

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 sensor measurements of related system 2 states. They can be used to derive fast and accurate estimates of system variables which cannot be 3 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 intro-5 duce the concepts and main methods of state estimation and review recent applications in improving 6 the sustainability of manufacturing processes. It is shown that state estimation algorithms can play a key role in manufacturing systems to accurately monitor and control processes to improve efficiencies, 8 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 10 and emerging trends in using state estimation as a framework for combining physical knowledge 11 with other sources of data for monitoring and control of distributed manufacturing systems. 12

Keywords: State Observer; Kalman Filter; Particle Filter; Sustainable Manufacturing; Soft Sensor; 13 Digital Twin 14

1. Introduction

Sustainable Manufacturing is now a very significant principle that industries must 16 adopt due to many factors driven by environmental issues, including more stringent legis-17 lation, higher energy costs, and consumer preference for environmentally benign products 18 and services [1]. Manufacturing processes have a direct impact on the consumption of 19 natural resources and their resultant emissions [2]. The emergence of Industry 4.0 provides 20 significant opportunities for the development of intelligent manufacturing environments 21 that have greater production flexibility and resource efficiency [3]. The deployment of 22 sensors, Internet of Things (IoT) and Cyber-Physical Systems (CPS) within manufacturing 23 is predicted to contribute to addressing some of the global challenges in respect to resource 24 and energy efficiency [4]. Greater sensorisation of manufacturing processes is a central 25 pillar of the Industry 4.0 concept and is critical to improving resource efficiency and sus-26 tainability. The ability to monitor key process variables in real-time enables tight control of 27 processes to avoid defects; eliminate waste of raw materials and energy in producing scrap; 28 prevent harmful environmental emissions, and facilitate processing of more sustainable 29 but difficult to process raw materials such as recyclates. However, it is not always feasible 30 to physically measure the critical variables in real-time due to e.g. lack of an available 31

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Copyright: © 2022 by the authors. Submitted to *Sustainability* for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). sensor technology, lack of sensor accessibility, high cost, poor accuracy, high latency etc. 32 In this case, concepts like soft sensing and data and sensor fusion may provide a solution, 33 enabling the variable(s) of interest to be inferred from available information in a connected 34 cyber-physical system. Often, this may be achieved through purely data-based approaches 35 via Machine Learning, however this will often require a large amount of historical training 36 data, high computational resources for model training and typically results in models 37 which do not generalise well to different systems/raw materials and which may exhibit 38 poor long-term robustness. An alternative in some situations is to use an observer-based 39 state estimation method, whereby the future value of the system states is predicted based 40 on the current value according to some model of the system. Then in the next time step, the 41 estimate is updated with measurement data available from the system - which may be indi-42 rectly related to the variables of interest and/or of limited reliability. This 'predict-correct' 43 structure, as illustrated in Figure 1, exploits, an often approximate, physical model of the 44 system to derive an algorithm which provides sufficiently accurate and fast estimates with 45 limited need for training data and with good robustness to variations in the process over 46 time. 47



Figure 1. Predict-Correct Structure of State Estimators.

State estimators can be deterministic ('observers') or stochastic (Bayesian filters such 48 as the Kalman filter and its extensions). In the stochastic case, uncertainties in models and 49 measurements are explicitly handled to derive an optimal estimate of the variable(s) of 50 interest together with a measure of the uncertainty in the estimate. These state estimation 51 methods have been applied to navigation problems since the late 1960s, with the Kalman 52 filter famously considered a key factor in the success of the Apollo 11 moon landing [5]. 53 The Kalman filter is the optimal state reconstructor for linear systems subject to white 54 noise, however this optimality is lost with nonlinear systems and/or systems with non-55 Gaussian noise distributions [6]. In recent decades, increasing computational power has 56 facilitated more sophisticated algorithms, which deal better with nonlinear systems and 57 more complex uncertainty distributions, which are fundamental to recent developments in 58 self-driving cars for example [7]. The concepts are less well known in some aspects of the 59 manufacturing community, however we show in this review that several studies indicate 60 the potential of various state estimation methods in manufacturing processes, moving from 61 automation of a defined task (Industry 3.0) to a wider systems-level approach (Industry 4.0). 62 As manufacturing enterprises are currently undergoing a period of considerable disruption, 63 driven on one hand by an urgent need to enhance sustainability and on the other hand enabled by progress in sensorisation, connectivity, and computation, state estimation 65 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 67 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: material processing, machining, additive manufacturing, semiconductor 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 79 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). 81 State variables are variables of the system whose values evolve over time depending on the current value of the variables and any external input to the system. For example, in 83 modelling a d.c. motor, motor position and speed are suitable state variables to capture 84 the system dynamics in response to changes in input voltage. The complete state space 85 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'), 87 which describes the relationship between the state variables and measurements (outputs) 88 of the system over time. Equations (1) illustrate the general form of a state space model for 89 a discrete linear system. We focus here on the discrete case due to the dominance of digital 90 systems in manufacturing. In simple terms, the values of the state variables at the next time 91 step are predicted by the state equation from the current values of the variables and the 92 current value of any input to the system. The relationship between the actual measurements 93 of the system and the state variables is described by the measurement equation.

$$\begin{aligned} x(k+1) &= A \, x(k) + B \, u(k) \\ y(k) &= C \, x(k) + D \, u(k) \end{aligned}$$
 (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 96 the unmeasured states are not independent from the measurements which can be checked by construction of an observability matrix derived from the system A and C matrices. 98 Provided a system is indeed observable, an observer can be constructed as in Figure 2 99 which depicts the discrete time Luenberger observer [8]. The values of the state variables at 100 the next time step are predicted from the current values and the input via the state equation, 101 and the measured values are then predicted from the estimated values of the state variables. 102 In the next time step, the predicted and measured values are compared and the error is fed 103 back to correct the estimates of the state variables. 104

$$\hat{x}(k+1) = A x(k) + B u(k) + L (y(k) - \hat{y}(k))$$
(2)

Provided the measurement equation is accurate (which is usually the case, as typically 105 the measurements are a subset of the whole state variables), the estimates converge to the 106 true values. The gain feedback matrix *L* requires careful design such that convergence can 107 be ensured to occur more rapidly than the dynamics of the plant (i.e. faster than the values 108 of the variables are themselves changing) but without introducing excessive noise into the 109 estimates. The Luenberger observer is a full-order observer, i.e. it estimates the values of all the state variables, not just the unmeasured ones. Reduced-order observers, in contrast, use 111 the system measurements to estimate only the 'hidden' states. They are more complicated 112 to design but can result in better performance [9]. 113

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

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Figure 2. The Luenberger observer.

Luenberger observers are however usually unable to estimate the plant states in pres-115 ence 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 117 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 119 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 121 particular feedback law which should be used at that instant in time. Provided a bound on 122 the magnitude of the disturbances is known, the ability to generate a sliding motion on 123 the error between the measured plant output and the output of the observer ensures that 124 a SMO can force the output estimation error to converge to zero in finite time, while the 125 observer states converge asymptotically to the system states. Consider 3 as an uncertain 126 linear system, where ξ is an unknown but bounded function representing the disturbance. 127

$$\dot{x}(t) = Ax(t) + Bu(t) + D\xi(t, y, u)$$

$$y(t) = Cx(t)$$
(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. The details of designing the sliding motion and surface can be found in [10].

