DOI: https://doi.org/10.20870/oeno-one.2024.58.4.8086

OPEN ACCESS

ORIGINAL RESEARCH ARTICLE

Modelling the climate changing concentrations of key red wine grape quality molecules using a flexible modelling approach

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Associate editor: João Santos

Received: 15 April 2024

Accepted: 28 September 2024

Published: 22 November 2024

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ABSTRACT

Grape (*Vitis vinifera*) composition is a weather-dependent determiner of wine quality. With changing climates, we can expect variation in wine-quality. To understand the extent of this we built path models to create a generalised Cabernet-Sauvignon grape quality model focusing on the total concentrations of six important molecular groups (sugar, pH, phenols, tannins, flavanols, anthocyanins). Path models statistically connect factors from input to output using a series of dependent models. As such, this modelling approach takes the output from one model and puts it into the next model as a chain. By varying climate inputs, we can simulate how changes in climate impact the final composition of the grapes throughout their ripening. We explore the impact of changes in composition under several climate change scenarios namely: changes in light, temperature, and rainfall by changing the climatic inputs to the path model. We find that, under moderate-projected climatic changes (a combination of RCP4.5 and SRES A2 and B2), we expect higher concentrations of sugars, lower acidity (a more neutral pH), and higher total concentrations of aromatic compounds (tannins, phenols, flavanols, and anthocyanins). We also find that an earlier start of ripening leads to the same result. These two results combined suggest the potential for stronger red wines in future, with more flavour-related compounds and in particular tannins which often give greater ageing potential.

KEYWORDS: climate change, grape molecular composition, modelling, path models, quality, simulation approach

INTRODUCTION

Changing climate conditions are impacting the quality of agricultural produce (DaMatta *et al*., 2010; Moretti *et al*., 2010), most notably perennial crops such as wine grapes [*Vitis vinifera]* (Jones *et al*., 2005; van Leeuwen & Darriet, 2016; Webb *et al*., 2008a). In these systems, crop value is more dependent upon quality than quantity. A major part of wine quality is determined by grape must composition: a more optimal composition of grapes at harvest generally gives better quality wines (Gutiérrez-Escobar *et al*., 2021). Naturally varying wine quality occurs due to variations in weather leading to an increased desire to understand the impacts of climate change on the composition of the grape. The precise optimal make-up of grape composition compounds is determined by the opinions of individual winemakers, with different winemakers preferring different must compositions depending on preference. Hence prediction tools must allow flexibility in output to allow for variation in individual preference. This paper seeks to understand and quantify the impact of changes in weather during the ripening period (véraison) on the composition of the grapes at harvest. In doing so it provides and demonstrates a flexible framework for the exploration of the accumulation of important compounds in perennial crops, thus demonstrating a technique by which important compounds can be modelled in any perennial crop globally.

This desire to understand climatic impacts on the composition of the grape is set in the context of changing climate suitability for winegrowing in current winegrowing regions. Winegrowing suitability in these areas is predicted to decrease by between 8 and 65 % under "conservative" climate change predictions [both under RCP 4.5] (Hannah *et al*., 2013; Sgubin *et al*., 2023). This large range indicates a range of potential outcomes depending on realised climate effects, and non-linearities in the outcomes (Sgubin *et al*., 2023). These models suggest a 1–2 °C increase in temperature in wine-growing regions globally and a large increase in variability of rainfall between regions, with some years and regions experiencing drought, and others experiencing an increase in strong rainfall events (Hannah *et al*., 2013; Millán, 2014; Sgubin *et al*., 2023; Webb *et al*., 2008b). However, little is known about the change in grape quality in such situations, with quantified changes in grape and wine composition not yet predicted. Qualitatively the general global impact of the aforementioned climate changes has been posited to lead to better and stronger wines, with higher concentrations of many aromatic compounds (Mira de Orduña, 2010; van Leeuwen *et al*., 2022; Wood *et al*., 2023).

A grape anatomically consists of three parts: pulp, skin, and seeds, each of which contains important compounds for quality (as seen in Table 1). These compound groups: sugars, acids, phenols, tannins, flavanols, and anthocyanins have previously been quantified chemically using laboratory and spectroscopic techniques. Spectroscopy has also subsequently been used to monitor the composition based on observed characteristics (Cozzolino *et al*., 2006; Fadock *et al*., 2016; Larraín *et al*., 2008; Schober *et al*., 2022).

Air temperature is frequently cited as having the greatest impact on ripening and maturity, with impacts on vigour, ripening rate and consequential harvest date (Jackson & Lombard, 1993; Montes *et al*., 2012). Accordingly, some models of grape maturity rely on temperature thresholds in growing degree days to help ascertain the maturity levels of the grapes and assist in the harvest of the grapes (Parker, 2012; Parker *et al*., 2011; Verdugo-Vásquez *et al*., 2017; Wolkovich *et al*., 2017; Yiou *et al*., 2012). These models evaluate the entirety of the grape as an ensemble, and thus incorrectly suppose that ratios between the compounds within the grapes change in concert (Zhu *et al*., 2020).

Temperature is not the only factor that affects the quality of the grape. Wine grapes require hot, dry summers and cool, wet winters, with plenty of sunshine (Coombe & Iland, 2004; Haddad *et al*., 2020; Johnson & Robinson, 2014; Patil *et al*., 1995; Robinson, 2006; Wood *et al*., 2023). Berry development during ripening is thought to require moderate temperatures (15–40 °C) coupled with high light and low humidity (Chaves *et al*., 2010; Coombe, 1995; Coombe & Iland, 2004; Correia *et al*., 2012; Costa *et al*., 2020; Haddad *et al*., 2020; Mira de Orduña, 2010; Patil *et al*., 1995; Talaverano *et al*., 2017). Each of these factors impacts different parameters of the grape differently (Cook & Wolkovich, 2016; Costa *et al*., 2020), as each set of compounds has a different biological purpose and property. Climate change is also leading to a decoupling of the impacts of drought and temperature (Cook & Wolkovich, 2016), with changes in extreme heat and water availability occurring differently. This has strong phenological effects and consequently changes in grape maturity and composition (Jones & Davis, 2000).

Chile is the 6th largest wine producer and the 8th largest country under vines (International Organisation of Vine and Wine, 2023). The wine growing area covers 8 of the 15 regions, with 87 % found in the 4 central regions of Maule, Valparaiso, Bio Bio and O'Higgins (SAG, 2021). Most of the grapes grown are for producing still red wine, with Cabernet-Sauvignon (39.3 %) making up the largest share of vineyard area (International Organisation of Vine and Wine, 2017; SAG, 2021). Accordingly, the same grape varieties are planted over a large geographic area, meaning that space for time comparisons can be used for determining the best climate and growing conditions. Whilst there exists a latitudinal gradient along these regions of Chile, there also exists an altitudinal gradient, with longitudinal variation existing as the coastal regions give way to the Andes mountains. As such there exists historic wine growing over a large longitude and altitudinal radius, with enough scope to explore the impact of weather on the grape composition over the ripening period.

