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Digital twins of food process operations: the next step for food process models?

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Food process modeling has matured with the development of multiscale, multiphase and multi-physics approaches. More comprehensive numerical tools and software platforms for improving insights and optimizing designs and processes have emerged. In the context of industrial digitalization and the advent of the Internet of Things, the concept of the digital twin has recently emerged as a means for more versatile process operational management. The digital twin is defined as a virtual replica of the real process operation, which is connected to the real world by sensor data and advanced big data analytical tools. While all elements are available for implementing digital twins, with the different types of models playing a central role, it will require a multidisciplinary approach for successful implementation and operation. The first agrofood applications still need to be demonstrated. This paper mainly focusses on the role more physics-based models can play, in addition to data-driven and hybrid models.

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Introduction

The agrifood sector needs to feed the future global population. It is inherently complex and extremely diverse in terms of types and origin of food, the way it is processed, preserved and delivered, as well as by the many different actors and stakeholders involved in the farm to fork supply chain. In response to questions related to food security, changing and diversifying needs, climate change, sustainability and consumer demands, the sector is forced to rethink methods to improve productivity, reduce waste, and increase traceability. To this end, it has been claimed that one way forward is the more intelligent use of data across the supply chain [1]. These data are becoming very abundant from an increasing amount of cheap sensors being deployed in the different processes and steps of production and supply chain.

Still, the agrifood actors are faced with the challenge on how to optimally use the large amount and diverse data being generated. To render successful frameworks for such task, tools from different areas of development are currently being explored. Internet of Things technologies facilitate transfer data from and to different sensors, computers and machines [2–4]. Cloud Computing offers ways to store, share and work with the data more effectively [5]. Data Mining and Artificial Intelligence allow to process the data in a smart and efficient way, more and more like the human brain does [6–8]. Apart from technological challenges of collecting and processing data, digitalized food production also poses other questions concerned with data sharing, such as transparency, trust and ownership. Any data-sharing platform should have the advantage of transparency, low transaction costs and instantaneous applications. To this end, there are initiatives such as blockchain, which is a decentralized database of records in the form of encrypted blocks of all transactions or digital events executed and shared among participating parties [9].

The methods presented above are typically developed in the domain of information and communication technology (ICT) and use software tools for digital data handling, inherent to the strategic initiative Industry 4.0 [10]. Therefore, the ensemble of tools is also referred to as the 'digitalization' of the agrifood sector, and the combined productivity-profitability-sustainability purposes for which these tools are deployed has been named Agrifood 4.0 [11].

So, the new Agrifood 4.0 era calls for more big data to be collected and analysed to provide improved insights, ultimately leading to better process control, supply chain management, traceability and ultimately decision making.

Digital data become intelligent only when they can be used to explain and predict the behavior of the underlying process. To this end, mathematical modelling has been shown to serve well, especially when implemented on computers [12–14].

The definition of a computer model has been formulated as the computer analog of physical reality, describing the real phenomena in terms of their mathematical description [12] and has been subject of research and development in food engineering for many decades [13,15•]. Still, this resembles very closely the definition of the recently put forward term Digital Twin that is making buzz in industry and research [16••,17]. So, what is new?

Computer models of food processes

Food engineers have since long attempted to develop mathematical models of agrofood processes. Models have improved understanding of the physical phenomena such fluid flow, heat and mass transfer and mechanical deformation that occur during food processing, and were used for designing new or optimizing existing food processes [12,13,18,19••].

