

Simulation of Biological Systems

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In 1991, the Agricultural Engineering Department at Virginia Tech changed the name of the undergraduate degree program to “Biological Systems Engineering.” Over the years, Agricultural Engineering, like other engineering disciplines, has expanded into new areas of activity. Activity focused on production agriculture is still a key component of the discipline, but it now coexists with a range of other activities. Changing the name to Biological Systems Engineering better communicates the *range* of activities in the Department and in the discipline.

A new curriculum was designed, primarily by refocusing on-going activity in the Department. This curriculum allows the student opportunity to choose electives which develop a “limited specialization.” The two specializations available are:

1. Land and Water Resource Engineering
2. Biological Engineering

Background

Land and Water Resource Engineering builds on a traditional strength in Agricultural Engineering. This limited specialization focuses on the stewardship of our land and water resource. Issues are soil conservation, water quality, non-point source pollution, precision farming, decision support systems for land use planning, and watershed management. Students who want to focus on environmental interactions in a biological system generally select the courses in the Land and Water Engineering limited specialization.

Biological Engineering was organized around on-going activities in food engineering (primarily thermal processing of biological materials into food products) and physical properties of biological materials. A new faculty member (Co-author, Agblevor) was hired to develop a program in “Bioprocess Engineering,” defined as the conversion of biological materials into non-food products (fuel and industrial chemicals). Future plans call for expansion of bioprocess engineering activity to include other, higher-value products.

The course described in this paper is titled, “Simulation of Biological Systems.” It is one of the courses designated as a core course for both limited specializations. This course provides the foundation which the students need for subsequent courses in their limited specialization. Organization of the course was a compromise between Biological Engineering students who do not want to spend too much time studying plants and Land and Water Engineering students who do not want to spend too much time studying microbial processes.

The faculty decided that mathematical description, and subsequent simulation, of a biological system provides understanding that is valuable to students in both specializations. For example,

effluent from a bioprocessing operation is processed in a wastewater treatment facility and released onto the land to grow new plants, which become the feedstock for the bioprocessing operation. Undergraduates need to be introduced (in a responsible way) to the upstream and downstream issues on either side of the problem they are solving. After all, they are being educated as Biological *Systems* Engineers.

There is a need for balance in a core course like “Simulation of Biological Systems.” Students need to identify part of the course as “my stuff.” Achieving balance was a key challenge in organizing the course. A second challenge was the amalgamation of the different techniques used to develop different types of models. There has to be a commonality in approach for students to learn at the pace dictated by a semester-length course.

Prerequisites

The course is taught during the spring semester of the junior year. Thermodynamics and fluid mechanics are prerequisites. Students have completed their mathematics through differential equations and their biology sequence. Organic chemistry is not a prerequisite, though many students will have completed this course when they take “Biological Systems Simulation.”

No text book was found that brought together the various topics that needed to be covered. Consequently, a set of classnotes were assembled using some material from other texts and some new material. Copywrite permission was obtained by the copy center where the notes are purchased by the students. The course was taught for the first time in spring, 1996. The notes were revised and a second draft is now available.

Course Outline

The course material is presented by summarizing each chapter in the classnotes. Much effort has been expended to reorganize the material so that it flows in a logical manner. Hopefully, this continuity is communicated by the relatively brief chapter summaries.

Chapter 1

Chapter 1 gives a brief introduction to the methodology of dynamic system analysis. Two biological systems are simplified to the point where they can be represented by first order differential equations. The student learns to apply the mathematics learned in calculus and ordinary differential equations to biological systems. Principles learned in fluid mechanics are applied to write a mass balance for a control volume. An energy balance for a control volume is written using principles learned in thermodynamics. Chapter 1 shows the student that all the engineering science courses are important in the analysis of biological systems.

All students at Virginia Tech take a common freshman year. They learn FORTRAN in their Engineering Fundamentals courses. In the future they may learn C; this decision is currently being debated. Since they know FORTRAN, the assignments require that everyone program in FORTRAN.

