

Building blocks for a digital twin of large cool store complexes

Hoang Minh PHAN^(a), Hans VAN CAUTEREN^(a), Maarten HERTOOG^(a), Bert VERLINDEN^(b), Bart NICOLAI^{(a)(b)}, Pieter VERBOVEN^{(a)*}

^(a) KU Leuven, division MeBioS, Postharvest Group,
Leuven, 3001, Belgium, hoangminh.phan@kuleuven.be

^(b) Flanders Centre of Postharvest Technology
Leuven, 3001, Belgium, bert.verlinden@vcbt.be

*Corresponding author: Pieter.verboven@kuleuven.be

ABSTRACT

Digital twins are virtual representations that serve as real-time digital counterparts of physical objects spanning their full lifecycle. In the context of postharvest horticulture, these represent infrastructure (storage plants including refrigeration and controlled atmosphere systems) and the produce being handled (fruit and vegetables). The aim of the digital twin is to be used in real-time to support decision-making throughout the logistic handling chain, considering targets for, among others, product quality, food losses, energy use, emissions, and costs. Working with biological produce involves accounting for the inevitable biological variance, but also uncertainty exists in terms of unforeseen temporal and spatial variations within cold rooms. This contribution will present a review of the state of the art of models that can be used for the digital twin for large cool store complexes, including fully resolved as well as reduced order models of heat and mass transfer, as well as kinetics models while addressing issues with uncertainty propagation at both the theoretical and applied levels. Challenges and solutions for sensor-digital twin integration are discussed.

Keywords: Storage, Energy Efficiency, Quality, Fruit and Vegetables, Kinetics, Heat and Mass Transfer, Modeling

1. INTRODUCTION

In recent years, the sustainability of the food supply chain has gained much attention, particularly in reducing energy consumption and greenhouse gas (GHG) emissions. The agrifood supply chain ranges from preharvest stages: cultivating, farming, and harvesting produce, to postharvest stages: storage, transportation, and commercialization. Each stage inherently involves many activities that influence not only earlier concerns but also the produce quality and the fruit/food loss (Defraeye et al., 2021). A cold chain is usually applied in postharvest stages to maintain fruit quality but requires considerable power consumption. For example, it was estimated that about 50 % of electric consumption in supermarkets resulted from their refrigeration system to keep the produce fresh (Mota-Babiloni et al., 2015).

The digital twin approach is emerging as a solution to help address such concerns involving multiple objectives and thresholds. However, with the increased attention, many definitions of a digital twin have been proposed, confusing applied scientists, technologists, and engineers (VanDerHorn and Mahadevan, 2021). To have a clear understanding, this paper considers a digital twin to be a virtual representation of a physical system with predefined behaviours between which information is exchanged (de Kooning et al., 2021). From this definition, it implies that not all aspects of the physical system will be necessarily included in the digital twin development. Furthermore, scientists and engineers can build digital twins on many different scales. For example, at the scale of fruits, digital twins of fruits can use the information of storage conditions to output the quality change during the storage period. On the other hand, the digital twin on the system scale, e.g., cool store complexes, can be used to keep track of energy use and control the system operation (Defraeye et al., 2019a).

Several reasons make digital twins promising in the agrifood supply chains. The first reason is the huge amount of data available throughout the supply chain, which provides more valuable information to make digital models more robust and accurate. Next, more realistic but complex models can be developed and implemented because the computation power and speed have increased significantly over the years. Finally, the development of the Internet of Things (IoT) and the increasing amount of cheap wireless sensors bring a solution to connect the physical system and the digital model to build the digital twins (Verboven et al., 2020).

This paper presents the concept of building digital twins for cool store complexes to control and predict the quality behavior of stored fruits during a long storage period. First, an architecture of suggested digital twins for the cool store complexes and the challenge of sensor-digital twin integration are introduced in section 2. Next, section 3 will give an overview of developing kinetic models for fruit quality and addressing the uncertainty propagation. In section 4, physical-based modelling for cool store systems will be discussed. Section 5 gives readers current and future applications of digital twins in predicting the firmness change of pears at different storage conditions. Finally, a conclusion is given in section 6.

2. DIGITAL TWIN FOR COOL STORE COMPLEXES

2.1. Digital twin architecture of cool store complexes

In general, the architecture of the digital twin consists of three main elements: the physical system, the virtual representation, and the interconnection between physical and virtual systems (de Ketelaere et al., 2022). The physical system and virtual representation of the cool store complexes will be mainly described in this subsection, while challenges to implementing the interconnecting part will be discussed in subsection 2.2.

Following VanDerHorn & Mahadevan (2021), the physical systems are determined by their structures and intended purpose within the digital twin. Each physical system has its boundary to separate itself from other physical systems in space and time. The physical environment, i.e., the outer space of the physical system, should sometimes be considered in developing the digital twin. For example, developing a digital twin to predict fruit quality change over the storage period should consider the storage conditions. On the other hand, in the digital twin of the cool room, the environment temperature, e.g., air and ground, should be considered for their thermal effect on the cool room. The virtual representations, like the physical system, are determined by digital twins' purposes and desired outcomes. Normally, the virtual representation will be idealized to some level of abstraction due to constraints about enabling technology, available measured data, infrastructures, and budget. Two main branches of modelling techniques are used to create virtual representations, i.e., physics-based/mechanistic and data-driven modelling. Physics-based/mechanistic modelling depends on understanding the physical reality related to physical laws and the physiological mechanism of the system, resulting in accuracy and robustness, which is good for prediction and system control. This type of modelling will be discussed in detail in sections 3 and 4. Data-driven modelling has been widely used recently due to the lack of understanding of several systems. Many techniques are involved in this branch, such as machine learning, deep learning, and statistical models. However, these model results are mainly valid in the range of training data, which sometimes is difficult to collect. Therefore, the operators should be aware of its drawback before making decisions (Defraeye et al., 2021; Verboven et al., 2020).