Depending on the complexity, different modeling approaches are used that can range from being completely observation-based to completely physics-based [19••]. Response surface models and neural networks are examples of somewhat more complex black-box models of the first category. Simple polynomial relationships can be obtained to link lumped food characteristics such as consumer acceptance and physical properties of a food [12]. Variables that are varying with time typically follow dynamics that can be modelled with ordinary differential equations; this could be the case for many quality and safety attributes of foods, such as for texture and color, in a semi-empirical approach. If space and time dependent variation of variables is important, one must rely on partial differential equations. This is usually the case for variables such as temperature. Depending on the complexity of the system, multiple equations can be involved for different variables of interest that could be coupled, meaning that parameters in an equation for one variable depend on the other variables, such as the local heat flux that depends on local flow velocity, or color change kinetics dependent on temperature.

modelling developments over the last decades have led to more or less formalized and standardized approaches for physics modelling in food processing that often need be combined. Computational fluid dynamics (CFD) models processes dominated by fluid flow, possibly involving turbulence, non-Newtonian fluids and multiple fluids, droplets and particles [20–23]. Multiphase deformable porous media modeling aims to resolve food product dynamics at different levels of complexity [12,18,24,25]. Multiscale modelling predicts the food material behavior by interconnected models at different spatial scales which allow the property-structure-composition relationships be formalized [13,26–29]. Still, more specialized modelling techniques could be appropriate for dedicated applications at specific scales. Discrete element modeling tackles particle body interactions [30–32]. Phase field modeling can resolve spatial phase dynamics such as in crystal formation [33]. Popular mesoscale methods include the lattice-Boltzmann method [34,35] and smoothed particle hydrodynamics [36]. At the nanoscale, molecular dynamics and Monte Carlo modelling can be used for obtaining macromolecules geometries that affect transport, and at subnanoscale resolution, density functional theory can be applied for the evaluation of different electronic properties of colloidal structures [37,38]. In fact, a general framework has already been proposed for applying the physics-based modeling approaches to any food process taking into account quality and safety evaluation [12]. Likewise, significant progress has been made with mechanistic models to describe biochemical processes [39].

The success of food process modelling has largely come with the development, from the 1970s onwards, of efficient numerical techniques to solve coupled systems of spatio-temporal differential equations. Particularly the finite element and finite volume techniques have led to the emergence of performant and user-friendly software for implementing and solving the model equations in a computer aided design (CAD) framework [15•]. For food engineers, this meant that the focus could be devoted to the resolving the physics and related phenomena, the food properties and 3D geometry of the systems rather than the tedious numerical implementation of the algorithms to solve the mathematical equations [12]. Furthermore, the improved efficiency and parallelization of the software codes has led to a drastic reduction of computation times, while, with increased memory came the possibility to cope with ever larger and more realistic problems [20]. Finally, more sophisticated experimental methods such as particle image velocimetry, positron emission particle tracking, X-ray computed tomography, magnetic resonance imaging and neutron imaging have been become more easily accessible to verify computations and increase robustness and reliability of the computer models at the same level of spatial and temporal detail [40–44].

The interested reader is referred to recent publications to explore a few further examples of more comprehensive physics-based models of food process operations and supply chains [45•,46–49].

Digital twins

A digital twin [50••] aims to expand computer simulations beyond their traditional scope of process or product design by virtual prototyping and optimization, which is an off-line effort with solutions implemented after the simulation study[5] . The digital twin incorporates the computer simulation into the actual operation, be it a particular process or a product throughout its lifecycle. This means that the digital twin should not only simulate accurately and realistically all relevant processes and their kinetics, as this would just fall under computational modeling and simulation. In addition, the digital twin also should be connected to the real-world product and processes by sensor data and analytical tools. The implication is that the model should run and update allowing results to be implemented by operational devices and/or personnel smoothly. As a result, the digital twin can elucidate important aspects of the ongoing process and product under development, just-in-time during real operation. The digital twin should also diagnose current and future performance and identify failures and their cause, reduce costs and downtimes for maintenance, predict future product quality and safety, and improve product and process designs and control.

In engineering and manufacturing fields, digital twins are already built and used for performance optimization and maintenance of engines, pumps, and turbines. Here, a numerical model provides unmatched insight in the internal operational behavior and is linked to the real-world process by real-time sensor data [16••,51–53,54•]. Similarly, in healthcare, digital twins are on the verge as *in silico* individualized copies of working organs for testing and optimizing medical treatments and therapies and training and assisting surgeons, while accelerating development of novel techniques for personalized medicine [55–57,58•].