Whilst Cabernet-Sauvignon is thought to have originated from Bordeaux (France) in the 17th century, it is now an "international variety" and makes up 5 % total world area under vines, the largest of any wine grape (International Organisation of Vine and Wine, 2021). These vines are thought to cover an area of approximately 341,000 hectares in countries from Chile and South Africa, to China, Italy, and

France (International Organisation of Vine and Wine, 2021). It is generally made into a still red wine, famed for its strong taste, full body, and ageing potential.

The key compounds of sugars, acids, phenols, tannins, flavanols, and anthocyanins together comprise the majority of aromatic and technical maturity in grapes. They are key compounds in the determination of when to harvest and contribute in a major way to the organoleptic quality of the grapes. Accordingly, these compounds groups were chosen to be modelled for their impact on quality. General reviews have predicted changes in each of the individual compound groups (Mira de Orduña, 2010), but little work has been done to quantitatively model them, especially to determine the impact of climate change on the composition of the grapes.

Path models statistically connect factors to create a model of multi-stage dependencies. In this way, they are a series of linked linear models which describe flow through a network from input to output, via any latent variables. They are highly flexible and agnostic to mechanism and hence can be used statistically to represent a series of undefined metabolic pathways. Other quantitative grape models seek to precisely mimic some parameters of grapevine behaviour. This can be either physiological through the flow of water (Godwin *et al*., 2002; Yang *et al*., 2023; Zhu *et al*., 2019) or biomass of the plant (Bindi *et al*., 1997; Faluomi & Borsi, 2019; Leolini *et al*., 2018; Schultz, 1992) or grape (Gutierrez *et al*., 1985). Other models explore quantitatively the impact of climate on the chemical structure of the grape through the plant's allocation of carbon to hexose sugar molecules (Lakso *et al*., 2008; Vivin *et al*., 2002; Wermelinger *et al*., 1991; Zhu *et al*., 2019). There are also models which seek to explore the impact of climate on grapevine phenology (Cameron *et al*., 2021; Fraga *et al*., 2023), as well as explore the optimal weather conditions for high-quality vintages (Wood *et al*., 2023). Conceptually, this work aligns with the multi-variate insights that were initiated by Costa *et al*. (2020) in their work on grape berry quality parameters. Whilst they did not simulate the predicted climatic changes based on their parameters, they captured some climatic variance and endeavoured to understand quality in a multi-variate way. In doing so they set out the framework for quantitative modelling of grape composition, especially by accepting that both technical and phenological maturity required consideration. By ignoring the multivariate biochemical nature of grape quality, other grape models fail to capture the metabolic complexity required for grapes to make compounds important for quality, taste, and flavour. In grapes, these metabolic reactions start with sugar being imported into the grape from the parent plant's phloem and then converted in the grape into myriad other molecules. Different compounds and observed characteristics are important for different wines, and thus any modelling approach which seeks to address quality must be flexible enough to deal with this. By using a path model and simulation approach we can therefore explore the impact of changes in climate on any potential compound or property, no matter the detail known about its metabolic synthesis.

This paper seeks to examine the impact of interannual variation in weather on the concentrations of quality-related compounds within the wine grape. It does this by creating linear models based on existing viticultural data which are subsequently used to estimate how projected climatic changes might affect the wine-grape composition in Chile by 2050. In doing so, this paper first demonstrates a generalised approach to determining the concentrations of important molecules within the grape. We use path models to create a generalised Cabernet-Sauvignon grape model focusing on the total concentrations of 6 key molecular groups (sugars, pH, phenols, tannins, flavanols, anthocyanins). We then explore the impact of changes in composition under several climate change parameters, namely changes in light, temperature, and rainfall.

METHODS

This study seeks to understand how weather influences the composition of the wine grape (*Vitis vinifera* subsp. 'Cabernet-Sauvignon') between the onset of ripening and harvest. It builds a mathematical simulation model which describes the linkage between weather and key metabolite groups within grapes ripening between veraison and the harvest period and then simulates outcomes based on weather regimes. The weather for this simulation is then manipulated to represent predicted climatic changes and the predicted change in grape composition are simulated. To parameterise this simulation, a statistical description of the system was built *via* a path model. This path model phenomenologically links the weather to the key metabolite groups which make up technical and phenological maturity. As it is a series of simple linked models, it is a highly flexible approach that could be applied to multiple systems across all perennial crops.

Simulation

We wanted to investigate how predicted changes in the climate would impact the composition of the wine. To do this, we simulated current (2000–2010s) and mid-century (circa 2040s) weather regimes for one location in El Boldo, Chile. Whilst we could have run the model for multiple different combinations of clones, rootstock, training systems, and quality productions, to explore the impact of climate change on quality we examined one singular grape-vine type in this location. This we selected as a vine of clone 170, with rootstock 110R, being grown in a cordon-libre training system, to produce premium wine. For this grapevine, we iterated the path model through the full ripening period (weeks 7 to 15 of the year in Chile). Grape values from one time step (t) were used alongside simulated weather at time t to predict the next time step (t+1). A single simulation took a vine from the point of entering veraison until ripeness, creating outputs for all 9 steps in the pathway. To run the model for other combinations of weather, grape-vine, and production system please see the Shiny application: https://andrewwood.shinyapps.io/Vitis_v1_PathModel/.

TABLE 1. Several important components of grapes for wine-making.