To illustrate the architecture of a digital twin, a single cool room is proposed, consisting of a physical system, a virtual system, and an interconnection between the physical and virtual systems, as illustrated in Fig. 1. Since the purpose is to predict and control fruit quality and operational performance of the cool room during the storage period, the physical system includes a single cool room and other components inside the rooms, such as pallets, bins, evaporators, and fruits stored in the room. In the virtual system, models for a cool room, an evaporator, and fruit quality are established to reflect the change in air temperature, relative humidity, gas composition, and fruit quality (e.g., firmness, colour) inside the physical cool room. The connection between the physical and virtual systems consists of two elements: a (wireless) sensor system and a data management platform, which play a role in the physical-to-virtual connection, and the virtual-to-physical connection, respectively (VanDerHorn and Mahadevan, 2021). A wireless sensor system will collect and

transmit storage conditions in the cool room to the virtual system. The output of the virtual system will be sent to the management interface platform on which operators or machine algorithms make decisions. The decisions aim to control and change the physical system's state to achieve the desired results.

Based on the mentioned architecture, the digital twin architecture of cool store complexes can be developed. Since the physical system is the cool store complex, the virtual representation should represent the interconnection between each cool room. Fig. 2 illustrates the architecture of the virtual representation of the cool store complexes, inspired by the work of Nahor et al. (2004). Specifically, as mentioned earlier, every cool room (the so-called cell) in the cool store complexes is built with a specific digital twin consisting of the cool room and fruit quality models. Then, these digital twins will be connected to model the interaction of each cell in the complex system. Furthermore, refrigeration units (e.g., a condenser, compressors) and gas-handling units (e.g., CO₂ and ethylene absorbers) will also be modelled to the extent of some abstraction level in order to better control the cool store complexes.

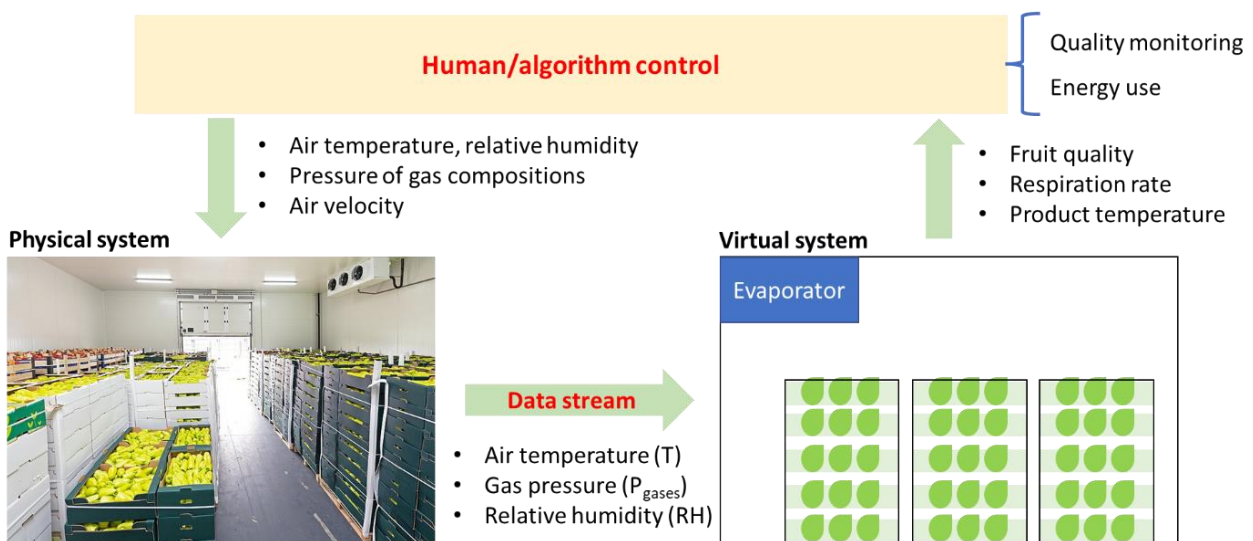


Figure 1. An architecture of a single cool room (one cell)

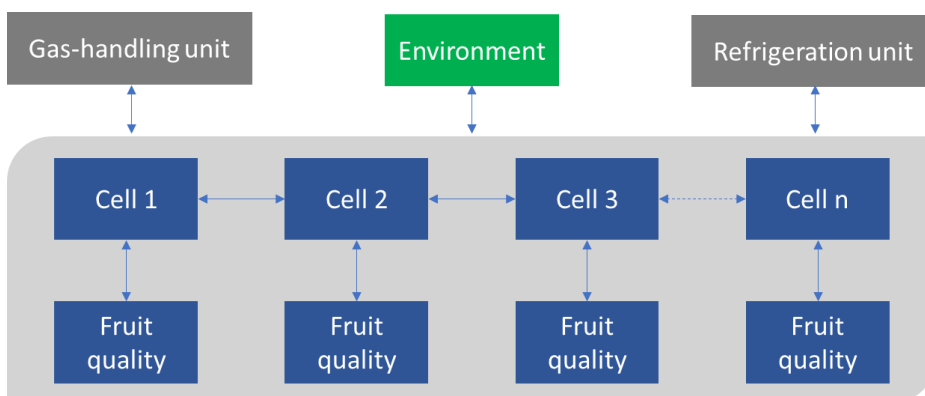


Figure 2. An architecture for a virtual representation of cool store complexes

2.2. A challenge of digital twin implementation: Sensor-digital twin integration

The connection between physical and virtual systems includes the physical-to-virtual connection and the virtual-to-physical connection (VanDerHorn and Mahadevan, 2021). The focus of this subsection is mainly on the physical-to-virtual connection, i.e., smart sensor technology, because it plays a vital role in successfully developing and implementing digital twins in practice.