A simplified carbon flow model for a plant leaf is shown in Figure 1. Some of the CO₂ captured by photosynthesis is used for respiration and some is converted to carbohydrate. Some of this carbohydrate is subsequently used for leaf cell growth, and some is translocated to the stem.

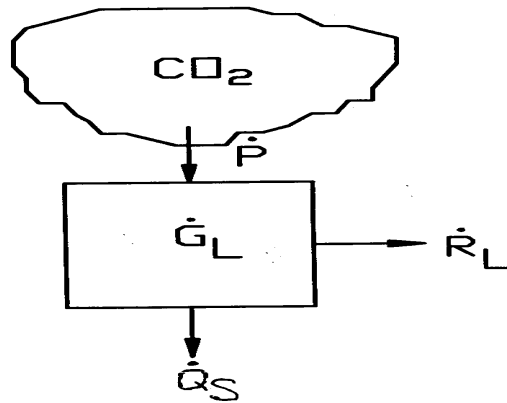


Figure 1. Simplified carbon flow model for a plant leaf.

The concept of mass flow into and out of a reservoir is shown in Figure 2. Here, water accumulates in the reservoir until the head (H) is large enough to cause flow, ($\dot{Q}_o = \dot{Q}_i$).

$$A \frac{dH}{dt} + k \sqrt{H} = \dot{Q}_i \quad (1)$$

Students use numerical integration to solve this equation and plot H vs t. The objective is to insure that they are never again intimidated by a non-linear differential equation. Most students need to review their programming skills, so a FORTRAN program is required.

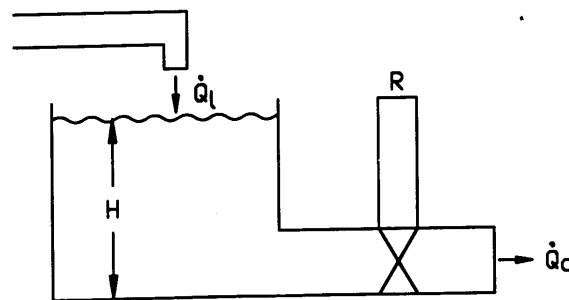


Figure 2. Model of mass flow into and out of a reservoir.

The concept of a control volume (Figure 3) is used for the derivation of an energy balance. The resulting equation is

$$\begin{aligned} \text{heat added} &= \text{change in internal energy} \\ &+ \text{work done} \end{aligned}$$

$$\Psi = \left(\frac{\partial E}{\partial t} \right)_{c.v.} + \int (h + \frac{v^2}{2} + gz) dM_{out} \quad (2)$$

$$- \int (h + \frac{v^2}{2} + gz) dM_{in} + P_{shaft} + P_{shear}$$

If flow is one dimensional, and the heat added and work done is expressed on a per unit mass basis, then Eq. (2) condenses to

$$Q = W + h_2 - h_1 + \frac{v_2^2 - v_1^2}{2} + g(z_2 - z_1) \quad (3)$$

In the problems solved in this course, velocity change and elevation change are not important. There is no work delivered to the surroundings, therefore, Eq. (3) reduces to

$$\text{heat added} = \text{change in enthalpy} \quad (4)$$

$$Q = h_2 - h_1$$

The review of principles learned in thermodynamics and fluid mechanics is done to show how these principles relate to the models that will be subsequently developed for biological systems. It requires about four lectures for the Chapter 1 material.

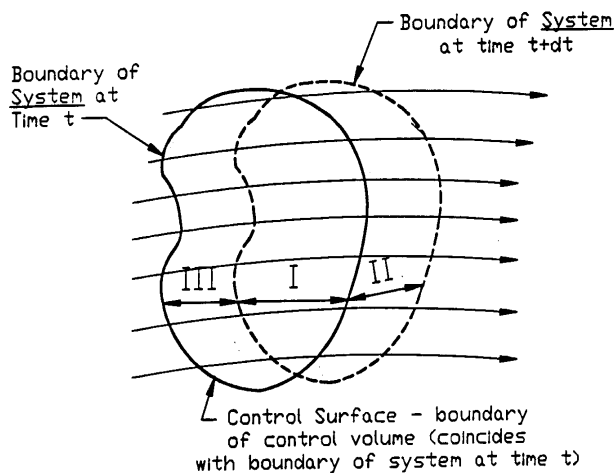


Figure 3. Definition of a control volume used for derivation of mass balance and energy balance.