Compound group	Molecules	Location in grape	Wine quality parameter	Maturity parameter
Sugar	Fructose, sucrose	Pulp	Alcohol and sweetness	Technical maturity
Acids (pH)	Malic acid, phenolic acids	Pulp	Acidity, balance with Sweetness, ageing potential (Gutiérrez-Escobar *et al.*, 2021)	
Simple (non-flavanoid) phenols	Hydroxybenzoic acids (Gallic acid)	Pulp	Astringency and flavour (Merkyte *et al.*, 2020)	Phenolic maturity
	Hydroxycinnamic acids (tartaric acid)	Pulp	Browning and aroma of wine (Nemzer *et al.*, 2021)	
Flavanoid phenols	Flavanols (myricetin and quercetin)	Skin	Stabilisation of the colour and flavour—primarily astringency and bitterness (Gutiérrez-Escobar *et al.*, 2021).	
	Anthocyanins [malvinidin and petunidin] (He *et al.*, 2012)	Skin	Colour of the wine, mildly bitter taste, astringent mouthfeel (Paissoni *et al.*, 2020)	
	Tannins [catechin, epicatechin, and proanthocyanidin] (Nemzer *et al.*, 2021)	Pips and skin	Structure (mouthfeel) and taste of wine	

For each of the 500 simulations run, a weather regime was created by sampling from a distribution, based upon historic weather data. To do this we extracted weekly weather per site over the past 25 years and then calculated the mean and standard deviation per site from the population. The normal distribution was used for both mean temperature and cumulative light, and the gamma distribution was used for the precipitation. The gamma distribution was used due to the high number of very low values of rainfall. For the gamma distribution, the shape parameter was calculated using the formula: $(\text{mean}/\text{standard deviation})^2$ and the rate parameter by: $\text{mean}/(\text{standard deviation})^2$. As the model was run stepwise, the inclusion of non-linear parameters was more freely possible, and thus the model was able to be better fitted to the training data. By using the natural logarithm in the models, we capture the non-linear change which is a pattern consistent with multiplicative growth forms and the non-linearity observed in the data.

For the middle-century predictions, distributions of each component of weather were altered depending on literature predictions of weather. Mean temperature increases of 1.5 degrees were predicted by Cabré *et al*. (2016), and a 35 % reduction in cumulative precipitation was predicted by Araya-Osses *et al*. (2020) and increases of light by 15 % were predicted by Zhang *et al*. (2021). These were all taken from moderate climate change scenarios, SRES A2 and B2 for Cabré *et al*. (2016), RCP 4.5 for Araya-Osses *et al*. (2020) and Zhang *et al*. (2021). Variability of all three was also predicted to increase, and we have therefore doubled the standard deviation in the climate change scenario to account for this. For each simulation, weather at a particular point of time is sampled from this new distribution which, as the mean and standard deviations are both larger, means that more extreme events occur. This was modelled both in concert, and independently, to explore the impact of coupled and decoupled climate effects.

A secondary impact of climate change is a change in phenology, most notably the beginning of the ripening period. To determine the impact of this change in the ripening period, we simulated changes in the start date of veraison. This was done by starting the simulation at the same sugar concentration and pH at different weeks around the mean veraison date but keeping the weather the same.

The first step in building the simulation was the creation of the statistical path model. This required three sets of data: weather, site (vineyard), and grape data.

Weather data

Historical weather data were extracted from the ERA-5 land reanalysis weather dataset (Muñoz Sabater, 2019) for each plot location using the KrigR package (Kusch & Davy, 2022) (see supplementary data for locations). ERA-5 land provides gridded interpolated data on a 0.1° grid at hourly time scales since 1st January 1950 (Muñoz Sabater, 2019). The data are interpolated from both Earth-based datasets (weather stations, buoys, aircraft, weather balloons, ships, and radar) and various satellite data (around 50 satellite datasets). We extracted the temperature (K) as a daily mean value, precipitation (m), soil moisture for 7 to 28 cm beneath the soil ($m^3\ m^{-3}$), and solar radiation ($J\ m^{-2}$) as daily cumulative totals, all in their standard untransformed units. From this, the mean temperature was extracted for a rolling window of either 7 or 30 days before the measurement was taken, allowing for the mean weather over the previous week or month to be calculated. Cumulative precipitation, soil moisture, and light were extracted using the same rolling window of 7 or 30 days previously. This soil moisture depth was chosen because it is the highest region of root density (Smart *et al*. 2006) and is not affected by soil surface dynamics which could lead to unrepresentative moisture levels due to increased evaporation.

Site data

Altitude data were extracted on a 0.1-degree resolution from the AWS terrain tiles using the *elevatr* package in R (Hollister *et al*., 2022). Four percentage measures of soil composition (percentages of clay, sand, silt and gravel/cfvo content) were extracted from the NCSS database on a 0.1-degree resolution using the *SoilDB* package (Beaudette *et al*., 2023), and values for composition extracted between the horizons 5–15 centimetres were used. Vertical autocorrelation was found to be very high in the gridded soil dataset (Table S5), and thus this depth was chosen as it is a region of high importance for the vine in terms of its root density (Smart *et al*., 2006) and high nutrient availability (Wilson *et al*., 2024) and also is not affected by soil surface dynamics.

Grape data

The climate and soil data were used as variables in models to better understand grape molecular composition. Two grape composition datasets were used for this work, both from commercial vineyards of Viña Concha y Toro (VCT) in Chile. Dataset 1 (harvest tracking) comprised maturity measures of weekly samples of sugar concentration and pH for 749 parcels of vines ("plots") across 35 vineyards during veraison (the ripening period, starting at the earliest date of 19/01 and finishing at the latest date of 03/05) between the years 2013 and 2021. The samples cover a 5.5-degree latitudinal range and a 1.7-degree longitudinal range and can be seen as purple triangles on the map below (Figure S1). Sugar and pH measurements were taken using the Dyostem Measuring system (*via* spectroscopic techniques) for 1600 plots for up to 10 years (see Table 1 for vineyard locations and Table 2 for years each region was sampled). This dataset consisted of 111,358 total samples.

Dataset 2 (high-performance liquid chromatography, HPLC) comprised 300 grape samples taken at harvest across three years (2018–2020), for 300 plots across the same vineyards (one bunch per plot) for a similar 6-degree latitudinal range and a 1.8-degree longitudinal range. Six important parameters of grape compositions were measured using standard protocols as per Schober *et al*. (2022) at the experimental winery of the VCT Centre for Research and Innovation [CII] (Schober *et al*., 2022). The parameters of grape composition measured were total concentrations of sugars (gL^{-1}), acidity (pH), total phenols (mgL^{-1}), tannins (mgL^{-1}), flavanols (mgL^{-1}), and anthocyanins (mgL^{-1}). In these measurements, individual phenolic compounds were analysed by HPLC, and total phenolic compounds were measured through UV-visualisation enzymatic assays, sugars, acidity and pH through their standard wet chemical techniques (Y15). For more details, see Schober *et al*. (2022).

Vineyard management data

For each plot where data were collected, two important management factors were recorded. The first was the trellising technique the grapes were grown under. The second was the distinct vineyard management corresponding to a specific quality level. In this way, quality levels denoted as generic or blend were for grapes being produced for bulk wine, and quality levels denoted as premium, super-premium, and ultra-premium were for the respective quality levels of Concha Y Toro wine.

