste and rework	[64]
Electroslag Remelting	Linear KF	Temperature distribution	Defect-free ingots and efficiency improvement	[65]
Vacuum Arc Remelting	PF	Solidification front	Production of defect-free ingots without heat treatment	[66]
Hot-rolled Strip Cooling	EKF	Transient Temperature distribution	Better control of microstructure resource efficiency and quality.	[67]
Heavy Plate Rolling	Full and reduced EKF	Plate temperature	Better control of microstructure. Reduction in material use and weight	[68]
Hot Sheet Metal Forming	EKF	Spatial-temporal Temperature distribution	Prediction of material properties and reduction in material use and weight	[69]
Metal Forming	PF	Physical properties (thickness, bend angle, etc.)	Improvement in production accuracy and efficiency	[70]

3.4. Machining Processes

Machining processes include milling, grinding, turning, drilling, etc., which contribute about 5% of the gross domestic product (GDP) in the developed world [71]. A significant factor in the cost of machining has been associated with suboptimal tooling setups, with cutting tool failure contributing to almost 20% of the machining downtime [72]. Machining processes are less efficient and consume unnecessary energy while working with faulty tooling. Machining processes account for approximately 33% of primary energy use in the manufacturing industry globally [73], but approximately only 25% of the energy consumed accounts for actual cutting [74]. Researchers have explored various methods to improve efficiency within the industry, with particular emphasis on improving monitoring methods for the condition of tools and various part quality indicators. The application of state estimation methods for predicting tool wear and part quality estimation in machining processes has become more prevalent over the past 10–15 years.

Tool wear is an important aspect of machining processes, as worn tools result in unnecessary energy consumption, waste generation, and process downtime. A number of researchers have explored the use of state observers and Bayesian methods with mathematical models of tool wear within machining processes.

Niaki et al. [75] developed a discrete linear model from a mechanistic model of tool wear to be used with a Kalman filter. While the true dynamic behavior of tool wear is nonlinear at the initial stages, linear at intermediate stages, and nonlinear at the final stages before catastrophic failure [76], their work focused only on the linear stage. From the mechanistic model of cutting, a linear relationship is derived between power consumption and tool wear. In-line measurements of spindle current allow for power consumption estimation, which is used to correct tool wear and tool wear rate estimates. In an experimental trial, the designed Kalman filter resulted in a maximum average error of 10% of tool flank wear using this low-cost method. Tiwari et al. [77] further extended the KF scheme proposed by Niaki [75] in an end milling process to incorporate machine vision measurements of the surface texture of the cut surfaces. Linear regression was used to formulate a measurement model of flank wear with the cutting force and image histogram variance as the measurement vector y . An alternative measurement model excluding cutting force

was also tested. In experimental trials, both KF implementations were able to predict the progression of tool failure, providing better accuracy than the standalone regression model (without the mechanistic model of tool wear progression). Both models provided adequate estimates of the flank wear, meaning that the force measurement could be neglected.

Zhang et al. [78] proposed the use of Least Squares Support Vector Machines (LS-SVM) in a Kalman Filter for tool wear estimation, also incorporating visual images into the measurement update. LS-SVM is used to train a tool wear prediction model from cutting conditions, cutting time and wear position based on a historical data set. A KF framework is implemented to 'correct' the LS-SVM model predictions using observed tool wear from visual images (LS-KF model). Because the model process noise and the measurement noise covariances are assumed to be fixed, the Kalman gain converges to a steady-state KF, which occurs after six time-steps. The steady-state KF was then used to update the LS-SVM model without actual tool wear images (LS-KF-S model). The KF approach significantly improved the prediction errors relative to the open-loop LS-SVM model alone. While the best performance is achieved using continual visual measurements of tool wear in the LS-KF model, LS-KF-S also provided good estimation performance. In this case, the KF framework facilitates significant improvements in LS-SVM predictions with a small set of images to correct the model.

Sadhukhan et al. [79] presented an unscented Kalman Filter (UKF) for flank wear estimation in a turning process. A discrete flank wear model is developed where two components of flank wear due to abrasion and diffusion are considered as state variables. The system model parameters are determined from experimental data. A linear measurement equation, derived via linear regression from the experimental data set, relates the state variables to the measured cutting force. Both a UKF and Extended Kalman Filter (EKF) were compared for tool wear estimation in a simulation. The simulation of both methods showed that flank wear estimation by UKF outperformed that of EKF with a 50% reduction in the error of UKF estimates relative to EKF.