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

An advantage of the SMO is that the applied observer injection signal (equivalent signal) 133 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]. 136

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 this recent reference [15] giving 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

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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.

$$x(k+1) = A x(k) + B u(k) + G w(k)$$

$$y(k) = C x(k) + D u(k) + e(k)$$
(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 the 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.

$$p(x \mid y) \propto p(x)p(y \mid x) \tag{6}$$

The concept is illustrated with a simple one dimensional example in Figure 3. The 156 previous estimate of the state variables, $\hat{x}_{k-1|k-1}$ (i.e. the estimate of x at sample k-1 given 157 all the information up to and including at sample k - 1), and its covariance $P_{k-1|k-1}$ is 158 propagated through the state Equation (5) to give $\hat{x}_{k|k-1}$ (i.e. the estimate of *x* at sample 159 k given all the information up to and including at sample k - 1). This step is sometimes 160 referred to as the 'time update'. The estimate $\hat{x}_{k|k-1}$ has a larger covariance $P_{k|k-1}$ as more 161 uncertainty is introduced due to the process noise term w(k) in the state equation. This 162 estimate is the prior distribution at sample k. The new measurement data y at sample k163 yields the likelihood function $p(y_k|x_k)$. The optimal (minimum variance) estimate of x 164 at sample k $\hat{x}_{k|k}$ is then determined from combining the prior and the likelihood in the 165 'measurement update' step. 166



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

The Kalman estimation equation can be written in terms of the Kalman gain matrix K: 167

$$\hat{x}(k|k) = \hat{x}(k|k-1) + K(y(k) - \hat{y}(k))$$
(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 the 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 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 175 multiple sources of measurement data according to their uncertainty. 176

The Kalman Filter applies to linear systems with an assumption that the model un-177 certainty and sensor noise can be described by a Gaussian distribution. A challenge in the 178 practical implementation is that the covariance matrices of the process and measurement 179 noises must be provided *a priori*, and this is a difficult task, particularly for the process noise 180 which is usually difficult to quantify [17]. To fulfil the requirement of achieving the filter 181 optimality, an adaptive Kalman filter (AKF) can be utilized for tuning the noise covariance 182 matrices [6]. Adaptive filters are based on dynamically adjusting the parameters of the 183 supposedly optimum filter based on the estimates of the unknown parameters. Another 184 solution to circumvent the system noise matrix specification is to parameterise the gain and 185 include its elements in the estimation process [18]. 186

The Kalman Filter has been extended to non-linear systems under two main approaches. 187 The first, the Extended Kalman Filter (EKF) involves linearisation of nonlinear system 188 equations using a Taylor series expansion and then applying the usual KF recursions [19]. 189 The classic EKF involves retaining only the first order terms of the Taylor series expansion, 190 however if the system behaviour is significantly nonlinear over the sample period or the 191 noise is high, then better performance may be achieved by including the second derivative 192 term in the Taylor series expansion. A drawback is that determination of the first and 193 second order derivative terms can be computationally intensive [20]. 194

An alternative approach is to use a nonlinear transformation and the Unscented 196 Kalman Filter (UKF) [21], which utilises the unscented transform, has emerged as a popular 197 alternative to the EKF. The unscented transform involves generating sigma points from 198 the distribution of the model input parameters. In the case of the UKF, these points are 199 the mean of the state estimates and symmetric deviations around the mean which are 200 computed from the covariance matrix. These sigma points are then propagated through 201 the nonlinear model and the mean and covariance of the model output (predicted state 202 estimates or predicted measurements) are estimated by applying weights to the sigma 203 points after the nonlinear mapping as illustrated in Figure 4. The UKF has the advantage of 204 not requiring the formation of derivative terms as needed for the EKF, and it may result in 205 better performance, depending on the form of the nonlinearity in the system. It should be 206 noted that the optimality of the Kalman filter is lost with EKF, UKF or any higher-order 207 filter. 208



Figure 4. 2D 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 the 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 of geophysical systems, instead 213 estimates the full covariance matrix using a sample of evolved states (the 'ensemble') 214 [23]. The EnKF is a Monte Carlo-based application of KF, propagating only the mean of 215 an ensemble of N < n state estimations through the KF recursions. The resulting mean 216 and covariance matrices are then estimated from the evolved samples. This method has 217 reduced computational complexity and can be applied to nonlinear state-space models and 218 non-Gaussian noise. For linear Gaussian systems if $N \to \infty$, the EnKF converges to the KF 219 results [24]. 220

2.3. Particle Filter

The particle filter was developed to deal with systems having multi-modal probability 222 distributions i.e. as opposed to the estimates having a normal (Gaussian) probability 223 distribution, there may be a distribution with more than one peak [25–27]. In navigation 224 problems, where the technique emerged, this would arise where there may be more than 225 one likely map location for a target vehicle based on the information available. In this 226 scenario, a numerical approximation of the distribution which can be propagated through 227 the prediction and correction recursions is needed. This can be done by representing the 228 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 230 particle filter in 5 general stages which can be described as: 231

- Weighted particles from last measurement update (usually sampled from a uniform distribution on initialization).
- 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. 236
- 3. Each particle is propagated through the state equation adding noise generated by sampling from the distribution for the process noise w(k), to give the time update (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. 240
- The states are estimated by e.g. 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 245

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State estimator	Advantages	Limitations
Luenberger observer	 Simple to design and implement Suitable for well-defined linear systems 	1.Poor estimation in the presence of model uncertainties
Reduced-Order observer	 Better Performance Lower computational cost 	Complicated to design
Sliding Mode Observer	 Suitable for linear and nonlinear systems High robustness Fault detection capabilities 	 Chattering of the estimator Complexity of the design
Kalman Filter	 Suitable for noisy systems Allows fusion of different measurement sources 	 Suitable for linear system Not Suitable for non-Gaussian noise Not suitable for high order systems
Adaptive Kalman Filter	 Suitable for noisy systems Allows fusion of different measurement sources Suitable for unknown noise covariance 	 Suitable for linear system Not suitable for non-Gaussian noise Not suitable for high order systems
Extended Kalman Filter	 Suitable for noisy systems Allows fusion of different measurement sources Suitable for nonlinear systems 	 High computational time Not suitable for high order systems
Unscented Kalman Filter	 Suitable for noisy systems Allows fusion of different measurement sources Suitable for nonlinear systems Lower computational cost 	Not suitable for high order systems
Ensemble Kalman Filter	 Suitable for noisy systems Allows fusion of different measurement sources Suitable for nonlinear systems Low computational cost Suitable for high order systems 	Not suitable for non-Gaussian noise
Particle Filter	 Suitable for multimodal probability distributions Suitable for nonlinear systems 	High computational time and cost

Table 1. Comparison of different state estimators

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, and featured limited programmability, mostly featuring hydraulic and pneumatic arms, primarily used for heavy lifting. Throughout the late 1960s and early 1970s, industrial robotics gradually shifted away toward handling and precision work, as

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the need for automation of manpower-intensive tasks in manufacturing increased. Eventually, smaller electric robots with advanced controls, microprocessors, miniaturized motors, 265 gyros, and servos were realized, which were ideal for lighter assembly tasks, e.g., bolt and 266 nut tightening. As a natural progression, the capabilities of robots expanded further to 267 include tasks such as material transferring, painting, and arc welding, replacing humans in certain dangerous and hazardous scenarios, by the late 1970s [32]. 269

Advancements in sensors and machine vision, coupled with a substantial reduction 270 in the costs of computer hardware, has resulted in a steep of advancement in industrial 271 robotic capabilities. Through the application of high precision sensors, e.g., force sensors, 272 vision and lasers etc, combined with suitable observers and estimators and high compu-273 tational power, enhanced high fidelity perception of the robot workspace as well as the 274 surrounding environment become possible. Features attainable through such accurate reli-275 able perception includes enhanced safety through collision detection and implementation 276 of effective human-robot collaboration which ultimately paves the way forward towards more sustainable manufacturing. 278