Chapter 2

The drying of plant material is covered in Chapter 2. Here, the emphasis is on the energy balance for the process. Psychrometric equations are presented and used to describe the flow of mass (moisture) and energy (heat). Upon completion of the simulation assigned in this chapter, the student understands how to solve drying problems and can understand the handbook material used to design drying facilities for biological materials.

The simulation problem assigned is tobacco curing. During a tobacco cure, 15 to 30% of the initial dry matter is lost due to breakdown of compounds in the leaf. The energy released by these reactions must be accounted for in energy balance. Later in the course, the students simulate composting and have to account for the energy release. Plant cells release energy during tobacco curing and microorganisms release energy during composting. Using tobacco curing as the drying example, introduces a concept, which is later reinforced by the study of composting.

Equations given in ASAE D271.2 are used to write a psychrometric subroutine. Data sets are available from tobacco curing experiments conducted in Georgia during the late 1970s. The students use dry bulb temperature and relative humidity to calculate the humidity ratio and enthalpy of the ambient air. Exhaust air conditions are calculated using dry bulb and wet bulb data.

A control volume is defined to coincide with the external surface of the curing structure, and an energy balance is written.

$$\dot{Q}_p + \dot{Q}_r + \dot{Q}_f = \dot{Q}_x + \dot{Q}_s + \dot{Q}_m \quad (5)$$

where \dot{Q}_p = energy that enters (or exits) the control volume due to radiation exchange with surroundings,
 \dot{Q}_r = energy released as a by-product of chemical reactions in the leaf,
 \dot{Q}_f = supplemental heat added,
 \dot{Q}_x = exchanged air energy (exhaust-entering),
 \dot{Q}_s = conductive heat loss plus sensible heat stored in structural materials, and
 \dot{Q}_m = sensible heat stored in material being dried.

Expressions are derived in the notes and in class for each of the rate functions. Students are given the percentage of total moisture removed during each 24-h period of the 6-day (or 5-day) cure. They are asked to calculate the required air exchange rate (air changes/h) and the total supplemental heat required.

Three moisture removal schedules are given. The students generate air exchange schedules for each and compare the supplement heat requirement for each schedule in their reports. Two weeks are allowed for the assignment.

Chapter 3

Fermentation is the model for many bioconversions. New opportunities for the use of microorganisms to produce useful products are emerging. It is estimated that over 200 commercial products are currently produced with fermentations. For example, the distinctive look of stone-washed jeans is produced by an enzyme that breaks down the dye; the enzyme is produced by a fermentation process.

The Michaelis-Menten and Briggs-Haldane models for enzyme catalyzed reactions are derived. The notes contain a step-by-step analysis of competitive and non-competitive inhibition. The influence of partially competitive inhibition on reaction rate is not derived. Most of the material in Chapter 3 comes directly or indirectly from Lee⁵.

The first assignment for the enzyme kinetics material is the solution of three simultaneous differential equations.

$$\frac{dC_p}{dt} = k_3 C_{ES} \quad (6)$$

$$\frac{dC_{ES}}{dt} = k_1 C_s C_E - k_2 C_{ES} - k_3 C_{ES} \quad (7)$$

$$\frac{dC_s}{dt} = -k_1 C_s C_E + k_2 C_{ES} \quad (8)$$

The Advanced Continuous Simulation Language (ACSL, 1986) software is used to solve these equations. Students are given mainframe accounts and instructions on how to run an ACSL program. With a little one-on-one help, the students quickly learn how to create and run a program. Their assignment requires them to change the rate constants, run several simulations, and write a report discussing the results.

