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Blueberry supply chain: critical steps impacting fruit quality and application of a boosted regression tree model to predict weight loss

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Highlights

- Shipping, store display and consumer are critical steps, impacting quality and waste
- Boosted regression tree model predicted weight loss at the end of storage
- Vapour Pressure Deficit, time, and point in the supply chain influence weight loss

Abstract

Blueberries have increased in popularity in recent years due to their nutritional benefits and sensory characteristics. However, to preserve quality and extend shelf-life, they need to be maintained at refrigerated temperatures and high relative humidity, conditions that are not routinely met along the supply chain. Poor temperature management leads to quality deterioration, increasing waste/losses along the supply chain. This study examined the impact of each step along the supply chain on the physicochemical quality and shelf-life of blueberries, identifying the most critical steps from field to consumption. The following steps were identified as critical in the blueberry supply chain: shipping to distribution centre (DC) (72 h at 5 °C), store

display (48 h at 15 ^{o}C), and consumer (48 h at 20 ^{o}C). Given the economic importance of weight loss and its link to fruit quality and shelf-life, a boosted regression tree (BRT) model was built to predict weight loss using the post-harvest environmental conditions of a simulated supply chain applying different temperature-time scenarios. The model explained 84 % of the variance on the test set and highlighted the interactions of supply chain conditions on weight loss.

Keywords: Cold chain; Shelf-life; Machine learning; Biochemical properties; Post-harvest storage

1. Introduction

Food security is a worldwide challenge faced by the uncertainty of meeting future food demand for an increasing population. Increasing food production is challenging, and reports have revealed that reducing food waste can address food security challenges (Gustavsson et al., 2011). Fresh fruit and vegetables are among the most frequently wasted foods (Kelly et al., 2019). Emphasis has been placed on temperature management as one of the major causes of fresh produce losses (FAO, 2019; Lai et al., 2011). Improper display conditions, limited shelf-life, and aesthetic standards have been linked to waste occurring at the retail level. At the consumer level, waste occurs, among other reasons, due to improper storage (FAO, 2019; Porat et al., 2018).

Blueberries are now the second most economically important soft fruit grown worldwide (Giongo et al., 2013), labeled as "superfoods" (Peano et al., 2017) due to their nutritional value and benefits to human health (Manganaris et al., 2014; Wang et al., 2017). Their shelf-life ranges from one to five (Matiacevich et al., 2013) or a maximum of eight weeks (Duan et al., 2011), depending on several preharvest and post-harvest factors. Commonly, blueberries are being exported via long supply chains (Paniagua et al., 2014), 95 % of which is shipped by ocean transport (Beaudry et al., 1998; Moggia et al., 2016). Lobos et al. (2018) reported an increase in rejected Chilean blueberries at the destination over the last decade. Peano et al. (2017) reported blueberries kept under normal atmosphere conditions results in wastage in the range of 6-10 % per pallet unit.

Optimum storage conditions for blueberries are 0 °C and high relative humidity (RH) (Cantwell, 2002), while blueberries are often stored under a controlled atmosphere to maximise their shelf-life (Falagan et al., 2020; Terry et al., 2009). Deviations from optimum conditions occur due to logistical constraints of precooling, sorting, and transport (Paniagua et al., 2014) and at the retail and consumer level (Nunes et al., 2009; Porat et al., 2018; WRAP, 2008). Non-optimal conditions lead to increased weight loss, decay incidence, and softening (Paniagua et al., 2014) and affect biochemical characteristics of fresh fruit, such as vitamin C, sugars, and soluble solids content (Chiabrando et al., 2009; Kelly et al., 2019).

Weight loss is a key factor influencing the shelf-life of blueberries, as it causes shriveling, loss of brightness (Chiabrando & Giacalone, 2011), and softening (Bai et al., 2019; Moggia et al., 2016). Weight loss (primarily due to water loss) directly causes economic losses when sold based on fruit weight (Bai et al., 2019). Blueberries can suffer high water loss due to their small size (high surface area/volume ratio) (Wills et al., 1981). Sanford et al. (1991) reported that blueberries become non-saleable when weight loss is higher than 5-8 %. Another study reports that the maximum acceptable weight loss during a 2-3-week period (14-21 days) is between 5-7 % (Paniagua et al., 2014). Non-optimal temperature and/or RH conditions result in higher water loss due to increased transpiration caused by a larger water vapour pressure deficit (VPD)(Laurin et al., 2005).

Extensive literature exists in mathematical models used to describe the moisture and weight loss of fresh produce (Bovi et al., 2018; Joshi et al., 2018; Lufu et al., 2019; Xanthopoulos et al., 2017). They provide detailed information on all the process variables and have been paramount in describing the phenomena associated with weight loss and how they are influenced by environmental conditions such as storage temperature and RH. Application of such models can be found in designing efficient packaging, designing strategies for controlling weight loss, designing and studying MAP packaging and efficiency, etc. (Joshi et al., 2019; Mahajan et al., 2016; Song et al., 2002). These models often require the estimation of many experimental parameters, application of advanced calculation methods, and in-depth knowledge of the process mechanisms (Omari et al., 2018).

In recent years, artificial intelligence and machine learning algorithms have empowered data analysis in the agri-food sector. The learning ability of such algorithms is suitable for identifying the complexity of biological responses. Modeling and predicting biological functions is difficult due to non-linear responses and complicated relationships among input variables (Lin and Block, 2009) to which mathematical approaches are not easily applied. These data-driven models, although they lack the ability equation-driven mathematical models have, to describe process parameters such as heat or mass transfer coefficients or reaction kinetics (Zhang, 2010), are derived from measurements using system identification techniques and are ideal for control purposes (Farkas et al., 2000). Such algorithms' applicability is becoming prevalent due to their ability to learn, adapt and improve continuously, ease of use, and high accuracy

(Ojediran et al., 2020). They have been used in agri-food quality evaluation and shelf-life determination (Ktenioudaki et al., 2019; Meng et al., 2012; Santos Pereira et al., 2018; Zhang et al., 2016), modeling and controlling drying processes (Chen et al., 2020; Erenturk and Erenturk, 2007; Farkas et al., 2000; Qadri et al., 2020) and various other applications in food engineering (Wang et al., 2012; Younis et al., 2019).

Little information is available in the literature regarding the relative importance of each step of the supply chain on the quality and shelf-life of blueberries. Knowledge of the impact of each step on the overall quality and shelf-life of blueberries would allow proper decision making to address/prevent waste and facilitate actions so that high quality and nutritious food products reach the consumer. The objectives of the study were: i) to identify critical supply chain steps where a significant decline in physical and/or biochemical quality occurred by determining the impact level of each step along the supply chain, and ii) given the importance of weight loss in the blueberry industry to build a machine learning model predicting weight loss taking into account post-harvest environmental conditions.

2. Material and Methods

2.1 Plant material and experimental setup

'Jewel' blueberries were harvested on two occasions during the production season (April and May) from commercial fields in Florida, USA. Within one hour of harvest, approximately 28 kg of blueberries were brought to the USF-Food Quality Laboratory (transit temperature of approximately 15 ^{o}C), where 21 kg were randomly selected for uniformity of colour and freedom from defects.

The blueberry supply chain was divided into nine steps to include all steps from production to consumer. Each step was split into two conditions: Moderate (M) and Extreme (E). *Moderate* being conditions of small temperature deviation from optimum or shorter duration and *Extreme* being conditions of higher temperature deviation or longer duration (Fig.1). Simulated supply chain conditions were selected based on previous observations during blueberry handling: Blueberry optimum temperature storage conditions (1.0 °C) were selected based on published data (Nunes, 2008; Perkins-Veazy, 2016). Grading delays, grading temperatures were estimated based on previous observations during field operations; field temperatures (30 °C) were selected based on the average field temperatures measured in Florida between April and May (https://fawn.ifas.ufl.edu/); cooling times and temperatures (2 or 5 °C for 2 h), storage at the grower's facilities (2 or 5°C for 24 h), shipping to distribution centre (DC) (2 or 5 °C for 72 h), DC storage (2 or 5 °C for 24 h), shipping to stores (2 or 8 °C for 8 h) and store display (2 or 15 °C for 24 h) were selected based on previous observations during field operations. The time (104 h) used to simulate shipping from grower to distribution center (DC) was chosen based on the farthest distance in time from Florida to the Midwestern States or Eastern Canada. Finally, conditions used for consumer handling (4 or 20 °C for 24 h) were chosen based on the standard household refrigerator (Godwin et al., 2007) and countertop conditions (temperature and RH). Target RH for most steps (except Step 9E-Consumer at 20 ^{o}C) was set at 80 %. However, the achievable RH was dependant on the temperature as it was difficult, due to equipment limitations, to maintain a high RH at temperatures close to freezing point. Recorded RH and temperature conditions are shown in Figure 1 and Table 1. RH at Consumer(20 ^{o}C) step was 55 % to simulate countertop conditions.