To meet these expectations for food applications, a digital twin requires the following elements in place (Figure 1):

1. Sensor networks that measure essential variables and properties of the product, process, actuators, inputs, outputs and environment in real time;
2. A platform to connect the sensors, actuators with cloud-based data storage and high performance computing, big data analytics, and applications to be used by relevant users within and across enterprises, which is conveniently provided by the Internet of Things (IoT);
3. A digital twin simulation platform with computer models that use the data from the platform as inputs to perform computations for testing, design, optimization and control and providing output for improved data analysis, process performance and product quality, and therefore provide decision support.

The integration of the real process operation with the IoT platform and the digital twin serve to provide improved decision support, with

- Easy-to-use apps that provide operators and management with an overview of relevant process performance and impact parameters, warnings, advice for process optimization, maintenance, logistics and predictions of product quality in the further supply chain;
- Smart and optimized model-based algorithms for more accurate and reliable process control and robotics operations;
- Augmented reality monitoring of the process, where the digital twin acts as a true virtual duplication of the real process that can help with for example training and process maintenance.

The digital twin so will not only be a decision tool for design, but becomes part of operation and management, serving a variety of tasks (Figure 1). Three main elements of this digital food processing context are further commented below, with respect to their importance for establishing a true digital twin of a food process operation. While pure data-driven digital twins are possible, here we explore the benefits and conditions for implementing mechanistic digital twins.

Smart sensors and actuators

Concerning in-operation measurement technologies significant progress is being made. Cheap, simple, low power and wireless sensors are now more common for monitoring process conditions such as temperature, humidity, gasses, light, pressure, stress and flow rates [59]. Non-destructive sensors for monitoring product attributes, using a variety of techniques that exploit different parts of the electromagnetic spectrum, NMR and other spectroscopy and imaging techniques, are also becoming cheaper, more flexible and/or smaller [60–65]. Furthermore, sensors as well as the actuators (like processing equipment, controllers, machines, robots) should be smart, meaning that communication to the devices is both ways over the wireless network, thereby allowing not only to capture data, but also activation, programming and operation of the sensors and actuators over the network. It has become more easy to connect devices through sophisticated wireless network architectures for fast data transfer to a central hub, making use of the latest communication technologies, each with specific spatial ranges and data rates [66], leading to large sensor networks [2,67].