The effect of mass transfer resistance on reaction kinetics of an immobilized enzyme is discussed, first with a derivation of external resistance, then internal resistance. Assuming Michaelis-Menten kinetics, the following simultaneous equations are derived to describe internal mass transfer resistance.

$$\frac{dC'_s}{dr'} = Y \quad (9)$$

$$\frac{dY}{dr'} = \frac{-2}{r'} Y + \frac{9\phi^2 C'_s}{1 + \beta C'_s} \quad (10)$$

For all previous problems, the independent variable was time, t . Here the independent variable is the spatial variable, r' . ϕ relates reaction rate to rate of mass transfer by diffusion.

$$\phi = \frac{R}{3} \left(\frac{r_{\max}}{D_s K_m} \right)^{1/2}$$

where r_{\max} = maximum reaction rate,
 D_s = diffusivity, and
 K_m = substrate concentration when the reaction rate equals $r_{\max}/2$.

ϕ is small when reaction rate is slow or mass transfer (diffusion) rate is fast. Conversely, ϕ is large when reaction rate is fast or mass transfer is slow.

The assumptions used to derive Eqs. (9) and (10) are:

1. Kinetics of reaction is the same as observed for free enzyme.
2. Mass transfer through the immobilization structure occurs via molecular diffusion.
3. No mass-transfer limitation at the outer surface.
4. The immobilized enzyme can be modeled as a spherical particle.

If ϕ is small enough, the substrate will diffuse to the center of the particle. For this case, identified as Case 1, substrate concentration at $r' = 0$ (center of particle) will be greater than zero. If ϕ is large enough, identified as Case 2, the substrate will be consumed before it reaches the center. At some $r' = R_c$, $C_s^l = 0$.

For their second enzyme kinetics assignment, the students are asked to solve Eqs. (9) and (10) for $\phi = 0.1, 0.5, 1.0, 2.0, 5.0, 10.0, 20.0,$ and 50.0 . For Case 1, they have to guess C_{so}^l (concentration at center) and integrate to determine if $C_s^l = 1$ at $r' = 1$. They write the ACSL program with a logic statement in the Terminal section. C_{so}^l is incremented and the integration repeated until $C_s^l = 1$ at $r' = 1$. To solve Case 2, they have to guess R_c , the radius at which $C_{so}^l = 0$, and integrate to determine if $C_s^l = 1$ at $r' = 1$. The assignment is designed to reinforce their understanding of how mass transfer resistance can influence the actual reaction rate, and teach them that ACSL provides the user with an opportunity to insert a FORTRAN program in the Initial section and another program in the Terminal section. Very sophisticated simulations can be done taking advantage of the numerical integration programming in the Dynamics section and user-written programs in the Initial and Terminal sections.

Chapter 4

The simulation of composting is covered in Chapter 4. Principles for maintaining an optimum environment for microorganisms are illustrated, plus the student gains practical knowledge of an important waste treatment process. A small amount of time is spent on design considerations such as preparation of a windrow composting site to control runoff from the piles. The main

emphasis, however, is the development of a model to predict time for windrow turning, and then the development of a model for in-vessel composting with aeration, but no mixing. The student writes the program to calculate remix times but is given a FORTRAN program for the simulation of in-vessel composting.

Five simultaneous differential equations describe the heat and mass transfer in a compost bed (Keener⁴ et al.). The bed is divided into layers and the control volume is a single layer, the *j*th layer.

$$\frac{dm_c}{dt} = F(m_c, m_e, T, MC_c, O_2, \dots) \quad (11)$$

$$\frac{d m_{cw}}{dt} = -\dot{m}_{evp} - b_{cw} \frac{dm_c}{dt} \quad (12)$$

$$\frac{dm_{da}}{dt} = \dot{m}_{daj} - \dot{m}_{daj+1} - b_{ca} \frac{dm_c}{dt} \quad (13)$$

$$\frac{dm_{aw}}{dt} = H_e \dot{m}_{daj} + \dot{m}_{evp} - H_x \dot{m}_{daj+1} \quad (14)$$

$$\Delta h_c \frac{dm_c}{dt} = (h_{xi} - h_{ei}) \dot{m}_{da} + (m_c C_c + m_{cw} C_w) \frac{dT}{dt} \quad (15)$$

Derivation of these equations is related back to the drying problem; many of the concepts are similar. For example, the energy balance [Eq. (15)] is

$$\text{Energy released} = \text{Exchange air energy} + \text{change in sensible heat}$$

or, in the notation used for the drying problem,

$$\dot{Q}_r = \dot{Q}_x + \dot{Q}_m$$

The energy balance for the compost model is actually a simpler statement than the energy balance for the drying model.