The experiment consisted of 19 treatments [9 simulated supply chain steps x 2 conditions each (M + E) and 1 Control]. Temperature and humidity-controlled chambers (Forma Environmental Chambers Model 3940 Series, Thermo Electron Corporation, OH, USA) were used to store the samples. Control samples were kept at optimum temperature conditions (1.0 °C) and 66 % RH. As mentioned earlier, optimum RH conditions of above 80 % were challenging to attain due to the limited capability of the equipment used in maintaining high RH values at this low temperature. Each step (Fig. 1) is an individual supply chain condition, as only that step differed from the control. Before and after each of those different time-temperature treatments, the blueberries were kept at constant optimum temperature conditions. The quality of the fruit was evaluated initially (day 0) and at each step individually, after a total supply chain length of 278 h (≈ 12 d).

In total, 133 clamshells of 150 g of fruit were prepared and distributed to the chambers set at different temperatures and RH conditions depending on the supply chain step (Fig. 1 and Table 1). Four clamshells were taken from each treatment/step (4 replicates) after 278 h and were used for weight loss, appearance, colour, and texture evaluation; and three additional clamshells per treatment (3 replicates) were homogenized in a laboratory blender, and the resulting puree was immediately frozen and kept at -30 °C for biochemical analysis. On the day of harvest (day 0), four replicates of 150 g fruit were used for appearance, colour, and texture evaluation. Additional three replicates of 150 g fruit were immediately blended and frozen and subsequently used for biochemical analysis.

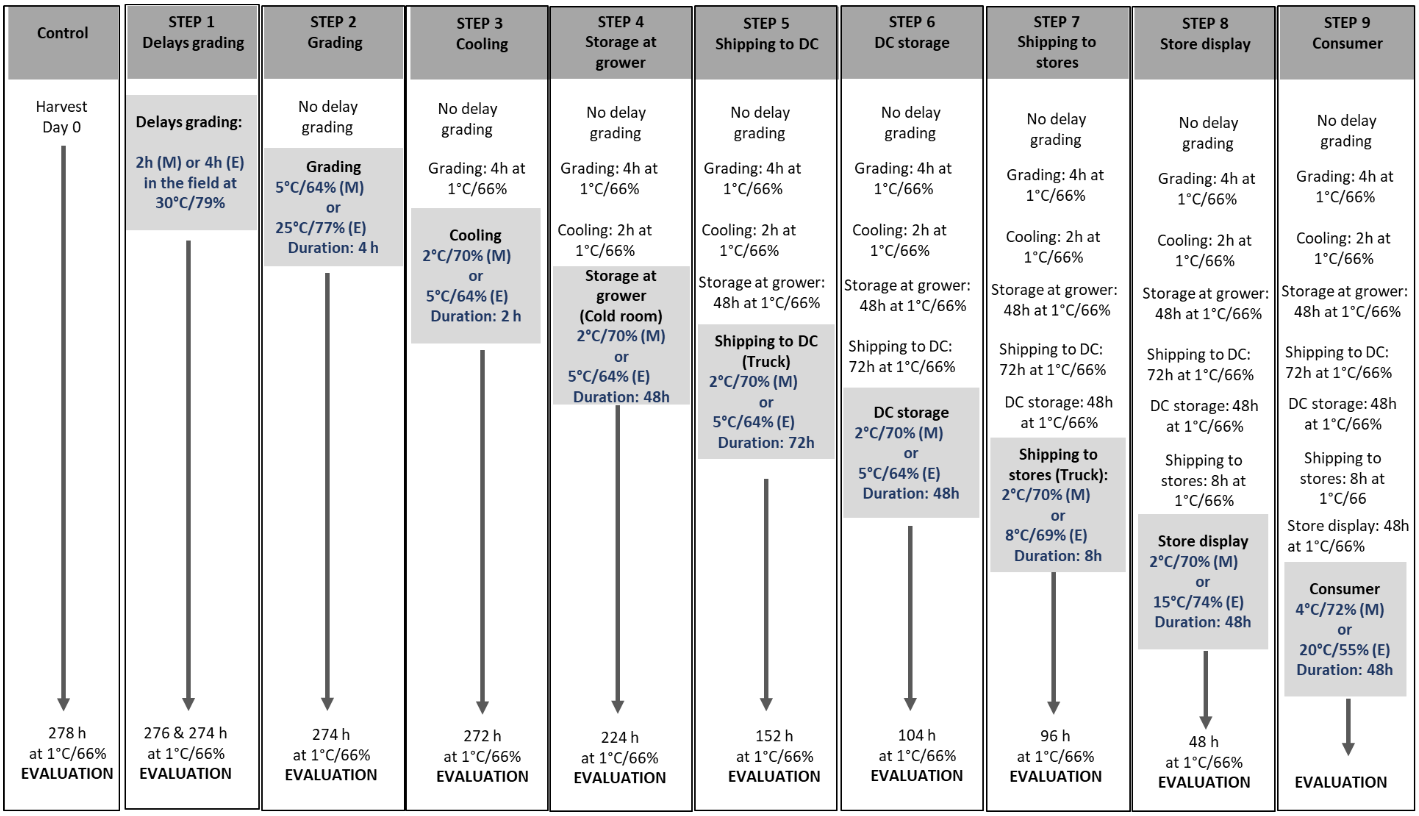


Fig. 1 Blueberry supply chain simulations from field to consumer. Each column represents a supply chain step, and within each step, moderate (M) and extreme conditions (E) were tested. DC: Distribution Centre

Table 1 Conditions of simulated supply chain steps

Samples/Steps		Conditions (Duration /Temperature/RH)	VPD* (kPa)	Point (h)	Time (h)
Control		278h / 1°C/ 66%	0.22 ± 0.00	0	0
	Simulated supply chain steps				
1M	Delays grading	2h / 30°C / 79%	0.934 ± 0.02	0	2
1E		4h / 30°C / 79%	0.934± 0.02	0	4
2M	Grading	4h / 5°C / 64%	0.31 ± 0.05	0	4
2E		4h / 25°C / 77%	0.75 ± 0.01	0	4
3M	Cooling	2h / 2°C / 70%	0.23 ± 0.02	4	2
3E		2h / 5°C / 64%	0.31 ± 0.05	4	2
4M	Storage at grower	48h / 2°C / 70%	0.23 ± 0.02	6	48
4E		48h / 5°C / 64%	0.31 ± 0.05	6	48

5M	Shipping to DC	72h / 2ºC / 70%	0.23 ± 0.02	54	72
5E		72h / 5ºC / 64%	0.31 ± 0.05	54	72
6M	DC storage	48h / 2ºC / 70%	0.23 ± 0.02	126	48
6E		48h / 5ºC / 64%	0.31 ± 0.05	126	48
7M	Shipping to stores	8h / 2ºC / 70%	0.23 ± 0.02	174	8
7E		8h / 8ºC / 69%	0.34 ± 0.01	174	8
8M	Store display	48h / 2ºC / 70%	0.23 ± 0.02	182	48
8E		48h / 15ºC / 74%	0.44 ± 0.03	182	48
9M	Consumer	48h / 4ºC / 72%	0.23 ± 0.04	230	48
9E		48h / 20ºC / 55%	1.05 ± 0.02	230	48

* M - moderate conditions of small temperature deviation from optimum or shorter duration, E - extreme conditions of higher temperature deviation from optimum or longer duration, VPD – Vapour Pressure Deficit, Point - point in the supply chain when a deviation from optimum conditions occurred (breach), Time - duration of breach

* VPD results shown are the mean (± standard deviation) of two harvests. VPD calculations were based on actual temperature and RH conditions recorded by the data loggers.

2.2 Temperature and relative humidity (RH) monitoring

Temperature and RH inside the chambers were monitored throughout the study using HOBO® brand U12 data loggers (Onset Computer Corporation, Pocasset, MA, USA), which records within an accuracy of ± 0.35 °C ± 2.5 % respectively.

2.4 Vapour pressure deficit (VPD)

VPD was calculated for all treatments based on the temperature and RH recordings of the data loggers. VPD was calculated according to equation 1:

$VPD = \upsilon p_{sat} * (1 - RH/100)$, (eq.1)

Where υp_{sat} is the saturation vapour pressure in kPa (obtained from psychrometric charts), RH is the relative humidity.

VPDt, the combination of VPD and Time (duration of breach), was calculated to show accumulated VPD during breach. The cumulative VPD (VPDt_total), which is the sum of the VPDt for the duration of the simulated supply chain (278 h), to express accumulated VPD during breach and control conditions.

2.5 Quality evaluation

Weight loss and dry weight. Weight loss was calculated from the initial weight of the fruit and after each supply chain (278 h). Weight loss was calculated as the percentage difference between the initial and the final net weight of the fruit in each clamshell. A digital balance (Denver Instruments, Timberline Series Model TP-3102) of 0.01 g of precision was used for this weight measurement.

