Essay

Mathematical modeling and simulation: a tool for crop protection

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Abstract

The consequences of climate change on crops are a cause for concern, as they cannot adapt quickly to new pathogenic threats. This article reviews the global use of mathematical models in plant health during the 2000-2020 period, through Scopus and Google Scholar. The objective of this study is to show modeling and simulation as an option in crop protection against meteorological risks or variations that occur due to global warming. Mathematical modeling is not an end in itself but a tool that helps in decision making for the sustainable management of crops. The prediction of the risk of occurrence of a pest or disease favors the reduction of the use of pesticides, thus reducing economic losses and damage to the environment. On the other hand, the simulation or numerical solution of mathematical models allows the exploration of hypotheses, it is an invaluable means in the research, since it allows exploring possible future scenarios and finding options of management systems that will be necessary at some point. In Mexico, it is necessary to carry out research for the generation and implementation of mathematical models that allow a lower cost of production and less negative impact on human health and the environment.

Keywords: computation applied to plant health, decision making, disease management.

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The consequences of climate change on crops are a cause for concern, as they cannot adapt quickly to new pathogenic threats (Garrett *et al*., 2013). To analyze the increase in the intensity and occurrence of pathogens and pests, it is necessary to consider that, historically, climatic variations show fluctuations, mainly in temperature with respect to the annual average (Mora-Aguilera *et al*., 2014). Actions that connect science with producers regarding the adaptation and control of pests in response to agrometeorological and climatic risks are urgently needed (López, 2014). The modeling of dynamic adaptive systems is a useful tool for the creation of models of simulation of complex systems, which allow the design of scenarios composed of various strategies, and the assessment of their results in the system (Martínez and Vargas, 2016).

Systems simulation is the numerical solution of the dynamic mathematical model of a system. This dynamic model is usually a set of differential equations or equations in differences, which have no exact solution but only numerical. It is necessary to develop dynamic models and simulate to control and optimize a system, as well as increase scientific knowledge (López, 2014) and apply it to pest and disease management based on forecast. For a disease to develop, three aspects known as plant disease triangle are required: a susceptible host plant, a conducive environment and a pathogenic agent. It becomes a pyramid when considering the human factor and its ability to influence some aspects of the plant, of the pathogen and of time (Téliz and Mora, 2007).

Mathematical modeling of systems

During the 60s-70s, the importance of the growing degrees days (GDD) was highlighted to understand the phenology of the plant and its relationship with pests (accumulation of heat units). Due to the abundance of data, analyses were carried out by means of computer systems, the dynamics of growth and production of plants, as well as their pests and the climatological data of the place, were estimated together, thus allowing the development of prediction models for decision-making in the management of cultural practices of the plant or in precise stages of the biology of the pest (Teliz and Mora, 2007).

De Wit and Penning de Vries (1982) proposed the classification of crop growth and development models of the Wageningen modeling school. It is a classification into four production situations: potential growth, water-limited growth, models for nitrogen-limited growth, and nutrient-limited production (Bouman *et al*., 1996). In the four situations, pests, diseases or weeds can further reduce field production. In practice, real production situations are difficult to assign to any of these four situations, but this practical simplification of schematizing specific situations allows progress, especially at the beginning of a study (De Wit and Penning de Vries, 1982).

The Wageningen group has a long tradition in crop modeling in its agroecological research program, based on the pioneering work of Wit (Van Ittersum *et al*., 2003). In the 1980s, scientists at Wageningen became involved in the development and application of crop models that could support rational decision-making about pesticide use. These include modeling perennial species in forest systems (Kramer, 1996) and the effects of yield-reducing factors such as weeds (Kropff, 1988), pests (Fransz, 1974), and decision-making support systems for pests and diseases (Rossing, 1993).

Studies such as that of Campbell and Madden (1990) highlighted the importance of predicting the increase of a disease before exceeding the threshold that causes economic losses in the crop. The forecast of the disease in days or weeks before an epidemic occurs allows producers to respond in a timely and efficient manner in the management of crops (Maloy, 1993). In addition, a prediction of low risk of disease occurrence may reduce pesticide use and environmental damage (De Wolf and Isard, 2007). Mathematical models and computational models allow representing the progress of a disease or an epidemic.

The quantitative description of epidemics provides information related to the amount of initial inoculum, environment, plant resistance, prediction system and crop management efficiency (Achicanoy, 2000). Ruiz (2020) classified the models according to their application into: a) teaching; b) research: hypothesis testing, genetic improvement, adaptation to climate change and optimization of inputs; and c) support systems for decision making: pest and disease forecasting, sowing dates, varieties, yield forecasting and irrigation and fertilization management.