The application of a particle filter framework for tool wear monitoring has been explored in a series of works [80–84]. A PF method for tool wear estimation in a milling process was proposed in [80] and further developed in [81]. This work proposes a physics-based analytical tool wear model for the prediction of the tool wear state, with the model parameters described by uniform probability distributions. A particle filter-based scheme is investigated to estimate the model parameters and the tool state based on online measurement. Tool vibration signals and force measurements are used as indirect measurements of the actual tool wear state. First, various features of the signal measurements (statistical, frequency-domain, and time-frequency domain) were extracted and analysed for the relationship with tool wear using an experimental dataset. It was found that wavelet energy in the x-direction of the force measurement has a strong linear correlation with the tool wear and, hence, it was selected as a single measurement for use in a particle filter measurement update. In [81], both an autoregressive (AR) model and support vector regression (SVR) were investigated to formulate the measurement model in order to predict the online measurement from the estimated tool wear state. In general, SVR outperformed the AR model. The use of a PF with an SVR or AR measurement model improved tool wear prediction by 2% compared to a PF using a simple linear measurement model. In [82], a similar scheme was explored with the addition of evaluating various dimension reduction techniques for improving the signal feature selection step of formulating an SVR measurement model. Principal Component Analysis (PCA), kernel Principal Component Analysis (k-PCA), and Locally Preserving Protection were explored with the best performance yielded by k-PCA. The performance of two different PF algorithms was explored in [84]. A Local Search Particle Filter (LSPF) is compared against a conventional sequential importance resampling (SIR) method. LSPF showed a reduction in prediction error by over 30% in comparison to the standard SIR approach, which suffered from the particle population diminishing too soon. In [83], the system model allows for time-varying machining settings and uses a particle filter for joint state and parameter estimation. A refined particle resampling strategy is

proposed for the implementation of the PF. In this work, the online measurements include acoustic emission (AE) data. Changes in the distribution of vibration and AE data were interpreted as indicators of tool wear. This method allows for good accuracy of tool wear prediction under changing settings of feed rate, cutting depth, and cutting speed.

Bayesian estimation methods have also been used to estimate the surface roughness of parts while they are being machined. Conventionally, surface roughness is measured post-manufacturing, which can result in waste due to rejects detected too late for corrective action to be taken. Moliner-Hereida et al. [85] examined three approaches for surface roughness monitoring of machined parts in real-time. In the first, they used an open-loop system to estimate surface roughness on the assumption that the surface roughness increases at a constant rate (as the cutting tool wears over time). In the open-loop scheme, the surface roughness is estimated based on an empirical model of the relationship between cutting parameters, surface roughness, and power consumption. In the second scheme, a steady-state Kalman filter was used for surface roughness estimation (i.e., both the process noise and the measurement noise covariances are assumed to be constant). The system model predicts both surface roughness and power consumption—again under the assumption that both increase at a constant rate, which depends on the cutting parameters. Actual power consumption measurements are obtained every ten parts and allow for the correction of state estimates. The third scheme incorporated surface roughness readings from a profilometer in addition to power consumption information at the same rate of every ten parts. The profilometer checks the surface roughness post-machining. All three approaches were compared in a simulation study. While the Kalman Filter implementation in scheme two improved results over the open loop system, significantly better performance was achieved by also including profilometer measurements.

Zhang et al. [86] examined tool wear estimation and surface roughness prediction in a micro-milling process with a particle filtering approach. An improved analytical surface generation model was developed from analysis of the process geometry-kinematics. The theoretical trajectory of tool wear including the non-linear behaviour of tool run-out was predicted. Using the particle filter framework, predicted tool wear was updated with tool vibration and dynamic cutting force measurements. The resulting stochastic model of the cutting process was used to predict surface roughness under five different machining conditions. The influences of the machining parameters on the stochastic surface generation were also analyzed. The model allows for the prediction of machined surface quality prior to the costly micro milling operations, and provides a basis for the optimization of machining parameters to improve quality and efficiency.

Table 3 summarises the studies undertaken using various state estimators in machining processes with the resulting impact on sustainability.

The application of state estimation approaches as presented in this section, has demonstrated greater accuracy in condition and part quality monitoring in machining processes compared to using open loop models. In many cases the proposed Bayesian filtering frameworks incorporate machine learning methods into the measurement update for dealing with complex high dimensional data, such as vibration and acoustic emission signals and visual images. The application of Bayesian inference is shown to improve over the use of machine learning approaches alone. The improved condition and part monitoring performance can result in greater control over the process, resulting in reduced downtimes due to unexpected tool failures and a reduction in energy use and waste generation from faulty tooling and components [87].

Table 3. State-estimator methods used improve sustainability of machining processes.

Machining Process	Method	Desired Output	Sustainability Impact	Refs
Milling	KF	Tool flank wear	Estimation of tool life and tool changes schedule	[75]
End-Milling	KF	Remaining tool life	Estimation of tool life, efficient tool changes and reduced waste	[77]
Milling	Least Square SVM and KF	Remaining tool life	Improve tool life prediction and process efficiency	[78]
Turning	Unscented KF	Remaining tool life	Tool life prediction, tool changes and process efficiency	[79]
Milling	PF	Wear width of the tool	Tool width estimation, tool change scheduling and process efficiency	[80]
Milling	PF	Remaining tool life	Tool life prediction, tool change scheduling and process efficiency	[81]
Milling	Augmented PF	Estimation of tool degradation	Tool life estimation and process efficiency	[82]
Milling	PF	Tool life estimation	Tool life monitoring, tool change scheduling and process efficiency	[83]
Milling	Local Search PF	Tool life estimation	Tool life monitoring, tool change scheduling and process efficiency	[84]
Milling	Model-based KF	Surface roughness	Improved part quality and efficiency improvement	[85]
Micro-Milling	PF	Surface roughness and Surface topology	Improved part quality and reduced waste	[86]

3.5. Semiconductor Manufacturing

Semiconductors have an invaluable role to play in meeting global climate goals as they are intrinsic to solar panels, wind turbines, electric vehicles, and many other green technologies. However, as the demand for computer chips continues to grow, semiconductor manufacturing itself has many challenges with regard to sustainability, as it requires significant input of energy and water and creates hazardous waste [88]. A recent analysis showed that the greatest source of carbon emissions in computing is from hardware manufacturing and infrastructure [89]. As a result, there is increasing attention on approaches to minimise resources and generation of waste in semiconductor manufacturing. State estimation plays an important role to this end as a persistent challenge in semiconductor manufacturing control is the lack of critical in situ sensors to provide real time information on the wafer status for feedback control and optimisation.