In the era of IoT, wireless sensors have become more popular, affordable, and less power-consuming. Furthermore, some non-destructive measurement techniques have become more feasible in the industry, such as electromagnetic spectrum, NIR spectroscopy, or imaging technique, providing more information for digital twin development (Verboven et al., 2020). However, implementing digital twins faces challenges in practice because not all of the information from the physical system can be collected due to technology limitations, budget constraints, or current infrastructure (Jedermann et al., 2022; VanDerHorn and Mahadevan, 2021). For example, while ethylene is an important gas in controlling fruit ripening, ethylene measurement is not often implemented in storage rooms due to lacking portable and reliable ethylene sensors suitable for a long storage period (Janssen et al., 2014; Wills and Golding, 2015). Also, measuring the flesh or core temperature for stored fruits is still challenging, while the fruit temperature is key to controlling fruit quality. To address this problem, artificial fruits that mimic the thermal properties of real fruits have been studied to reflect fruit temperature during storage (Hübner and Lang, 2012). Another challenge is that most sensors or artificial fruits can only measure the conditions at fixed locations within the cool rooms (Defraeye et al. 2021). Therefore, it is not easy and accurate to formulate representative storage conditions from the measured signals. One solution is using a worst-case approach, i.e., measurement at locations with extreme conditions, but the sensor accessibility and layout of sensor installation should be thoroughly considered. Finally, measurement of the energy flow in and out of individual storage rooms is currently not done. However, it could prove vital for warnings, maintenance and operational management and could relate to the fruit's respiration status.

Besides signal measurement by smart sensors, the physical-to-virtual connection also involves other steps, such as measurement frequency and signal processing. Related to the measurement frequency, although most definitions of digital twins state the real-time synchronization of information, it should be emphasized that not all measured properties are necessary for a real-time update. Furthermore, the measured signal should be processed and filtered noises and errors before entering the virtual system. These steps should be carefully considered for sensor integration with digital twins, and they mainly depend on the use cases and desired outcomes of digital twins (Jedermann et al., 2022; VanDerHorn and Mahadevan, 2021).

3. MODELING OF FRUIT QUALITY CHANGE

3.1. Kinetic modelling of fruit quality

Cool storage aims to maintain the fruit quality as high as possible since the quality criteria (such as color, firmness, taste, aroma, and defect absence) are key in influencing consumers' purchase decisions. However, fruit quality changes during storage time, and depend on storage temperature and atmosphere. Developing a fruit quality model is necessary to use the digital twin to draw any conclusions on fruit quality (Nicolai et al., 2005). As mentioned in section 2, this section will mainly focus on mechanistic modelling, but it should be noted that the data-driven approach is still being used ((Cao et al., 2014; Han et al., 2022).

Mechanistic models on fruit quality are based on the fundamental kinetics of (bio)chemical reactions. However, the concept can be extended to model physical properties, texture, or microbial growth in the food industry (van Boekel, 2008). A general form of a kinetic model can be proposed as

$$\frac{dA}{dt} = -kA^n$$

In which A is the concerned attribute that changes over time (t), k is the rate constant, and n is the order of the change. In fruit quality, the order of the change is usually zero-order ($n= 0$), first-order ($n= 1$), or second-order ($n= 2$) (Defraeye et al., 2019b). Furthermore, some attributes, especially fruit firmness or color, can be described as logistic behaviours (Hertog et al., 2004a, 2007b).

In reaction kinetics, the rate of the attribute change mainly depends on temperature following the Arrhenius law. However, in the case of fruit quality, it is well-known that not only storage temperature but also gas composition are involved as main factors affecting quality deterioration (Nicolai et al., 2005; Tijssens and

Schouten, 2021). Hertog et al. (2001) proposed a model approach to describe the softening behaviour of 'Braeburn' apples incorporating the effect of atmospheres. This study used the Michaelis-Menten equation to describe the effect of a modified atmosphere on gas exchange and then integrate it into the kinetic model of softening behaviour. Subsequently, Hertog et al. (2003) extended the approach to a 'Hass' avocado quality model, including the effect of both gas conditions by the Michaelis-Menten equation and temperature by Arrhenius law.

Apart from the effect of temperature and respiratory gases on fruit quality, ethylene also plays a vital role in ripening and fruit quality, especially for climacteric fruits, such as apples and pears. However, the developed models above were not linked with the ethylene effect. In other words, the effect of ethylene, such as inducing the synthesis of pectin-degrading enzyme for softening process, was lumped into the model parameters and was not evaluated separately (Hertog et al., 2001). Gwanpua et al. (2012) successfully developed a model of firmness breakdown in 'Braeburn' apples that did explicitly integrate the ethylene effect. To reduce the complexity of enzymatic reactions, the model lumped these into a simple reaction catalyzed by a single enzyme. The biosynthesis of endogenous ethylene was modelled by the Michaelis-Menten equation, and it was assumed that ethylene plays a role in inducing the synthesis of this single enzyme. Finally, the temperature dependence was integrated into the rate constants following the Arrhenius law. This approach was extended to model the skin color of 'Jonagold' apples with some modifications to illustrate the autocatalytic ethylene production (Gwanpua et al., 2014).

3.2. The importance of uncertainty propagation

In postharvest management, one usually considers an average behaviour of a fruit batch to make further decisions on that batch. Additionally, most developed kinetic models to control fruit quality were deterministic, meaning that the model output referred to the average quality. However, when one is dealing with biological entities such as fruit and vegetable, the biological entities are exposed inherently to biological variance, which means that individual fruit from the same batch can behave differently during storage. Therefore, using the average behaviour can lead to inappropriate decisions in management and undesired fruit losses (Hertog et al., 2007a; Tijskens et al., 2003). Since biological variance is present widely and unavoidable, understanding and estimating biological variance can further enhance postharvest quality management (Tijskens et al., 2003).