Traditionally, industrial robots operate within a safety fence without any human inter-280 action. 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 effec-282 tively results in bringing together the best of each partner, robot and human, by combining 283 coordination, dexterity and cognitive capabilities of humans with the robots' accuracy, 284 agility and ability to produce repetitive work [33]. They utilize advanced technology, including force-limited joints and computer vision to detect the presence of humans in their 286 environment. Cobots are often much smaller and lighter than traditional industrial robots, 287 easily moveable, and trainable to perform specific tasks. Robots' external perception relies 288 on sensing technology, thus, capturing accurate sensor information is vital for ensuring 289 robotic security and improving human-machine interaction performance. Amongst other 290 sectors, the manufacturing industry has benefited significantly by using mobile robots to 291 increase efficiencies and reduce costs while operating autonomously alongside humans, 292 including for material handling [34]. However, to allow the mobile robot to navigate its 203 environment, self-localization is critical autonomous mobile robots. SLAM algorithms 29 serve exactly this purpose and are thus the most widely used strategy for self localization in 295 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 297 the simultaneous (i) estimation of the state of a robot equipped with on-board sensors and (ii) the construction of a map (grid of obstacles) of the environment as perceived by 200 onboard robot sensors. While usually the robot state is described by its pose (position and orientation), the map is a representation of aspects of interest (e.g., position of land-301 marks, 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 304 classified as 'AI' or 'stochastic'. The latter group encompassing Bayesian filtering and 305 Dempster-Shafer evidence theory, while the former includes fuzzy algorithms, neural networks and fuzzy-neuro approaches. Kalman filtering has been applied for robot po-307 sitioning [37–39], while the particle filter is shown to give accurate positioning together 308 with consistent mapping of the 3D environment of the robot via simultaneous localisation 309 and mapping [34,40–43]. In their recent review, Ding et al. [36] conclude that the stochastic 310 algorithm approaches are accurate and mature while the AI approaches currently have limitations in practical cobot applications. 312

Recently, Li et al. [44] developed an Augmented Reality (AR) teleoperation method 314 to monitor and control a robot in real-time using a Kalman filter. Precise teleoperation 315 can facilitate the use of robots in applications where high precision is required and in 316 environments where human safety is compromised. In this work, a LeapMotion sensor is 317

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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. 320

3.2. Chemical Process Industries

While state observer concepts were initially applied and developed in tasks related to 333 localisation, tracking and navigation, such as in the field of robotics, the same algorithms 334 were later applied to various other state estimation problems. In particular, state estimation 335 methods have been of considerable interest in process industries since the 1990s. Many 336 industrial chemical processes have a high degree of variability and a large number of 337 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 330 using physical sensors and as such require sensorless control. A 'soft sensor' measurement 340 can yield lower cost, increased reliability, lower maintenance requirements, and thereby 341 increased sustainability [45]. 342

State estimation concepts in monitoring and controlling industrial chemical processes has been the subject of previous reviews e.g. [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. 344

3.2.1. Polymerisation

Polymerisation is a chemical process for the synthesis of polymers, which are long-348 chained molecules made of repeating monomer units. Although traditionally synthesised 349 from petroleum-based products, much research activity is ongoing to replace such poly-350 mers with those derived from more sustainable and eco-friendly plant sources such as 351 polylactide (PLA), which can be synthesised from natural feedstocks including corn starch, 352 rice, potatoes, sugar beet and seaweed [49]. The process of manufacturing polymers via 353 chemical polymerisation has inherent nonlinear and time-varying dynamics which are 354 a challenge to control [50]. Various studies have been carried out to model and control 355 the dynamics of polymerisation processes to improve yield, improve product quality and 356 reproducibility, and enhance safety and sustainability [51]. 357

Salas et al [52] applied an EKF for approximation of the nonlinear behaviour in semi-358 batch polymerisation to track the molecular weight (Mw) trajectories. Molecular weight is 350 critical to the properties of the resulting polymer product but can only be directly measured 360 off-line using time consuming techniques such as gel permeation chromatography (GPC). 361 They used a state-space mathematical model for the free radical polymerisation process and 362 followed the proposed approach by Crowley [53] for the calculation of molecular weight 363 distribution (MWD). They tested the method in an open-loop system to estimate Mw and 364 MWD and good estimation capability was confirmed with offline GPC analysis. They 365 compared closed-loop control of the polymerisation process using a PID controller with 366 and without the EKF state estimation. The result showed that with the incorporation of the 367 EKF there was approximately a 50% reduction in the absolute error between the actual and 368 the set point of the Mw trajectory after initialisation of the experiment. The experiments 369

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confirm that the nonlinear state estimation provides the opportunity of achieving full 370 polymer characterization in real-time. 371

Zhao et al [54], proposed a method using data fusion and cubature KF for nonlinear 373 state estimation with delayed measurement. The cubature KF is equivalent to a UKF with 374 specific parameters for generating the sigma points. For the delayed measurement, they 375 introduced and compared two data fusion methods; excluding mutual information (EMI) 376 and covariance intersection (CI). These data fusion methods were then combined with 377 cubature KF to incorporate delayed measurements, for example measurements from off-378 line testing which are only available post-production. They implemented their proposed 379 method in the nonlinear chemical polymerisation process. The results illustrated that the 380 combination of EMI and cubature KF has a higher speed, while CI is more accurate for non-381 linear and complex systems. Under classic state estimation approaches, data from delayed, 382 off-line measurements cannot be incorporated, although these are usually more accurate. 383 The proposed method offers a potential framework to improve the accuracy of real-time 384 estimation of unmeasured process states by exploiting these delayed measurements. 38

Luo et al. [55] studied batch-to-batch polymerisation and proposed an adaptive hing-386 ing 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 388 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 390 batches. A sequential quadratic programming method (SQP) was applied, to solve the opti-391 mal control of each batch. The method was implemented for the polymerisation of styrene 392 to achieve the desired values for number-average and weight-average chain length. The 393 method resulted in improved accuracy and stability for the estimated process behaviours. 394

Recently, Rangegowda et al. [56], used a new approach, receding-horizon KF (RHKF), 396 to estimate the state of methyl methacrylate polymerisation. RKF is a combination of 397 moving window-based methods, such as moving horizon estimator (MHE), and Bayesian 398 estimators. It has the advantages of both methods, including simultaneous smoothing and 300 filtering with a relatively low computational cost. The RHKF applies simultaneous state 400 and parameter estimation in a moving-window. They also compared partial likelihood 401 and complete likelihood parameter estimations for the measurement update in RHKF. 402 Results in polymerisation illustrated that RHKF based on complete likelihood parameter 403 estimations performed better and this method required much less computational time and produced accurate state estimations. 405

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, resource efficient and at the same time 408 remain competitive. As a fundamental step in the lifecycle of many products and systems, 409 efficiency in material processing is paramount, as is increasing capability in processing 410 '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. 413 In this section, we review the application of state estimation methods in material processing 414 towards zero-defect sustainable manufacturing 415

3.3.1. Injection Moulding

Injection moulding involves melting a polymer and injecting it at high pressure into a 417 mould. It is one of the most used industrial processes for the formation of polymer products. 418 Improvements in monitoring and control of the process can reduce energy consumption 419 and waste generation as well as enable the processing of more complex, sustainable raw 420

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material streams [57].