Semiconductor processing consists of many different operations to create the finished product. Due to physical constraints, it is not feasible to conduct the high precision metrology needed for quality validation until after a step is completed. However, processes such as lithography are subject to many sources of variation caused by environmental changes, regular maintenance, and operational drift over time. Therefore, metrology steps are integrated into the production line to minimise the delay as much as possible [90]. Typically, each main processing step utilises ‘run-to-run’ (R2R) control, which integrates process control theory with statistical process control (SPC). In R2R, wafer measurements following a run of a unit process are used to update the process settings for the next run in order to achieve the required quality targets. The basic structure of a run-to-run controller consists of a process model, a state estimator, and a control law. The successful implementation of R2R control in commercial facilities has been achieved for processes including chemical mechanical polishing, chemical deposition, and plasma etching and it has proven that it can efficiently improve the product yield and reduce scrap, rework, and cycle time [91]. Exponential weighted moving average (EWMA) control (composed of EWMA filtering followed by a deadbeat controller) is the established method of R2R control and has been shown to be optimal for processes subject to integrated moving average (IMA)

disturbances, which is the most common type of disturbance signal in semiconductor manufacturing. Kim et al. [92] explored a Kalman filter based R2R controller and compared performance against an EWMA controller for minimising variation in the quality variables of the product under different types of process disturbance signals. The Kalman filter provides the optimal one-run-ahead prediction of the model parameters perturbed by the disturbance, and the controller computes the control input for the next run to compensate for the effect of the disturbance. For IMA and integrated white noise (IWA) disturbances, the EWMA and Kalman filters have the same structure and show identical performance. However, for integrated auto-regressive (IAR) and auto-regressive integrated moving average (ARIMA)-type disturbances, the Kalman filter R2R controller outperformed the EWMA controller.

Disturbance observers aim to identify the specific nature of a disturbance in a system and to subtract this from the control input in order to reject disturbance. This involves feeding the output y of a plant through an inverse model of the plant and subtracting the input signal u to estimate the disturbance signal. Disturbance observers have been shown to be effective in high precision motion control for mechatronic stages in semiconductor processes including lithography and chip packaging [93–96]. The disturbance observer concept has also been applied to run-to-run control to deal with some of the shortcomings of EWMA control. If there is severe aging of a production tool or the process drifts, EWMA control produces an offset in the process output, which can be corrected by different means such as a predictor corrector controller (PCC) or double EWMA controller. Lee et al. [97,98] proposed an output disturbance observer (ODOB) structure as a unified framework for these controllers and provided a systematic method to obtain the optimal parameters for guaranteed optimal nominal performance. They showed in simulation studies that the performance of the controllers was improved using this method.

A challenge for R2R control is the trend towards high-mix manufacturing; i.e., a single machine may process several different products at different times, and products with the same specification may be fabricated on different machines in different lots. This led to the introduction of ‘threaded’ R2R control, which partitions historical data into different ‘threads’ based on the specific manufacturing context (tool, product, etc.). However, as product mixes are becoming increasingly diversified, this can result in too many threads, some of which have insufficient data. A long delay between adjacent lots in one thread may make the estimation unreliable for infrequently manufactured products. Furthermore, a lack of information sharing on data relating to tool degradation means that all the threads using the same tool must address this shift disturbance separately [99]. To address this, several non-threaded state estimation methods have been proposed, which involve an observer to identify the contribution from different production contexts. Of these methods, the Kalman filter is one of the most important [91]. Haririchi et al. [99] proposed a modified Kalman filter to overcome the problem that in a non-threaded system, the model structure can be such that the system states may not be completely observable. Wang et al. [100] proposed a modified, simple-to-implement Kalman filter scheme (involving periodic reset of the P covariance matrix) that considers the fact that if a context item is not involved in a process run, then its state does not change. The method was shown to be robust to uncertainty in the disturbance parameter and to outperform the conventional KF scheme for common IMA-type disturbances.

A drawback of KF methods is that the nominal performance of the controller can only be maintained when the disturbance model is known. In recent work, an extended state observer (ESO) was investigated for R2R control in semiconductor manufacturing [101]. ESO algorithm disturbances, including plant-model mismatch, are lumped into a total disturbance, which is set as a new state. An advantage of ESO is that the disturbance can be reconstructed without an accurate model. A threaded ESO R2R controller was shown to outperform other threaded approaches in a photolithography process fabricating five different products. The authors further developed a discrete sliding mode observer for the same process, which estimates disturbance without using a process model. The system

was shown to outperform EWMA and double EWMA controllers in the rejection of IMA disturbances with a shift or drift (as occurs in tool aging). It also performed better under plant–model mismatch and had better tolerance for metrology delay [102].