To predict the uncertainty propagation caused by biological variance, random variables are introduced to deterministic models, which then become stochastic. A random variable is a mathematical concept describing and quantifying a biological variability using mean, (co)variances, (joint) probability density functions, and confidence intervals. However, solving the stochastic model will become challenging if many random parameters are introduced. Therefore, model parameters should be screened by a sensitivity analysis to assign only important parameters as random variables. Several popular techniques to deal with stochastic models have been reported, such as Monte-Carlo simulation, stochastic kinetic modelling, the Fokker-Planck equation, and variance propagation algorithms (Hertog et al., 2007a).

The Monte-Carlo simulation is a well-known method to estimate uncertainty propagation. Its principle is to generate the simulated output with randomized parameters from certain distributions in many simulation runs. However, its drawback is time-consuming, making it infeasible in real-time applications (Gwanpua et al., 2013). It has been applied in postharvest studies, such as Gwanpua et al., (2013 and 2014)). Stochastic kinetic modelling was proposed by Hertog (2002) and Schouten et al. (2004). The general idea is due to an assumption that if a distribution of random variables is known, one can transform the probability density function of random variables via a known algebraic equation to obtain the probability density function of a response variable. However, since this technique was based on an analytical solution, it was not easy to deal with some models containing more than three random variables (Hertog et al., 2007a). Next, the Fokker-Planck equation and variance propagation algorithm were proposed by Scheerlinck et al. (2004) to model uncertainty propagation for the soluble solids content of apples. It is worth noting that while the Fokker-Planck equation requires the knowledge of the parameters' distribution for its solution, the variance propagation algorithm can approximate the mean and (co)variance of a response variable without that

requirement. Furthermore, the variance propagation algorithm was reported to require less computation demand than the Monte-Carlo simulation (Hertog et al., 2007a).

4. PHYSICAL-BASED MODELING OF COOL STORAGE SYSTEMS

4.1. Computational fluid dynamics (CFD.)

Computational Fluid Dynamics (CFD) is a computational simulation tool to study cooling processes both on a small and large scale, from individual packages up to industrial cool rooms (A. Ambaw et al., 2014; Defraeye et al., 2014). In this modelling approach, fundamental conservation laws for mass, momentum and energy are solved throughout the domain of interest (i.e., the cool room) using numerical discretization methods that can employ unstructured meshes which can be suitably refined in regions where large gradients are expected, such that the computations can be performed accurately and efficiently. Specific information that is otherwise hard to obtain experimentally can so be gathered at a high spatiotemporal resolution (Ambaw et al., 2013; Duan et al., 2020), providing not only information about the condition and consequent quality distribution of the stored products but also the performance of the storage room as a whole, such as the net energy use (Gruyters et al., 2017).

CFD models of cool rooms have been successfully developed by our team (Alemayehu Ambaw et al., 2014; Gruyters et al., 2016). The focus has been largely on applications of temperature uniformity and optimization of postharvest treatments using porous media models of which parameters are identified by experiments. Previous research on long-term storage and transportation employing the porous medium approach (Verboven et al., 2006) includes application cases for chicory roots (Delele et al., 2009), pears (Delele et al., 2012) and apples (Gruyters et al., 2019). With dedicated experiments or explicit CFD models with fruit shape models (Gruyters et al., 2020), the airflow resistance coefficients for these situations were estimated, and approximate heat transfer was solved. To elaborate the CFD model towards dynamic controlled atmosphere storage applications, models for gas exchange and respiration kinetics will need to be included. A complete model will need to be developed considering comprehensively the fruit metabolism and diffusion in the 3D fruit shape, the transport and exchanges in fruit filled storage containers and the airflow in the cool room, accounting for fruit variability (Delele et al., 2019). For upscaling from individual fruit to large rooms, homogenization approaches will need to be implemented (Ho et al., 2013).

4.2. Reduced order models

While CFD models are the most comprehensive tools for evaluating the heat and mass transfer in storage rooms, their computational demand and time-consuming setup may not yet be compatible with the digital twin concept, certainly when considering large cooling complexes consisting of several tens of storage rooms. Therefore, other approaches have been proposed to provide insight into the thermal performance of the rooms. So-called reduced order model (R.O.M.) formulations have been proposed and validated (Nahor et al., 2005). In their simplest form; these models ignore the spatial gradients inside the rooms and use coupled lumped models of heat and mass transfer of the different main elements inside the rooms, such as the evaporator, room air and the product; and can be coupled to models of the refrigeration and gas handling systems to provide a complete cooling complex simulation model. To resolve gradients that may exist in storage rooms, for example, between different pallets, zonal models have also been proposed (Laguerre et al., 2015) at the expense of introducing semi-empirical model parameters that may be more difficult to identify. It is expected that the combination of distributed measurements of relevant quantities such as temperature, humidity, gas concentrations and air velocity using cheap sensor networks inside rooms provide a means to, in real-time, identify these model parameters and continuously improve the model predictions (Geyer et al., 2018; Praeger et al., 2020). Another interesting approach would be to elaborate the heat and mass transfer ROMs in a stochastic modelling framework (as discussed in section 3.2) to account for the effects of spatial non-uniformity. Finally, the progress in machine learning algorithms to solve efficiently spatially resolved models could circumvent the current limitations of CFD solvers and provide real-time spatially resolved predictions (Wu et al., 2022). However, such an approach still requires careful training and testing using large datasets, for which off-line CFD computations will need to be performed.

5. CURRENT AND FUTURE APPLICATIONS OF DIGITAL TWINS

5.1. Experimental data and quality kinetics model

To demonstrate the potential of the kinetic model for digital twin development, a kinetic model of firmness softening for Conference pears is developed and calibrated by historical datasets of storage of Conference pears in 2014 and 2016. The information on the pear fruit is presented in Table 1. After harvest, pears were divided into three groups. The first group was stored at shelf-life conditions (18 °C and regular atmosphere), and pear firmness was measured over 14 d, considered a harvest experiment. The other two groups were stored in two storage conditions, i.e., controlled atmosphere (CA) and dynamic controlled atmosphere (DCA), except for batch 1622, which was only stored in DCA. CA storage aims to reduce O₂ and increase CO₂ to a predetermined point for the pear storage (3 % O₂ and 0.7 % CO₂) and then keep them fixed during storage. In contrast, DCA aims to adjust O₂ and CO₂ dynamically to avoid fruit hypoxia, which may induce fruit physiological disorders (e.g., internal browning) during low O₂ storage. During storage, fruit were taken out every three months for season 2014 and every four months for season 2016. Then, they were put in shelf-life conditions to measure firmness change during 14 d using an LRX Universal Testing Machine.