Liu et al. [58] used an EKF to improve the part quality in a micro-injection moulding 423 process by controlling the pressure signature. The pressure signature is generated by a 424 pressure transducer as the plastic melt passes through the nozzle. Electromagnetic noise on 425 the pressure signature can lead to short-shot (under-filling the mould) or flashing (overfill-426 ing the mould) because of incorrect control of injection volume. The authors proposed an 427 adaptive EKF based on F-distribution to track the pressure signature around the nozzle. The 428 experimental results on a real microinjection moulding process showed that the adaptive 429 EKF performed well in eliminating the noise and tracking the true pressure signature at 430 both high and low injection speeds. Cao et al. [59] combined KF with iterative learning 431 control to consider the effect of disturbances and random noises from batch to batch in 432 repetitive processes like injection moulding. First, they used a KF to estimate the current 433 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 435 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 437 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 439 suboptimal controllers (combining conventional KF with iterative learning control) are able 440 to reject the batch-to-batch noises and disturbances in injection moulding. 441

In the injection moulding process in order to change from the filling phase (veloc-443 ity control scheme) to the packing phase (pressure control scheme), a switch-over point A A A exists. The switch-over point is determined empirically by experiment, however if ap-445 plied at the wrong time the cavity pressure profile is affected, resulting in defects in the 446 injection moulded parts. Stemmler et al. [60] proposed a cross-phase controller method 447 to eliminate this switch-over point and replace it with a continuous pressure trajectory. 448 They first derived a model for the filling and packing stages of the process. Then the 449 model was piece-wise linearised. The proposed model was applied in an EKF to estimate 450 the states in an MPC (Model Predictive Controller) for optimization. Based on the EKF 451 predictions, the MPC specifies the controller output corresponding with the reference 452 input. The comparison of the proposed approach to a PID controller in an actual injection 453 moulding process resulted in superior performance of the cross-phase controller method. 454 Recently, they further developed the work to propose a modelled-based norm-optimal 455 iterative learning controller to track a desired reference for the cavity pressure (based on 456 PVT-optimisation) to optimise the part weight during an injection moulding cycle [61]. 457 They used the piece-wise linearised steady-state model for injection moulding based on 458 their previous work [60]. EKF was applied to track the desired cavity pressure and estimate the process state. The experimental set-up with the embedded pressure sensors resulted in 460 manufacturing injection moulded parts that weighed 50% less than the non-optimised ones. 461 The approach has the potential to achieve significantly higher efficiency in raw material use. 462

Chen et al. [62] proposed a method to detect the presence of a foreign body in an 464 injection mould and minimise the 'detected distance' (i.e., the amount which a detected 465 foreign body is compressed by the mould closure). Such a system can prevent damage 466 to the mould which results in defective parts, downtime, and costly repair. A state-space 467 model is derived for the toggle mechanism, driven by a servo system (which closes the 468 mould), and an EKF was used to filter the electric current readings of the drive for the 469 toggle mechanism, which was then used to self-adapt the mould protection system to keep 470 the current in a safe range. The system showed a reduction in the detected distance of 471 foreign bodies of 22%. As damaged tools result in the fabrication of poor-quality parts and 472 harm to the whole injection moulding machine, this approach can enhance the lifespan of 473 the equipment as well as reducing scrap. 474

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3.3.2. Other Forming Processes

Extrusion is a continuous process for forming polymer or metal products by forcing 476 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, 478 as incorrect operating conditions can waste large amounts of energy, time, and material. 479 Melt viscosity is one of the most important parameters relating to the product quality, 480 but is challenging to measure online with physical sensors. Liu et al. [63] implemented a 481 non-linear state observer approach to estimate the melt viscosity. Viscosity and pressure 482 were modelled by a Genetic Algorithm (GA)-based dynamic Gray-box model with NFIR 483 (nonlinear finite impulse response) structure. The viscosity was predicted from the process 484 input parameters and the predicted viscosity was then used to estimate the barrel pressure. 485 The error between the predicted and measured barrel pressure was used to correct the 486 viscosity estimation. The proposed method was applied to a real extrusion process with six 487 different polymers and resulted in an RMS (root mean square) error of less than 1%. The 488 method is proposed for use in the production of consistent products from recycled polymer 480 feedstock despite having inherently variable viscosity behaviour. 490

Amoaoui et al. [64] developed an observer for the liquid composite molding process 492 which is a method for fabricating large composite parts with complex geometries, such as in 493 the aerospace industry. This process suffers from issues of void formation at the flow front during resin impregnation which reduces the mechanical performance. An observer was 495 developed for monitoring the system pressure (output) and the permeability (unmeasured state) which is inaccessible to physical measurement. They first derived a steady-state 497 model for the process and designed a non-linear state observer using a Lyapunov theory and a linear matrix inequalities technique. The performance of the observer was demon-499 strated through simulation which showed that the estimated permeability values converge 500 to the true state values. Application of the method to real-time monitoring of void forma-501 tion has the potential to reduce production of scrap parts which do not meet the required 502 specifications. 503

Remelting is a process to produce homogeneous metal ingots. The ingots should be 505 defect-free with a fully dense and desired grain structure, as defects cannot be removed 506 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 508 distribution in the electrode of the electroslag remelting process. They proposed a reduced-509 order melting model for the process and estimated the temperature using three different 510 estimators; EKF, UKF and steady-state nonlinear estimators. The controller with UKF had the best performance as it had less overshoot, undershoot, and responded to disturbances 512 better. Lopez et al. [66] studied the Vacuum Arc Remelting Process, used in aerospace 513 applications. A dynamic model capturing the melting and solidification stages was used 514 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, 516 meaning a lot of particles are required for high accuracy. They applied the PF with a GPU 517 containing a large number of processors to enable parallelisation. The PF outperformed a 518 KF when used with a large number of particles. 519

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 e.g. 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. Precise control of the cooling curve is therefore extremely 528

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important but is hampered by the difficulty in physically monitoring the temperature distribution. Various studies have been done to estimate the internal spatial temperature 530 distribution in sheet rolling using state estimation concepts. 531

Zheng et al. [67] used EKF to estimate the transient temperature distribution in the hot-532 rolled strip cooling process. They developed a nonlinear high-dimension (14 state variables) 533 state space model from a thermodynamic model of partial differential equations using a 2D 534 finite volume scheme. Validation of the method with numerical simulation resulted in an 535 accurate temperature estimation with EKF. Speicher et al. [68] used full and reduced EKF to 536 estimate plate temperature in heavy plate rolling based on a few thermocouples' measure-537 ments. They used a similar approach to discretise a partial differential equation model of 538 the thermodynamics using a finite difference method. As quantification of the process noise 539 is the major practical challenge in implementing an EKF, they propose a systematic method 540 for tuning of the process noise covariance matrix via analysis of the extended dynamic 541 system. The approach was tested in an industrial rolling mill and successfully estimated the temperature. The reduced and full EKF performed similarly in estimation, however the 543 reduced EKF simplifies the simulation and reduces the computational time.

Kloeser et al. [69] examined spatio-temporal estimation of temperature distribution in 545 the hot sheet metal forming process. Rather than using a course grid finite difference method to derive the state space model, they instead designed a dynamical Reduced Order 547 Model (ROM) from a high-dimensional thermo-mechanical model by proper orthogonal 548 decomposition (POD). Starting with a refined model of several thousand states they use 549 POD to project the states onto a reduced order state space model which preserves the most 550 important dynamics in the system. A disturbance model was added to EKF to address the 551 simplifications and modelling errors. The approach was validated in the simulation of the 552 hole-flanging process by reduction of the states from 17000 to 30. The experimental results 553 confirmed the approach in the estimation of spatial-temporal temperature distribution in 554 real-time by using sparse local temperature measurements.

