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FAST-TRACKING SCIENTIFIC RESEARCHES THROUGH MODELLING AND SIMULATION

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ABSTRACT
The role of modeling and simulation in scientific research was presented in this paper the application of models to study several concepts is growing in acceptance and utilization. The difficulty in measuring some components of research has prompted the use of simulation models to investigate the processes involved. Simulation models integrate levels of knowledge about separate parts of a system and they can be used as exploratory tools to investigate solutions to problems that in agriculture and other allied sciences are normally site-specific. Models are simplified representations of the real system and must be used with precaution.

KEYWORDS:Modelling, Simulation, Simulation Models, Scientific Research, Mechanistic models, Deterministic Models

1.0 INTRODUCTION

Manyresearchers have tried from the turn of the 20thcentury to develop data and information bases that when interpreted can be used to improve the management of systems(Martin, 2014). Early on, researchers recorded and published descriptions that, for the most part, were observations of situations involving abnormal and unusual occurrences. With the invention of adding machines and calculators, scientists began to define and determine relationships. With the advent of computers, engineers and scientists began to consider continuous and discrete happenings with respect to time. Beginning in the late 1950s, descriptive and mathematical modelling of processes evolved. These mimics were called simulations (Robert and Bruce, 1998).

Simulation is the imitation of the operation of a real-world process or system over time. The act of simulating something first requires that a model be developed; this model represents the key characteristics or behaviors/functions of the selected physical or abstract system or process. The model represents the system itself, whereas the simulation represents the operation of the system over time(Loucks*et al.,* 2015).Simulation is used in many contexts, such as simulation of technology for performance optimization, safety engineering, testing, training, education, and video games. Often, computer experiments are used to study simulation models. Simulation is also used with scientific modelling of natural systems or human systems to gain insight into their functioning. Simulation can be used to show the eventual real effects of alternative conditions and courses of action. Simulation is also used when the real system cannot be engaged, because it may not be accessible, or it may be dangerous or unacceptable to engage, or it is being designed but not yet built, or it may simply not exist(Loucks*et al.,* 2015).

Key issues in simulation include acquisition of valid source information about the relevant selection of key characteristics and behaviours, the use of simplifying approximations and assumptions within the simulation, and fidelity and validity of the simulation outcomes.

Procedures and protocols for model verification and validation are an ongoing field of academic study, refinement, research and development in simulations technology or practice, particularly in the field of computer simulation(Kuczera and Diment, 2015).Technically, models are equations and rules defining and describing a system, Simulation involves calculating values over time in dynamic fashion (Jones *et al.,* 1979).They are useful tools for research, decision making, education, training and technology transfer (Igbadun, 2010).The objective of this paper is to explore the role of modeling and simulation in research and also to create some level of awareness, to sensitize and encourage researchers towards development and application of these models in researches and training.

2.0 MODEL TYPES AND THEIR FUNCTIONS

A model is a representation of a real-world which is defined as a system, they can be broadly classified into two: Physical models (Physical representation of the system; e.g., prototypes, pictures, sculptures, miniaturized representations and Conceptual models (A representation of the idea or principles in operation/ governing the system (Igbadun, 2010).

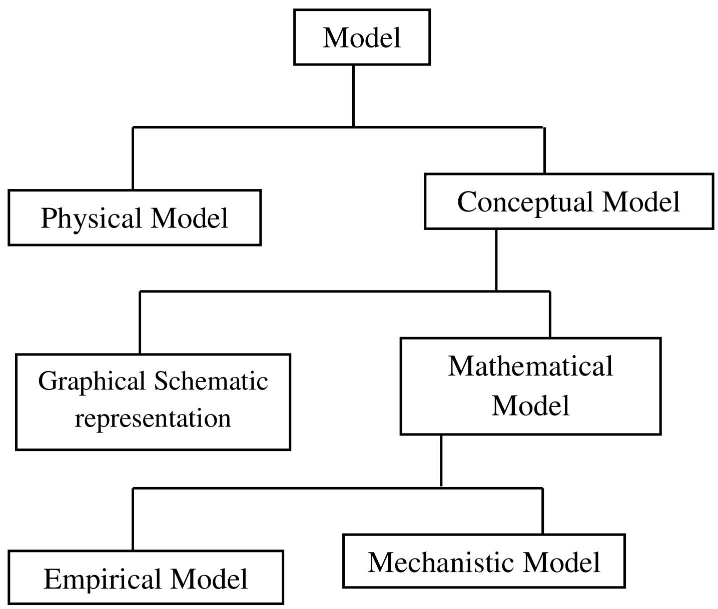

Figure 1: Model categorization

Types of Models

Depending upon the purpose for which it is designed the models are classified into different groups or types. A few of them are:

A **conceptual model** is a model made of the composition of concepts, which are used to help people know, understand, or simulate a subject the model represents. Some models are physical objects; for example, a toy model which may be assembled, and may be made to work like the object it represents(Kuczera and Diment, 2015).The term *conceptual model* may be used to refer to models which are formed after a conceptualization or generalizationprocess. Conceptual models are often abstractions of things in the real world whether physical or social. Semantics studies are relevant to various stages of concept formation and use as Semantics is basically about concepts, the meaning that thinking beings give to various elements of their experience(Kennington and Helgason, 2016).