Table 1. Information on 'Conference' pear dataset

Year	Location	Harvest date	Temperature (°C)		Batch identifier
			Storage	Shelf-life	
2014	Rotselaar	27/08/2014	-0.5	18	1410DCA and 1410CA
2016	Rotselaar	13/09/2016	-1	18	1610DCA and 1610CA
	Kortenaken – Region 1	09/09/2016	-1	18	1621DCA and 1621CA
	Kortenaken – Region 2	22/09/2016	-1	18	1622DCA

The model of pear softening is described as logistic behavior below.

$$\frac{dF}{dt} = -k(F_{-\infty} - F)(F - F_{+\infty})$$

In which F is pear firmness (N) changing over time (t , d), $F_{-\infty}$ and $F_{+\infty}$ are asymptotes of firmness (N) at negative and positive infinite time, and k is a rate constant of softening process (N⁻¹.d⁻¹). The rate constant, k , is governed by the energy production rate of the fruit during the storage period, which depends on storage conditions, such as temperature, oxygen, and carbon dioxide. Therefore, a general form of the rate constant, k , is written below:

$$k = f(T, O_2, CO_2)$$

Herein T is storage temperature (°C), O₂ and CO₂ are partial pressure of oxygen and carbon dioxide (kPa), respectively, using Arrhenius and Michaelis-Menten kinetics. Given, during DCA, the O₂ and CO₂ levels are changing over time, k becomes a time variable as well.

This research used the experimental data from 2016 for model calibration. The parameters k and $F_{+\infty}$ were considered generic and estimated by the whole data, while $F_{-\infty}$ was considered a batch-dependent parameter and estimated for specific batches. Next, the calibrated model was validated with the datasets in 2014. Since the batch-dependent parameter, $F_{-\infty}$, was involved, firmness at harvest measurement was used to estimate $F_{-\infty}$ again, corresponding with the validation datasets. Then, the storage measurements of the validation dataset were used to validate the model. The calibration and validation processes were conducted

in OptiPa, a MATLAB-based software developed by our group for modelling in postharvest applications (Hertog et al., 2007c).

5.2. Discussion and potential applications

Fig 3A and B illustrate the firmness changes of batch 1610CA (model calibration) and batch 1410DCA (model validation), respectively. The simulated behavior seems to fit quite acceptably with the experiment data. However, since this model only considered the effect of respiration and a lumped enzyme system on softening process, the model could not explain all variations in experimental data. The model calibration showed that R^2 was around 0.774, while the calibrated model could explain approximately 77.2 % of the variation in the validation data. It is well-known that ethylene and its biosynthesis have a vital effect on quality change during storage and shelf-life. Therefore, the proposed model can be improved by including the ethylene effect in further research.

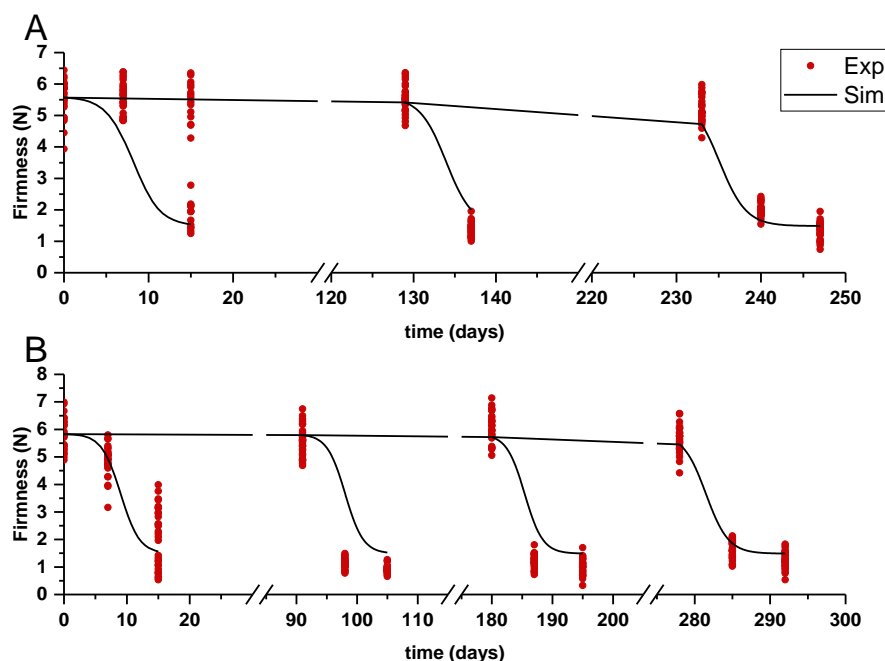


Figure 3: Experimental data (Exp) and simulated results (Sim) of pear firmness change during storage and shelf-life periods of A) batch 1610CA (model calibration) and B) batch 1410DCA (model validation)

In the case of practical implementation, the batch-dependent parameter $F_{-\infty}$ should be calibrated using a harvest experiment of each fruit batch. As a result, the accuracy of estimating this parameter is highly dependent on the data accuracy and the quality change in the shelf-life condition at harvest. For example, if the quality change in the shelf-life condition is not significantly large at harvest, the parameter $F_{-\infty}$ can be estimated inaccurately, leading to a poor prediction for the future. However, generally, the model of pear softening is good and simple enough to be applied in practice since it only requires the initial firmness measurement at harvest and condition data (temperature and gas composition) as the model inputs.

