Potential of mathematical modeling in fruit quality

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A review of mathematical modeling applied to fruit quality showed that these models ranged in resolution from simple yield equations to complex representations of processes as respiration, photosynthesis and assimilation of nutrients. The latter models take into account complex genotype-environment interactions to estimate their effects on growth and yield. Recently, models are used to estimate seasonal changes in quality traits as fruit size, dry matter, water content and the concentration of sugars and acids, which are very important for flavor and aroma. These models have demonstrated their ability to generate relationships between physiological variables and quality attributes (allometric relations). This new kind of hybrid models has sufficient complexity to predict quality traits behavior.

Key words: Mathematical modeling, fruit quality, respiration, photosynthesis and assimilation of nutrients.

INTRODUCTION

Fruit quality is a complex issue defined as a sophisticated chain of biological processes (Genard et al., 2007). These processes (transpiration, respiration, photosynthesis) involve exchanges between the fruit and its environment. Quantitative integration of these processes to monitor fruit’s behavior is a task involving physiological modeling. Nowadays, the interest in mathematical modeling about the quality changes during fruit maturation has increased (Wegehenkel and Mirschel, 2005). It is possible through simulation to evaluate the quality of final products in order to identify critical points during post-harvest handling and to adjust or improve the decision making related to harvest dates and product commercialization. Adequate models should be mechanistic enough to give a representative description of physiological processes and explain variations in some quality traits.

Recently, models have become more accurate and better able to predict the outcome of complex issues such as genotype-environment interactions. Furthermore, efforts have been made to define fruit quality and integrating it with crop growth models. These models are based on accurate descriptions of early stages of growth, including fresh fruit mass, dry matter content and concentration of sugars. The goodness-of-fit of a proposed model for each crop is evaluated taking into account the criterion of the root mean squared error (RMSE). This is a common parameter used to quantify the mean difference between predicted model and experimental data for the case of non-linear models (Quilot et al., 2005; Kobayashi and Us Salam, 2000).

The global goodness-of-fit of a model is computed by averaging the relative RMSE (RRMSE) of all experiments (Quilot et al., 2004). Spearman’s rank correlation coefficients could also be calculated. These coefficients compare the ranking of experiments on the basis of observed and predicted values (Quilot et al., 2005). Given the economic importance of these quality traits, their
prediction by mathematical modeling based on underlying physiological principles should have priority.

MATHEMATICAL MODELING

A mathematical model is an abstraction of reality which describes processes and whose aim is the study and analysis of a system under different conditions (Mason and Dzierzon, 2006; De Wit, 1982). In order to realize a successful mathematical model, the modeler needs to chose what mathematical principles and techniques to use and the solution also needs to be checked against experimental data (Crouch and Haines, 2004). Models sometimes simplify the system in order to reduce the dataset required to estimate parameters (Lisson et al., 2005; Lentz, 1998).

Mathematical models allow prediction of the system behavior under specific handling and environmental influences, especially when it is too expensive to perform certain types of studies or in which long term effects may be difficult to monitor (Fraisse et al., 2006). By this way it can be demonstrated that there is a mutual dependency between basic crop physiology research and model development (Lisson et al., 2005).

APPLICATION OF MATHEMATICAL MODELS TO DESCRIBE GROWTH AND YIELD IN PLANTS

For the last decades, crop modeling has become an important tool in horticulture as in other areas of plant production (Gary et al., 1998). Such success has been encouraged by the progress in crop physiology, crop ecology and computer technology which enhances the versatility of this technique (Bouman et al., 1996; Colbert, 1995).

The quantification and prediction of the potential effects of agricultural management practices on crop growth and yield is an essential task in any agro-ecological research (Wegehenkel and Mirschel, 2005). Growth, development and yield have been simulated as a function of weather, soil conditions and crop management by integrating scientific knowledge from diverse agronomic disciplines (Hoogenboom et al., 2004). By mathematical modeling, the production of some crops has been improved taking into account climate variables such as radiation, salinity, temperature, moisture, atmospheric carbon dioxide (CO₂), temporal and spatial climatic variability (Karlsberg et al., 2006; Pearson et al., 2008; Ewert et al., 2005; Tao et al., 2009) and recently satellite-derived meteorological inputs (de Wit and van Diepen, 2008). Changes in crop productivity depend on different biophysical and socioeconomic factors which are difficult to assess. Process-based biophysical models are increasingly used to estimate productivity and food supply under different climatic factors, but have several limitations due to inherent complexity (Ewert et al., 2005). The best level of resolution for growth and yield models has been highly debated. With the use of extremely complex models the compounded errors are increased (Mason and Dzierzon, 2006).