There are three types of mathematical models of systems: empirical models, teleonomic models and mechanistic models (Thornley and France, 2007). A mechanistic model is defined by a set or system of nonlinear ordinary equations in differences or differential equations, which describe the behavior of the state variables of the system, those variables that represent the relevant properties or attributes of the system under consideration. Explanatory models are more appropriate for expressing hypotheses mathematically and thus provide a quantitative description and explanation of the most important processes that occur in a biological system. Mechanistic models simulate systems as functions of measured or estimated environmental variables. They are considered more promising to solve the problem, but they are also difficult to develop.

Research in crop protection can be grouped into: a) basic research. It characterizes crop growth and development, biological enemies, factors that determine their adaptation, and predictive models of the behavior of harmful organisms; and b) applied research. Phytosanitary problems are monitored through applications that use simulation models and climate databases. It includes methods and procedures for the assessment of the damage caused by the pest (SIAFEG, 2010).

Researchers in the agricultural area should promote knowledge of systems and control theory (Van Straten, 2012). A system is a simplified representation of a portion of reality. It is a series of selected and chosen elements, with specified limits and predetermined time characteristics (Savary and Willocquet, 2014). There is currently a lot of software available that can help build and run models.

Extensible modeling systems are modeling packages that allow the user to add a specific code if the methods are not sufficient for their purposes (Voinov, 2008). For example, the Stella® program allows focusing only on the components, structure, relationships, and behavior of the system, rather than on the program code itself (ISEE Systems, 2010). Vensim® has the same basic characteristics for modelling as Stella, with the addition of some important functions, such as calibration (automatically adjusts parameters to get the best correspondence between model behavior and data), optimization (the effective algorithm), Kalman filter, Monte Carlo analysis, causal tracing (a tree diagram shows a selected variable and variables that ‘cause’ its change) (Voinov, 2008).

Fortran simulation translator (FST®) is a simulation environment that allows the researcher to develop concepts in terms of mathematical equations. This computer system can be run using subroutines of standard mathematical libraries and developed by the user in the Fortran programming language, so it is a valuable tool, both for research and education (Van Kraalingen *et al*., 2003). Globally, there are models of growth and yield in climate change scenarios (Noriega-Navarrete *et al*., 2021). Specific simulation models for a crop; for example, Ceres-wheat in wheat, Corngro in corn, or they can be generic and applied to different species using specific parameters for each crop: Daisy, Epic, Wofost, Cropsyst, and Stics (Steduto, 2006).

There are microclimate models (Pohlheim and Heiβner, 1996; Ruiz, 2009). There is a new family of models called structural-functional models (Boudon, 2012), they use 3D representations of plant architecture to simulate different types of physical, physiological or eco-physiological processes in plants and allow evaluating the effects of these processes on the functioning, development and shape of plants (Rongier *et al*., 2017) and their interaction with pathogens (Hanan *et al*., 2002).

The L-systems formalism was introduced by biologist and botanist (Lindenmayer, 1968). In L-systems, the plant is represented by a chain in square brackets, whose elements, called modules, represent the components of plants (metamers, meristems, flowers, etc.). Modules consist of a symbolic name and an optional set of parameters. A set of rules defines how each module transforms over time (Prusinkiewicz, 2021).

Dynamic models

Dynamic models predict how variables of interest change over time. López (2014) describes, according to the theory of dynamical systems, the general procedure of modeling a system (Rabbinge *et al*., 1989; Van Straten, 2012; López, 2014): 1) definition of a problem and its analysis; 2) development of a conceptual representation of the model through relational or Forrester (1971) diagrams, based on existing knowledge in the literature. This is a qualitative model of the system; 3) the quantitative model can be generated by two options: black box models (BBM) and transparent or mechanistic models (TMM). In BBMs, real experiments are designed and carried out to obtain an empirical model, based on measurements of variables called inputs and outputs of the system.

In the case of TMMs, the set of dynamic equations (differential equations or equations in differences), also called the structure of the model, is postulated (Thornley and France, 2007), based on the conceptual model, the objectives of the model, the theories and data existing in the literature, as well as the existing constraints (data, time, among others).