Statistical analysis (path model)

The data was then used to build a path model. A path model is a series of linked linear models, each assuming a Gaussian distribution of the predictor variable and an identity link function (Formula *S*1). Each step connected the inputs to a parameter of grape composition. Below are the nine steps which formed the steps in the pathway, with the output (target, dependent, y) variable, in bold:

1. From climate and vineyard (C+V) to **soil moisture**;
2. From soil moisture and C+V to **sugar concentration**;
3. From sugar concentration, soil moisture and C+V to **pH**;
4. From sugar concentration, pH, soil moisture and C+V to **reflectance at 520 nm wavelength**;
5. From sugar concentration, pH, soil moisture and C+V to **reflectance at 280 nm wavelength**;
6. From sugar concentration, pH, soil moisture, reflectance at 280 and 520 nm wavelengths, and C+V to the concentration of **total anthocyanins**;
7. From sugar concentration, pH, soil moisture, reflectance at 280 and 520 nm wavelengths, and C+V to the concentration of **total tannins**;
8. From sugar concentration, pH, soil moisture, reflectance at 280 and 520 nm wavelengths, and C+V to the concentration of **total phenolics**;
9. From sugar concentration, pH, soil moisture, reflectance at 280 and 520 nm wavelengths, and C+V to the concentration of **total flavanols**.

Each step mimics a transfer of energy, starting with an external process (the soil moisture) and then moving to the characteristics of the grape that define the technological maturity (sugar concentrations, pH). From this technological maturity, two spectroscopic measurements were analysed as intermediaries (the reflectance at 280 nm and 520 nm), and then from these, the analysis considered the aromatic maturity characteristics (total concentrations of tannins, flavanols, anthocyanins, and phenols). The spectroscopic measurements were chosen to represent the growth of the pulp and the skin respectively.

The statistical analysis found that the relationship between both sugar concentrations and time (in weeks of veraison), and pH and time (again, in weeks of veraison), as well as the two spectroscopic measures (DO580 and DO280), are a non-linear curve of diminishing returns. As the model was stepwise it was more flexible as lagged components reduced the variance to be explained in the model. We also added a non-linear time parameter to the path model (the natural logarithm of the time since veraison had started). This meant that non-linear dynamics were more precisely captured, and the model was a better statistical fit for the data.

For each step in the pathway, a fully connected model was created between the output variable and the named input parameters detailed in Table S1, with the linear models encoded as in Formula S1. There are two issues with just running the model as per this fully connected model. The first is covariance. To remove this from the model, a correlation pairs plot was created, and variables which were co-linear above the 0.4 covariance threshold (Pearson's correlation coefficient) were removed from possible models, such that no two covarying variables were allowed in the same model.

The second is the high number of redundant non-significant terms in the model. To remove this, the statistically significant variables ($p < 0.05$) were fixed in the model evaluation, and all other possible models were evaluated (dredge function, *MuMIn)* used to. The model chosen was that with the lowest AIC value. Model goodness of fit was also examined for each linear model using plots of predicted values against true values, coupled with R^2 values.

Validation

Models were validated in several ways. Before model building, the analysis of co-variance between input factors ensures that the model is not biased or distorted by highly correlated variables, and thus improves the fit of the model. The goodness of fit was further improved by examining both the R^2 and AIC values of the models fitted and by examining the plots of predicted against true data for each step of the path model. The R^2 value is also known as the coefficient of determination and denotes the proportion of variance in the dependent variable which is explained by the model. The AIC (Akaike Information Criterion) is a different measure of model fit which helps to identify the model that best balances complexity in terms of the number of parameters, as well as the fit of the model. Finally, the plots of predicted against true data are a direct measure of model validation. They explore the relationship between a test dataset and the patterns explained by the model, demonstrating the model captures the underlying patterns.

RESULTS

The path model is a statistical understanding of the network of factors that impact the composition of the grape. The linear models built during the statistical analysis suggest a statistically robust and complex network of inputs from across terroir–from climate, human management, and soil. Figure 1 shows the statistically significant ($p < 0.05$) connections in the most parsimonious (lowest AIC) models for each output or latent variable (interior node in the graph). There are 67 connections in the network, out of a possible 130 connections, making the graph 51.54 % connected. No output variable has fewer than 4 predictors (the minimum is anthocyanin concentration), up to a maximum of 9 predictors (for both tannin and flavanol concentrations), as seen in Table S4. The most connected input variables are altitude and the cumulative monthly precipitation, with 7 connections each. This indicates that grape composition is a complex phenomenon, with many influencing factors that each contribute additively to the final composition of the grapes.

The statistical analysis indicates that there exists a strong link between the environment of the grapevine and the concentrations of key molecular compounds within the

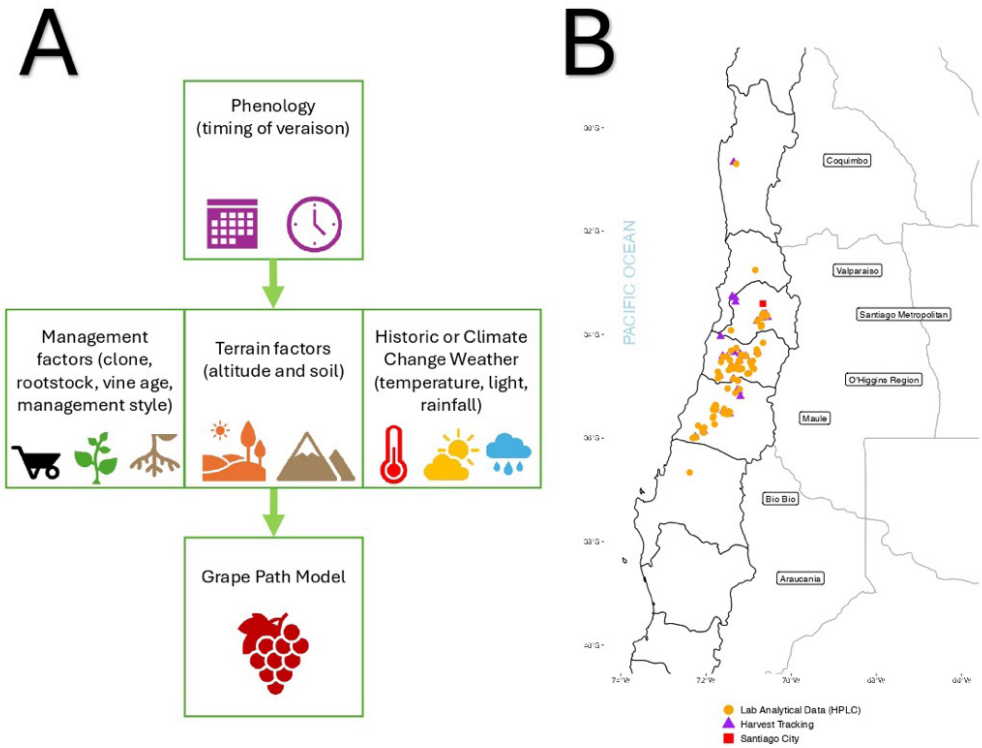


FIGURE 1.

grape. The model's predictions all sit on the y = x line of the predicted against true value plots (Figure 2), suggesting a strong link and good fit of the models. The mean R^2 value of the models is 0.86 (Table S4), meaning that on average 86 % of the variance within the data is captured by each model. The high R^2 value of the models (Table S4), coupled with the straight Predicted-Actual Plots (Figure 2), suggests that the linear models are a good fit for the data, and suitable over a breadth of variation in climate and soil space.