EVALUATION OF PHYSIOLOGICAL TRAITS THROUGH MODELING

The development of a plant is the result of processes working at a hierarchy of scales. The representation of these processes and interactions in a model is a big challenge. Ecophysiological orientation is needed to predict composition and plant functioning on the basis of physiological traits (van Wijk, 2007). There are a few studies on variability of crop traits related to biomass production and final yield such as leaf area size, spatial distribution and senescence, light interception capacity, radiation use efficiency and biomass partitioning. These traits have been used in the search of maize genotypes with improved performance for nitrogen capture and use (Cirilo et al., 2009). The modeling of physiological traits can help to improve yield and to make decisions that optimize use of available resources (Soltani et al., 2001). Crop growth models exist for many horticultural crops. Often, descriptive and mechanistic models are distinguished (Pronk et al., 2003). Descriptive models reflect little or none of the mechanisms that are the cause of a system behavior, whereas mechanistic models consist of quantitative description of these mechanisms (Penning de Vries et al., 1989).

Descriptive models

Until 1960, agricultural research almost completely relied on experimental and empirical work, combined with statistical analysis (Van Ittersum et al., 2003). These models, in a first stage, were designed to describe and analyze plant growth without any model underlying the physiological processes being classified as function-oriented models (Renton et al., 2005). Descriptive models have a short computing time and they usually contain a few stated variables (Mirschel et al., 2004). Although the predictive value of descriptive models can be high, there are important limitations. This is so because they are not able to simulate plant adaptability and response to different conditions; due to the fact that adding new input factors means building a new model based on an extended data set (Renton et al., 2005). Unlike descriptive, mechanistic models are ruled by biological principles and involve breaking down the system into components that are modeled separately. In general, descriptive models only describe relationships between response and predictor variables as economically as possible for a particular dataset. Essentially, descriptive models are descriptions of observational data, most often associated with
Mechanistic models

Mechanistic models are used for testing hypotheses and synthesizing knowledge of complex systems on the basis of physiological processes such as photosynthesis, assimilation and respiration which respond to climatic conditions (Brainard and Bellinder, 2004; Huang, 2004; Thornley and Cannell, 2000) (Figure 1). The use of these models is increasingly being used to investigate the impacts of weather and climate variability on crop growth and production (Tao et al., 2009).

Photosynthetic active radiation (PAR) is the driving force for evapotranspiration and photosynthesis (Dutilleul et al., 2007; Sentelhas and Gillespie, 2008). In photosynthesis-based models, the interception of light by leaf area is used to simulate the production of photosynthates which consists of carbon leaf assimilation plus the carbon mobilized from reserves, carbon is allocated according to organ demands. Subsequently, the use of photosynthates for respiration, conversion into structural dry matter (DM) and finally, the fresh weight can be estimated from the dry weight (Jordan-Meille and Pellerin, 2004). Using the model of Genard et al. (2003), the fruit flesh carbon is then partitioned into several compounds: sugars, other fruit compounds and respired CO$_2$. These processes are described in terms of a set of differential equations.

In the SUCROS models, the rate of CO$_2$ assimilation is calculated from daily incoming radiation, temperature and leaf area index. This model is based on time of radiation and on exponential light extinction (Beer-Lambert Law) (Monsi and Saeki, 1953). Prediction of the leaf area index is required to estimate interception of solar radiation and biomass production (Soltani et al., 2006). In field crops, there is often a linear relationship between cumulative intercepted PAR and accumulated biomass (Zhang et al., 2008). Insufficient nitrogen (N) levels promote a diminishing in leaf area development, decreased mass accumulation and early maturity (Sinclair et al., 2003). Temperature can affect plant leaf area via its effects on rate of leaf appearance (Singels et al., 2005).

Respiration is one of the main energy sources in growing plants and it has been hardly studied compared to photosynthesis (Kuretz et al., 2003). Respiration has been modeled according to the concept of growth and maintenance (Albrizio and Steduto, 2003). Short-term observations generally show that respiration is highly sensitive to temperature variations and CO$_2$ may affect the growth coefficient (Challinor and Wheeler, 2008). In simulation models, the growth coefficient is usually independent of environmental factors (Urban, 2003; Bannayan et al., 2005).
Mathematical models that successfully predict product composition as a function of climatic variables would be a useful tool to achieve more desirable sensorial characteristics in the final crop product (Heredia and Andres, 2008).