These techniques are useful for describing all aspects related to agricultural systems, among them the development of pests and diseases; 4) once the nonlinear ordinary differential equations or equations in differences have been generated, they are solved numerically using digital computers through simulation; 5) uncertainty analysis allows quantitatively evaluating the variability in the parameters or input variables of the model, by deducting uncertainty distributions for each variable that the model predicts; 6) a sensitivity analysis of the model is then done to observe how its initial conditions, input variables and parameters affect the behavior of state variables and output variables; 7) through an identifiability analysis, it can be known if the parameter vector of the dynamic model can be determined uniquely from the input variables and output variables.

The methods used in practical identifiability of models are: Monte Carlo simulation, correlation matrix or calculation of the Fisher information matrix and methods based on sensitivity analysis; and 8) parameter estimation or model calibration is performed using existing information in the literature, data from experiments and the results obtained from sensitivity analysis. This is to bring as close as possible the predictions of the state variables and output variables of the model to measurements obtained from the real system.

In both MMs and BBMs, several data sets can be used and a calibrated model can be satisfactorily achieved; 9) the following is the evaluation (validation) stage of the model, this consists of using independent data sets to study the behavior of the model, using the values of its parameters obtained during the calibration phase; and 10) once an evaluated model is obtained, it can be used for some application or carry out another uncertainty analysis. A crucial stage in the development of a model is the verification process, it consists of verifying that the model is 'as real as life itself' (Taylor, 2003). The procedure of system modeling is an iterative process that allows returning from one stage to another until the mathematical model is an acceptable representation of the behavior of the real system.

System simulation

Mahalanabis (1982) considers the following stages in systems engineering: modeling, analysis, simulation and design. Simulating is the act of running a mathematical model and obtaining results on the variables of interest (Ruiz, 2020). It is necessary to explore different scenarios through simulation models, to analyze and find crop management options to maintain or increase productivity.

In the simulation of the effect of pests, it should be considered that they can cause great losses, when: the host population is susceptible and genetically uniform, the hosts are grouped or very close together, the pathogen increases rapidly due to its reproductive capacity; the climate and other factors are appropriate for its spreading and development and the period of favorable conditions is optimal to sustain the epidemic (Jarvis, 2000).

Simulation models have become important tools in epidemiology, they allow the exploration of hypotheses, and are an invaluable means of guiding research (APS, 2018). They help solve specific questions (Zadoks and Rabbinge, 1985) and explore the available knowledge of a system. This is due to the link that exists between the levels of integration in biological systems (Rabbinge *et al*., 1989). Simulation as a scientific approach is unique since it allows the exploration of possible futures. The dependence of agriculture on the climate is of particular importance, due to its high sensitivity to global climate change and climate variability, which makes it essential to understand the interactions between climate change and agricultural production for the stable development of society (Hui *et al*., 2013).

Simulation can provide a practical and intuitive analysis of plant disease systems and allows exploring the sensitivity of phytopathogenic systems to some of their specified components (Savary and Willocquet, 2014). According to Ruiz (2020), the challenges of crop modeling are: 1) improve the predictive quality of models (fewer models, but better); 2) generate and make accessible meteorological, soil and crop information, necessary to carry out the simulations; 3) develop models for irrigation and fertilization management, considering a public not specialized in modeling; 4) incorporate crop simulation into the study programs of agronomic engineering degrees; and 5) greater collaboration between specialists from different areas for the development, improvement and dissemination of simulation models.

Evaluation (validation) is a demonstration that a model, within a specific application domain, has acceptable predictive precision in that domain (Thornley and France, 2007). Currently with the help of computers, simulations of climate, pest population growth, crop development can be run, generating data for phytopathologists to use in the forecast and management of diseases.

Models applied to plant health

A case of modeling with a phytosanitary approach is that of the apple moth, in which heat units are counted to know the diapause of insects and thus be able to establish optimal moments for efficient control (Jacobo *et al*., 2005). Other examples of mathematical models for crop protection from pests (*Spodoptera frugiperda* (Yáñez *et al*., 2019); *Meloidogyne incognita* - *Trichoderma* sp., (Miranda *et al*., 2016); *Lobesia botrana* (Dagatti and Becerra, 2015); *Liriomiza* (Hernández *et al*., 2009); *Aeneolamia postica* (García *et al*., 2006); *Spodoptera exigua* and *Helicoverpha zea* (Cabello and Carreño, 2002); *H. zea*, *Helicoverpa armigera* and *Bemisia tabaci* (Gámez *et al*., 2000) and diseases (*Phytophthora ramorum* (Magarey, 2007); *Phytophthora infestans* (Rebellón *et al*., 2020); *Xanthomonas campestris* (Rocha, 2020); *Cladosporium cladosporioides* (Romero *et al*., 2016); *Altenaria tenuissima* (Moschini *et al*., 2014); *Gibberella zeae* and *Magnaporthe grisea* (Fernandes *et al*., 2011); *Mycosphaerella fijiensis* (Freitez *et al*., 2009); *Phytophthora infestans* (Gómez *et al*., 2002); *Botrytis cinerea* (Vidal *et al*., 2001)), as well as ecological niche models that have been used when modeling species distribution (*Moniliophthora roreri* (Vilchez, 2021); *Colletotrichum acutatum* (Quishpe, 2020); *Xylella fastidiosa* (Gutiérrez, 2019); *Rhagoletis* sp., (Samano, 2019); *Phyllophaga ravida* (Aragón *et al*., 2018)), can be found in the literature.