Tsai et al. [103] developed a discrete sliding mode observer to estimate the core temperature of multi-layer metal plates in semiconductor manufacturing process for real-time (rather than run-to-run) thermal control. While the middle and top layers are monitored by thermocouples, the middle layer is not accessible to physical measurement. This can result in either excessive heating, which can damage the material, or heating which is insufficient to result in the desired metal phase change. A state space model was developed from the physics of the heat transfer processes. A sliding mode observer was proposed due to the high robustness of the approach to plant-model mismatch and external disturbances. The system was shown via experiment to accurately estimate the core temperature of the system despite being influenced by unknown external cooling temperatures.

In summary, state estimation has a powerful role in semiconductor manufacturing due to the problems in achieving physical measurements relative to the required precision in situ. State estimation methods are combined with SPC approaches in run-to-run control to minimise the effect of process disturbances. Sophisticated algorithms have been devised, which can enable tight quality tolerances to be achieved, despite many sources of variation in fabrication sites having a high product mix. Most recent developments show the potential for good performance without an accurate model of the process disturbances, making practical implementation more feasible. Due to the high environmental impact of semiconductor manufacturing (energy and water use, and toxic waste products), the ability to produce wafer products ‘right first time’ can reduce scrap, rework, resource use, and emissions.

3.6. Additive Manufacturing

Additive manufacturing (AM) is the fabrication of objects from computer-aided design (CAD) data by translating 3D CAD data into 2D cross-sectional profiles. Material is then deposited layer-by-layer following the form of the generated 2D cross-sections, which fuse to form the 3D object. Early applications of additive manufacturing were for rapid prototyping of non-functional models. However, with advances in materials and technology, AM is now widely used in various industries to produce products that offer both form and function, and it is no longer limited to basic model creation [104].

AM processes are near net-shape; that is, the initial fabrication of the product is very close in size and shape to the final requirements, meaning minimal material removal is required. Compared to conventional and subtractive manufacturing such as machining, additive manufacturing is significantly more resource efficient and can reduce the need for additional, energy-intensive post-processing steps [105]. The main advantage of AM over conventional machining methods is that it can produce complex parts with geometries not possible through conventional methods with a high degree of precision. AM can be used to manufacture one-off bespoke products, such as customised medical devices, cost-effectively and close to the point of use, eliminating distribution steps. However, challenges remain in production of defect-free parts by AM processes and the development of inline process monitoring and control of critical features is still at an early stage, with most commercial systems having only open-loop temperature regulation schemes [106].

There are different types of AM processing techniques, which can be classified into seven general categories: powder bed fusion, material jetting, vat polymerization, sheet lamination, fused deposition modelling, binder jetting, and directed energy deposition [107]. Within these, there are three main classes that have the greatest application in manufacturing processes, namely Powder Bed Fusion (PBF), Directed Energy Deposition (DED), and Fused Deposition Modelling (FDM) (see Figure 6).

In the PBF process, the parts are built from a bed of powder particles (polymer or metal) that are fused together selectively by a heat source, layer by layer. This heat source can be a laser or electron beam [108]. The DED process fabricates components by melting

the material, in the form of powder or wire, with a focused laser beam [109]. The last class, FDM, also known as fused filament fabrication (FFF), feeds a polymer filament through a nozzle, which heats it to a molten state. This molten filament extrudes through the nozzle, which deposits the polymer onto a build plate based on the 2D cross-sectional layers of the 3D design [110].

These three classes have a lot of process parameters and design criteria which affect the quality of the additively manufactured parts. These include material selection and properties, melt pool temperature, melt pool width, laser power, support structure design, bed adhesion, layer height, wall thickness, infill parameters, etc. A number of recent studies have explored improving the quality of the process and final printed parts with real-time monitoring by using KF, PF, and other state observers to improve on the limitations of physical measurement.

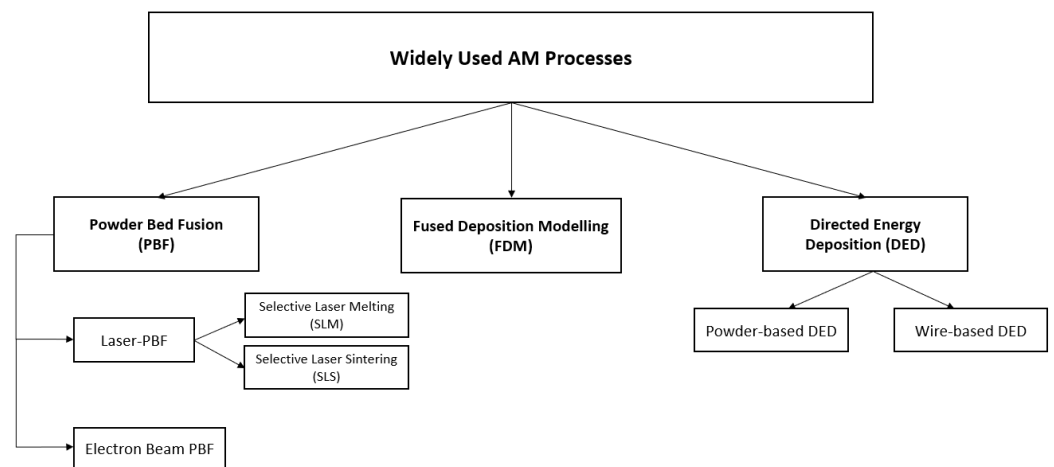


Figure 6. Classes of AM widely used in manufacturing industries.