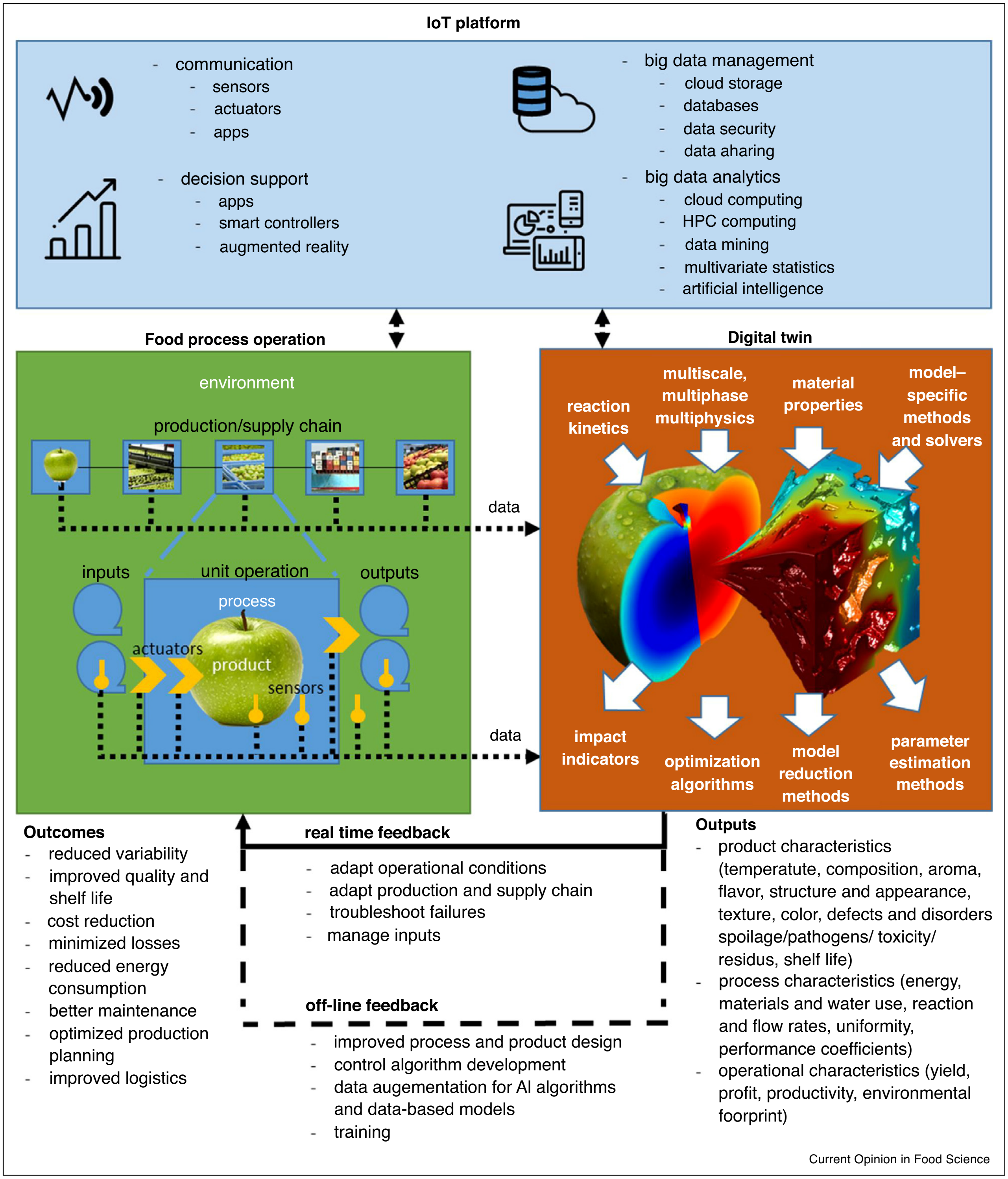
Typical of food processes is that a large variety of different data types are generated that need further analysis for proper interpretation. Needless to say that this poses questions about how to manage and make optimal use of these big data, as detailed below. Still, not everything that is required to comprehensively understand food process operations what is going on can yet be measured in-line and non-invasively. Thereto, the digital twin will have a unique role to play.

Big data analytics

The Internet is a real-time accessible platform with tools to manage communication, data, analysis and interface

[5] White Paper: The new age of manufacturing: Digital twin technology and IIoT. https://www.seebo.com/digital-twin-technology/ 2019.

Figure 1



Concept and elements of a digital twin of food process operations, with focus on the potential contribution of physics-based models. The digital twin is a collection of efficient computational models that present a virtual replica of the actual product, process and operation. The data collected in the process by sensors are used to feed the digital twin that runs food process models along with the actual process, providing in real time relevant outputs of product process and operation for process control, troubleshooting and operational and supply chain management, but also to optimize processes for uniformity, performance and sustainability, develop new designs and feedback outputs to advanced data analysis into hybrid data-based an artificial intelligence models. The IoT platform provides the necessary framework and tools for the integrated sensor communication, data storage, data analysis and decision support that links reality and digital twin.

applications. When it incorporates communication with not only people but also with sensors and actuators, it becomes the Internet of Things (IoT) [3,4,68]. An IoT platform operates mainly in the cloud, making use of ease of connectivity and abundant availability of low cost storage and computing infrastructure, but can also easily connect to local computer hubs for data storage and processing. It is thereby ideally suited to implement and manage advanced big data analytical and data sharing tools. IoT services are provided by different operators, including Amazon, Microsoft, IBM, GE and SAS [68]. Most providers also ensure data security and basic tools for big data analysis.