In this simulation study, the proposed model was used to generate the firmness change of 'Conference' pears during an 8-month storage and 14-day shelf-life period. The effect of DCA and CA storages on firmness would be compared at different temperatures (-1°C and 5°C). The profile of O_2 and CO_2 to simulate DCA storages was taken from a 2018 DCA dataset on 'Conference' pear stored at -1°C . Therefore, the DCA simulation at 5°C may be different in real life. Furthermore, the fruit maturity related to optimal and late harvest dates was assessed to see their influence on firmness behaviour. Hereto, the batch-dependent parameter $F_{-\infty}$ was assumed to be the same in the two fruit batches, so the difference in the fruit maturity only resulted from the initial firmness of the two batches. The results of different simulations: (-1°C , DCA, optimal), (5°C , DCA, optimal), (-1°C , CA-3% O_2 , optimal), and (-1°C , DCA, late) are shown in Fig. 4. It is clear in Fig. 4A that at the same temperature (-1°C) and fruit maturity, the DCA storage maintained pear firmness better than the CA

storage. In particular, after 8 months, the DCA storage retained 96 % firmness, compared to 79.7 % firmness for CA storage. In a comparison between -1 °C and 5 °C, the higher temperature significantly facilitated the softening process of pears. However, pear firmness after 5-month DCA storage at 5 °C was similar to that after 8-month CA storage at -1 °C. It implies that in certain cases, DCA storage at a higher temperature for a shorter storage period can achieve comparable firmness while saving energy consumption, as compared to CA storage. Finally, Fig. 4B indicates that fruit maturity affected softening of pear fruit. However, in this case, we assumed that $F_{-\infty}$ was the same for the optimal- and late-harvested batches. In practice, the $F_{-\infty}$ should be re-estimated with a harvest experiment, so the result may be different. However, with this simulation, this model can still demonstrate its power to be used in different scenarios and help postharvest managers gain more insights to support their decision-making.

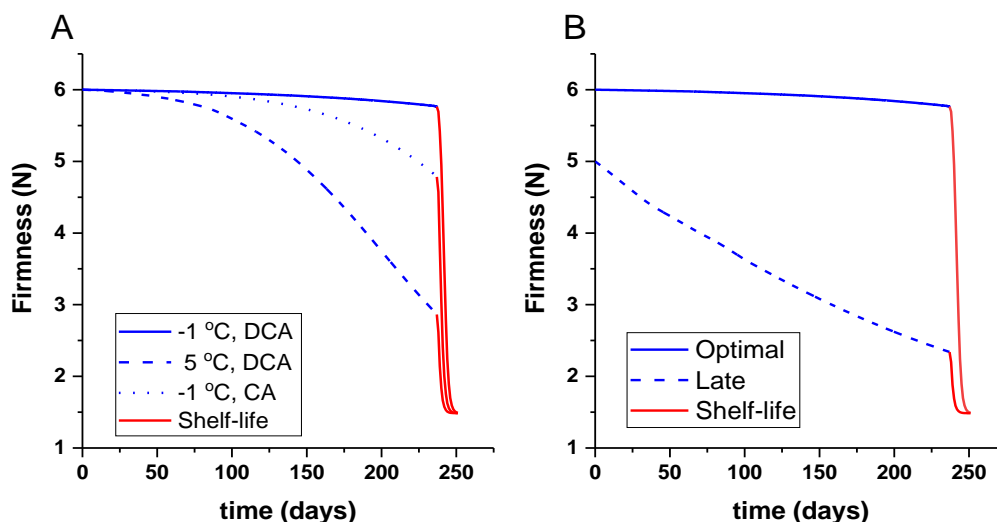


Figure 4. Simulation results of firmness change of Conference pears in storage and shelf-life periods at different storage conditions: A) optimal harvested fruit at (-1 °C, DCA), (5 °C, DCA), and (-1 °C, CA 3% O₂); B) optimal and late harvest fruit at (-1 °C, DCA)

Furthermore, in the practical application of DCA/CA storage, opening storage rooms to assess fruit quality is not feasible as it disrupts storage conditions and poses a suffocation risk to workers. Therefore, the fruit quality model that is then extended to the digital twin can enable real-time prediction to enhance postharvest warehouse management. By properly integrating the quality model with the physics-based models of storage rooms and a refrigeration system, a complete virtual system of the cool storage system can be obtained. Herein, dynamic states of the system (i.e., energy consumption and room temperature) and fruit quality can be monitored, controlled, and predicted thoroughly.

6. CONCLUSIONS

This paper provides an overview of the requirements to set up a comprehensive digital twin of cooling and storage complexes for fruit vegetables. While significant progress has been made in the different aspects, particularly with the modelling, the integrated real-time execution of the models with sensor-based inputs and model-based decision making remains to be implemented and demonstrated. Finally, a concept to develop a digital twin of fruit quality is introduced together with a discussion about the digital twin potential to virtualize a complete cool storage system in the postharvest chain.