**QUALITY IN HORTICULTURAL PRODUCTS**

Recently, fruit crop models have been developed beyond fruit dry mass accumulation but including fruit quality (Struik et al., 2005). Fruit quality is a complex issue. It involves a set of traits such as fruit size, overall composition, taste, aroma, texture and proportion of edible tissue (Genard et al., 2007; Gruda, 2005). Fruit growers must produce high-grade quality fruits in terms of these traits to satisfy consumer demands (Sivakumar and Korsten, 2007; Nicolai et al., 2008). The links between environmental control and quality traits have been extensively investigated (Wu et al., 2002; Challinor et al., 2004). These studies have limited explanatory power of models since they focus on these links without explicitly considering the underlying mechanisms. Current methodologies for prediction of changes in product quality are based on deterministic simulations (Qin and Lu, 2009; Di Scala and Crapiste, 2008). Even though every process involved in fruit physiology cannot be integrated into a model, a real degree of complexity is needed since fruit exchanges energy and mass with its environment and it is composed of a large number of diverse components (different sugars, acids, etc.) which interact with each other non-linearly (Genard et al., 2007). Taste mainly results from the accumulation of sugars and acids in fruit cells.

This accumulation can be controlled through the intensity of metabolic transformations. These processes are well known and have been extensively described in the literature (Ho, 1988; Wink, 1993). On this basis, Genard et al. (2003) designed a mechanistic model called SUGAR to predict changes in sugar composition during each fruit development. In this model, sugars are either directly stored in the cells, transformed into other sugars, or used to synthesize other compounds. Lobit et al. (2006) designed two models predicting fruit acidity, the first one described citric acid production and degradation through the citrate cycle. In the second, malic acid content was modeled mainly on thermodynamic conditions of its transport from cytosol to vacuole.

Important quality traits were manifested at the fruit scale (Figure 2). This is especially true for fruit size, dry matter content and percentage of edible tissues. Fruit size and dry matter result from exchange of resources with the plant and the atmosphere. For tomatoes, the dry matter content is an important attribute to determine fruit quality. It can be predicted from net photosynthesis and correlated to the sugar content (Cooman and Schrevens, 2006). The carbohydrate supply has been modeled according to the source/sink concepts (Lechaudel et al., 2005). Recent studies tend to improve models for dry matter content and its partitioning between the different organs in tomato crop (Dimokas et al., 2009) and in response to variations in light intensity. This situation led tomato crop to strong morphological adaptations (Dong et al., 2008). Several models have been developed during the last two decades to simulate the growth, development and yield of a tomato crop, but their results were not well correlated with quality attributes in order to develop the quality models (Cooman and Schrevens, 2006; Schouten et al., 2007; Dimokas et al., 2009).

Quality in tomato is a difficult issue and sensory studies have not clearly established the importance of the analytical variables (Ruiz et al., 2006). Considerable progress has been made in the identification of important components, but additional information is required regarding the optimal concentrations of sugars, acids and other components required for good flavor (Causse et al., 2003). Compounds such as vitamins and carotenoids are essential for the nutritional quality of fruits. Their biosynthetic pathways are often known (Carrari and Fernie, 2006), but the lack of knowledge on their regulation strongly limits the modeling capacity. So, more quantitative studies are needed before undertaking the modeling. There is a real challenge for the future here.

**FUTURE TRENDS IN MATHEMATICAL MODELING OF FRUIT QUALITY**

Fruit breeders must satisfy two requests concurrently: the production of high quality fruits and the use of sustainable practices (Li et al., 2009; Quilot et al., 2005; Kropff and Struik, 2002). Globalization of markets has increased competitiveness, highlighting the need for products of high quality (Dimokas et al., 2009), following a pre-established delivery data for these products. Crop development should therefore, be programmed so that it follows a desired growth profile by considering various crop features and climatic conditions, as well as the consumer demands to satisfy quality traits (Pucheta et al., 2006). These quality traits in harvestable parts, in terms of human requirement, are diverse and crop-specific, but by sensory analysis data, they can be modeled considering the balance of carbon, sugar, water, acid content and their correlation with aroma and flavor (Figure 2).

Recent advances in genetics and molecular plant biology can play a key role in crop modeling by improving crop responses to environmental conditions and management factors (Bannayan et al., 2007). The crop development showed a phenology strongly determined by temperature and photoperiod. Both are the principal modulators of visible manifestations of the genetic programming, while crops showed an allometry of reproducible constancy (Misle, 2006). Allometric models are based on correlations between biomass and morphological characters (Nafus et al., 2009). This simulation approach provided
simple descriptions of crop growth with a high level of empiricism (Marcelis, 1993).

**CONCLUSION**

A new generation of models should enable us narrow the gap between genes and complex phenotypes. Concerning fruit quality, this new generation is really needed to accompany the advances in fruit genomics (Baxter et al., 2005). An approach for the understanding of physiological and genetic phenomena has been the dissection of the quality traits into elementary processes. This approach has helped to highlight the main processes responsible for variations in complex fruit systems (Figure 3). The combined models can be used for practical purposes such as predicting the genotypic variations of a plant response to environmental conditions (Yin et al., 2003).