Monitoring and control of processing temperatures is one of the most vital factors in metal AM since it affects metallurgical phase formation and thereby the microstructure of the printed part [111]. The energy to melt the material in PBF and DED processes is localised in a small melt pool, and as a result, the temperature gradients are extremely large. This causes differential thermal contraction and local micro-distortions, which can integrate to form large milliscale distortions [112]. It is not possible to place a physical temperature sensor on the surface being built; thus, temperature measurement must always be remote. Most commercial systems have a thermocouple in the build plate but the temperature here is hundreds of degrees lower than at the melting plane. Some more expensive systems use digital camera-based pyrometer systems to monitor the melt pool or to obtain a thermal image of the top surface.

In a low-cost approach, Oakes et al. [113] proposed a two-step Kalman filter in Laser Metal Deposition (a DED method) to monitor the melt pool temperature in a closed-loop model-based controller. They compared the performance of a temperature controller with and without KF on two different temperature references (time-varying and constant). A comparison of the results showed a reduction in average absolute error by almost 32% and 23% for the constant and time-varying references, respectively. Despite the high system uncertainty, KF performed well in estimation of the melt pool temperature.

Research undertaken by Jiang et al. [114] used a Kalman filter to control the temperature of the powder bed in a PBF process. They introduced a multi-zone temperature control in which nine temperatures from different locations of the powder bed were extracted by infrared cameras and each of them were fed back to a separate PID controller. They compared the results: first to a single loop controller that used only one average temperature reference and one PID controller; and secondly, to a Model Predictive Control (MPC) controller. For all methods, KF was used to filter the measurements with large noise covariances. They

demonstrated that multi-zone control has a superior performance compared to single-loop and provided similar performance as MPC. However, it had the advantage that it reduced the computational cost in comparison to MPC.

In addition to control of temperature, research has also been performed on the control of other quality factors within AM processes. Lopez et al. [115] studied uncertainty identification and propagation in the prediction of melt pool width in a Laser PBF process. They further developed a thermal model from a laser cladding process [116] to be applied to PBF for melt pool width prediction. They validated their model using a case study of printed overhanging structures and showed how thermographic monitoring is effective in uncertainty identification and reduction. A KF was used for process estimation using the noisy measurements of melt pool width. The approach has the potential to be applied to control the melt pool dimensions in real-time.

The high laser power in PBF evaporates and fuses the metal powder. If the boiling point is reached, a vapour plume arises in the melt pool that causes the formation of a void in the printed parts. The evaporation also generates sparks, known as spatter, that can lead to instability in the melt pool and discontinuity at the surface. Hence, real-time monitoring of plume and spatter can aid better control of the process to avoid such defects [117]. Zhang et al. [118] monitored and extracted various features from the melt pool in laser PBF, including plume and spatter, with an off-axis vision monitoring system employing a high-speed camera. The contrast of images from the camera was enhanced using an optical filter. They introduced a novel image processing method to segregate melt pool, plume, and spatter from each other. They also used KF tracking to find the exact location of the melt pool. Various features such as melt pool intensity, plume area, plume orientation, spatter area, direction and velocity were extracted in four different single-track scenarios using this approach. These features are the potential indicators that assist with the investigation of and decisions on printed part quality.

As the temperature history directly influences phase formation, the ability to estimate the complete temperature history of the entire part, and not only the melt pool, would be extremely valuable for process validation and precise control over resulting part properties. Wood et al. [106] conducted investigations using state observation for the estimation of temperature states throughout the printed part itself from the measurement of surface temperature in the laser PBF process. Here, a Finite Element Method (FEM) was utilised to model the complex spatio-temporal temperature dynamics of the process. A high-dimensional state-space model (196 state variables) was extracted from the FE model, from which the KF temperature state observer was defined. They successfully estimated temperature evolution in several simulated test parts.

They further developed their work in later research to estimate internal temperature distribution and proposed a two-dimensional linear model with FEM not only for a laser heat source (L-PBF) but also for electron beam PBF (E-PBF) [119]. They applied an ensemble KF to this system to deal with high dimensionality. In their research, the EnKF estimates temperature by correcting the linear model temperature prediction to agree with measurements extracted from a Finite Element model in lieu of physical measurement data. In simulation tests, they assessed the EnKF estimation error for E-PBF and L-PBF systems when the assumed material properties matched the FEM simulation and when they differed. Figure 7 presents the L_∞ -norm of the temperature errors (i.e., comparison of the maximum errors) for E-PBF (labelled 3) and L-PBF (labelled four) for the open loop and EnKF estimates for 304 stainless steel (SS) at low temperature (Figure 7a) and elevated temperature (Figure 7b). The EnKF scheme presented up to a 44% reduction in the L_∞ -norm of the temperature field error relative to the open-loop FE model predictions when the material properties differed. The method has the potential for exploitation in a closed-loop control scheme to modulate laser power in order to ensure that the desired microstructure is achieved despite uncertainty in the raw material properties.