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REFERENCES

- Ambaw, A., Delele, M.A., Defraeye, T., Ho, Q.T., Opara, L.U., Nicolai, B.M., Verboven, P., 2013. The use of CFD to characterize and design post-harvest storage facilities: Past, present and future. *Comput Electron Agric* 93, 184–194.
- Ambaw, A., Verboven, P., Delele, M.A., Defraeye, T., Tijssens, E., Schenk, A., Verlinden, B.E., Opara, U.L., Nicolai, B., 2014. CFD-based analysis of 1-MCP distribution in commercial cool store rooms: porous medium model application. *Food Bioproc Tech* 7, 1903–1916.
- Ambaw, Alemayehu, Verboven, P., Delele, M.A., Defraeye, T., Tijssens, E., Schenk, A., Verlinden, B.E., Opara, U.L., Nicolai, B.M., 2014. CFD-Based Analysis of 1-MCP Distribution in Commercial Cool Store Rooms: Porous Medium Model Application. *Food Bioproc Tech* 7, 1903–1916.
- Cao, Y., Jiang, Y., Gao, H., Chen, H., Fang, X., Mu, H., Tao, F., 2014. Development of a model for quality evaluation of litchi fruit. *Comput Electron Agric* 106, 49–55.
- de Ketelaere, B., Smeets, B., Verboven, P., Nicolai, B., Saeys, W., 2022. Digital twins in quality engineering. *Qual Eng* 34, 404–408.
- de Koning, J.D.M., Stockman, K., de Maeyer, J., Jarquin-Laguna, A., Vandeveld, L., 2021. Digital twins for wind energy conversion systems: A literature review of potential modelling techniques focused on model fidelity and computational load. *Processes*.
- Defraeye, T., Lambrecht, R., Delele, M.A., Tsige, A.A., Opara, U.L., Cronjé, P., Verboven, P., Nicolai, B., 2014. Forced-convective cooling of citrus fruit: Cooling conditions and energy consumption in relation to package design. *J Food Eng* 121, 118–127.
- Defraeye, T., Shrivastava, C., Berry, T., Verboven, P., Onwude, D., Schudel, S., Bühlmann, A., Cronje, P., Rossi, R.M., 2021. Digital twins are coming: Will we need them in supply chains of fresh horticultural produce? *Trends Food Sci Technol*.
- Defraeye, T., Tagliavini, G., Wu, W., Prawiranto, K., Schudel, S., Assefa Kerisima, M., Verboven, P., Bühlmann, A., 2019a. Digital twins probe into food cooling and biochemical quality changes for reducing losses in refrigerated supply chains. *Resour Conserv Recycl* 149, 778–794.
- Defraeye, T., Tagliavini, G., Wu, W., Prawiranto, K., Schudel, S., Assefa Kerisima, M., Verboven, P., Bühlmann, A., 2019b. Digital twins probe into food cooling and biochemical quality changes for reducing losses in refrigerated supply chains. *Resour Conserv Recycl* 149, 778–794.
- Delele, M.A., Bessemans, N., Gruyters, W., Rogge, S., Janssen, S., Verlinden, B.E., Smeets, B., Ramon, H., Verboven, P., Nicolai, B.M., 2019. Spatial distribution of gas concentrations and RQ in a controlled atmosphere storage container with pear fruit in very low oxygen conditions. *Postharvest Biol Technol* 156, 110903.
- Delele, M.A., Schenk, A., Ramon, H., Nicolai, B.M., Verboven, P., 2009. Evaluation of a chicory root cold store humidification system using computational fluid dynamics. *J Food Eng* 94, 110–121.
- Delele, M.A., Vorstermans, B., Creemers, P., Tsige, A.A., Tijssens, E., Schenk, A., Opara, U.L., Nicolai, B.M., Verboven, P., 2012. CFD model development and validation of a thermonebulisation fungicide fogging system for postharvest storage of fruit. *J Food Eng* 108, 59–68.
- Duan, Y., Wang, G.B., Fawole, O.A., Verboven, P., Zhang, X.R., Wu, D., Opara, U.L., Nicolai, B., Chen, K., 2020. Postharvest precooling of fruit and vegetables: A review. *Trends Food Sci Technol*.

- Geyer, M., Praeger, U., Truppel, I., Scaar, H., Neuwald, D., Jedermann, R., Gottschalk, K., 2018. Measuring device for air speed in macroporous media and its application inside apple storage bins. *Sensors* 18, 576.
- Gruyters, W., Ambaw, A., Schenk, A., Gwanpua, S.G., Geeraerd, A., Verboven, P., Nicolai, B., 2016. A CFD study of adapting on-off cooling cycles in apple cold stores for energy saving, in: *Refrigeration Science and Technology*.
- Gruyters, W., Defraeye, T., Verboven, P., Berry, T., Ambaw, A., Opara, U.L., Nicolai, B., 2019. Reusable boxes for a beneficial apple cold chain: A precooling analysis. *International Journal of Refrigeration* 106.
- Gruyters, W., van de Looverbosch, T., Wang, Z., Janssen, S., Verboven, P., Defraeye, T., Nicolai, B.M., 2020. Revealing shape variability and cultivar effects on cooling of packaged fruit by combining CT-imaging with explicit CFD modelling. *Postharvest Biol Technol* 162.
- Gruyters, W., Verboven, P., Delele, M., Gwanpua, S.G., Schenk, A., Nicolai, B., 2017. A numerical evaluation of adaptive on-off cooling strategies for energy savings during long-term storage of apples. *International Journal of Refrigeration* 85, 431–440.
- Gwanpua, S.G., Verlinden, B.E., Hertog, M.L.A.T.M., Bulens, I., Van de Poel, B., Van Impe, J., Nicolai, B.M., Geeraerd, A.H., 2012. Kinetic modeling of firmness breakdown in “Braeburn” apples stored under different controlled atmosphere conditions. *Postharvest Biol Technol* 67, 68–74.
- Gwanpua, S.G., Verlinden, B.E., Hertog, M.L.A.T.M., van Impe, J., Nicolai, B.M., Geeraerd, A.H., 2013. Towards flexible management of postharvest variation in fruit firmness of three apple cultivars. *Postharvest Biol Technol* 85, 18–29.
- Gwanpua, S.G., Vicent, V., Verlinden, B.E., Hertog, M.L.A.T.M., Nicolai, B.M., Geeraerd, A.H., 2014. Managing biological variation in skin background colour along the postharvest chain of “Jonagold” apples. *Postharvest Biol Technol* 93, 61–71.
- Han, J.W., Ren, Q.S., Ji, Z.T., Yang, X.T., 2022. Mathematical model of postharvest variation in tomato color based on optimized response surface methodology. *J Sci Food Agric* 102, 2972–2980.
- Hertog, M.L.A.T.M., 2002. The impact of biological variation on postharvest population dynamics. *Postharvest Biol Technol* 26, 253–263.
- Hertog, M.L.A.T.M., Lammertyn, J., de Ketelaere, B., Scheerlinck, N., Nicolai, B.M., 2007a. Managing quality variance in the postharvest food chain. *Trends Food Sci Technol* 18, 320–332.
- Hertog, M.L.A.T.M., Lammertyn, J., Desmet, M., Scheerlinck, N., Nicolai, B.M., 2004. The impact of biological variation on postharvest behaviour of tomato fruit. *Postharvest Biol Technol* 34, 271–284.
- Hertog, M.L.A.T.M., Lammertyn, J., Scheerlinck, N., Nicolai, B.M., 2007b. The impact of biological variation on postharvest behaviour: The case of dynamic temperature conditions. *Postharvest Biol Technol* 43, 183–192.
- Hertog, M.L.A.T.M., Nicholson, S.E., Banks, N.H., 2001. The effect of modified atmospheres on the rate of firmness change in “Braeburn” apples. *Postharvest Biol Technol* 23, 175–184.
- Hertog, M.L.A.T.M., Nicholson, S.E., Whitmore, K., 2003. The effect of modified atmospheres on the rate of quality change in “Hass” avocado. *Postharvest Biol Technol* 29, 41–53.
- Hertog, M.L.A.T.M., Verlinden, B.E., Lammertyn, J., Nicolai, B.M., 2007c. OptiPa, an essential primer to develop models in the postharvest area. *Comput Electron Agric* 57, 99–106.
- Ho, Q.T., Carmeliet, J., Datta, A.K., Defraeye, T., Delele, M.A., Herremans, E., Opara, L., Ramon, H., Tijssens, E., van der Sman, R., van Liedekerke, P., Verboven, P., Nicolai, B.M., 2013. Multiscale modeling in food engineering. *J Food Eng* 114, 279–291.