To determine the change in composition caused by climate change we first simulate a baseline of the current weather patterns. The output from the simulation using the current weather regime indicates a general increase in concentrations of most molecules throughout the ripening period (except for tannins, flavanols, and phenols). Weekly cumulative soil moisture remains constant for the first 10 weeks, before increasing in an almost exponential fashion (Figure 3, solid line). Sugar concentration, pH, and anthocyanins rise in a logarithmic growth curve throughout the season, never completely reaching the stationary phase but declining in rate of accumulation after week 10. Tannin, flavanol, and phenol concentrations rise slowly to begin with but then decline, with tannins ending in week 15 at a concentration lower than they started, phenols ending slightly higher, and flavanols at about the same concentration. The variance for the baseline (depicted as shaded areas in Figure 3 centred on each line), is quite small, suggesting a high degree of certainty around these trends, however, it is worth noting that particularly for tannins, flavanols, and phenols, there is a larger variation than for sugar and pH. This leads to the potential for some variation within these concentrations. The evolution of grape composition throughout ripening indicates that grapes change dramatically in quality and flavour over time, with wet weather having a negative effect on the final harvest concentration and warm weather having a positive effect on the final harvest concentration.

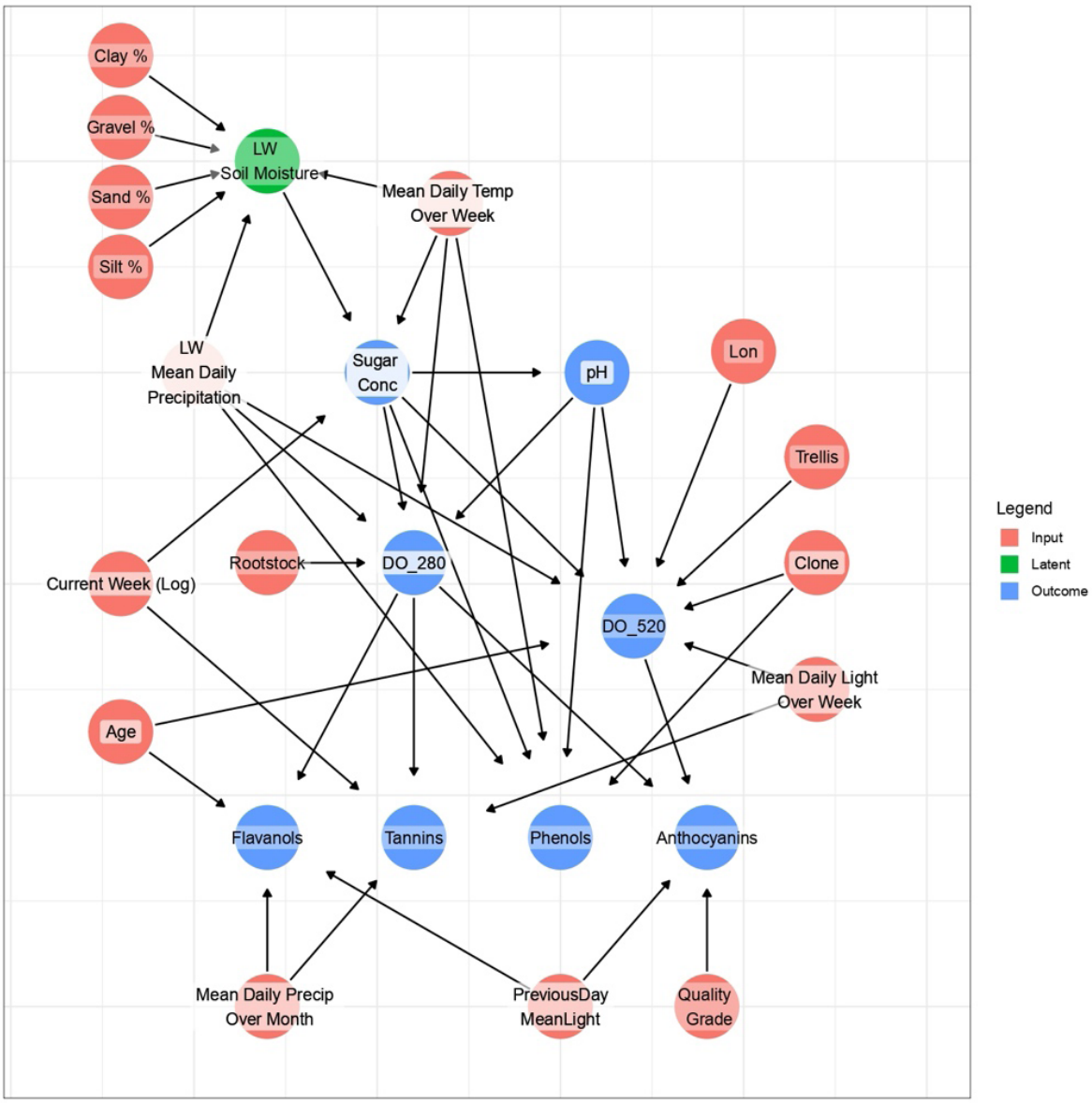


FIGURE 2.

We then hold all other factors aside from the weather regime constant (soil, altitude, rootstock, and scion clone) and re-run the simulations with the literature-predicted weather changes. Under this climate change scenario, there is lower soil moisture across the whole growing period (Figure 2, dotted lines). The concentration of all molecules is found to increase at a faster rate in this simulation. The increase in concentration also continues until it reaches a higher total concentration. This is particularly interesting in the case of the more variable compounds (tannins, flavanols, and phenols) which show a clear increase in the climate change scenario. The notable exception to this increase is acidity, which, as pH increases more, suggests a faster and greater decrease in acidity. This indicates that grapes are higher in sweetness, lower in acidity, and higher in compounds which give flavour and structure to wine. In short, the grapes are riper, which could therefore lead to stronger wines.