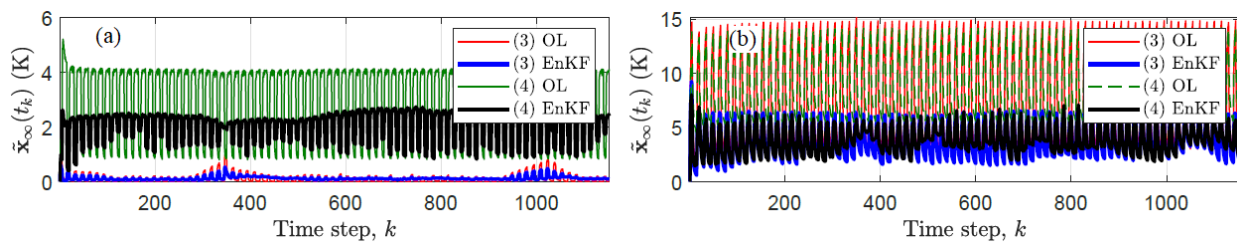


Figure 7. Comparison of L_{∞} -norm error of open loop with EnKF for E-PBF (3), L-PBF (4) with (a) 304 SS at low temperature and (b) high temperature

Several studies have also been conducted to investigate the processing parameters and part quality of polymer printed parts. Kim et al. [120] proposed a digital twin method for part temperature measurement in FDM. Similarly to the work of Wood et al. [106,119], they defined a spatio-temporal thermal model here using the finite difference method. They fused this model with sensor data (IR camera) using a linear KF to estimate temperature. The verification of the method was performed with a virtual experiment setup, which demonstrated that this closed-loop approach can estimate the temperature and related uncertainties accurately.

Garanger et al. [121] proposed an optimal control law to control the mechanical properties in leaf springs produced by fused deposition modelling. They printed the stacked leaves with a simple FDM printer using PLA filament and used a KF framework to estimate the stiffness of parts. The KF was applied to update the stiffness estimates following a physical test of the stiffness of each printed leaf. The proposed KF method resulted in higher accuracy in stiffness estimation in comparison with an unfiltered open-loop prediction model. They later followed a similar approach to estimate the stiffness in a printed cantilever beam [122]. They proposed a dynamic model for the printing process of the beam and fused this model with force sensor data in an optimal control law with KF. Comparison with an open-loop system showed an improvement in predicted stiffness error of about 94% and a reduction in noise by almost 80%.

Table 4 summarises the studies that have been performed to date in AM with state estimators and their related sustainability impacts. State estimators enable inline monitoring of process parameters which cannot be directly measured or for which only noisy measurements are available. Enhanced monitoring of the process and online estimation of part quality indicators can reduce defects in the printed parts such as delamination and warpage. Hence, as the failures are predictable, there will be less wasted material, energy, and time and greater practical realisation of the benefits of AM.

Table 4. State-estimators used to improve sustainability of AM processes.

AM Process	Method	Desired Output	Sustainability Impact	Refs
DED	Two-step KF	Melt pool temperature	Better estimation of the process and efficiency improvement	[113]
PBF	PID and KF	Temperature of powder bed	Enhance the profits by reduction of computational cost	[114]
Laser PBF	KF	Melt pool width	Part quality and efficiency enhancement by less waste and rework	[115]
Laser PBF	Image processing and KF	Various features of melt pool, plume, and spatter	Part quality and efficiency enhancement by less waste and rework	[118]
Laser PBF	State-observer	Temperature estimation of underlying layers of the part	Higher precision part and less rework	[106]

Table 4. *Cont.*

AM Process	Method	Desired Output	Sustainability Impact	Refs
E-PBF and L-PBF	Ensemble KF	Internal Temperature fields	Higher part quality and waste reduction	[119]
FDM	Linear KF	Printed part Temperature	Uncertainty estimation and process quality enhancement	[120]
Polymer AM	KF	Stiffness of the printed part	Part quality and efficiency enhancement by less waste and rework	[121]
Polymer AM	KF	Stiffness of a printed cantilever beam	Part quality and efficiency enhancement by less waste and rework	[122]

4. Discussion

State estimation is an important concept in manufacturing, providing a suite of tools for improved monitoring and control of manufacturing systems. In this review, we have highlighted recent advances and applications of state estimation in industrial robotics, chemical processes, material forming, machining, semiconductor manufacturing, and additive manufacturing sectors. In particular, Bayesian filtering concepts have emerged as a popular approach to estimate system variables which cannot be measured directly or for which only noisy, uncertain, and/or latent information is available. Compared to deterministic state observer approaches, the Bayesian methods have enhanced flexibility in facilitating the incorporation of knowledge about the uncertainty of both system and measurement models and different sources of data about the process. This means that not only is the most accurate estimate of the system states derived under a probabilistic framework but also a measure of the associated uncertainty is derived, which provides useful information to operators and manufacturing managers about the appropriateness of corrective action. Particle filtering is more flexible than the Kalman filter as it can deal with non-Gaussian probability distributions, and advances in computing power mean that it is now a feasible approach in systems where dimensionality is relatively low. Kalman filtering and particle filtering have been shown to improve the precision, speed, and perception of industrial robotics, improving the capability of robots to work alongside humans for more efficient, flexible, and safer manufacturing processes. These Bayesian filtering methods have also found wide application in the estimation of product quality variables in material synthesis and processing (see Table 2), tool condition and part quality monitoring in machining processes (Table 3), compensation of process disturbances in high precision semiconductor manufacturing (Section 3.5), and for quality monitoring and control in additive manufacturing processes (Table 4). Below, we outline the main challenges and limitations in the implementation of state estimation approaches in manufacturing and discuss emerging and future trends in the context of sustainable manufacturing.