- Hübert, T., Lang, C., 2012. Artificial fruit: Postharvest online monitoring of agricultural food by measuring humidity and temperature. *Int J Thermophys* 33, 1606–1615.
- Janssen, S., Schmitt, K., Blanke, M., Bauersfeld, M.L., Wöllenstein, J., Lang, W., 2014. Ethylene detection in fruit supply chains. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 372.
- Jedermann, R., Singh, K., Lang, W., Mahajan, P., 2022. Digital twins for flexible linking of live sensor data with real-time models. *Sensoren und Messsysteme*.
- Laguerre, O., Duret, S., Hoang, H.M., Guillier, L., Flick, D., 2015. Simplified heat transfer modeling in a cold room filled with food products. *J Food Eng* 149, 78–86.
- Mota-Babiloni, A., Navarro-Esbrí, J., Barragán-Cervera, Á., Molés, F., Peris, B., Verdú, G., 2015. Commercial refrigeration - An overview of current status. *International Journal of Refrigeration* 57, 186–196.
- Nahor, H.B., Scheerlinck, N., Verboven, P., van Impe, J., Nicolai, B.M., 2005. A continuous/discrete simulation of controlled atmosphere (CA) cool storage systems: Evaluation of plant performance/design and product quality evolution. *International Journal of Refrigeration* 28, 471–480.
- Nahor, H.B., Scheerlinck, N., Verboven, P., Van Impe, J., Nicolai, B.M., 2004. Continuous/discrete simulation of controlled atmosphere (CA) cool storage systems: Model development and validation using pilot plant CA cool storage. *International Journal of Refrigeration* 27, 884–894.
- Nicolai, B.M., Hertog, M.L.A.T.M., Lammertyn, J., Scheerlinck, N., Veraverbeke, E.A., Verboven, P., Verlinden, B., 2005. Quality kinetics and modelling, in: *Acta Hort*. 687. pp. 23–32.
- Praeger, U., Jedermann, R., Sellwig, M., Neuwald, D.A., Hartgenbusch, N., Borysov, M., Truppel, I., Scaar, H., Geyer, M., 2020. Airflow distribution in an apple storage room. *J Food Eng* 269, 109746.
- Scheerlinck, N., Peirs, A., Desmet, M., Schenk, A., Nicolai, B.M., 2004. Modelling fruit characteristics during apple maturation: A stochastic approach. *Math Comput Model Dyn Syst* 10, 149–168.
- Schouten, R.E., Jongbloed, G., Tijssens, L.M.M., Van Kooten, O., 2004. Batch variability and cultivar keeping quality of cucumber. *Postharvest Biol Technol* 32, 299–310.
- Tijssens, L.M.M., Konopacki, P., Simcic, M., 2003. Biological variance, burden or benefit? *Postharvest Biol Technol* 27, 15–25.
- Tijssens, P., Schouten, R., 2021. What I always wanted to know about kinetic modelling, but..., in: *Acta Hort* 1311. International Society for Horticultural Science, pp. 1–13.
- van Boekel, M.A.J.S., 2008. Kinetic modeling of food quality: A critical review. *Compr Rev Food Sci Food Saf* 7, 144–158.
- VanDerHorn, E., Mahadevan, S., 2021. Digital Twin: Generalization, characterization and implementation. *Decis Support Syst* 145.
- Verboven, P., Defraeye, T., Datta, A.K., Nicolai, B., 2020. Digital twins of food process operations: the next step for food process models? *Curr Opin Food Sci*.
- Verboven, P., Flick, D., Nicolai, B., Alvarez, G., 2006. Modelling transport phenomena in refrigerated food bulks, packages and stacks: basics and advances. *International Journal of Refrigeration* 29, 985–997.
- Wills, R.B.H., Golding, J.B., 2015. Reduction of energy usage in postharvest horticulture through management of ethylene. *J Sci Food Agric* 95, 1379–1384.
- Wu, X., Zhang, X., Huang, X., Xiao, F., Usmani, A., 2022. A real-time forecast of tunnel fire based on numerical database and artificial intelligence. *Build Simul* 15, 511–524.