The independent changes to the weather regime were conducted as a form of sensitivity analysis, and have a more varied effect, as seen in Figure S3. For sugar, pH, and anthocyanins the largest single effect comes from changes in mean light, for tannins, flavanols, and phenols it comes from increases in mean temperature. This indicates that light and temperature are more important in the development of higher concentrations of key grape compounds, and hence for the potential of making stronger wine.

Climate changes are, however, not confined to specific weeks of the year, and hence lead to changes in the phenology of the vine. Most importantly for this simulation, we changed

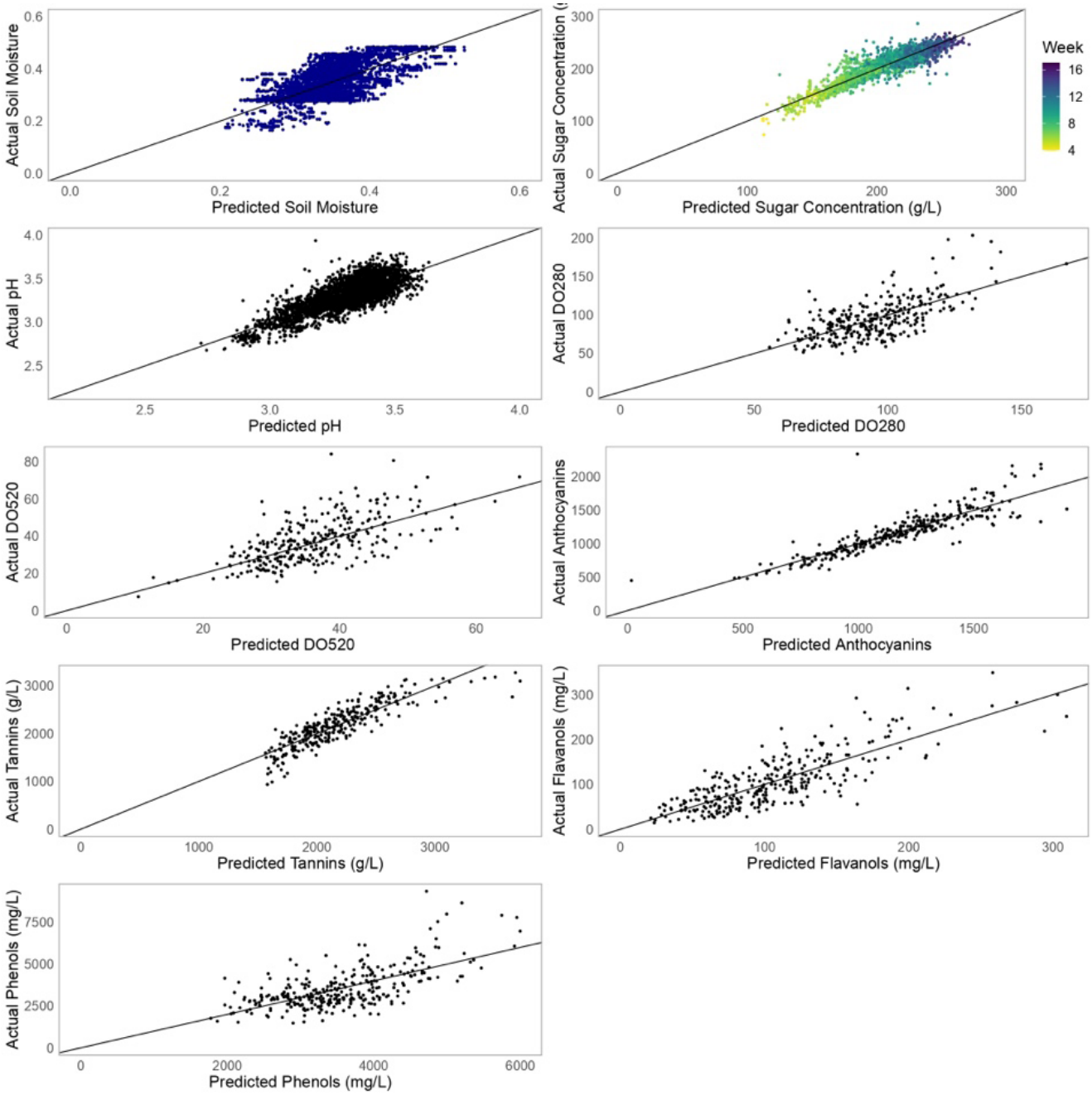


FIGURE 3.

the start date of the simulation to change the timing of the onset of ripening. We find that the soil moisture remains approximately the same in trend throughout the simulation, however, there is a consistent trend of later starts leading to consistently lower concentrations of the grape molecules (Figure 4, with error Figure S3). Each week that the delay occurs reduces the maximum reached by a constant amount. Comparing the earliest with the latest starts to ripening it can be seen that there is a comparable rate of accumulation of sugars and increase in pH (decrease in acidity). A similar trend is seen for anthocyanins and phenols, with sharp increases occurring post-onset which do not catch up with the earlier ripening berries. Tannin concentration starts lower when ripening is delayed and as it declines at a similar rate (and all simulation outputs plateau between weeks 10 and 13 before declining again), parity is not reached until approximately week 15 (early April). This is similar to the other molecules too, with parity not being reached by the extremes in ripening times until this time. The phenological changes suggest that earlier onset of ripening will also lead to stronger grape concentrations, and hence the potential for stronger wines.

Combining the two parameters of the scenario leads to the potential for much stronger concentrations of important flavour molecules in grapes under the predicted climate changes in Chile. This leads to the potential for stronger, higher-flavour wines, with greater structure, and potentially longer ageing potential.