For data analysis, different tools are available. Pure black-box statistical approaches include statistical process control (SPC), multivariate statistics (MVS), data mining (DM), machine learning (ML) and deep learning (DL). SPC is a collection of mainly monitoring methods using directly measured process line data and that allow detection of anomalies in the process affecting final outcome, thereby also targeting reduced variability [69]. In processes where sensor signals are more complex, MVS and DM techniques will be required to achieve successful qualitative monitoring, discrimination as well as classification using a variety of techniques including ML and DL methods and empirical modeling [70]. Such decision support models will require careful training and validation in lab conditions [71], thus usually performed offline. Current developments in data augmentation, unsupervised and reinforcement learning hold the prospect to perform this during process operation [8,72].

A mechanistic digital twin, if needed operating in a stochastic mode to account for biological and process variability, will have the benefit of predicting additional process or product variables and impacts that cannot be directly measured to incorporate in the data analysis, provided the model is sufficiently lean to produce the outputs timely [73,74]. The digital twin then becomes not only a virtual sensor, but a true digital replica of the actual process. The model so will become a central engine for comprehensive process analysis that pure statistics or artificial intelligence will not be able to provide. Physical models can be used to generate large datasets that are used to train more efficient models using artificial intelligence methods such as machine and deep learning, but optimally they run in real time along with the actual real life operation, providing on the go support for current and future operations.

Elements of the digital twin

So far the mindset of the food process modelling community has largely been to use models for improving knowledge and computer aided design and engineering purposes [12,15•]. This has meant using comprehensive models as an off-line design and evaluation tool, disconnected from the real world, solved on a powerful computer with considerable memory, often taking hours to days to solve the millions of equations involved, even with efficient numerical solvers. The accessibility and performance of commercial software codes for multiphysics simulation such as NUMECA, ANSYS, STAR-CCM + and Comsol, but also programming languages such as Matlab and Phyton, have been very instrumental in this respect [12,15•]. Modelers have taken advantage of the drastic increase in computing power to develop ever more realistic but also more complex models with more parameters to identify and longer computation times. As a consequence, the use of computer models have often been limited to what-if exploration of the spatio-temporal processes and come up with design or operational guidelines, within the bounds of validity of the model [45•,46]. Further improvement of computation speed is expected from large scale parallelization on high performance computers (HPC) from industry oriented cloud-based platform services, such as ANSYS Cloud running on Microsoft Azure[6] and Siemens Cloud Solutions[7], or the completely cloud-based platform SimScale[8], while most research organisations have access to HPC infrastructure where parallelized solvers can be deployed. Still, several challenges remain:

- for many food applications, still specific programming is required to deal with complex material properties and the multiscale, multiphase and multiphysics coupling in combination with mechanistic kinetics of biological and chemical processes involved; this also means that food process models are highly fragmented in the domain and one general implementation approach such as for CFD, although advocated [12], is not available today;
- the more complex integration of different modeling methods operating at different scales and corresponding solvers is not feasible today within single available commercial software suites, that are mostly based on a performant solver engine for the numerical techniques of the finite element method (FEM) or the finite volume method (FVM), at best incorporating a discrete element method (DEM) solver (as in STAR-CCM+); true multiscale model simulation has so far hardly been implemented, rather it has been often a discrete iterative effort, taking results of simulations on one scale to predict parameters of models at a higher level [13]. It should also be noted that these types of models will be hard to solve in real time today. Therefore, in the next

[6] Simulation in the Cloud: The New Imperative: https://www.ansys.com/-/media/ansys/corporate/resourcelibrary/whitepaper/simulation-in-the-cloud.pdf?la=en&hash=50C9F994EA779E929FBA4A7F65EB9243700E420D, 2019.

[7] CAD in the Cloud | Siemens - Thought Leadership. https://blogs.sw.siemens.com/thought-leadership/CAD-in-the-Cloud-how-does-it-fit-in-your-digitalization-efforts/, 2019.