If Eq. (11) is assumed to be a first-order reaction, these five equations can be solved with a FORTRAN program. (The students have some basic knowledge of reaction kinetics at this point, based on what they learned in Chapter 3.) Results are given in Figure 4. The diamond-shaped dots show the times when remixing is needed. Water is added at each remixing to bring the moisture content back to 0.615 (w.b.). The solid curve shows how compost dry matter changes over time.

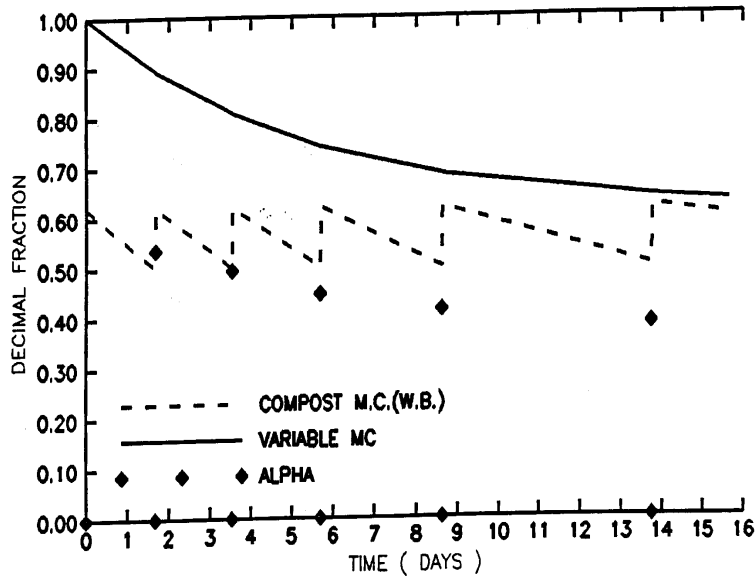


Figure 4. Remix schedule predicted for a yardwaste mixture where moisture is controlled between 0.615 and 0.50 w.b.

A model developed by Stombaugh and Nokes⁶ is used to simulate in-vessel composting. Aeration is provided, but no mixing.

The differential equations derived for in-vessel composting are summarized below. The control volume is an individual layer.

Growth rate of microorganisms:

$$\frac{dX}{dt} = (\mu - k_d) X \quad (16)$$

where $\mu = \mu_{\max} \frac{C_s}{K_M + C_s} \times \frac{O_2}{k_{O_2} + O_2} \times ktemp \times kH_2O$, assuming Monod kinetics

Rate of substrate consumption:

$$\frac{dC_s}{dt} = \frac{1}{Y_{X/S}} \frac{dX}{dt} - \eta X \quad (17)$$

where $\eta = \eta_{\max} \frac{C_s}{K_M + C_s} \times \frac{O_2}{K_{O_2} + O_2} \times k_{temp} \times k_{H_2O}$

Rate of change of oxygen concentration:

$$\frac{dO_{2j}}{dt} = Y_{O_2/S} \frac{dC_s}{dt} + \frac{\dot{v}}{V_L} (O_{2j-1} - O_{2j}) \quad (18)$$

Rate of change of water concentration:

$$\frac{dm_{wj}}{dt} = -Y_{w/S} \frac{dC_s}{dt} - \frac{\dot{v} \rho_a}{V_L} (H_{xj} - H_{ej}) \quad (19)$$

Energy balance for layer:

$$Q_{mj} \frac{dT}{dt} = \Delta h_c \frac{dC_s}{dt} - \frac{\dot{v} \rho_a}{V_L} (h_{xj} - h_{ej}) - Q_{lj}/V_L \quad (20)$$

The structure for the FORTRAN program to solve Eqs. (16) - (20) is provided. The program must sequence through the layers, then increment time and repeat the sequence. It is too much to ask the student to invest the time to write a program with this complexity.