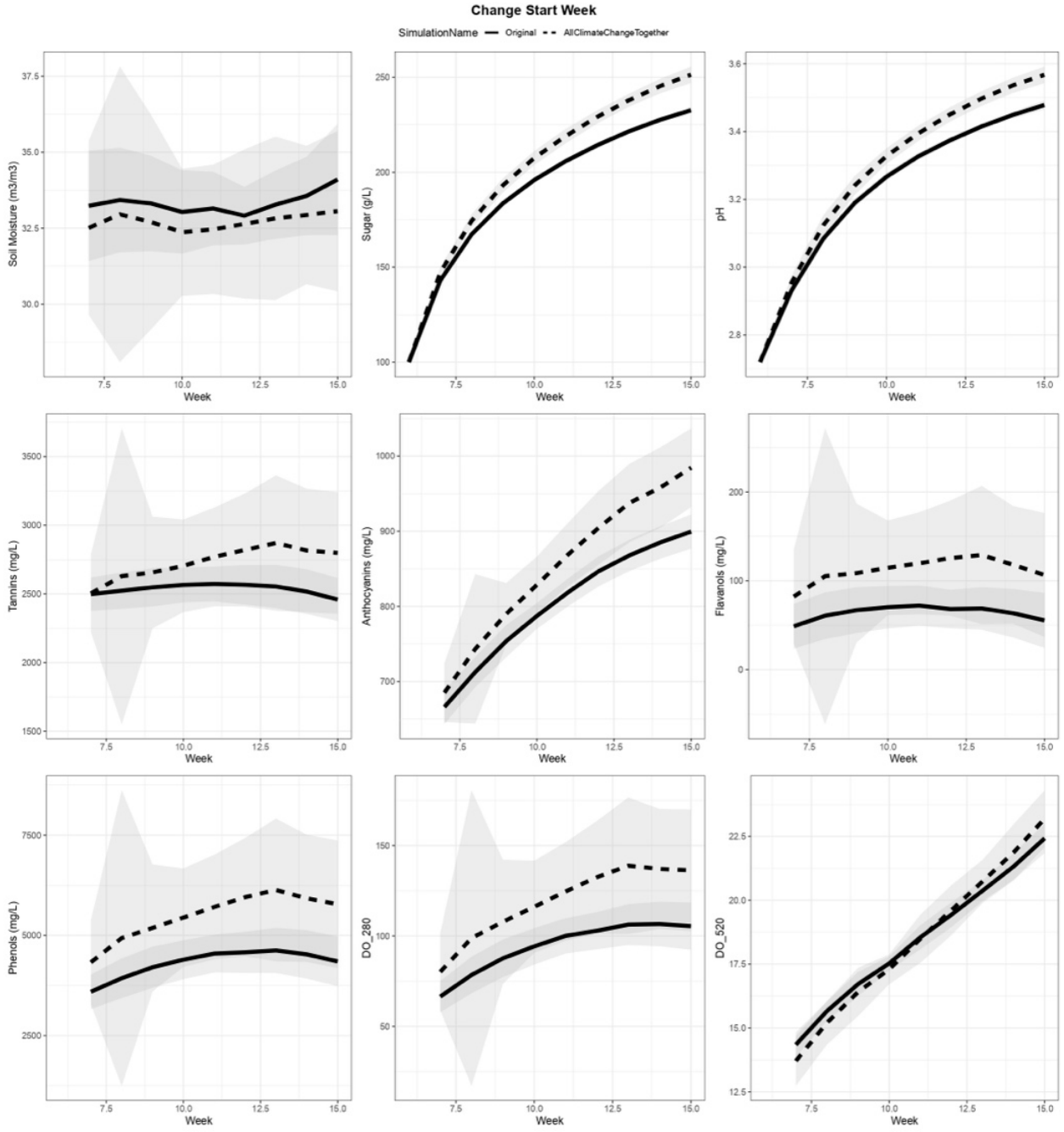


FIGURE 4.

DISCUSSION

This paper suggests a quantitative method of forecasting the composition of major components within a wine grape that contributes to quality. It uses a path model method to determine how climate change will impact the composition of grapes at harvest. It finds that, under the projected climatic changes the reduced rainfall, and increased temperature and light will lead to higher concentrations of sugars; lower acidity (a more neutral pH), and higher total concentrations of phenolic compounds (tannins, phenols, flavanols, and anthocyanins). It also suggests that phenological changes are important too, with an earlier start to ripening resulting in the same as the 2040s climate change scenario–higher total concentrations are reached (with a more neutral pH). These combined suggest the potential for stronger red wines in future, with higher concentrations of flavour-related compounds and in particular tannins which give longer ageing potential.

The simulation findings are in accordance with previous qualitative and synthesis works. van Leeuwen *et al*. (2022) suggest in their recent synthesis that climate change in wine-growing regions may lead to stronger wine flavours, with deeper

