Understanding Modeling & Simulation in Agriculture

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1. What is Modeling & Simulation?
2. Why use Modeling & Simulation?
3. What approaches are used to create a model?
4. What Methodology is used?
5. How reliable are their forecasts?

Examples:
1. Crop Model Systems
2. Agricultural Processing
Modeling & Simulation

INPUTS

Crop
Soil
Weather
Management

OUTPUTS

Agricultural Systems Model

Yield (kg/ha)
What is Modeling & Simulation?

- Capture the behavior of a system or process on a computer
  - Only those relevant to the model’s purpose
- Based on Scientific principles
  - Highly developed in the physical sciences (physics, chemistry and engineering)
  - Biological sciences still catching up (Why?)
- Usually involves lots of calculations
Have you done any modeling?
My Background

B.S. Chemical Eng, UP Los Baños, M.S. Chemical Eng, UP Diliman
Ph.D. Biological & Environmental Eng. & Postdoc, Cornell Univ, NY

Equipment Design

Space Kitchen

Space Dryer

Velocity (m s$^{-1}$)
(Inside galley)

Inlet velocity (m s$^{-1}$)

Mean bed temperature

Mathematical Modeling
Real-time PCR method to measure fungal biomass in food components of space trash

(Arquiza and Hunter, 2014)

- A species–specific real–time PCR biomass assay for fungi growing on solid media was developed
- Specific growth rates measured at different water activities using rt–PCR are reported for the first time
Solid-state fermentation for bioproducts (chemicals, enzymes, biocontrol agents)

Growth kinetics of *Trichoderma reesei* RUT-C30 (cellulase producer)

**Bioreactor design**

*Trichoderma reesei* RUT-C30 with *Aspergillus niger*

Engineered Consortia (microbial ecology, ‘omics)
Modeling in Agriculture

THE CHALLENGE

RESEARCH QUESTION
Given historical hybrid (inbred by tester) performance data across years and locations, how can we create a model to predict/impute the performance of the crossing of any two inbred and tester parents?

Agricultural Production Systems sIMulator

- Simulate biophysical processes in agricultural systems
- Relate to the economic and ecological outcomes of management practices in the face of climate risk
- Explore solutions for food security, climate change adaptation and mitigation and carbon trading problem domains
Biophysical modules that simulate biological and physical processes in farming systems

Management modules to specify management rules and control for the scenario being simulated

Data input and output modules

A simulation engine that drives the simulation process and facilitates communication between the independent modules
Crop Module Documentation

AgPasture
Barley
Canola
Canopy (Intercropping)
Chickpea
Cotton
Cowpea
Fababean
FieldPea
Growth (E. Grandis, E. Melliodora, E. Populnea)
HorseGram
LabLab
Lucerne
Lupin
Maize
Millet
Mucuna
Mungbean
OilPalm
Peanut
PigeonPea
Plant
Rice (Oryza2000)
Slurp
Sorghum
SoyBean
Sugar
Weed
Wheat

Also available as a downloadable PDF
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The **System** to be Modeled

- **Defined** to study a part of the real world
  - **Components**
  - **Interrelationships** among components

Mathematical Model

- Mathematical representation of the system
  - interrelationships among components
  - Environmental effects
- Equations of processes that cause changes
- Environmental variables that affect system
- Properties of the system’s components
- Assumptions made by the model
Simulation

- **Numerical solution** of the system model
- Produce values of variables for the system components
  - Time
  - Space \((x,y,z)\)
- Large number of variables and equations
- Calculations done by computer
  - Computational model
- Results compared with experimental data to validate the model
Scientific principles

Real Model

Real World Problem

Simplify

Interpret

Abstract

MOST IMPORTANT

1. Mechanistic
2. Functional

Assumptions

Variables f(x,y,z,t)

Equations

Systems of Differential equations

Mathematical Model

Calculate

Simulate

Values of variables at x,y,z,t

Conclusions

Computer Model

Program
Why model?

- Scientific understanding
  - How a process happens (Mechanisms)
  - Functional relationship among variables

- Decision or policy support
  - Compare different courses of action
  - Effect of bad weather
  - Long-term results of Climate Change
Computational Modeling & Simulation

Three developments

1. Efficient & accurate numerical methods that can be programmed (e.g. finite element method)

2. Inexpensive computers with powerful, high-speed processors, large memories and long-term storage

3. Software packages (CAD, meshing, solvers, postprocessing, graphics...)
Modeling & Simulation example

- Predicting path of hurricanes/typhoons
Modeling & Simulation example

- Climate Models – predicting climate change

General Circulation Models (GCMs) are full 3-D representations of Earth’s surface and atmosphere, represented by individual grid boxes (Ruddiman, 2000)
Model Predictions

IPCC Projected Temperature Changes for Various Emission Scenarios
Observed global average temperature changes versus simulations via the HadGEM1 GCM assuming only natural forcing factors, human factors, or the sum of the two. The gray band denotes the uncertainty of the GCM simulation. The baseline is the average for the whole period.