In a context of multicriteria objectives, combined models integrated the knowledge and potentialities of physiology, genetics and mathematical modeling to enhance the understanding of plant functioning (Quilot et al., 2005). Another modeling approach which involves relationships between the relative growth rates of two or more plant organs is the allometric modeling (Antunes et al., 2008). This method has the advantage of being inexpensive, rapid, reliable and a non-destructive alternative for growth estimations (Litton, 2008). These descriptive models could be correlated to mechanistic models to enhance the comprehension of the physiological processes involved in fruit quality. In particular, models have been extended to lower organizational levels, such as cell metabolism and biochemical pathways. Furthermore, efforts have been made to define plant systems biology and to broaden its scope by integrating it with crop models (Hammer, 2004). Together, these developments create opportunities for applying understanding at a lower organizational level to analyze complex phenotypical behavior at crop level and improve the quality of crops and harvestable products (Struik et al., 2005).
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**REFERENCES**

Antunes WC, Pompelli MF, Carretero DM, DaMatta FM (2008). Allometric models for non-destructive leaf area estimation in coffe (Coffea Arabica and Coffea canephora). Ann. Appl. Biol. 153: 33-40.

Brainard DC, Bellinder RR (2004). Assessing variability in fecundity of Amaranthus powellii using a simulation model. Weed Res. 44: 203-217.

Bannayan M, Kobayashi K, Marashi H, Hoogenboom G (2007). Gene based modeling for rice: An opportunity to enhance the simulation of rice growth and development. J. Theor. Biol. 249: 593-605.

Bannayan M, Kobayashi K, Kim HY, Liefering M, Okada M, Miura S (2005). Modeling the interactive effects of atmospheric CO₂ and N on rice growth and yield. Field Crops Res. 93: 237-251.

Bouman BAM, Van Keulen H, Van Laar HH, Rabbinge R (1996). The School of de Wit crop growth simulation models: a pedigree and historical overview. Agric. Syst. 52: 171-198.

Colbert JJ (1995). Models as links between empiricism and theory in insect ecology. Comput. Electron. Agric. 13: 87-90.

Cooman A, Schreven E (2006). A Monte Carlo approach for estimating the uncertainty of predictions with the tomato plant growth model: Tomgro. Biosyst. Eng. 94: 517-524.

Crouch R, Haines C (2004). Mathematical modeling: Transitions between the real world and the mathematical model. Int. J. Math. Educ. Sci. Technol. 35: 197-206.

De Wit AJW, van Diepen CA (2008). Crop growth modeling and crop yield forecasting using satellite-derived meteorological inputs. Int. J. Appl. Earth Observation Geoinformation, 10: 414-425.

Di Scala K, Crapiste G (2008). Drying kinetics and quality changes during food drying of red pepper. LWT, 41: 789-795.

Domijan K, Jorgensen M, Reid J (2006). Semi-mechanistic modeling in nonlinear regression: A case of study. Aust. N.Z.J. Stat. 48: 373-392.

Dutilleul P, Han L, Smith DL (2007). Plant light interception can be explained via computed tomography scanning: Demonstration with pyramidal cedar (Thuja occidentalis, Fastigiata). Ann. Bot. 101: 19-23.

Ewert F, Rousevall MDA, Reginster I, Metzger MJ, Leemans R (2005). Future scenarios of European agricultural land use I. Estimating changes in crop productivity. Agric. Ecosyst. Environ. 107: 101-116.

Fraisse CW, Breuer NE, Zierden D, Bellow JG, Paz J, Cabrera, VE, García y García A, Ingram KT, Hatch U, Hoogenboom G, Jones JW, O’Brien JJ (2006). AgClimate: A climate forecast information system for agricultural system for agricultural risk management in the southeastern USA. Computers Electronics Agric. 53: 13-27.

Gary C, Jones JW, Tchamitchian M (1998). Crop modeling in horticulture: State of the art. Sci. Hortic. 74: 3-20.

Genard M, Lescouret F, Gomez L, Habib R (2003). Changes in fruit sugar concentrations in response to assimilate supply, metabolism and dilution: a modeling approach applied to peach fruit (Prunus persica). Tree Physiol. 23: 373-385.
Exp. Bot. 44: 231-246.
Wu B, Genard M, Lescourret F, Gomez L, Li S (2002). Influence of assimilate and water supply on seasonal variation of acids in peach (cv. Suncrest). J. Sci. Food Agric. 82: 1829-1836.
Yin X, Stam P, Kropff MJ, Schapedonik HCM (2003). Crop modeling, QTL mapping and their complementary role in plant breeding. Agron. J. 95: 90-98.

Zhang L, van der Werf W, Bastiaans L, Zhang S, Li B, Spiertz JHJ (2008). Light interception and utilization in relay intercrops of wheat and cotton. Field Crops Res. 107: 29-42.