Havinga et al. [70] used a PF with on-line force measurements to estimate the physical 556 state (sheet thickness, friction, angle after bending etc) of the product in a metal forming 557 process in real-time for mass production, based on force measurements. They built a 2D 558 FEM model of the bending process and then applied POD along with Radial Basis Func-559 tion interpolation to create a fast model. The proposed approach was used in numerical 560 simulation of the bending process and successfully predicted the state changes based on 561 variation in process forces. 562

The application of state estimators in polymer synthesis and material processing, and the resulting potential impact on sustainability is summarised in Table 2. 565

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 & 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 & 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]
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 & 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]

Table 2.	State-estimators	used to im	prove material	synthesis and	forming processes
				- /	

3.4. Machining Processes

Machining processes include milling, grinding, turning, drilling etc. which contribute 567 about 5% of the gross domestic product (GDP) in the developed world [71]. A significant 568 factor in the cost of machining has been associated with sub-optimal tooling setups, with 569 cutting tool failure contributing to almost 20% of the machining downtime [72]. Machining 570 processes are less efficient and consume unnecessary energy while working with faulty 571 tooling. Machining processes account for approximately 33% of primary energy use in the 572 manufacturing industry globally [73], but approximately only 25% of the energy consumed 573 accounts for actual cutting [74]. Researchers have explored various methods to improve 574

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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 585 nonlinear at the initial stages, linear at intermediate stages, and nonlinear at the final stages 586 before catastrophic failure [76], their work focused only on the linear stage. From the 587 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 589 estimation which is used to correct the tool wear and tool wear rate estimates. In an experimental trial, the designed Kalman filter resulted in a maximum average error of 10% 591 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 593 measurements of the surface texture of the cut surfaces. Linear regression was used to 594 formulate a measurement model of flank wear with the cutting force and image histogram 595 variance as the measurement vector y. An alternative measurement model excluding cutting force was also tested. In experimental trials, both KF implementations were able 597 to predict the progression of tool failure, providing better accuracy than the standalone 598 regression model (without the mechanistic model of tool wear progression). Both models 599 gave adequate estimates of the flank wear, meaning that the force measurement could be neglected. 601

Zhang et al. [78] proposed the use of Least Squares Support Vector Machines (LS-602 SVM) in a Kalman Filter for tool wear estimation, also incorporating visual images into the 603 measurement update. LS-SVM is used to train a tool wear prediction model from cutting 604 conditions, cutting time and wear position based on a historical data set. A KF framework 605 is implemented to 'correct' the LS-SVM model predictions using observed tool wear from 606 visual images (LS-KF model). Because the model process noise and the measurement 607 noise covariances are assumed to be fixed, the Kalman gain converges to a steady-state 608 KF, which occurs after six time-steps. The steady-state KF was then used to update the LS-SVM model without the actual tool wear images (LS-KF-S model). The KF approach 610 significantly improved the prediction errors relative to the open-loop LS-SVM model alone. 611 While the best performance is achieved using the continual visual measurements of tool 612 wear in the LS-KF model, the LS-KF-S also gave good estimation performance. In this case the KF framework facilitates significant improvement in the LS-SVM predictions with a 614 small set of images to correct the model. 615

Sadhukhan et al. [79] presented an unscented Kalman Filter (UKF) for flank wear 616 estimation in a turning process. A discrete flank wear model is developed where two com-617 ponents of flank wear due to abrasion and diffusion are considered as state variables. The 618 system model parameters are determined from experimental data. A linear measurement 619 equation, derived via linear regression from the experimental data set, relates the state 620 variables to the measured cutting force. Both a UKF and Extended Kalman Filter (EKF) 621 were compared for tool wear estimation in a simulation. The simulation of both methods showed flank wear estimation by UKF outperformed that of EKF with a 50% reduction in 623 the error of the UKF estimates relative to EKF. 624

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 prediction of the tool wear state, with the model parameters described by uniform probability distributions. A particle filter based scheme is 630 investigated to estimate the model parameters and the tool state based on online measure-631 ment. Tool vibration signals and force measurements are used as indirect measurements of 632 the actual tool wear state. First, various features of the signal measurements (statistical, 633 frequency-domain, time-frequency domain) were extracted and analysed for relationship 634 with tool wear using an experimental dataset. It was found that wavelet energy in the 635 x-direction of the force measurement has a strong linear correlation with the tool wear 636 and hence it was selected as a single measurement for use in a particle filter measurement 637 update. In [81] both an autoregressive (AR) model and support vector regression (SVR) 638 were investigated to formulate the measurement model in order to predict the online mea-639 surement from the estimated tool wear state. In general, SVR outperformed the AR model. 640 The use of a PF with an SVR or AR measurement model improved the tool wear prediction 641 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 643 improving the signal feature selection step of formulating an SVR measurement model. Principal Component Analysis (PCA), kernel Principal Component Analysis (k-PCA) and 645 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 647 Particle Filter (LSPF) is compared against a conventional sequential importance resampling 648 (SIR) method. LSPF showed a reduction in prediction error by over 30% in comparison to 649 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 651 particle filter for joint state and parameter estimation. A refined particle resampling strategy 652 is proposed for the implementation of the PF. In this work the online measurements include 653 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 655 prediction under changing settings of feed rate, cutting depth, and cutting speed. 656

Bayesian estimation methods have also been used to estimate the surface roughness 658 of parts while they are being machined. Conventionally, surface roughness is measured 659 post-manufacturing, which can result in waste due to rejects detected too late for corrective 660 action to be taken. Moliner-Hereida et al. [85] examined three approaches for surface 661 roughness monitoring of machined parts in real-time. In the first, they used an open-loop 662 system to estimate the 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, 664 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, 666 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 668 system model predicts both surface roughness and power consumption - again under the 660 assumption that both increase at a constant rate, which depends on the cutting parameters. 670 Actual power consumption measurements are obtained every ten parts and allow for 671 correction of the state estimates. The third scheme incorporated surface roughness readings 672 from a profilometer in addition to power consumption information at the same rate of 673 every ten parts. The profilometer checks the surface roughness post-machining. All three 674 approaches were compared in a simulation study. While the Kalman Filter implementation 675 in scheme two improved results over the open loop system, significantly better performance 676 was achieved by also including the profilometer measurements. 677

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, the predicted tool wear was updated with

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]

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

tool vibration and dynamic cutting force measurements. The resulting stochastic model of the cutting process was used to predict surface roughness under 5 different machining conditions. The influence of the machining parameters on the stochastic surface generation are also analyzed. The model allows for prediction of the machined surface quality prior to the costly micro milling operations, and provides a basis for optimization of the machining parameters to improve quality and efficiency.

Table 3 summarizes the studies undertaken using various Machining technologies and
applying state estimators and it captures desired outputs and the sustainability impacts.689

The application of state estimation approaches as presented in this section, has demon-691 strated greater accuracy in condition and part quality monitoring in machining processes compared to using open loop models. In many cases the proposed Bayesian filtering frame-693 works incorporate machine learning methods into the measurement update for dealing with complex high dimensional data, such as vibration and acoustic emission signals and 695 visual images. The application of Bayesian inference is shown to improve over use of the machine learning approaches alone. The improved condition and part monitoring 697 performance can lead to greater control over the process, resulting in reduced downtimes 698 due to unexpected tool failures and a reduction of energy use and waste generation from 699 faulty tooling and components [87].

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 manu-707

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facturing and infrastructure [89]. As a result, there is increasing attention on approaches to minimise resources and the production 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 optimization.