Mexico has a National Laboratory of Modeling and Remote Sensing, which is responsible for offering agricultural producers' real-time meteorological information to make decisions in their production systems and reduce the risks caused by adverse climatic conditions (INIFAP, 2021). In the country, some studies aimed at the use of modeling in the area of pests and diseases have been carried out (Guzmán *et al*., 1999; Jacobo *et al*., 2005; Hernández *et al*., 2009; Hernández *et al*., 2013; Duran *et al*., 2017; Hernández *et al*., 2020). López *et al*. (2021; 2022a); López *et al*. (2022b) generated dynamic models of the development of phytophagous thrips and biological control thrips in avocado, with these, one can simulate the progress of prey populations in their different biological stages and quantify the number of predators that must be introduced for effective biological control.

It is necessary to transfer knowledge through current computational tools and thus support the producers of the different crops in decision-making. Figure 1 shows that the use of simulation models in crops associated with pests and diseases is increasing over time. This is due to the easy access to information, to the use of technology for data analysis and to the rapid processing of the information that relates: elements of the climate, the growth and development of the crop, as well as the behavior of pests and diseases.

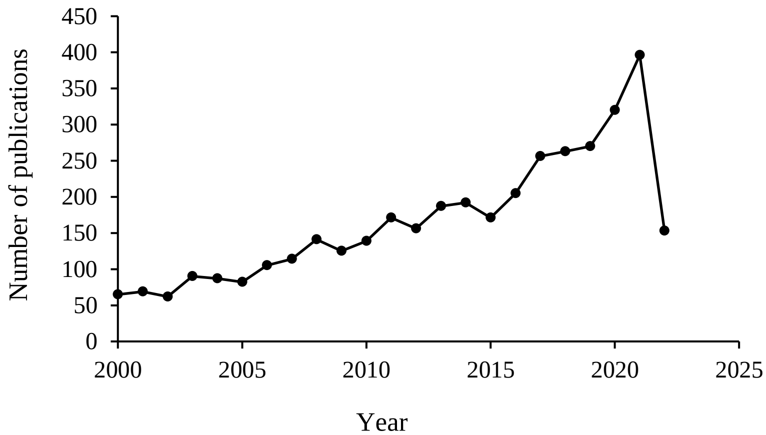

Figure 1. Number of publications related to modeling applied to crop protection.

The countries that publish the most on modeling applied to plant health are the United States of America, China, England and France. The institutions that have the most publications on this topic are: United States Department of Agriculture, Wageningen University and University of Florida. The scientific journals that publish the most models of pests and diseases are Pest Management Science, Journal of Economic Entomology, Applied and Environmental Microbiology, Environmental Entomology and Ecological Modelling (Scopus, 2022).

Conclusions

The main economic benefit of modeling and simulation of systems is the savings that producers can have by applying only the indispensable number of sprays. Modeling can favor better crop management, less environmental damage, and safe production, which meets the most demanding standards of current and new export markets for some products, such as the European and the Asian where there is a large population and purchasing power.

The type of model will depend on the problem being studied, it can be useful to understand the dynamics of infections or as a forecasting instrument. Therefore, a good understanding of the biological system to be studied and defining data collection in accordance with the objectives of the model is necessary. Systems simulation is a tool that allows the exploration of possible future scenarios and the understanding that some components may have a greater or lesser effect on the plant-pathogen system over time. It can be useful in the analysis of the resistance of the host plant because it allows tracing through time processes that cannot be seen and that can be linked to current advances in molecular improvement.

The temporal-spatial distribution of pests and diseases in agroecosystems can simulate and evaluate scenarios for efficient and sustainable management.

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