4.1. Limitations and Practical Issues

A problem with the practical implementation of Bayesian methods is that model uncertainty is often difficult to quantify, particularly with regard to process noise. In practice, the measurement noise is usually estimated from experimental data (comparing sensor measurements to known ground truth values) and the process noise covariance is tuned until good filtering performance is achieved. In operation, the estimates should be monitored for divergence over time—if the difference between the predicted measurements and actual measurements is significantly higher than the expected covariance, then the reason for the divergence should be investigated. If it is due to sensor errors (outliers and missing data) or numerical issues, then the filter should be restarted. However, if divergence is due to model errors then the filter should be redesigned. Reference [28] provides useful information on troubleshooting these practical issues. A useful starting point for model uncertainty analysis is to examine the sensitivity of model predictions for

initial conditions and/or model parameters. A sensitivity analysis will reveal what model outputs are most influenced by different states/parameters and can reveal weaknesses in the information flow—for example, to identify where in the process sensors should be located and if additional sensor data are needed (see for example [123–125]). That said, the Bayesian filtering approaches have limitations where the actual nature of the system uncertainty is unknown, as is the case with manufacturing systems which may be subject to different sources of variability in the interval between measurement data being available. This arises particularly in the case of semiconductor manufacturing where high precision metrology for analysis of part quality can only be conducted after each run and used to update the process settings for the next run. In this context, the application of a disturbance observer framework (where the system output measurements are input to an inverse model of the plant to estimate the disturbance signal directly) has been found to be useful in improving control performance. Furthermore, the sliding mode observer, which has the property of high robustness to unknown disturbances, has shown excellent potential for practical applications where accurate models of process disturbances are unavailable.

4.2. Spatio-Temporal Monitoring

While state observers and Bayesian filters have traditionally been used to estimate system states which vary over time at a particular point, recent developments have extended the approach to observe dynamic variables which are spatially distributed—taking inspiration from approaches applied in geostatistics. This has been investigated in additive manufacturing and metal forming where a number of works have applied Bayesian filtering methods to estimation of spatio-temporal temperature dynamics [119,120]. In these processes, physical measurements of temperature are limited by physical accessibility. However, the temperature profile is directly related to the quality of both metal and polymer parts affecting microstructure and void formation in the former, and the resulting residual stresses and warpage in both. Due to complex spatio-temporal dynamics, the system model in these cases is derived from numerical finite element models. In metal forming, this has been addressed by either (i) using a coarse 2D grid with low spatial resolution or (ii) using a reduced order model which allows for a more complex model and higher spatial resolution but preserves only the most important dynamics of the system. In AM, a very high number of state variables from an FE approach were preserved and an Ensemble Kalman Filter (EnKF) proposed to deal with the high dimensionality [120]. However, this work is still in its early stages and has only been tested in simulation and on 2D models to date.

4.3. Relationship between State Estimators and Machine Learning in Manufacturing

The literature points to an emerging trend in combining machine learning with model-based state estimation, and this has been pursued in monitoring and control of machining processes in particular. Physics-based models of cutting have been exploited to predict the progression of tool wear and increasing surface roughness in milling and turning processes, while available machine measurements such as cutting force power consumption are used to correct predictions. However, increasingly indirect measurements including visual images, vibration signals, and acoustic emission data are used to provide information on the tool and/or part state, and it can be difficult to derive physical relationships between changes in these types of signals and the wear of the tool. A number of recent works have, therefore, applied machine learning to develop a suitable measurement model for applications in a Bayesian filtering framework. Notably, the combination of a system model which predicts the progression of tool wear and/or part roughness together with measurement information from the process is shown to outperform machine learning models on their own [78]. In the case of robot perception, Bayesian filtering is also currently regarded as a more accurate and mature approach than AI-based methods such as ANN and neuro-fuzzy approaches [36].

4.4. Systems-Level Approach

A trend in recent works on state estimation in manufacturing is a greater tendency towards a more holistic systems level approach to evaluating, optimising, and controlling a manufacturing system. It is shown that a predict-correct state estimation framework can perform the following: (1) incorporate post production inspection and QA data into real-time monitoring and process control (e.g., [54]); (2) exploit historical data for process modelling via machine learning where physical relationships are not well defined; and (3) integrate computational models typically used for product design/process setup into the process monitoring and control scheme. State estimation algorithms have also been applied to the issue of cybersecurity in the context of industrial Internet of Things. While IoT is an enabling technology for the capture, sharing, storage, and utilisation of data in distributed industrial control systems, it also makes industrial processes vulnerable to cyber attacks, which can result in economic and environmental damage as well as risks to human safety and health. In [126], a Kalman filter is proposed for time-series prediction of process states in a petroleum gas oil treatment process. KF is shown in the simulation to be effective for rapid anomaly detection in a framework which facilitates automated control action to correct the plant operation to safe levels. Other research works examined Kalman filter-based fault detection and isolation methods to enhance the cyber security of water treatment plants and found that these state estimation methods excel in certain types of attack but have limitations in others and cannot always effectively isolate and correct the system [127,128]. There remain several challenges in secure state estimation and control of cyber-physical systems, and further research on data-driven and AI-based secure state estimation approaches is anticipated [129].