The students use the program provided, add their psychrometric subroutine, and simulate 240 hours of in-vessel composting. Average moisture content (Figure 5) and substrate concentration (Figure 6) are shown as sample output. When the various layers dry out, the microbial population dies and no more substrate is consumed. In Figure 6, the substrate concentration at 240 hours is higher in Layer 1 than in Layer 5. Layer 1 dries out quickly, thus the microbial population dies before consuming a significant amount of substrate.

Examining results like Figures 5 and 6 helps the student to understand how the composting process changes throughout the bed. When these results are discussed in class, a portion of the lecture is used to relate the layer simulation technique to thin-layer drying of grain. Very similar procedures are used.

Total time spent on composting is about four weeks. This material is of direct interest to the Biological Engineering Students and the Land and Water Engineering students.

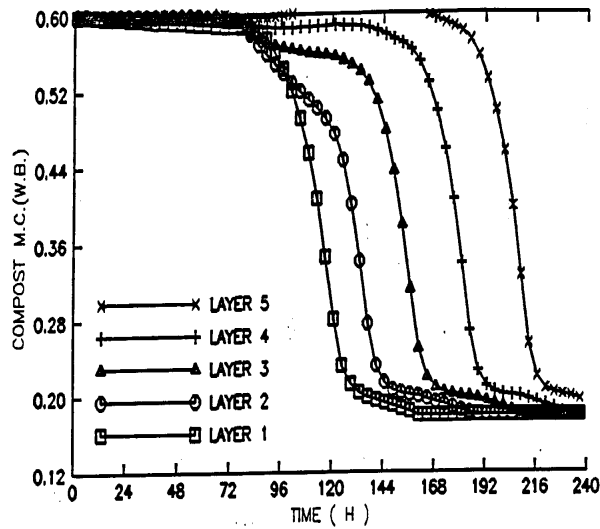


Figure 5. Average moisture content in each layer.

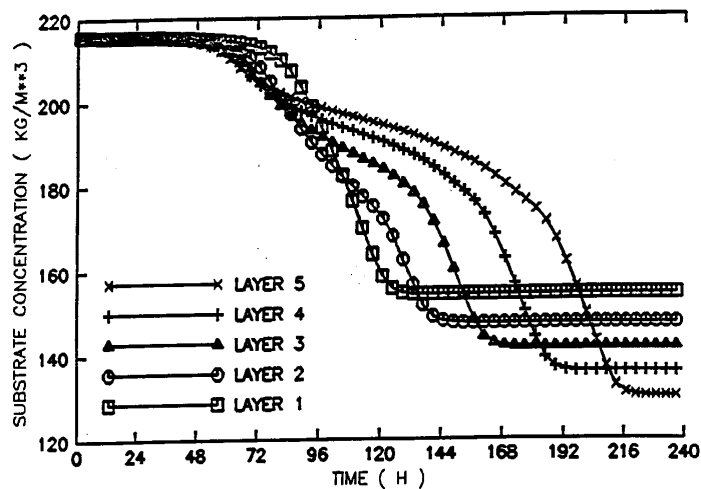


Figure 6. Substrate concentration in each layer.

Chapter 5

Chapter 5 presents a review of photosynthesis. Radiant energy is converted to chemical energy when a plant converts CO₂ to carbohydrate. Subsequent plant growth is the basis for all life on planet earth.

The reference for Chapter 5 is Barden² *et al.*, and since two of the authors are on the faculty at Virginia Tech, it is convenient to ask one of them to present three lectures to review photosynthesis, photorespiration, and respiration.