Empirical Models: These are direct descriptions of observed data and are generally expressed as regression equations (with one or a few factors) and are used to estimate the final yield. This approach is primarily one of examining the data, deciding on an equation or set of equations and fitting them to data. These models give no information on the mechanisms that give rise to the response. Examples of such models include those used for such experiments as the response of crop yield to fertilizer application, the relationship between leaf area and leaf size in a given plant species and the relationship between stalk height alone or coupled with stalk number and/or diameter and final yield(Kennington and Helgason, 2016).

Mechanistic Models: A mechanistic model is one that describes the behaviour of the system in terms of lowerlevel attributes. Hence, there is some mechanism, understanding or explanation at the lower levels (e.g. Cell division). These models have the ability to mimic relevant physical, chemical or biological processes and to describe how and why a particular response occurs. The modeller usually starts with some empirism and as knowledge is gained additional parameters and variables are introduced to explain crop yield. The system is therefore broken down into components and assigned processes(Jensen and Barnes, 2017).

Static and Dynamic Models: A static model is one that does not contain time as a variable even if the endproducts of cropping systems are accumulated over time. In contrast dynamic models explicitly incorporate time as a variable and most dynamic models are first expressed as differential equations(Jensen and Barnes, 2017).

Deterministic Models: A deterministic model is one that makes definite predictions for quantities (e.g. crop yield or rainfall) without any associated probability distribution, variance, or random element. However, variations due to inaccuracies in recorded data and to heterogeneity in the material being dealt with are inherent to biological and agricultural systems (Brockington, 1979). In certain cases, deterministic models may be adequate despite these inherent variations but in others they might prove to be unsatisfactory e.g. in rainfall prediction. The greater the uncertainties in the system, the more inadequate deterministic models become.

Stochastic Models: When variation and uncertainty reaches a high level, it becomes advisable to develop a stochastic model that gives an expected mean value as well as the associated variance. However, stochastic models tend to be technically difficult to handle and can quickly become complex. Hence, it is advisable to attempt to solve the problem with a deterministic approach initially and to attempt the stochastic approach only if the results are not adequate and satisfactory(Jensen and Barnes, 2017).

Simulation Models: These form a group of models that is designed for the purpose of imitating the behaviour of a system. Since they are designed to mimic the system at short time intervals (daily time-step), the aspect of variability related to daily change in weather and soil conditions is integrated. The short simulation time-step demands that a large amount of input data (climate parameters, soil characteristics and crop parameters) be available for the model to run. These models usually offer the possibility of specifying management options and they can be used to investigate a wide range of management strategies at low costs.

Computer Simulation Model (CSM)

When a computer program is developed to handle the computation and dynamic iterations of the processes in the modelled system, the model built is referred to as computer simulation model(Hula, 2018).

Development and application of water management models requires a thorough understanding of:

- the role of the models in the overall water resources management decision-making process and the questions to be answered by the modeling exercises,
- the real-world processes being modeled and the capabilities and limitations of methods for representing these processes with mathematical equations,
- computational techniques for solving the equations,
- data availability and limitations,
- model calibration and verification techniques,
- the availability of computer software and hardware and the skills required to use these tools, and
- the communication capabilities required to assure that model development and application is responsive to water resources planning and management needs and that model results are effectively incorporated into decision-making processes.

Optimizing Models

These models have the specific objective of devising the best option in terms of management inputs for practical operation of the system. For deriving solutions, they use decision rules that are consistent with some optimizing algorithm. This forces some rigidity into their structure resulting in restrictions in representing stochastic and dynamic aspects of agricultural systems(Hula, 2018).

Three types of simulations

Simulations generally come in three styles: live, virtual and constructive. A simulation also may be a combination of two or more styles. Within these styles, simulations can be *science-based* (where, for example, interactions of things are observed or measured), or involve interactions with humans. Our primary focus at IST is on the latter— *human-in-the-loop* — simulations.