4.5. State Estimation and ‘Digital Twins’

A digital twin is a computational representation of a physical process where there is exchange of data in real-time between the real and virtual processes. Digital twins are seen to be a vital tool for design, optimisation, control, virtual testing, and predictive maintenance of industrial processes [130]. A digital twin must be capable of processing real-time data for monitoring a system, and ideally can generate optimal control inputs to the system to ensure product quality and process efficiency. However for many manufacturing processes, an accurate computational model requires complex systems of partial differential equations, which can only be solved via finite element and computational fluid dynamics (CFD) approaches. These approaches are widely developed and deployed for exploring process design and setup; however the high computational resources required mean that such models cannot typically be deployed in real-time for the purposes of monitoring and control. Hence, the development of methods to generate low-dimensional ‘surrogate’ models from high-fidelity computational models of nonlinear, multi-physics, and multi-scale dynamic systems for use as a digital twin is currently a very active area of research. State estimation algorithms can then provide a framework for the integration of such models with available sensor data for process monitoring and control. Surrogate models or ‘emulators’ can be developed using machine learning to derive a simpler and faster model from physics-based models, with Gaussian Process regression (GPR or ‘kriging’) being one of the most successful [130]. A Kalman filtering framework for the spatio-temporal dynamics of uncertain systems captured by Gaussian process models using a network of distributed sensors has recently been proposed and may have significant potential for complex, distributed manufacturing systems [131]. An alternative emerging approach to develop model surrogates which can be used in real-time state estimation and process control, is the model order reduction approach (MOR) approach. MOR aims to compute a reduced order model (ROM) of low dimension that captures the important characteristics of the original high dimensional model. Under this approach the physics of the problem is embedded in the reduced-order representation, typically using a projection-based method such as proper orthogonal decomposition (POD), which requires less training data and greater generalisation capacity relative to purely data-driven machine learning

approaches [132–134]. Such methods have recently been explored for state estimation in structural health monitoring [135], hydraulic systems [136,137] and, as discussed here, metal forming [69,70]. The extension of the state observer/Bayesian filter framework to utilise surrogate model approaches has great potential for process monitoring and control of complex manufacturing problems with uncertain spatial dynamics, for example, in additive manufacturing, and promises to be a rewarding avenue for future research.

5. Conclusions

A review of recent works in the development and application of state estimation methods in manufacturing demonstrates that such algorithms play an important role in soft sensing and sensor fusion to improve product quality; reduce material use, waste, and downtime; and improve efficiency and safety in manufacturing. As manufacturing industries are under increasing pressure to improve sustainability through greater resource efficiency, reduction in pollutants and greater use of ‘circular’ materials, state estimation algorithms can be an important tool to use alongside developments in sensorisation, computing, and IoT in advanced manufacturing. Bayesian filtering, in particular, is a popular and flexible approach capable of integrating physical knowledge and various data sources of information in an optimal manner. The framework provides a natural way to synthesise both physics and data-based modelling approaches with real-time data in a connected cyber-physical system under the Industry 4.0 concept. Recent works have highlighted how state estimation algorithms such as the Kalman filter can incorporate complex partial differential equation models through a variety of approaches for real-time monitoring and control of systems with spatial and temporal dynamics. Further research on the integration of state estimation methods in digital twin approaches promises to be a vital tool in the optimisation and control of complex manufacturing systems.

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Abbreviations

The following abbreviations are used in this manuscript:

IoT	Internet of Things;
SMO	Sliding Mode Observer;
KF	Kalman Filter;
EKF	Extended Kalman Filter;
EnKF	Ensemble Kalman Filter;
UKF	Unscented Kalman Filter;
PF	Particle Filter;
SLAM	Simultaneous Localisation and Mapping;
AI	Artificial Intelligence;
ROS	Robot Operating System;
AMCL	Adaptive Monte Carlo Localisation;
Mw	Molecular Weight;
EMI	Excluding Mutual Information;

CI	Covariance Intersection;
MPC	Model Predictive Controller;
APF	Augmented Particle Filter;
AHH	Adaptive Hinging Hyperplane;
RHKF	Receding Horizon Kalman Filter;
PID	Proportional Integral Derivative;
LS-SVM	Least Square Support Vector Machine;
SSKF	Steady-State Kalman Filter;
SVR	Support Vector Regression;
GDP	Gross Domestic Product;
PCA	Principle Component Analysis;
K-PCA	Kernel Principle Component Analysis;
LSPF	Local Search Particle Filter;
R2R	Run to Run;
SPC	Statistical Process Control;
EWMA	Exponential Weighted Moving Average;
IMA	Integrated Moving Average;
IAR	Integrated auto-regressive;
PCC	Predictor Corrector Controller;
ESO	Extended State Observer;
AM	Additive Manufacturing;
CAD	Computer-aided Design;
PBF	Powder Bed Fusion;
DED	Directed Energy Deposition;
FDM	Fused Deposition Modelling;
FFF	Fused Filament Fabrication;
L-PBF	Laser beam Powder Bed Fusion;
E-PBF	Electron beam Powder Bed Fusion;
FEM	Finite Element Method;
MOR	Model Order Reduction;
ROM	Reduced Order Model;
POD	Proper Orthogonal Decomposition.

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