General methodology

Theory

Mathematical model

Computational model

Simulation (Run the model in a computer)

Results

Experiments

Verification and Validation
Examples:

1. Crop Growth Models
2. Agricultural Processing
Crop Growth Models

- Crop
- Soil
- Weather
- Management

Model

Yield (kg/ha)
Plant growth model

defining factors
- CO₂
- radiation
- temperature
- crop characteristics
  - physiology, phenology
  - canopy architecture

limiting factors
- water
- nutrients
  - nitrogen
  - phosphorus

reducing factors
- Weeds
- Pests
- Diseases
- Pollutants

Potential  Water and/or nutrient limited  Actual

How do we get the mathematical equations for the Model?
Modeling plant biomass
Most of the mass of the tree came from

a) the air
b) the soil
c) substances dissolved in the water taken by the roots
d) the surrounding grass
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Photosynthesis

\[ 6\text{CO}_2 + 6\text{H}_2\text{O} \xrightarrow{\text{Light}} \text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \]

Carbon dioxide + Water \[\xrightarrow{\text{Light}}\] Sugar + Oxygen
How it happens

Derive equations for all processes?

Mechanistic Model
Enzyme Reaction Example

Rate of reaction vs. [glucose]

Equation: regression fit

Parameters

Function: $y = -216.55x^2 + 126.5x + 1.9984$

High-fructose corn syrup

Effect of concentration of glucose on reaction rate at constant temperature
Enzyme Mechanistic Model

**Mechanism**

\[
E + S \xrightarrow{k_1} E \cdot S
\]

\[
E \cdot S \xrightarrow{k_2} E + S
\]

\[
E \cdot S + W \xrightarrow{k_3} P + E
\]

\[
r_P = k_3 (E \cdot S)(W) = \frac{k_{cat} E_t S}{k_2 + k_3 W + S}
\]

\[
r_P = V_{max} \frac{S}{K_m + S}
\]

**Rate of reaction vs. glucose concentration**

**Parameters**

- \( V_{max} \)
- \( K_m \)

**Michaelis–Menten eqn.**
Which is better? Mechanistic or Functional?
Photosynthesis: Functional Model

\[ P = f(LAI) \cdot f(PAR) \cdot \text{Min}\{f(VPD), f(REW)\} \cdot f(T) \cdot f(T_{min}) \cdot f(S) \cdot f(CO2) \]

- \( P = \) flux of carbon from photosynthesis
- \( f(\ ) = \) function that describes the individual effect of each factor

- \( LAI = \) leaf area index
- \( PAR = \) Photosynthetically available radiation
- \( CO2 = \) carbon dioxide (CO2)
- \( VPD = \) air humidity
- \( Tmin = \) days of minimum temperature
- \( S = \) temperature history
- \( REW = \) soil moisture

http://www.hiilipuu.fi/articles/how-model-photosynthesis
**LAI** = "Leaf Area Index“, amount of leaves
- More leaves produce more photosynthesis
- Not all leaves are the same because leaves shade each other
- Also resources are allocated differently to leaves in different places

\[
f(LAI) = \frac{1}{K} \times (1 - e^{-(K \times LAI)})
\]
Giant Leap for Gene-Based Testing Estimates Risk of Heart Disease, Breast Cancer and Others

This research, 6.6 million — that’s how many spots on the human genome Sekar Kathiresan looks at to calculate a person’s risk of developing coronary artery disease. Kathiresan has found that combinations of single DNA-letter differences from person to person in these select locations could help to predict whether someone will succumb to one of the leading causes of death worldwide. It’s anyone’s guess what the majority of those As, Cs, Ts and Gs are doing. Nevertheless, Kathiresan says, “you can stratify people into clear trajectories for heart attack, based on something you have fixed from birth”.
ORYZA: A crop growth simulation model for rice

ORYZA version 3 (ORYZA v3), or simply ORYZA, is an ecophysiological model which simulates growth and development of rice including water, C, and N balance (Bouman et al., 2001; IRRI, 2013) in lowland, upland, and aerobic rice ecosystems. It works in potential, water-limited, nitrogen-limited, and NxW-limited conditions. And it was calibrated and validated for 18 popular rice varieties in 15 locations throughout Asia.

Since 2009, ORYZA2000 has been modified from a crop model toward a cropping model aimed mainly at abiotic stress. The modeling group in International Rice Research Institute encourages tests and applications of ORYZA and welcomes feedback. The modeling group also provides minor tech support to users.

https://sites.google.com/a/irri.org/oryza2000/about-oryza-version-3
Analysis of different scenarios
- Estimate weather-constrained rice growth & yield
- Estimate actual growth & yield for water- and/or nitrogen-limited conditions
- Study rice cropping management on water (irrigation), nitrogen fertilizer, sowing and transplanting date, etc.