Live simulations typically involve humans and/or equipment and activity in a setting where they would operate for real. Think *war games* with soldiers out in the field or manning command posts. Time is continuous, as in the real world. Another example of live simulation is testing a car battery using an electrical tester.

Virtual simulations typically involve humans and/or equipment in a computer-controlled setting. Time is in discrete steps, allowing users to concentrate on the important stuff, so to speak. A flight simulator falls into this category.

Constructive simulations typically do not involve humans or equipment as participants. Rather than by time, they are driven more by the proper sequencing of events. The anticipated path of a hurricane might be "constructed" through application of temperatures, pressures, wind currents and other weather factors. Science-based simulations are typically constructive in nature.

Steps involved in developing simulation models

The steps involved in developing a simulation model, designing a simulation experiment, and performing simulation analysis are:

Step 1. Identify the problem.
Step 2. Formulate the problem.
Step 3. Collect and process real system data.
Step 4. Formulate and develop a model.

Step 5. Validate the model.
Step 6.Document model for future use.
Step 7. Select appropriate experimental design.
Step 8. Establish experimental conditions for runs.
Step 9. Perform simulation runs.
Step 10. Interpret and present results.
Step 11. Recommend further course of action.

Although this is a logical ordering of steps in a simulation study, much iteration at various sub-stages may be required before the objectives of a simulation study are achieved. Not all the steps may be possible and/or required. On the other hand, additional steps may have to be performed. The next three sections describe these steps in detail.

3.0 MODEL TESTING AND EVALUATION

This involve procedures necessary to ensure that the model is working and produces expected outputs which are similar to those of the real world (the system) it is designed to represent.

Four very important procedures:

- Verification
- Calibration
- Validation
- Sensitivity analysis

Verification

Verification involves the evaluation of the accuracy with which thecomputer code represents the mathematical model and the programmer'sintentions. Verification also involves the careful checking ofmathematical manipulations, units and their conversions, and programminglogic and code to ensure that neither the mathematicalmodel nor its translation into one or more computer programs haserrors in it(Feldman, 1981, Frevert, *et al.,* 1994).

Calibration

Calibration consists of making adjustments to model parameters togive the best fit between simulated results and results obtained frommeasurements on the real system. In other words, calibration involvesadjusting certain model parameters by systematically comparing simulatedresults with observations of state variables. Model structureremains the same, and parameters are adjusted to more closely describeobserved behaviour, For example, suppose that partitioning ofnew crop growth to leaves varies with variety all else being equal.An experiment could be conducted in which the total crop and leafdry matter are measured and a leaf partitioning parameter estimatedfor each variety by fitting simulated results to match observed data.Calibration should be conducted only within the confines of a givendata set. In many cases, calibration is the only practical way to estimatesome parameter values that are used in biological models(Feldman, 1981, Frevert, *et al.,* 1994).

Validation

Validation is the process of comparing simulated results to real systemdata not previously used in any calibration or parameter estimationprocess. The purpose of validation is to determine if themodel is sufficiently accurate for its application as defined by objectivesof the simulation study. Simulated state variables are comparedwith measured values of state variables. Usually in crop simulationstudies only a few state variables out of many possibilities are measured,and thus a complete comparison is usually not possible(Feldman, 1981, Frevert, *et al.,* 1994).

Sensitivity Analysis

Sensitivity analysis involves exploring the behaviour of the model fordifferent values of parameters. This is done to determine how mucha change in the value of a parameter influences the important outputsfrom the model.

4.0 ADVANTAGES AND DISADVANTAGESOF SIMULATION

Main advantages of simulation include:

- Study the behavior of a system without building it.
- Results are accurate in general, compared to analytical model.
- Help to find un-expected phenomenon, behavior of the system.
- Easy to perform ``What-If'' analysis.

Main disadvantages of simulation include:

- Expensive to build a simulation model.
- Expensive to conduct simulation.
- Sometimes it is difficult to interpret the simulation results.

Interest in simulations

Technically, simulation is well accepted. The 2006 National Science Foundation (NSF) Report on "Simulation-based Engineering Science" showed the potential of using simulation technology and methods to revolutionize the engineering science. Among the reasons for the steadily increasing interest in simulation applications are the following:

1. Using simulations is generally cheaper, safer and sometimes more ethical than conducting real-world experiments. For example, supercomputers are sometimes used to simulate the detonation of nuclear devices and their effects in order to support better preparedness in the event of a nuclear explosion. Similar efforts are conducted to simulate hurricanes and other natural catastrophes.
2. Simulations can often be even more realistic than traditional experiments, as they allow the free configuration of environment parameters found in the operational application field of the final product. Examples are supporting deep water operation of the US Navy or the simulating the surface of neighbored planets in preparation of NASA missions.
3. Simulations can often be conducted faster than real time. This allows using them for efficient if-then-else analyses of different alternatives, in particular when the necessary data to initialize the simulation can easily be obtained from operational data. This use of simulation adds decision support simulation systems to the tool box of traditional decision support systems.
4. Simulations allow setting up a coherent synthetic environment that allows for integration of simulated systems in the early analysis phase via mixed virtual systems with first prototypical components to a virtual test environment for the final system. If managed correctly, the environment can be migrated from the development and test domain to the training and education domain in follow-on life cycle phases for the systems (including the option to train and optimize a virtual twin of the real system under realistic constraints even before first components are being built).