Semiconductor processing consists of many different operations to create the finished 714 product and due to physical constraints it is not feasible to conduct the high precision 715 metrology needed for quality validation until after a step is completed. However, processes 716 such as lithography are subject to many sources of variations caused by environmental 717 changes, regular maintenance and operational drift over time. Therefore metrology steps 718 are integrated into the production line to minimise the delay [90]. Typically, each main 719 processing step utilizes 'run-to-run' (R2R) control which integrates process control theory 720 with statistical process control (SPC). In R2R, the wafer measurements following a run of a 721 unit process are used to update the process settings for the next run in order to achieve the 722 required quality targets. The basic structure of a run-to-run controller consists of a process 723 model, a state estimator, and a control law. Successful implementation of R2R control 724 in commercial facilities has been achieved for processes including chemical mechanical polishing, chemical deposition, and plasma etching and has proven that it can efficiently 726 improve the product yield and reduce scrap, rework, and cycle time [91]. Exponential 727 weighted moving average (EWMA) control, (composed of EWMA filtering followed by a 728 deadbeat controller), is the established method of R2R control and has been shown to be 729 optimal for processes subject to integrated moving average (IMA) disturbances, which is 730 the most common type of disturbance signal in semiconductor manufacturing. Kim et al., 731 [92] explored a Kalman filter based R2R controller and compared performance against an 732 EWMA controller for minimising variation in the quality variables of the product under 733 different types of process disturbance signals. The Kalman filter provides the optimal 734 one-run-ahead prediction of the model parameters perturbed by the disturbance, and 735 the controller computes the control input for the next run to compensate for the effect 736 of the disturbance. For IMA and integrated white noise (IWA) disturbances the EWMA 737 and Kalman filter have the same structure and show identical performance. However for 738 integrated auto-regressive (IAR) and auto-regressive integrated moving average (ARIMA) 739 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 the disturbance. This involves 743 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 shown 745 to be effective in high precision motion control for mechatronic stages in semiconductor processes including lithography and chip packaging [93–96]. The disturbance observer 747 concept has also been applied to run-to-run control to deal with some of the shortcomings 748 of EWMA control. If there is severe aging of a production tool or the process drifts, EWMA 749 control produces an offset in the process output, which can be corrected by different means 750 such as a predictor corrector controller (PCC) or double EWMA controller. Lee et al., [97,98] 751 proposed an output disturbance observer (ODOB) structure as a unified framework for 752 these controllers and provided a systematic method to obtain the optimal parameters for 753 guaranteed optimal nominal performance. They showed in simulation studies that the 754 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

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product mixes are becoming increasingly diversified this can lead to too many threads, some of which have insufficient data. A long delay between adjacent lots in one thread may 763 make the estimation unreliable for infrequently manufactured products. Further, a lack of 764 information sharing on data relating to tool degradation means that all the threads using 765 the same tool must address this shift disturbance separately [99]. To address this, several 766 non-threaded state estimation methods have been proposed which involve an observer 767 to identify the contribution from different production contexts. Of these methods, the 768 Kalman filter is one of the most important [91]. Haririchi et al., [99] proposed a modified 769 Kalman filter to overcome the problem that in a non-threaded system, the model structure 770 can be such that the system states may not be completely observable. Wang et al., [100] 771 proposed a modified, simple to implement, Kalman filter scheme (involving periodic reset 772 of the *P* covariance matrix), which considers the fact that if a context item is not involved 773 in a process run, then its state does not change. The method was shown to be robust to 774 uncertainty in the disturbance parameter and to outperform the conventional KF scheme 775 for the common IMA-type disturbances. 776

A drawback of the KF methods is that the nominal performance of the controller can 778 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 780 [101]. In the ESO algorithm disturbances, including plant-model mismatch, are lumped into 781 a total disturbance which is set as a new state. An advantage of ESO is that the disturbance 782 can be reconstructed without an accurate model. A threaded ESO R2R controller was shown to outperform other threaded approaches in a photolithography process fabricating 784 five different products. The authors further developed a discrete sliding mode observer 785 for the same process, which estimates the disturbance without using a process model. The 786 system was shown to outperform EWMA and double EWMA controllers in rejection of 787 IMA disturbances with a shift or drift (as occurs in tool ageing). It also performed better 788 under plant-model mismatch and had better tolerance for metrology delay [102]. 789

Tsai et al. [103] developed a discrete sliding mode observer to estimate the core tem-791 perature of multi-layer metal plates in semiconductor manufacturing process for real-time 792 (rather than run-to-run) thermal control. While the middle and top layers are monitored by 793 thermocouples, the middle layer is not accessible to physical measurement. This can result 794 in either excessive heating which can damage the material, or heating which is insufficient 795 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 797 high robustness of the approach to plant-model mismatch and external disturbances. The system was shown in experiment to accurately estimate the core temperature of the system 799 despite being influenced by an unknown external cooling temperature.

In summary, state estimation has a powerful role in semiconductor manufacturing due 801 to the problems in achieving physical measurements to the required precision in situ. State 802 estimation methods are combined with SPC approaches in run-to-run control to minimise 803 the effect of process disturbances. Sophisticated algorithms have been devised which 804 can enable tight quality tolerances to be achieved, despite many sources of variation in 805 fabrication sites having a high product mix. Most recent developments show potential for 806 good performance without an accurate model of the process disturbances making practical 807 implementation more feasible. Due to the high environmental impact of semiconductor 808 manufacturing (energy and water use, toxic waste products), the ability to produce wafer 809 products 'right first time' can reduce scrap, rework, resource use and emissions. 810

3.6. Additive Manufacturing

Additive manufacturing (AM) is the fabrication of objects from computer-aided design (CAD) data, by translating the 3D CAD data into 2D cross-sectional profiles. Material is then deposited layer by layer following the form of the generated 2D cross-sections,

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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 820 close in size and shape to the final requirements, meaning minimal material removal is 821 required. Compared to conventional and subtractive manufacturing such as machining, 822 additive manufacturing is significantly more resource efficient and can reduce the need for 823 additional, energy-intensive post-processing steps [105]. The main advantage of AM over 824 conventional machining methods is that it can produce complex parts with geometries not 825 possible through conventional methods with a high degree of precision. AM can be used to 826 manufacture one-off bespoke products, such as customised medical devices, cost-effectively 827 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 829 monitoring and control of critical features is still at any early stage with most commercial 830 systems having only-loop temperature regulation schemes [106]. 831

There are different types of AM processing techniques, which can be classified into 833 seven general categories: powder bed fusion, material jetting, vat polymerization, sheet 834 lamination, fused deposition modelling, binder jetting and directed energy deposition [107]. 835 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 837 Fused Deposition Modelling (FDM) (see Figure 6). 838 In the PBF process, the parts are built from a bed of powder particles (polymer or metal) 839 that fuse together selectively by a heat source, layer by layer. This heat source can be a 840 laser or electron beam [108]. The DED process fabricates the components by melting the 841 material, in the form of powder or wire, together with a focused laser beam [109]. The 842 last class, FDM, also known as fused filament fabrication (FFF), feeds a polymer filament 843 through a nozzle which heats it to a molten state. This molten filament extrudes through 844 the nozzle, which deposits the polymer onto a build plate based on the 2D cross-sectional layers of the 3D design [110]. 846

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.