The following formula was used for water loss corrections: [chemical components (fresh weight) × 100 g/(dry weight) + weight loss during storage (g)]. The dry weight was determined by drying three weighed aliquots of homogenized fruit tissue at 80 °C until the weight stabilized. Concentrations of chemical constituents were expressed in dry weight to show the differences between treatments that might be obscured by differences in water content and water loss during storage (Kelly et al., 2018).

Overall appearance. Subjective quality evaluation of blueberry was performed at harvest (initial) and the end of each supply chain step (278 h), always by the same trained personnel. Four replicated samples of 150 g were evaluated for overall appearance/marketability based on colour, firmness, shrivelling, and decay (Table 2). A score of 3 was considered the lower limit of acceptability for sale (Sanford et al., 1991; Nunes, 2015). The time (days) between harvest and this lower limit of acceptability (score of 3) determined the shelf-life of the fruit.

Table 2. Visual quality scores and descriptors for blueberry

	Scores and description				
	1	2	3[a]	4	5
	Very poor	Poor	Acceptable	Good	Excellent
Colour[b]	Extremely dark; overripe or senescent	Very dark blue/purplish	Fully dark blue	Bluer, less bright	Bright blue colour
Firmness[c]	Berry rupture on touch	Berry surface very depressed on touch but no rupture	Berry surface depressed on touch, softer than firmer	Slight depression on touch	Firm berry, not yielding to touch
Shrivelling [d]	Extremely wilted and dry	Severe shrivelling	Shrivelling evident but not serious	Slight signs of shrivelling	Field-fresh, fruit appear very fresh and turgid
Decay [d]	76 -100% decay, severe to extreme decay	51-75% decay, moderate to severe decay	26-50% decay, slight to moderate decay	1-25% decay, probable decay (brownish/greyish sunken minor spots)	0%, no decay

[a] Score of 3 was the minimum acceptable quality before blueberries become unmarketable.
[b] Modified from Jackson et al. (1999); Sapers et al. (1984).
[c] Modified from Sanford et al. (1991).
[d] Nunes et al. (2004).

*Instrumental colour (L*a*b*) analysis.* Ten surface measurements (L*a*b*) were taken directly in the bulk of blueberries with a hand-held tristimulus reflectance colorimeter (Model CR-400, Konica Sensing Americas, NJ, USA) using standard illuminant D65. The measurement took place directly from the clamshell. The blueberries were spread out evenly throughout the clamshell. Colour was recorded using the CIE-L*a*b* uniform colour space (CIE-Lab), L* (lightness), a* (redness), and b* (yellowness) values. Numerical values of a* and b* were converted into hue angle and chroma using the CR-400 Utility Software (Konica Minolta Sensing Americas, NJ, USA).

Texture analysis. Firmness of blueberries was measured after conditioning the samples at room temperature for approximately one hour, using a TA.XT Plus Texture Analyzer (Texture Technologies Corp., NY, USA) equipped with a 50 kg load cell. Three replicated samples of 30 g each were placed into three-100 mL plastic beakers. The fruit was then compressed to a depth of 30 mm using a 38 mm diameter and 20 mm high acrylic cylinder probe, driven at 1 mm/sec crosshead speed, and the compression force was recorded in N (Sanford et al. 1991; Nunes, 2015).

Biochemical analysis. Frozen pureed samples were thawed at 4 ˚C overnight, and samples were analysed for sugar content, ascorbic acid (AA), total phenol content (TPC), and total anthocyanins (ANC) content as described by Kelly et al.(2019). All values are expressed in g kg^{-1} on a dry weight basis. Total sugars were calculated as the sum of individual sugars. TPC is expressed as g kg^{-1} gallic acid equivalents (GAE), ANC is expressed as g kg^{-1} pelargonidin 3-glucoside equivalents. Titratable acidity (TA), pH, and soluble solids content (SSC) were determined, according to Kelly et al. (2019). TA and SSC are expressed in % on a dry weight basis.

2.6 Boosted Regression Tree

A boosted regression tree model (BRT) was used to predict fruit weight loss using the recorded simulated supply chain storage conditions. Decision tree algorithms are popular as they present information in the form of a tree and are easy to visualize with straightforward rules (Elithet al., 2008; Santos Pereira et al., 2018). BRT combines a large number of simple tree models adaptively to improve the performance of the model (Elith et al., 2008).

The objective was to explore whether the BRT model can be used to predict weight loss by using commonly recorded storage conditions (temperature and RH). Cumulative VPD was calculated, showing the total VPD the fruit was subjected to during the simulated supply chain. Cumulative VPD and Point - point in the supply chain when a deviation from optimum conditions (breach) occurred were the two independent variables of the model.

The model was fitted in R version 3.4.4 and R Studio 1.2.5001 (R Core Team, 2017) using the Caret and gbm packages. The hyperparameters were tuned using a 10fold cross-validation technique. These hyperparameters (n.trees = 150, interaction depth = 3, shrinkage = 0.1, n.minobsinnode = 3) were then used to fit a model with and to acquire the partial plots using the gm.plot function. The data was divided through random stratified sampling in training and test set (75:25 split ratio) and Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and R-squared (R^2) were used as model metrics. The gbm library was used to identify variable importance and build the partial effect plots. The model was tested on new splits (n=10) to examine data randomness, and the mean and standard deviations of RMSE, MAE, and R^2 are presented.

2.5 Statistical and data analysis

One-way ANOVA analysis was carried out using R version 3.4.4 and R Studio 1.2.5001 (R Core Team, 2017). Where ANOVA indicated significant differences were present, the Tukey pairwise comparison of the means (and 95% confidence intervals) was used to identify where the sample differences occurred. Significant differences in the physicochemical properties were identified between the two harvests, and the results were treated separately. Algorithms investigated included regression trees, support vector regression (SVR) and generalised additive models (GAMs), but the boosted regression tree had the best performance in this study. The following R packages were used to perform the data analysis: Agricolae (Mendiburu, 2015), Caret (Kuhn, 2019), gbm (Greenwell et al., 2019), pdp (Greenwell, 2017), caTools (Tuszynski, 2019), Metrics (Hammer & Frasco, 2018), writexl (Ooms, 2018).

3. Results & Discussion

Significant differences in the initial biochemical properties of blueberries were observed between the two harvests, possibly due to variability in pre-harvest conditions that can affect the concentration of chemical components in fruit or variability in the degree of ripeness. Overall, fruit from the first harvest H1 exhibited higher acidity, TPC, ANC, total sugars, and AA; and lower pH and SSC (see section 3.3).

3.1 Impact of supply chain steps on weight loss

Weight loss of blueberries was observed regardless of the storage conditions (Fig. 2). The conditions in many steps of the simulated supply chain resulted in significantly higher weight loss than the control (3.5 ± 0.4 % and 3.8 ± 0.5 % in H1 and H2, respectively). Differences in weight loss between moderate and extreme conditions within each step were not significant except for steps 3, 8, and 9 in H1 and step 9 in H2. In these cases, blueberries stored in extreme conditions (higher temperatures and/or longer exposure times) exhibited higher weight loss. In H1 and step 5, the weight loss was significantly higher in moderate conditions (lower temperature) and the highest observed in the study. Due to this unjustified and unusual high value, data from this step was considered an outlier and excluded from further analysis. Our results are within the range of weight loss values reported in previous studies. For example, Chiabrando and Giacalone (2011) reported a weight loss of 1.55 and 2.64 % on years 1 and 2, respectively, for blueberries stored at 0 ^{o}C and 90-95 % RH. In contrast, Paniagua et al. (2013a) reported a 10 % weight loss after 21 days of storage at 0 ^{o}C. Temperature and RH and their interaction affect weight loss. Furthermore, the rate of weight loss has been linked to VPD, based on the principle that transpiration rate is dependent on VPD (Lufu et al., 2019); and higher VPD will lead to higher rates of water loss. All supply chain steps caused an increase in VPD compared to the control. During step 9E-Consumer, for example, VPD increased to 1.05 kPa, resulting in an approximately 5 times higher rate of water loss than control (VPD= 0.22 kPa). Fig. 3 shows the cumulative VPD for each step of the simulated supply chain and the deviation from control. There were significant increases in cumulative VPD during steps 8E-Store Display and 9E-Consumer, and smaller increases in steps 4E-Storage at the grower, 5E-Shipping to DC, 6E-DC Storage for both harvests.

Similarly, in steps 8E-Store Display and 9E-Consumer, significantly higher weight loss was noted compared to control in both harvests. The cumulative VPD variation alone did not explain the weight loss results because weight loss is a complex process influenced by many physiological and environmental factors. However, as discussed further in section 3.5, cumulative VPD could indicate with accuracy where and when the most water loss will occur, which is valuable information for perishable goods moving through a cold supply chain.