5.0 APPLICATIONS OF SIMULATION MODELS

Simulation modeling is increasingly being applied in research, teaching, farm and resource management and policy analysis and production forecasts. They can be applied, namely, research, crop system management, and policy analysis(Gilbert and Shane, 1982).

- **Research understanding:** Model development ensures the integration of research understanding acquired through discreet disciplinary research and allows the identification of the major factors that drive the system and can highlight areas where knowledge is insufficient. Thus, adopting a modeling approach could contribute towards more targeted and efficient research planning
- **Integration of knowledge across disciplines:** Adoption of a modular framework allows for the integration of basic research that is carried out in different regions, countries and continents. This ensures a reduction of research costs (e.g., through a reduction in duplication of research) as well as the collaboration between researchers at an international level.
- **Improvement in experiment documentation and data organization:** Simulation model development, testing and application demand the use of a large amount of technical and observational data supplied in given units and in a particular order. Data handling forces the modeler to resort to formal data organization and database systems.
- **Site-specific experimentation:** Specific site selection can be using the models and can be used to predict the performance of a system in regions.
- **Yield analysis:** When a model with a sound physiological background is adopted, it is possible to extrapolate to other environments. Simulation models are used to climatically-determined yield in various crops. Through the modeling approach, quantification of yield reductions caused by non-climatic causes (e.g., delayed sowing, crop spacing, soil fertility, pests and diseases) becomes possible. Simulation models have also been reported as useful in separating yield gains into components due to changing weather trends, genetic improvements and improved technology(Giles and Wunderlich, 1981).
- **Climate change projections:** The variability of our climate and especially the associated weather extremes is currently one of the concerns of the scientific as well as general community. The application of crop models to study the potential impact of climate change has been widely used across the continents. The increased concentration of carbon dioxide and other greenhouse gases are expected to increase the temperature of earth. Crop production is highly dependent on variation in weather and therefore any change in global climate will have major effects on crop yields and productivity.
- **Scoping best management practices:** Simulation can be done to determine the best management practices under a certain cropping system. In the past, the main focus of agronomic research has been on crop production. Recently, in addition to profitable crop production, the quality of the environment has become an important issue that agricultural producers must address. Agricultural managers require strategies for optimizing the profitability of crop production while maintaining soil quality and minimizing environmental degradation.
- **Yield forecasting:** Reasonably precise estimates of crop yield over large areas before the actual harvest are of immense value to both the researcher and the farmer in terms of planning. In this approach the model is run using actual weather data during the cropping season for the geological region of interest. Weather years for typical years are used to continue simulations until harvest.
- **Breeding and introduction of a new crop variety:** Development and release of a variety is a complex process that may extend over a period of 5 – 15 years. Since the modeling systems approach integrates different components of agro ecosystems, it can be used to

conduct multi-location field experiments to understand genotype by environment (G x E). Such studies can help in reducing the number of sites/seasons required for field evaluation and thus increase the efficiency of the process of variety development.

6.0 CONCLUSION

As a research tool, model development and application can contribute to identify gaps in our knowledge, thus enabling more efficient and targeted research planning. Models that are based on sound physiological data are capable of supporting extrapolation to alternative cropping cycles and locations, thus permitting the quantification of temporal and spatial variability. Most models are virtually untested or poorly tested, and hence their usefulness is unproven. Indeed, it is easier to formulate models than to validate them. Many agronomists have been confused by the situation. They are discouraged by the complexity of the models, the lack of model testing, and the inevitable inaccuracies that arise when such testing is done. Consequently, they have seriously doubted the usefulness of crop models in agronomy. Unfortunately, this confusion is caused partly by those who are naively optimistic that crop modelling is the panacea for agricultural problems and apply crop models indiscriminately. Because most agronomists do not fully understand the concept of crop growth modelling and systems-approach research, training in this area is required. An intensely calibrated and evaluated model can be used to effectively conduct research that would in the end save time and money and significantly contribute to developing sustainable agriculture that meets the world's needs for food.

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