Monitoring and control of processing temperatures is one the most vital factors in 856 metal AM since it affects the metallurgic phase formation and thereby the microstructure 857 of the printed part [111]. The energy to melt the material in PBF and DED processes is 858 localised in a small melt pool, and as a result the temperature gradients are extremely large. 859 This causes differential thermal contraction and local micro-distortions which can integrate 860 to form large milliscale distortions [112]. It is not possible to place a physical temperature 861 sensor on the surface being built, so temperature measurement must always be remote. Most commercial systems have a thermocouple in the build plate but the temperature here 863 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 865 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 the KF on two different temperature references (time-varying and constant). Comparison of the results showed a reduction of 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 tempera-874 ture of the powder bed in a PBF process. They introduced a multi-zone temperature control in which nine temperatures from different locations of powder bed were extracted by in-876 frared cameras and each of them were fed back to a seperate PID controller. They compared the result, first to a single loop controller that used only one average temperature reference 878 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 880 demonstrated that multi-zone control has a superior performance compared to single-loop 881 and provided similar performance as MPC. However, it had the advantage that it reduced 882 the computational cost in comparison to MPC. 883

Besides control of temperature, research has also been done into the control of other 885 quality factors within AM processes. Lopez et al. [115] studied uncertainty identification 886 and propagation in the prediction of melt pool width in a Laser PBF process. They further 887 developed a thermal model from a laser cladding process [116] to be applied to PBF for 888 melt pool width prediction. They validated their model using a case study of printed 880 overhanging structures and showed how thermographic monitoring is effective in uncer-890 tainty identification and reduction. A KF was used for process estimation using the noisy 891 measurements of melt pool width. The approach has the potential to be applied to control 892 the melt pool dimensions in real-time. 893

The high laser power in PBF evaporates and fuses the metal powder. If the boiling 895 point is reached, a vapour plume arises in the melt pool that causes formation of a void in the printed parts. The evaporation also generates sparks, known as spatter, that can lead to 897 instability in the melt pool and discontinuity at the surface. Hence, real-time monitoring 898 of plume and spatter can aid better control of the process to avoid such defects [117]. 899 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 901 high-speed camera. The contrast of images from the camera was enhanced using an optical 002 filter. They introduced a novel image processing method to segregate melt pool, plume, and 903 spatter from each other. They also used KF tracking to find the exact location of the melt 904 pool. Various features such as melt pool intensity, plume area, plume orientation, spatter 905 area, direction and velocity were extracted in four different single-track scenarios using 906

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this approach. These features are the potential indicators that assist with the investigation of, and decisions on printed part quality. 908

As the temperature history directly influences the phase formation, the ability to esti-910 mate the complete temperature history of the entire part, not just the melt pool, would be 911 extremely valuable for process validation and precise control over resulting part properties. 912 Wood et al. [106], explored using state-observation for the estimation of temperature states 913 throughout the printed part itself from the measurement of surface temperature in the 914 laser PBF process. Here a Finite Element Method (FEM) was utilized to model the complex 915 spatio-temporal temperature dynamics of the process. A high-dimensional state-space 916 model (196 state variables) was extracted from the FE model, from which a KF temperature 917 state observer was defined. They successfully estimated the temperature evolution in 918 several simulated test parts. 919

They further developed their work in later research to estimate internal temperature 921 distribution and proposed a two-dimensional linear model with FEM, not only for a laser 922 heat source (L-PBF) but also for electron beam PBF (E-PBF) [119]. They applied an ensemble 923 KF to this system to deal with the high dimensionality. In their research, the EnKF estimates temperature by correcting the linear model temperature to agree with measurements 925 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 927 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) 929 for E-PBF (noted as 3) and L-PBF (noted as 4) for the open loop and EnKF estimates for 304 930 stainless steel (SS) at low temperature (Figure 7 (a)) and elevated temperature (Figure 7 (b)). 931 The EnKF scheme presented up to a 44% reduction in the L ∞ -norm of the temperature field 932 error relative to the open-loop FE model predictions when the material properties differed. 933 The method has the potential for exploitation in a closed-loop control scheme to modulate 934 laser power in order to ensure the desired microstructure is achieved despite uncertainty in 935 the raw material properties. 026



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 done to investigate the processing parameters and part 938 quality of polymer printed parts. Kim et al. [120], proposed a digital twin method for 939 part temperature measurement in FDM. Similar to the work of Wood et al. [106,119], they 940 defined a spatio-temporal thermal model, here using the finite difference method. They 941 fused this model with sensor data (IR camera) using a linear KF to estimate the tempera-942 ture. Verification of the method was performed with a virtual experiment set-up, which 943 demonstrated that this closed-loop approach can estimate the temperature and measure 944 the related uncertainties accurately.

Garanger et al. [121] proposed an optimal control law to control the mechanical prop-947 erties in leaf springs produced by fused deposition modelling. They printed the stacked 948 leaves with a simple FDM printer using PLA filament and used a KF framework to estimate 949 the stiffness of the parts. The KF was applied to update the stiffness estimates following 950 a physical test of the stiffness of each printed leaf. The proposed KF method resulted 951

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Polymer AM

Polymer AM

KF

KF

	1	y 1		
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]
E-PBF & L-PBF	Ensemble KF	Internal Temperature fields	Higher part quality and waste reduction	[119]
FDM	Linear KF	Printed part Temperature	Uncertainty estimation and	[120]

Stiffness of the printed part

Stiffness of a printed cantilever beam

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

in higher accuracy in stiffness estimation in comparison with an unfiltered open-loop 952 prediction model. In 2020, they followed a similar approach to estimate the stiffness in a 953 printed cantilever beam [122]. They proposed a dynamic model for the printing process 954 of the beam and fused this model with force sensor data in an optimal control law with 955 KF. Comparison with an open-loop system showed an improvement in predicted stiffness 956 error of about 94% and a reduction in noise by almost 80%. 957

process quality enhancement

and efficiency enhancement

and efficiency enhancement by less waste and rework

by less waste and rework

Part quality

Part quality

Table 4 summarises the studies that have been done to date in AM with state estimators 959 and their related sustainability impacts. State estimators enable inline monitoring of process parameters which cannot be directly measured or for which only noisy measurements 961 are available. Enhanced monitoring of the process and on-line estimation of part quality 962 indicators can reduce defects in the printed parts such as delamination and warpage. Hence, 963 as the failures are predictable, there will be less wasted material, energy, and time and greater practical realisation of the benefits of AM. 965

4. Discussion

State estimation is an important concept in manufacturing, providing a suite of tools 967 for improved monitoring and control of manufacturing systems. In this review, we have 968 highlighted recent advances and applications of state estimation in industrial robotics, 969 chemical processes, material forming, machining, semiconductor manufacturing and ad-970 ditive manufacturing sectors. In particular, Bayesian filtering concepts have emerged 971 as a popular approach to estimate system variables which cannot be measured directly 972 or for which only noisy, uncertain and/or latent information is available. Compared to 973 deterministic state observer approaches, the Bayesian methods have enhanced flexibility 974 in facilitating the incorporation of knowledge about the uncertainty of both system and 975 measurement models and different sources of data about the process. This means that 976 not only is the most accurate estimate of the system states derived under a probabilistic 977

[121]

[122]

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framework, but also a measure of the associated uncertainty is derived, which provides 978 useful information to operators and manufacturing managers about the appropriateness of 979 corrective action. Particle filtering is more flexible than the Kalman filter as it can deal with 080 non-Gaussian probability distributions and advances in computing power mean that it is 981 now a feasible approach in systems where the dimensionality is relatively low (i.e. in the 982 order of two state variables). Kalman filtering and particle filtering have been shown to 983 improve the precision, speed and perception of industrial robotics, improving the capability 984 of robots to work alongside humans for more efficient, flexible and safer manufacturing 985 processes. These Bayesian filtering methods have also found wide application in estimation 986 of product quality variables in material synthesis and processing (see Table 2), tool condi-987 tion and part quality monitoring in machining processes (Table 3), compensation of process 988 disturbances in high precision semiconductor manufacturing (Section 3.5), and for quality 989 monitoring and control in additive manufacturing processes (Table 4). Below we outline the main challenges and limitations in implementation of state estimation approaches 991 in manufacturing, and discuss emerging and future trends in the context of sustainable 992 manufacturing. 993