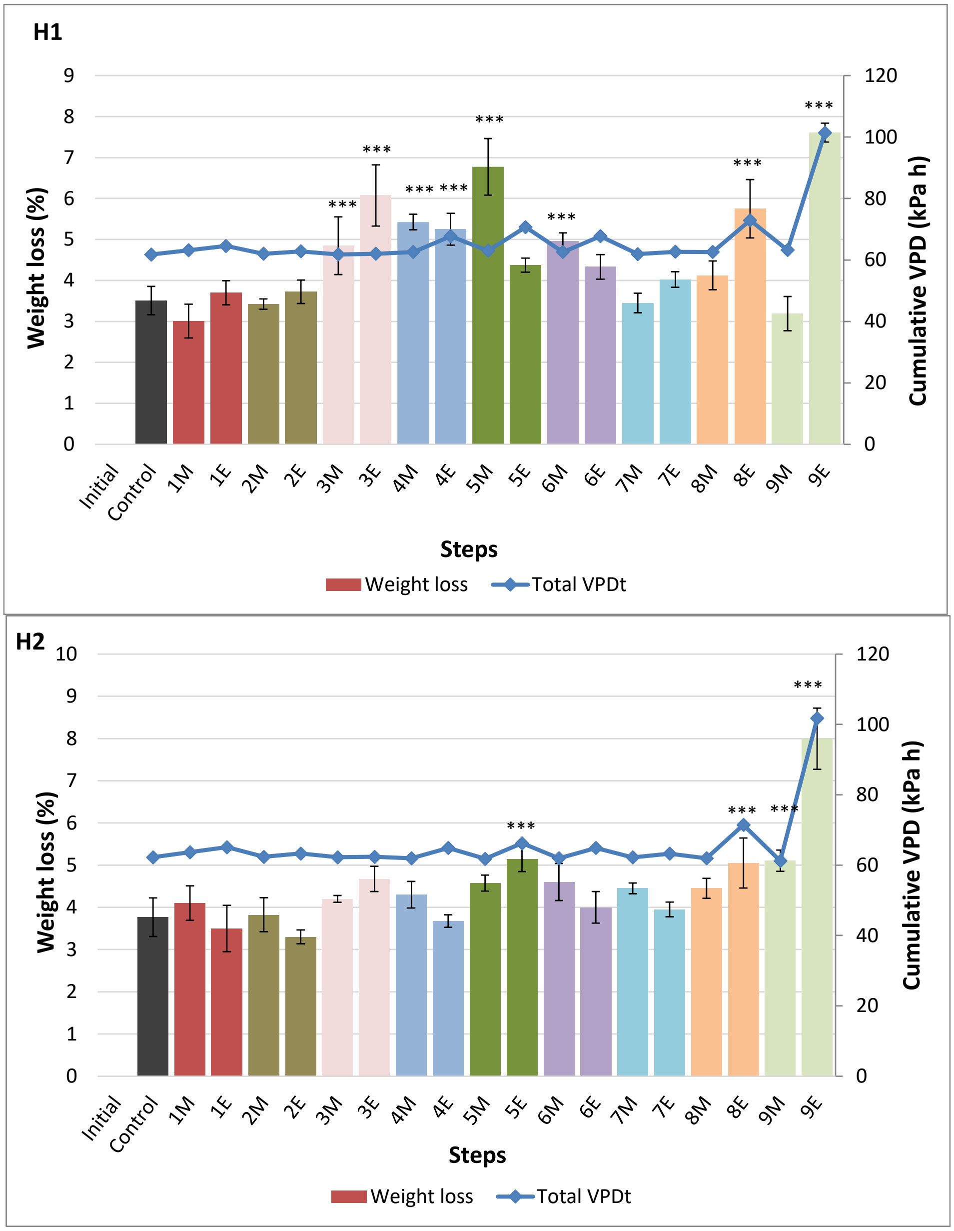


Fig. 2 Impact of simulated supply chain steps (moderate (M) and extreme conditions (E)) on weight loss of fresh blueberries after 278 h of storage in harvest 1 (H1) and harvest 2 (H2). Error bars show standard deviation between replicates (n = 4). Asterisks indicate significant differences ($p \leq 0.0001$) between control and supply chain steps. Cumulative Vapour Pressure Deficit (VPD) in each step is also shown.

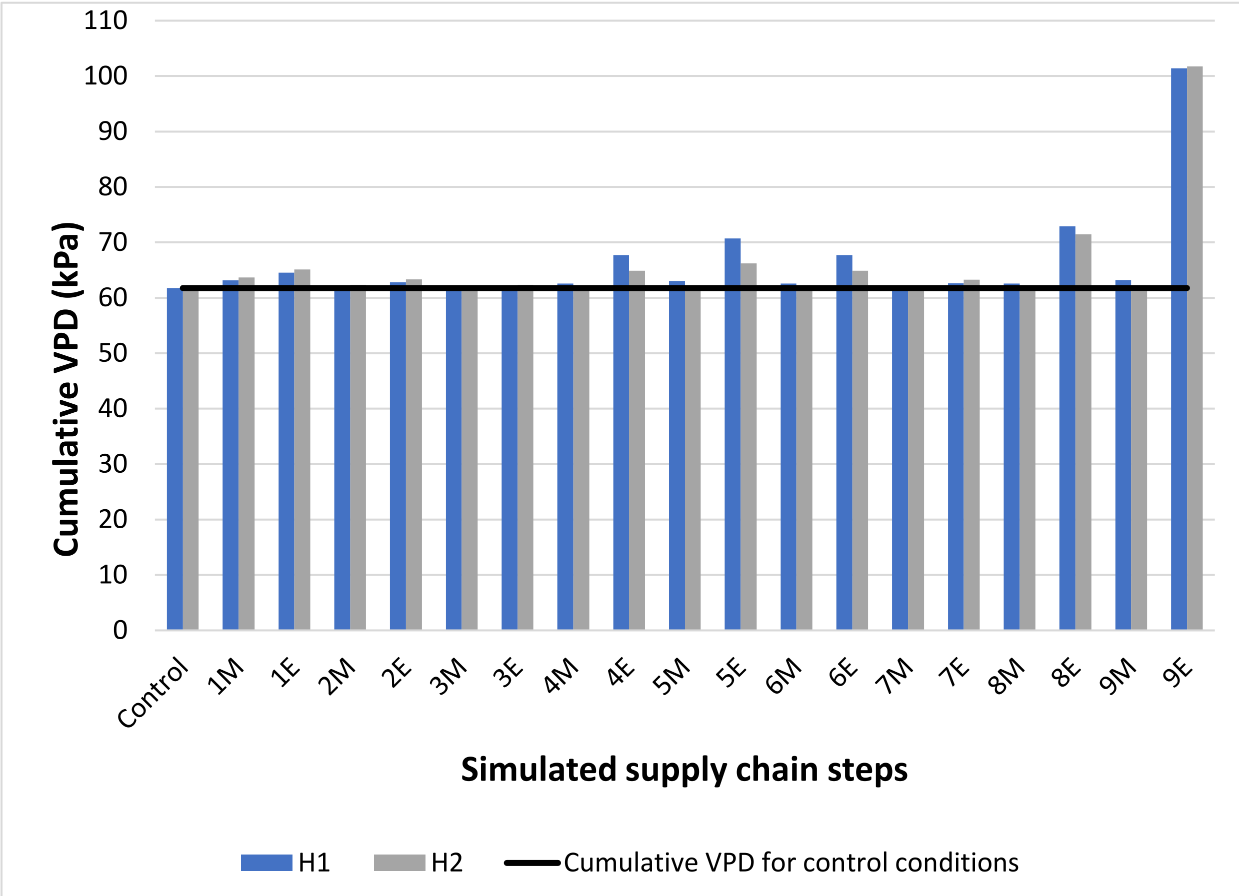


Fig. 3. Cumulative Vapour Pressure Deficit (VPD) for each step (moderate (M) and extreme conditions (E)) of simulated supply chain.Results from two harvests are shown (Harvest 1 - H1 and harvest 2 - H2).

3.2 Impact of supply chain steps on physical quality attributes

Fruit appearance, an important quality attribute that influences shelf-life and waste, declined during storage for all treatments. Blueberries kept at control conditions scored higher in both harvests (mean score of 4.6) than the fruit exposed to simulated supply chain conditions (scores ranged between 3.6 to 4.5, Fig. 4). Most blueberries exposed to extreme (E) simulated supply chain conditions received lower scores, but not all differences were significant.