[8] https://www.simscale.com/.

years it is expected that more simple Multiphysics-based models will be first used in digital twins, which need to be carefully parameterized and validated.
- Prediction of changing material properties of foods is feasible [13,75]; however, a general comprehensive platform that can be integrated with modeling software is not available yet.

More formal optimization of processes using models has been implemented much less widespread with elaborate physics-reaction based models of food processes, because of computational effort required while facing challenges with multi-objective optimization of multi-variate distributed non-linear numerical problems [19••]. To this one should add the complexity of predicting food properties [75,76] and a lack of links between the model and the actual process control variables or impacts [19••,77]. For model-based control purposes, linking the model to the real process, much simpler, lumped type of models have been derived, with the consequence of having to remove or parameterize certain details of the process, such as the spatial distribution of variables [77,78,79•,80,81,82•]. All major computer simulation software suppliers have started to provide tools for parameterized exploration, optimization and model reduction that can be exploited next. Typical examples are ANSYS DesignXplorer and the FINE/Design3D Module of NUMECA. More versatile reduced order models for process simulation and optimization typically are typically provided in specialized simulation software, such as ASPEN HYSYS and gPROMS [83] that are not straightforwardly integrated with CFD software codes.

So, as with for the modeling approaches themselves, more holistic frameworks will be required for optimization, allowing model reduction and multi-criteria decision making [19••]. In this context, proper definitions of impacts will be instrumental, and models or indicators need to developed for these, including for:

(1) kinetics of degradation and/or development of relevant food quality and safety attributes [39,84,85]; it should be recognized that these properties are highly dependent on the particular food, thus require proper parameterization [86], and have considerable variability [74];
(2) impacts on nutrition and health, still a highly under-explored area that should consider oral processing and gastric digestion [87],
(3) environmental impact that could make use of life cycle analysis (LCA) methods [83] and thermodynamics to quantify energy streams [88].

Finally, existing computer models of food applications are also mostly limited to a particular part or scale of the process (for example one food product, one cool room, one section of a dryer), often not incorporating the complete apparatus, its operation and control, nor its interaction with the process line, the environment, the complete processing plant or the supply chain at large. It is clear that a true digital twin will need to consist of different models of products, processes, equipment, logistics and chains that are combined to unravel all relevant aspects of the food process. Today only few examples exist that incorporate such system or chain wide dynamics in the models [81,88,89].

Still, with different elements more or less in place, the first applications of digital twins are now emerging in the field of fresh product supply chain management, where there is ample scope for providing data to producers, exporters, retailers, and consumers, to support logistics decisions and marketing strategies [90••]. The fact that this application works on relatively long time scales, makes the speed of computer models and data analysis much less stringent.

Conclusions

While the elements for digital twins of agrofood processes are available, it remains to be demonstrated that the implementation of such holistic digital tools are feasible and affordable for the diverse agrofood industry. Advantages to demonstrate include reduced interproduct variability, improved quality and shelf life, mimized losses, reduced use of resources, better maintenance, cost reduction, optimized production planning, improved logistics, energy savings and higher transparency. This clearly goes beyond the scope of food process modeling today that mostly has had pure design optimization targets.

A first important step will be to integrate the essential elements of a digital twin in representative applications for demonstration. Such applications still need to be identified properly for food process operations, but it is expected that most benefit can be expected for complex and difficult to access processes and chains where limited sensor data are available. The first applications are demonstrated in the fresh product supply chain.

Implementation of a digital twin will require expertise beyond that of the food process modeler: specialists in sensor technology, ICT, programming, optimization, statistics and artificial intelligence need to work together with the industrial food experts (including modelers but also operators, management and other stakeholders in the supply chain that will potentially use the IoT apps). The success with which the entire digital twin workflow will be implemented with respect to ease of use and reliability, will determine whether digital twins will survive for food processing operations.

Conflict of interest statement

Nothing declared.

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