4.1. Limitations and practical issues

A problem with the practical implementation of the Bayesian methods is that the model uncertainty is often difficult to quantify, particularly with regard to process noise. In 997 practice, the measurement noise is usually estimated from experimental data (comparing 998 sensor measurements to known ground truth values) and the process noise covariance is 999 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 1002 reason for the divergence should be investigated. If it is due to sensor errors (outliers, 1003 missing data) or numerical issues then the filter should be restarted. However, if the 1004 divergence is due to model errors then the filter should be redesigned. Reference [?] 1005 provides useful information on troubleshooting these practical issues. A useful starting 1006 point for model uncertainty analysis is to examine the sensitivity of the model predictions to 1007 initial conditions and/or model parameters. A sensitivity analysis will reveal what model 1008 outputs are most influenced by different states/parameters and can reveal weaknesses 1009 in the information flow - for example to identify where in the process sensors should 1010 be located and if additional sensor data is needed (see for example [123–125]. That said, 1011 the Bayesian filtering approaches have limitations where the actual nature of the system 1012 uncertainty is unknown, as is the case with manufacturing systems which may be subject 1013 to different sources of variability in the interval between measurement data being available. 1014 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 1016 update the process settings for the next run. In this context, the application of a disturbance 1017 observer framework (where the system output measurements are input to an inverse model 1018 of the plant to estimate the disturbance signal directly) has been found to be useful in 1019 improving control performance. Further, the sliding mode observer, which has the property 1020 of high robustness to unknown disturbances, has shown excellent potential for practical 1021 application where accurate models of process disturbances are unavailable. 1022

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 1029

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filtering methods to estimation of spatio-temporal temperature dynamics [119,120]. In 1030 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 1032 polymer parts affecting microstructure and void formation in the former, and the resulting residual stresses and warpage in both. Because of the complex spatio-temporal dynamics, 1034 the system model in these cases is derived from numerical finite element models. In metal 1035 forming this has been addressed by either (i) using a course 2D grid with low spatial 1036 resolution, or (ii) using a reduced order model which allows for a more complex model and 1037 higher spatial resolution but preserves only the most important dynamics of the system. 1038 In AM a very high number of state variables from an FE approach were preserved and 1039 an Ensemble Kalman Filter (EnKF) proposed to deal with the high dimensionality [120]. 1040 However, this work is still in its early stages and has only been tested in simulation and on 1041 2D models to date. 1042

4.3. Relationship between state estimators and machine learning in manufacturing

The literature points to an emerging trend in combining machine learning with model- 1045 based state estimation, and this been pursued in monitoring and control of machining 1046 processes in particular. Physics-based models of cutting have been exploited to predict the 1047 progression of tool wear and increasing surface roughness in milling and turning processes, 1048 while available machine measurements such as cutting force power consumption are used 1049 to correct predictions. However, increasingly indirect measurements including visual 1050 images, vibration signals and acoustic emission data are used to provide information on 1051 the tool and/or part state and it can be difficult to derive physical relationships between 1052 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 applica- 1054 tion in a Bayesian filtering framework. Notably, the combination of a system model which 1055 predicts the progression of tool wear and/or part roughness together with measurement 1056 information from the process is shown to outperform the machine learning models on their 1057 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 1059 approaches [36]. 1060

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4.4. Systems-level approach

A trend in recent works on state estimation in manufacturing is a greater tendency 1003 towards a more holistic systems level approach to evaluating, optimising and controlling a 1064 manufacturing system. It is shown that a predict-correct state estimation framework can: (1) 1055 incorporate post production inspection and QA data into real-time monitoring and process 1066 control (e.g. [54]); (2) exploit historical data for process modelling via machine learning 1007 where physical relationships are not well defined; and (3) integrate computational models 1008 typically used for product design/process set-up into the process monitoring and control 1009 scheme. State estimation algorithms have also been applied to the issue of cybersecurity in 1070 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 1073 and environmental damage as well as risks to human safety and health. In [126] a Kalman 1074 filter is proposed for time series prediction of process states in a petroleum gas oil treatment process. The KF is shown in 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 1078 methods to enhance cyber security of water treatment plants, and found that these state 1079 estimation methods excel in certain types of attack but have limitations in others and cannot 1000 always effectively isolate and correct the system [127,128]. There remain several challenges 1091 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 1085 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 1087 maintenance of industrial processes [130]. A digital twin must be capable of processing realtime data for monitoring a system, and ideally can generate optimal control inputs to the 1000 system to ensure product quality and process efficiency. However for many manufacturing 1090 processes, an accurate computational model requires complex systems of partial differential 1091 equations which can only be solved via finite element and computational fluid dynamics 1002 (CFD) approaches. These approaches are widely developed and deployed for exploring 1093 process design and set-up, however the high computational resources required mean that 1094 such models cannot typically be deployed in real-time for the purposes of monitoring 1005 and control. Hence, the development of methods to generate low-dimensional 'surrogate' 1006 models from high-fidelity computational models of nonlinear, multi-physics and multi- 1007 scale dynamic systems for use as a digital twin is currently a very active area of research. 1008 State estimation algorithms can then provide a framework for the integration of such 1000 models with available sensor data for process monitoring and control. Surrogate models 1100 or 'emulators' can be developed using machine learning to derive a simpler and faster 1101 model from physics-based models, with Gaussian Process regression (GPR or 'kriging') 1102 being one of the most successful [130]. A Kalman filtering framework for spatio-temporal 1103 dynamics of uncertain systems captured by Gaussian process models using a network 1104 of distributed sensors has recently been proposed and may have significant potential for 1105 complex, distributed manufacturing systems[131]. An alternative emerging approach to 1106 develop model surrogates which can be used in real-time state estimation and process 1107 control is the model order reduction approach (MOR) approach. MOR aims to compute a 1108 reduced order model (ROM) of low dimension that captures the important characteristics 1109 of the original high dimensional model. Under this approach the physics of the problem is 1110 embedded in the reduced-order representation, typically using a projection-based method 1111 such as proper orthogonal decomposition (POD), which requires less training data and 1112 greater generalisation capacity relative to purely data-driven machine learning approaches 1113 [132–134]. Such methods have recently been explored for state estimation in structural health monitoring [135] and hydraulic systems [136,137] and, as discussed here, metal 1115 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 1117 complex manufacturing problems with uncertain spatial dynamics, for example in Additive Manufacturing, and promises to be a rewarding avenue for future research. 1119

5. Conclusions

A review of recent works in the development and application of state estimation 1121 methods in manufacturing demonstrates that such algorithms play an important role in 1122 soft sensing and sensor fusion to improve product quality, reduce material use, waste 1123 and downtime, and improve efficiency and safety in manufacturing. As manufacturing 1124 industries are under increasing pressure to improve sustainability through greater resource 1125 efficiency, reduction of pollutants, and greater use of 'circular' materials, state estimation 1120 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 1128 flexible approach capable of integrating physical knowledge and various data sources of 1129 information in an optimal way. The framework provides a natural way to synthesise both 1130 physics and data-based modelling approaches with real-time data in a connected cyberphysical system under the Industry 4.0 concept. Recent works have highlighted how state 1132 1130

1120

	equation models through a variety of approaches for real-time monitoring and control of	1134	
systems with spatial and temporal dynamics. Further research on the integration of s			
	estimation methods in digital twin approaches promises to be a vital tool in optimisation	1136	
	and control of complex manufacturing systems.	1137	
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	Connets of interest. The autions declare no connet of interest.	1145	
	Abbreviations	1146	
		1140	
	The following appreviations are used in this manuscript:	1147	
		1148	

[h] 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 Localization
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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