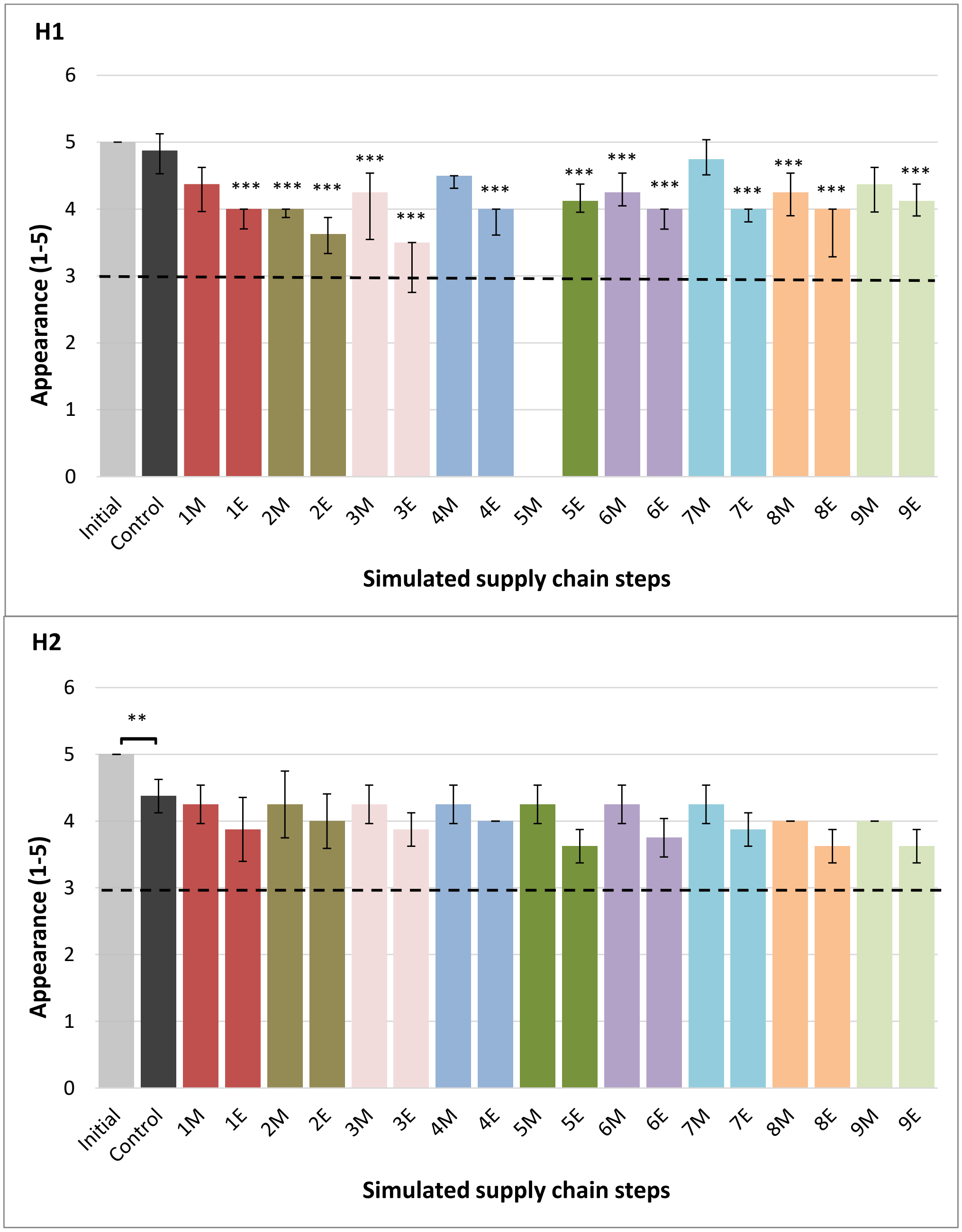


Fig. 4. Impact of simulated supply chain steps (moderate (M) and extreme conditions (E)) on appearance of fresh blueberries after 278 h of storage in harvest 1 (H1) and harvest 2 (H2). Error bars show standard deviation between replicates (n = 4). Asterisks indicate significant differences (***$p \leq 0.0001$, **$p \leq 0.001$) between control and supply chain steps. Dashed straight line represents the minimum acceptable quality before blueberries become unmarketable (rating 3).

The colour of blueberries depends on maturity level, and the colour-appearance of the fruit is affected by the presence of bloom. Higher L* values were generally observed for fruit on day 0 than the control samples after 278 hours of storage, indicative of a lighter color or presence of bloom (Eum et al., 2013). There was variability in L* for samples exposed to simulated supply chain conditions varied from 27.8 to 33.6 in H1 and 23.3 to 34.4 in H2 (results not shown). Hue values slightly increased during storage, indicating a change to a blue-purple colour.

Firmness changes during storage have been linked to changes in the primary cell wall components (Liu et al., 2019). Variable behaviour was observed with most steps leading to a decrease in firmness compared to the control and initial values; however, in some cases increase in firmness was also noted. Significantly lower firmness was observed between step *2-Grading(E)* (10.2 ± 1.6 N), *3-Cooling(E)* (11.0 ± 3.1 N), and control samples (21.8 ± 6.6 N) in H1, whereas the increase in firmness observed was not significant. No significant differences were observed in H2; firmness varied between 9.12 ± 1.7 N (step *2-Grading(E)*) and 15.2 ± 3.5 N (Initial). The firmness of control blueberries was 13.3 ± 2.15 after 278 hours. Variable firmness behaviour during storage has also been reported previously (Paniagua et al., 2013b). Many studies have linked weight loss to the decrease of firmness (Chen et al., 2017;Paniagua et al., 2013b) with Paniagua et al. (2013b), suggesting a threshold of 8 % weight loss over which extensive softening can occur. An increase in firmness during storage has also been observed and associated with low weight loss (Paniagua et al., 2013b). Different theories have been proposed to explain this phenomenon (i.e., thickening of parenchyma and epidermal cell wall (Allan-Wojtas et al., 2001) due to moisture loss reduction on the outer cell layers (Paniagua et al., 2013b)

3.3 Impact of supply chain steps on biochemical quality attributes

Soluble solids content (SSC) decreased from day 0 for all samples regardless of the simulated supply chain conditions (Table 3). There was variability during H1, as blueberries exposed to simulated supply chain conditions showed both significantly higher and lower contents compared to the control. Variability in the maturity of harvested blueberries could be the reason for the variability in the responses observed. Eum et al. (2013) did not report any significant differences in the SSC of blueberries due to temperature treatments, while Chiabrando and Giacalone (2011) found a slight increase in SSC for the first weeks followed by a decline, but overall no consistent change was found.

Acidity was significantly lower for all samples exposed to simulated supply conditions compared to the control in H1, and five steps significantly impacted blueberry acidity in H2 (lower than control) (Table 3). A decrease in titratable acidity during storage has been associated with organic acids being substrates for respiratory metabolism (Gol et al., 2013). This is a possible explanation for the lower TA observed in the samples subjected to the simulated supply chain conditions. On average, in both harvests, pH varied from 2.74 to 3.41.

Table 3 Soluble solids content (SSC) and acidity values for samples measured on day 0 (Initial) and after 278 hours (control and simulated supply chain steps)