Application-oriented research analysis
- Explain yield gaps
- Optimization of crop management
- Effects of climate change on crop growth
ORYZA Rice modeling

Level of variable

Rate of transport or transformation

Material flow

information flow
WHAT IS ORYZA

Overview

The ORYZA Online 2.0 is an ORYZA interface that aims to simplify the use of the ORYZA rice crop model for basic simulations.

This is an online web tool for beginners in crop modeling to familiarize themselves with the input files needed, to run a basic simulation, and to visualize the results of the simulation.

Note that the basic simulation for ORYZA v3 does not include calibration and validation.

START NOW

http://oryzawebinterface.irri.org/
ORYZA Input File Templates

Input file templates include:
- control.dat for control file.
- standard.crp for crop file.
- standard.exp for experiment file.
- standard.sol for soil file.
- reruns.rer for rerun file, and
- phi1.008 for the weather file.

The easiest way to prepare these input files for user’s simulation is to get these template files, make necessary changes in parameter values, and save each as a new file.

However, the user must follow the correct syntax and variable data types in order to minimize errors. Refer to the General Rules in Writing Input Files.

Please select and click each of the standard input templates, export each, then modify to create your own simulation input files.

http://oryzawebinterface.irri.org/home/scripts/learnOryza.html
Validation
Agricultural Processing
My Background

Food systems for Space Exploration
9 tropical storms make landfall, another 10 enter Philippine waters (average per year)

Earthquakes, volcanic eruptions, climate change, armed conflicts
Evacuation centers

Quezon City

Cagayan de Oro

Legazpi, Albay

Marawi
Space food → food for disasters

Ready-to-eat

Add water

Natural form

Beverages

NASA Advanced Food Project

(http://www.nasa.gov/centers/johnson/slsd/about/divisions/hefd/project/advanced-foods.html)
Eating rice on Mars (3 ways)

Prepackaged

Bulk prepackaged

Bioregenerative

Planting

Harvest/Postharvest

Processing

Cooking
Plant experiments

Space Station
Multi-purpose Space Dryer (Prototype)

Three thermoelectric porous-media condensers

Dryer Vessel
Low-Temperature, Low-Humidity Drying System (LTLH) 2015

DOST-FNRI LTLH Dryer (Utility Model application pending)

Physical Appearance

Top view

Fresh and LTLH Dried mango samples
(1-inch squares, 5 mm thick)
Vitamin C content (mg/100g) of LTLH dried mango vs commercial dried mango

Vitamin C content, mg/100g

No heating, 6 hrs: 278
60°C, 4.5 hrs: 265
70°C, 4 hrs: 239
Commercial dried mango: 76
Other dried products

- Fresh vs LTLH Dried Carrots
- Fresh vs LTLH Dried Papaya
- Fresh vs LTLH Dried Cabbage
- Fresh vs LTLH Dried Malunggay
- Fresh vs LTLH Dried Pineapple
- Fresh vs LTLH Dried Baguio beans
LTLH Dried vegetables can be rehydrated
LTLH Dried vegetables for instant cup noodles

After 3 mins, the LTLH dried vegetables were rehydrated and cooked

Much Cheaper than freeze-dried
2018: Packaging & Shelf-life
The Scale-up problem

Lab Prototype → Small or Pilot → Medium or Commercial

Scale-up: Modeling & Simulation Virtual Prototyping
Modeling & Simulation

LTLH Drying

Top view

Side view

Fresh Mango Sample

Free flow domain

Velocity
Temperature
Humidity

Porous domain containing water vapor and liquid water

Air flow simulation

Time=36000 s  Surface: Velocity magnitude (m/s)
6 hours

Mango, 0.5 cm thick, 2.54 cm long
Mango, 0.5 cm thick, 2.54 cm long

6 hours

Mango, 0.5 cm thick, 5.08 cm long

8.5 hours
Simulation of airflow inside LTLH dryer

Surface: Velocity magnitude (m/s)
Arrow Surface: Velocity field

Free flow domain

Velocity
Temperature
Humidity

Porous domain containing water vapor and liquid water
Thank you!
Questions?

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Modeling in Science

**THEORETICAL**
- Assumptions
- Predictions
- Theory A vs. Theory B

**MODELING**
- Numerical Experiments
- Simulation results
- Theory A or Theory B?

**EXPERIMENTAL**
- Actual data
- Theory A or Theory B?
Cropping system model:

Components

- Crop
- Soil
- Weather
- Management


Decision Support System for Agrotechnology Transfer (DSSAT)
Drying of a product

Variables (z, t)
\[ T_a, T_b, \mathcal{H}, M \]

Input Data
- Physical Properties
- Drying curves
- Water vapor concentration at solid-gas interface

Initial Conditions

Boundary Conditions
- Conservation of Mass
- Conservation of Energy \( T_a, T_b \)

Governing Equations
- Water in product, \( M \)
- Water vapor in air, \( \mathcal{H} \)

Evaporation

Transfer coefficients
- \( hA \)
- \( k_mA \)

Equilibrium Moisture Curve

Subscripts:
- \( a = \text{air} \)
- \( b = \text{product} \)