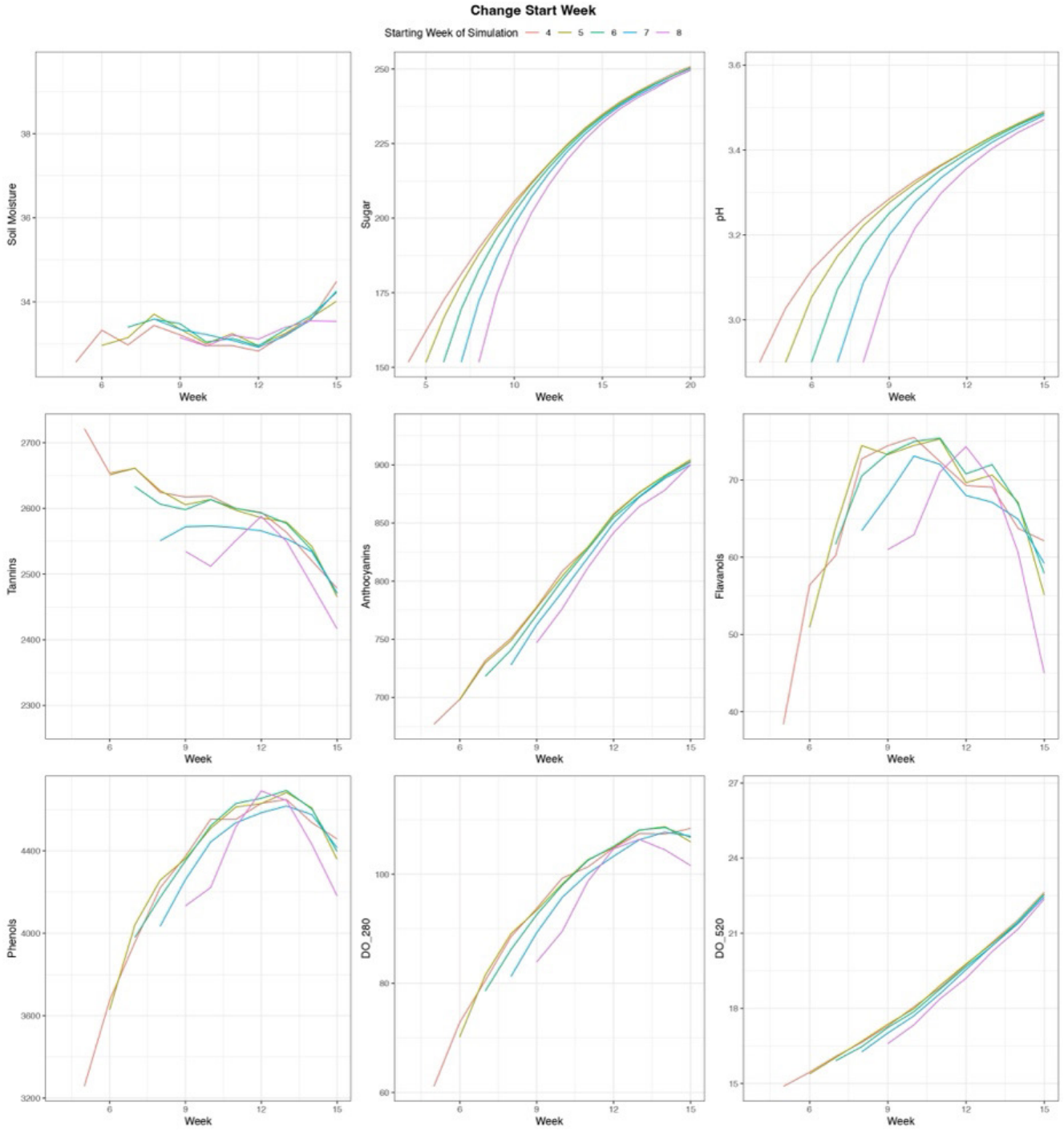


FIGURE 5.

colours and greater structure (van Leeuwen *et al*., 2022). This is in line with their previous work, which shows that "hotter" climates give stronger wines (Deloire *et al*., 2005a; Deloire *et al*., 2005b; van Leeuwen & Destrac-Irvine, 2017). Costa *et al*. (2020) in their experimental work in Northern Portugal showed that in interannual weather variation, stronger wines come from hotter places, with higher pH and sugar (potential alcohol). They found no heating trend in the phenolics and anthocyanins across temperature gradients between regions but found a difference between high and low maturity years. This is similar to what we find in our model (Figure 3), with higher sugar and pH in hotter climates, and higher variation in the phenolics, anthocyanins, tannins, and flavanols. Unlike Costa *et al*. (2020) we do find a general climate change effect in the aromatic compounds, however, this may be due to the differing location, or specific changes in climate factors, such as changes in light intensity. This is similar to the changes suggested by Mura de Orduña (2010) in their review on the topic, with increased climate leading to increases in concentrations of sugars, acids, and aromatic compounds, until such a point that it reaches a physiological limitation. We, therefore, suggest that in this instance the environment that this model system is parameterised on has not reached its physiological limitation. The linear nature of the simulations means that the system cannot predict this threshold of decline, as the data from which it has drawn has not had that occur. The large sample size within this dataset means that many events have been captured in the data, but non-linearity means that at extreme values outside those currently seen the model will not perform as well as for scenarios within which it has been parameterised.

The path model and simulation framework form a general model of Cabernet-Sauvignon grapes. As such, it is also possible to use it to predict the composition of the grapes several weeks into the future in any given year and, thus, it could be useful for the planning of harvesting of the grapes. Quality is a subjective measure which depends on the desired outcome of the viticultural management team, and the desires of the winemakers utilising the grapes. Hence by predicting the composition of the grape, rather than the date of harvest itself or the status of the vine, we can give choice to the vineyard managers and winemakers as to when they would like to pick their own grapes.

As well as understanding the potential impacts of unmitigated climate change on a single vineyard, the model is also useful for understanding the potential impacts of climate change interventions. As we have demonstrated through our climate change forecasting, by understanding the impact of the intervention on the environment that the grape vines experience can understand the changes of the intervention to the composition of the grape. For example, a sun canopy would reduce light and precipitation but may increase temperature around the vine, and thus the model could be parameterised to see what impact this intervention would have on the grapes. This tool could, therefore, be used to understand the impact of these interventions on the composition of the grape. It is worth noting that, due to the high co-linearity between temperature and light, there is no information gained by using both variables in a given statistical model and hence the path model built was constrained such that only one was included per statistical model built. It is also worth noting that whilst the current non-linear relationship between the historic weather experienced by the vines and data collected from them is a good fit, but may not extend to future scenarios should the relationship significantly change. As we have demonstrated in this paper, however, it is also possible to model the impact of changes in each of them separately, allowing for future changes in the covariance structure between the two climate variables to be accounted for (Cook & Wolkovich, 2016). Of course, this work is based upon climate models which contain inherent uncertainties (Chacón-Vozmediano *et al*., 2021; Reis *et al*., 2020; Fraga *et al*., 2020; Fonseca *et al*., 2023). Such future climate projections are subject to variability and may not capture the full dynamics of local climate events. As such, the predictions in this paper are not for vines in a given year or weather regime. They are instead a demonstration of the capabilities of these models and the outcome of the current understanding of climate-vine interactions projected to our current understanding of mid-21st century climate.

However, this paper is not just about the specific regional results for one specific variety of wine grapes. The model parameters are both globally relevant and easily calculable for any grape variety, and the gridded input data used in the model is available to be used for any point on the planet. Further, whilst we explore the impact of climate on one set of quality parameters–namely the total concentrations of many quality component compounds, this framework is flexible enough to accommodate any target variables. This flexibility means any combination of possible molecules could be modelled and predicted, potentially in any crop. Staying with viticulture, white wines would require different characteristics to be tracked than red wines, with tannings and anthocyanins being less important and aromatic compounds being more important. For example, naphthalene compounds give Riesling wines their characteristic petrol smells and thus are particularly important for quality in this specific wine grape variety. Thus, when Riesling grapes are growing it is important to know their concentration to determine when to harvest. This modelling approach would be able to do just this by adding napthalenes as an output predictor in the model.

As a flexible statistical modelling approach, our path model framework can be used for any crop, and in particular for any crop in which quality is more important than yield. The structure used in our path model is based on the underlying metabolism, which is conserved across many perennial crop species. Thus, the same structure, with sugar being fixed first and then other compounds and properties evolving from it, would be a highly possible new method for modelling the composition of perennial fruits and hence crop qualities.

Growing perennial crops under changing climate conditions requires new tools and new approaches. The use of models such as the ones we have developed suggests that there is a new future for perennial crop quality. With warming climates

dramatically altering the composition of the grapes at harvest, the quality of the wines made from these grapes will also vary. This new modelling strategy allows important parameters of the grape to be estimated and serves as a potential platform for interventions to be planned. The metabolic-style structure of the model also allows for great flexibility in the model applications, with the potential here to model target variables of interest, both within wine grapes and beyond into other perennial crops. In the case of Cabernet-Sauvignon in Chile, from our simulations, it appears that the predicted climate changes will lead to stronger concentrations of grape metabolites in the future. This should allow winemakers to make wines with a relative increase in their complexity, structure, and concentration of aromatic compounds. These wines should have both great flavour and ageing potential and hence suggest an increase in desirability in wines in the future from this region.

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