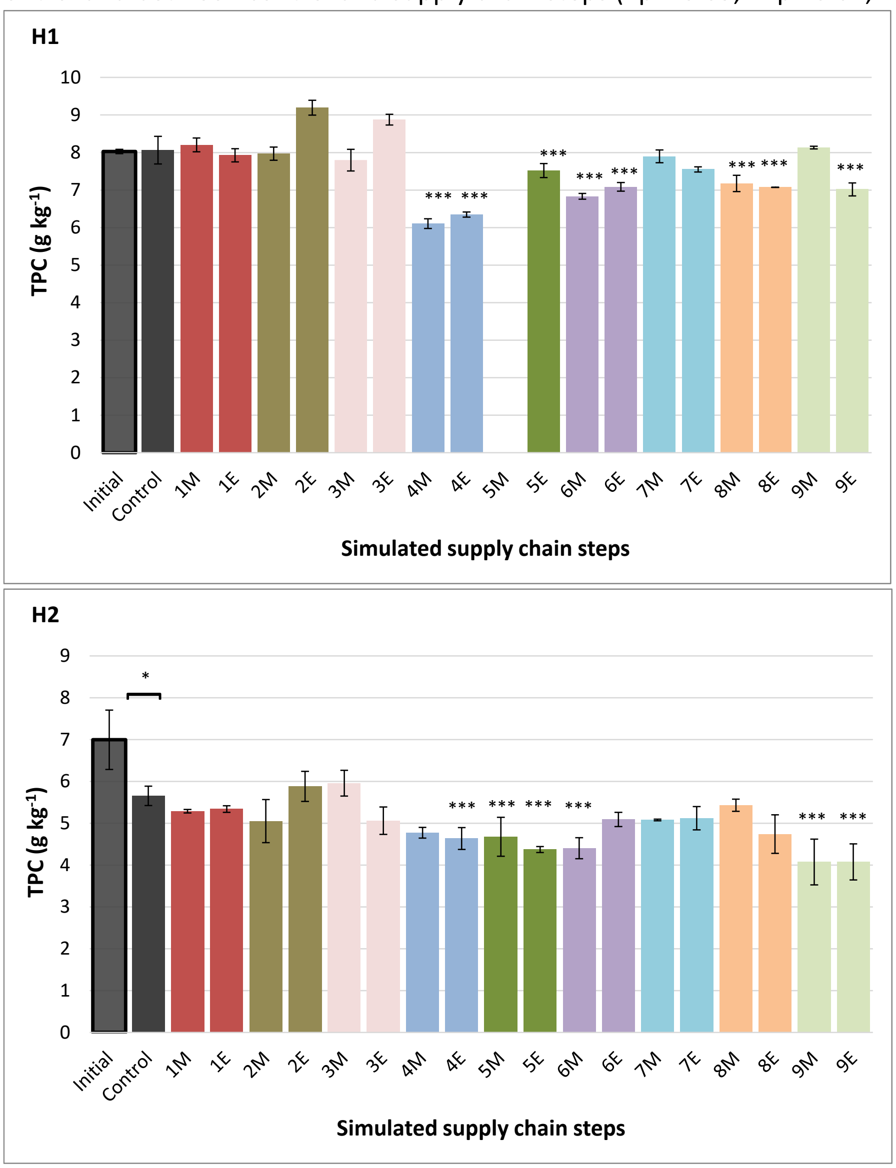
	Harvest 1		Harvest 2	
Treatment / Step	SSC (%)	Acidity (%)	SSC (%)	Acidity (%)
Initial (Day 0)	89.5 ± 0.8 *	8.05 ± 0.1	82.4 ± 1.3 *	6.69 ± 0.2 *
Control	64.2 ± 6 ^{efg}	8.7 ± 0.4 ^{a}	59.8 ± 1.4 ^{abcd}	5.6 ± 0.2 ^{a}
1M	82.2 ± 0.6 ^{a}	7.6 ± 0.1 ^{b}	57.1 ± 1.5 ^{bcdef}	5.6 ± 0.5 ^{a}
1E	70.7 ± 0.3 ^{cd}	5.5 ± 0.1 ^{fgh}	60.4 ± 3.8 ^{abc}	5.9 ± 0.3 ^{a}
2M	74.6 ± 0.6 ^{bc}	5.8 ± 0.0 ^{efg}	57.2 ± 1.9 ^{bcdef}	5.9 ± 1.1 ^{a}
2E	82.3 ± 0.6 ^{a}	6.5 ± 0.1 ^{cd}	57.8 ± 2.7 ^{bcdef}	5.6 ± 0.9 ^{a}
3M	67.8 ± 0.6 ^{def}	5.9 ± 0.1 ^{defg}	55.3 ± 1.2 ^{cdefg}	5.4 ± 0.2 ^{a}

3E	77.9 ± 1.4 ^{ab}	6.1 ± 0.1 ^{def}	51.7 ± 1.3 ^{g}	5.4 ± 0.4 ^{a}
4M	62.3 ± 0.3 ^{gh}	4.2 ± 0.2 ^{j}	57.6 ± 0.6 ^{bcdef}	5.0 ± 0.2 ^{a}
4E	62.6 ± 0.5 ^{fgh}	4.0 ± 0.2 ^{jk}	59.4 ± 3.4 ^{abcde}	5.1 ± 0.2 ^{a}
5M	-	-	54.4 ± 0.9 ^{defg}	5.0 ± 0.1 ^{a}
5E	58.8± 0.6 ^{hi}	6.1 ± 0.3 ^{def}	52.4 ± 1.0 ^{fg}	4.8 ± 0.1 ^{a}
6M	61.9 ± 0.5 ^{gh}	4.1 ± 0.0 ^{j}	55.7 ± 2.4 ^{cdefg}	4.5 ± 0.9 ^{abc}
6E	63.3 ± 1.7 ^{fgh}	4.3 ± 0.1 ^{iJ}	56.2 ± 1.1 ^{cdefg}	5.2 ± 0.4 ^{a}
7M	62.4 ± 0.3 ^{fgh}	6.4 ± 0.2 ^{cde}	62.3 ± 1.9 ^{ab}	3.5 ± 0.2 ^{bcd}
7E	58.6 ± 1.5 ^{hi}	6.5 ± 0.2 ^{cde}	64.6 ± 0.8 ^{a}	3.3 ± 0.2 ^{cd}
8M	76.9 ± 1.5 ^{ab}	3.2 ± 0.1 ^{l}	54.1 ± 0.4 ^{efg}	5.3 ± 0.1 ^{a}
8E	69.1 ± 3.0 ^{de}	3.4 ± 0.5 ^{kl}	61.9 ± 1.1 ^{ab}	2.6 ± 0.2 ^{d}
9M	67.3 ± 1.6 ^{defg}	6.8 ± 0.2 ^{c}	59.5 ± 1.0 ^{abcde}	3. 4 ± 0.2 ^{cd}
9E	53.9 ± 0.3 ^{i}	4.9 ± 0.1 ^{hi}	53.2 ± 0.6 ^{fg}	2.5 ± 0.1 ^{d}

M - moderate conditions of small temperature deviation from optimum or shorter duration, E - extreme conditions of higher temperature deviation from optimum or longer duration.Values with different letters indicate significant difference ($p<0.05$). Asterisk (*) indicates significant difference between initial and control.

Eight supply chain steps in H1 and six steps in H2 impacted total phenolic content (TPC), resulting in significantly lower values compared to the control (Fig. 5). In H1, the TPC of control samples did not change significantly from day 0, whereas a significant decrease was observed in H2. In some cases, blueberries exposed to simulated supply chain conditions showed higher TPC. This could be due to sample variation or a result of the stress response (Van de Velde et al., 2017). The highest decrease in TPC was observed for step *9E-Consumer* in both harvests. This was the most abusive step in Point, Time, and Temperature and was also the step with the highest weight loss. Duan et al. (2011) also reported a decrease in TPC after one week of cold storage. However, results were dependant on variety. The decrease in TPC has been attributed to the oxidation of phenolic compounds catalyzed by polyphenol oxidase and peroxidase (Verma and Joshi, 2000) during post-harvest storage. Loss of water leads to membrane collapse, which allows for enzymes like polyphenol oxidase to come in contact with polyphenols; hence a reduction in TPC is observed (Nunes et al., 2005). This could explain the higher decrease in TPC observed in step 9E-Consumer.

Fig. 5. Impact of simulated supply chain steps (moderate (M) and extreme conditions (E)) on TPC of fresh blueberries after 278 h of storage in harvest 1 (H1) and harvest 2 (H2). Error bars show standard deviation between replicates (n = 3). Asterisks indicate significant differences between initial quality at harvest and control and between control and supply chain steps (*p ≤ 0.05, **p≤ 0.01, ***p≤ 0.001).



The main sugars present in blueberries were fructose and glucose (data not shown). Falagan et al. (2020) found a sharp decrease in sucrose and fructose content during the storage of blueberries at 0 °C, whereas glucose showed a small increase. In our study, total sugars decreased with time for most samples with significantly lower values than the control in H1 and H2 (Fig. 6). Sugars are substrates in the respiratory metabolism (Falagan et al., 2020); Saltveit, 2019). The significantly lower sugar content in blueberries in the simulated supply chain was most likely caused by differences in the respiratory behaviour due to the different storage conditions. In four supply chain steps in H1 total sugar content was higher than the initial value on day 0, but none of the differences was significant. An increase in sugars during storage has been previously reported due to sucrose metabolism and decomposition into glucose and fructose (Wang et al., 2020). However, in this experiment, sucrose content was low; the increase observed was not significant and most likely due to sampling variability during harvest.

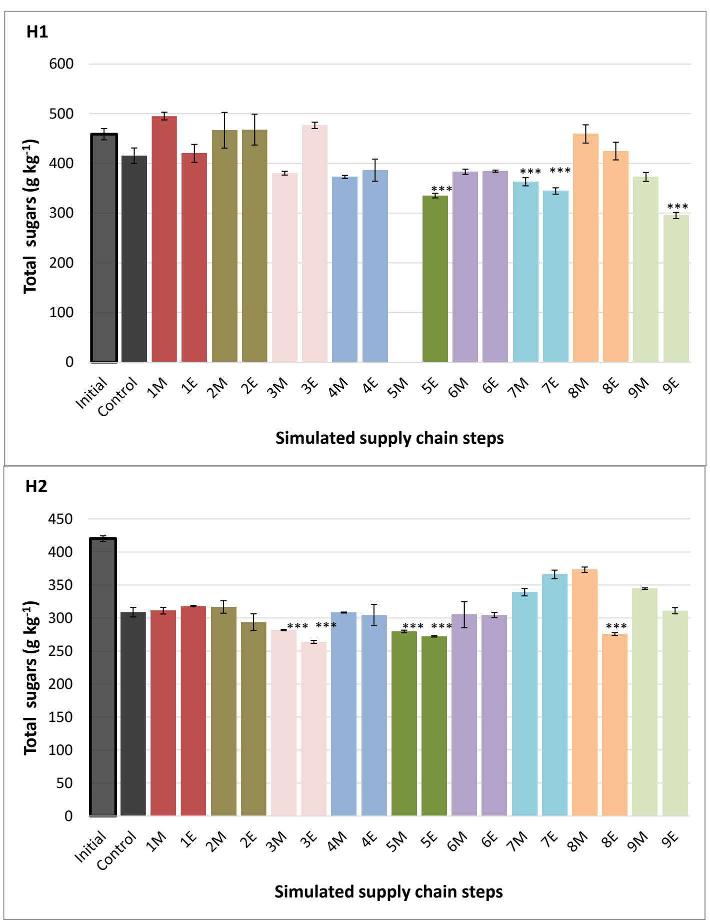


Fig. 6. Impact of simulated supply chain steps (moderate (M) and extreme conditions (E)) on total sugars content of fresh blueberries after 278 h of storage in harvest 1 (H1) and harvest 2 (H2). Error bars show standard deviation between replicates (n = 3). Asterisks indicate significant differences between initial quality at harvest and control and between control and supply chain steps (*$p \le 0.05$, **$p \le 0.01$, ***$p \le 0.001$).

Ascorbic acid (AA) decreased significantly in both harvests with storage, regardless of the supply chain step. In H1, AA decreased by 41.7% in the control and, on average, by 46.4% in blueberry samples subjected to simulated supply chain conditions. In H2 initial ascorbic acid levels were significantly lower than H1 (0.6 g kg^{-1} compared to 1.06 g kg^{-1}), and it decreased by 14.2% and 15.7% for the control and samples subjected to the simulated supply chain, respectively. Many studies have reported a loss of AA during storage for fresh fruits (Falagan et al., 2020; Ktenioudaki et al., 2019) and have been attributed to tissue degradation, cell wall damage, enzymatic oxidation, and water loss (Nunes et al., 1998; Klein, 1987). The lowest AA content was observed for step 9E-Consumer (0.49 g kg^{-1}) of the supply chain in H1 and step 2M-Grading (0.47 g kg^{-1}) of the supply chain in H2. Blueberries exposed to the simulated supply chain conditions had lower AA content compared to control samples. Still, only two steps in H1 was the decline significant (5E-Shipping to DC, and 9E-Consumer, data not shown).

Anthocyanin (ANC) content varied from 3 ± 0.2 g kg^{-1} to 6.1 ± 0.5 g kg^{-1} in H1 and decreased after 278 h of storage for most samples. In H2there was no significant change in ANC content; it varied from 3.1 ± 0.3 g kg^{-1} to 5.6 ± 0.1 g kg^{-1}. There were no significant differences between the ANC content of the control and the samples subjected to the simulated supply chain

3.4 Critical supply chain steps

A supply chain step was deemed critical based on whether a blueberry quality attribute had significantly declined after 278 hours of storage compared to the control. Table 4 shows the critical steps listed in order of importance, depending on the number of attributes they affected and the affected quality attributes. Only the steps that impacted at least three quality attributes are listed. In H1, the top critical step was 9E-C*onsumer*, affecting seven quality attributes, and in H2, the top critical steps were 5E-S*hipping to DC* and 9E-C*onsumer,* affecting four quality attributes each.

Steps 5E-S*hipping to DC*, 8E-*Store Display,* and 9E-*Consumer* were common in both harvests and were thus considered the most critical steps of the supply chain under the conditions used in our study. Step 5E was characterised by a considerably small temperature deviation from optimum (4 ^{o}C); however, the duration of the steps is high (72 h). Steps 8E and 9E were characterised by high deviations from optimum temperature and equally high durations (48 h). The most common negatively impacted quality attributes in both harvests were weight loss, acidity, SSC, total sugars, and TPC. The effect of various individual supply chain steps on quality attributes has been previously considered but separately. For example, Paniagua et al. (2013a) reported that delays of 20 h at 10 ^{o}C cause a significant effect in softening and weight loss in blueberries, whereas Eum et al. (2013) reported that fruit was not suitable for sale after 6 days at room temperature or 16 days at 10 ^{o}C during transport. A similar methodology as presented in our study was applied to strawberries (Kelly et al., 2019) and the critical supply chain steps identified were storage at consumer (20 ^{o}C), shipping to stores (8 ^{o}C), and storage at the grower (5 ^{o}C). The last step in the supply chain (i.e., consumer) has been highlighted as the step with higher losses than retail (Golan and Buzby, 2015) as over 65 % of consumers store fresh produce at unsuitable temperatures (i.e., ambient temperatures) (WRAP 2008).

Table 4 Critical supply chain steps based on the number of quality attributes impacted

Step	N^{o} of quality attributes impacted	Quality attributes impacted
Harvest 1		
9E - Consumer (48 h at 20^{o}C) *	7	Appearance, weight loss, AA, TS, TPC, Acidity, SSC
5E - Shipping to DC (72 h at 5 ^{o}C) *	5	Appearance, AA, TS, Acidity, SSC
8E - Store Display (48 h at 15^{o}C) *	4	Appearance, weight loss, TPC, Acidity
3E - Cooling (2 h at 5 ^{o}C)	4	Appearance, weight loss, Texture, Acidity
4E - Storage at grower (48 h at 5^{o}C)	4	Appearance, weight loss, TPC, Acidity
6M – DC Storage DC (48 h at 2^{o}C)	4	Appearance, weight loss, TPC, Acidity
7E- Shipping to stores (8 h at 8^{o}C)	4	Appearance, TS, Acidity, SSC
4M - Storage at grower (48 h at 2^{o}C)	3	Weight loss, TPC, Acidity
3M - Cooling (2 h at 2 ^{o}C)	3	Appearance, weight loss, Acidity
6E - DC Storage DC (48 h at 5^{o}C)	3	Appearance, TPC, Acidity
8M - Store Display (48 h at 2^{o}C)	3	Appearance, Acidity, SSC
3M- Cooling (2 h at 2^{o}C)	3	Appearance, Acidity, Weight loss
Harvest 2		
9E - Consumer (48 h at 20^{o}C) *	4	Weight loss, TPC, Acidity, SSC
5E - Shipping to DC (72 h at 5 ^{o}C) *	4	Weight loss, TS, TPC, SSC
8E - Store Display (48 h at 15^{o}C) *	3	Weight loss, TS, Acidity
9M - Consumer (48 h at 4^{o}C)	3	Weight loss, TPC, Acidity

[a] AA = ascorbic acid content (AA), TS = total sugar content, TPC = total phenolics content, SSC = soluble solids content.
[b] E = extreme conditions of higher temperature deviation from optimum or longer duration.
[c] M = moderate conditions of small temperature deviation from optimum or shorter duration
* Asterisk indicates common steps in both harvests.

3.5 BRT model

A gradient boosted model was built to predict weight loss using environmental data from the simulated supply chain conditions. The BRT model explained 84 % of the variance in weight loss on the test set (R^2 = 0.84 ± 0.02, RMSE = 0.44 ± 0.05, MAE= 0.40 ± 0.04) and 89 % on the training set (R^2 = 0.89 ± 0.01, RMSE = 0.37 ± 0.01, MAE= 0.28 ± 0.01). Cumulative VPD and Point (point in the supply chain when a breach occurred) were the two predictors used in the model, and the results showed that Point had a 23 % influence on the model, noting it as an important factor in the estimation of weight loss.

Fig. 7. shows the Partial Dependency Plot (PDP) with the marginal effect of the two variables on weight loss. It can be observed that blueberries exposed to cumulative VPD between approximately 60 and 70 kPa h will lose less than 5 % of their weight in 278 hours, those exposed to cumulative VPD of 70 – 87 kPa h approximately will lose between 5 and 6.5 % of their weight, whereas finally at higher cumulative VPD ranges weight loss will be over 7 %. This information can be useful in extended supply chains where due to logistic constraints, storage/ shipping conditions deviate from optimum, and blueberries can become unsalable by the time they reach their destination.

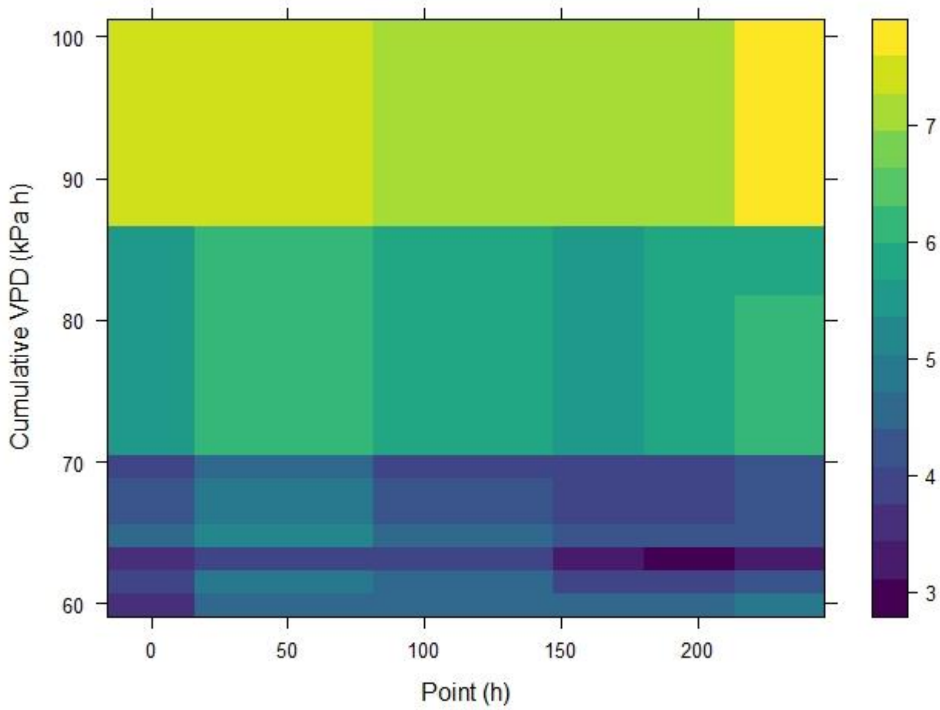


Fig. 7. Partial dependency plot showing the marginal effect of cumulative Vapour Pressure Deficit (VPD) and Point - point in the supply chain when a deviation from optimum conditions occurred (breach) on predicted weight loss. Colour scale refers to % weight loss.

The effect of Point in the supply chain on weight loss is not apparent from Fig. 7. To investigate this further, and since there was a significant relative influence on the model, the BRT model was built using the following variables: VPD (as in VPD at point of breach), Point (point in the supply chain where a breach occurred) and Time (duration of breach). Fig. 8 shows the PDP plots of the three variables and the marginal effect on weight loss. It can be observed that if a breach occurred in the first 24 hours, regardless of the duration, it is unlikely that it will have a significant effect on the weight loss. At later stages of the supply chain, when VPD was > 0.4 kPa, weight loss was likely to be higher than 6-7 %, especially when the duration of the unfavourable conditions is longer (top and bottom right boxes). Finally, VPD values > 1 are likely to lead to maximum weight loss > 8 % regardless of time and duration of the breach. However, these results were influenced by the design of the simulated supply chain used in the study, where the last step (9E-*Consumer*) was the most abusive in terms of temperature, RH, and duration. Hence, it can influence this representation. More data would be required to verify the effect of Point on weight loss.

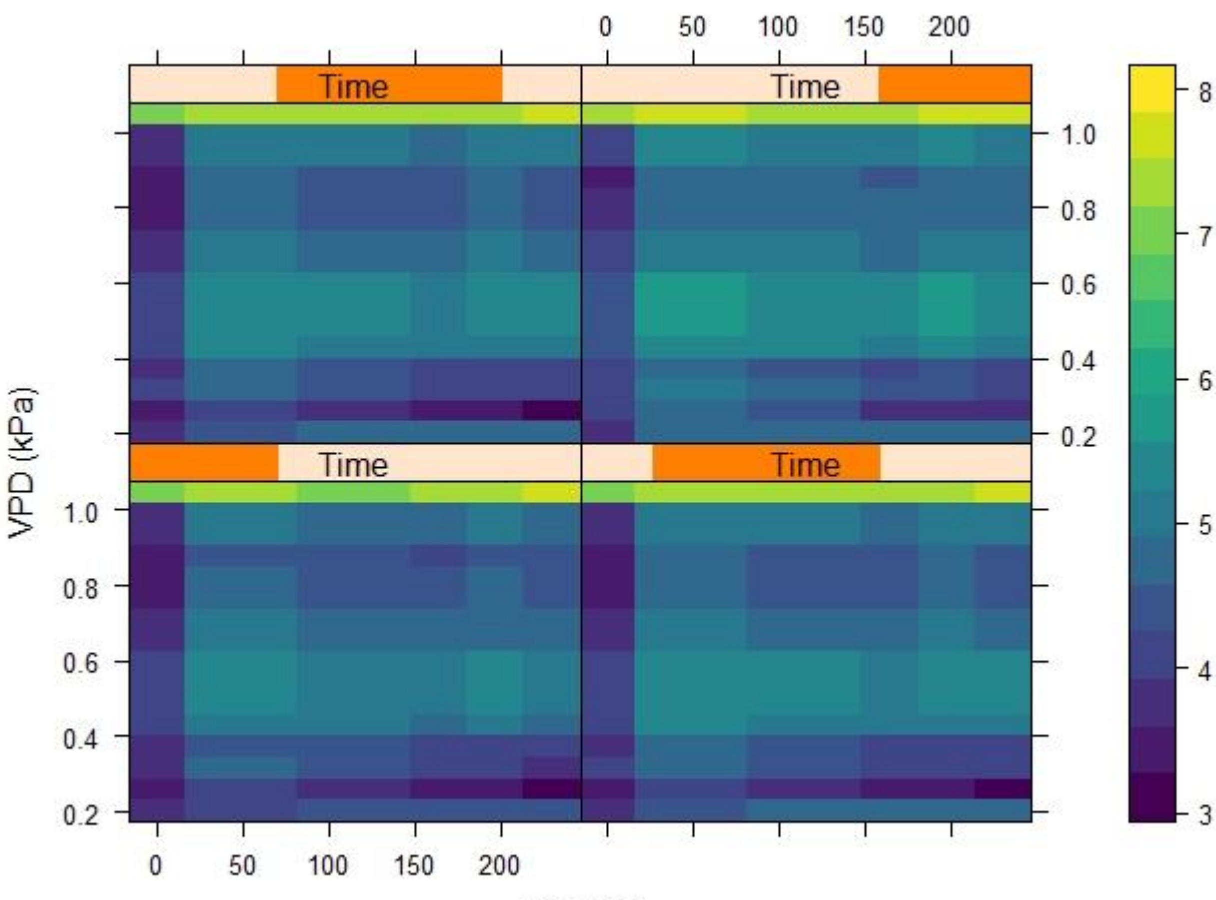


Fig. 8. Partial dependency plot showing the marginal effect of VPD, Point, and Time on predicted weight loss. Time is continuous, therefore it is first converted to a shingle; in this case, four groups with 10% overlap. Colour scale refers to % weight loss.

Respiration and transpiration have long been identified as the primary sources of weight loss in fresh fruit and vegetables (Bovi et al., 2018). Maguire et al. (2000) described weight loss in apples as a function of initial weight, respiration and transpiration rates, fixed water vapour permeance, saturated water pressure at air temperature, and fruit surface area. The model highlighted the importance of transpiration and respiration in weight loss and identified more factors (e.g., respiration dependence on RH, variable water vapour permeance) to be accounted for weight loss predictions. Hertog (2002) expanded this model to include fruit-to-fruit variation accounting for individual fruit differences in skin permeate to water. Another study (Lufu et al., 2019) reported that most of the weight loss in fresh pomegranate was explained by the vapour pressure deficit (VPD) and concluded that temperature, RH, and time must be considered in weight loss predictive models.

The analysis used in this study showed that the BRT algorithm could be used to accurately predict the expected weight loss of blueberries depending on the supply chain conditions. The model was also effective in identifying and explaining the influence of each variable and their interactions on weight loss.

4. Conclusions

This study shows the importance of monitoring and maintaining appropriate conditions throughout each step along the supply chain to minimise waste and ensure a good quality product reaches the consumer. The critical steps identified in this study with the highest impact on the quality (physical and biochemical) of blueberries were Shipping to DC (72 h at 5 ^{o}C), Store Display (48 h at 15^{o}C), and Consumer (48 h at 20 ^{o}C).

Furthermore, from this study, a BRT model was developed to predict weight loss. The model used data suitable for supply chain control purposes (i.e., temperature, RH, duration, expressed as cumulative VPD, and point of breach) and accurately predicted the range of weight loss expected at the end of the simulated supply chain. Cumulative VPD did not explain all the variation in weight loss, so more data from diverse simulated supply chain scenarios are needed to verify the predictive power of cumulative VPD and the model. The advantage of the BRT model is that it can adapt and improve continuously as more data is accumulated.

The analysis presented in this study provides valuable insightson which blueberry quality attributes are impacted along the supply chain. It also highlights the importance of supply chain monitoring and the potential benefits of real-time data analysis to aid stakeholders in making informed decisions concerning required actions to prevent product, quality, and monetary losses.

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Declaration of interests

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

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