The net equation for the production of a glucose molecule by the Calvin Cycle (Figure 7) is

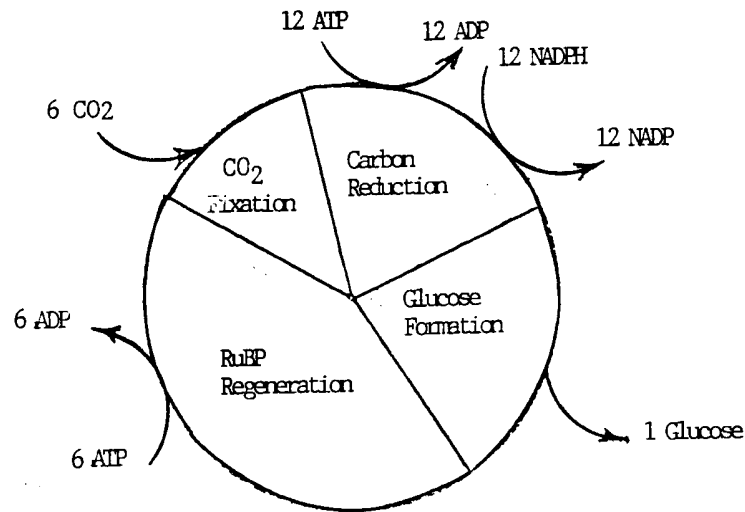
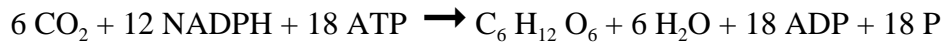


Figure 7. Simplified Calvin cycle.

The purpose for Chapter 5 is to reinforce the student's understanding of how a plant captures, uses, and stores energy. This understanding is essential to the modeling of plant growth.

Chapter 6

Plant growth models are reviewed in Chapter 6. SIMED, a carbon flow model for simulation of alfalfa growth (Holt³ *et al.*), and SORGF, a grain sorghum growth model (Arkin¹ *et al.*), are discussed in more detail. Several parameters derived for corn growth modeling are also discussed. Two lectures are used to discuss EXNUT, an expert system for peanut production developed by USDA-ARS.

Historically, average yield of major crops in the United States have increased about 2% per year. These yield increases were primarily achieved using the following methods.

1. Develop higher yielding varieties
2. Develop varieties with insect and disease resistance
3. Develop improved management practices

The implementation of these methods is complicated by the fact that many variables interrelate in the growing of a plant. A high-yielding variety at one location may do very poorly at another location. Often, different locations with different environments require different management practices.

Sorghum is determinate, meaning that the individual plants produce a genetically predetermined number of leaves. Alfalfa is not determinate; the plant continues to put on leaves until it is killed by frost. Alfalfa is a C₃ legume and sorghum is a C₄ grass. Studying models of these two very different species gives the student a wide range of experience.

Considerable time is spent in Chapter 6 studying mathematical expressions for physiological processes. The study does not reveal significant opportunity for a manager to influence maximum crop yield. Ambient temperature and humidity, defined by the weather pattern, are uncontrolled inputs, as is solar radiation. The one variable that can be controlled is soil moisture. Biological Systems Engineers are very concerned with soil moisture levels, movement of water through the soil, and removal of moisture by a growing crop.

Models developed in Chapter 6 use a multiplicative factor to reduce plant growth when soil moisture is limiting. In SORGF, net CO₂ fixed during the *i*th day is

$$P_i = P_{oi} P(T) P(S) - N_i \quad (21)$$

- where P_{oi} = net CO₂ fixed during *i*th day for nonlimiting moisture and temperature conditions,
 $P(T)$ = multiplicative factor between 0 and 1 associated with a temperature limiting condition,
 $P(S)$ = multiplicative factor between 0 and 1 associated with a soil moisture limiting condition, and
 N_i = Nighttime respiration losses.

The $P(S)$ factor is 1 when extractable soil water is above 20%. Studies on sorghum, a drought-tolerant crop, have shown that when approximately 80% of the extractable soil water is depleted by evapotranspiration, net photosynthesis is reduced. SORGF requires the following input: soil water holding capacity, initial available water, and rainfall. These inputs are used, along with calculated evapotranspiration losses, to determine extractable soil moisture available each day.

SIMED deals with physiological and environmental factors in a much more detailed way than SORGF. This model attempts to partition the carbon that is captured by photosynthesis as structural and nonstructural carbohydrate in the leaf, stem, and root (Figure 8). The rate equations for the leaf processes are shown as examples.

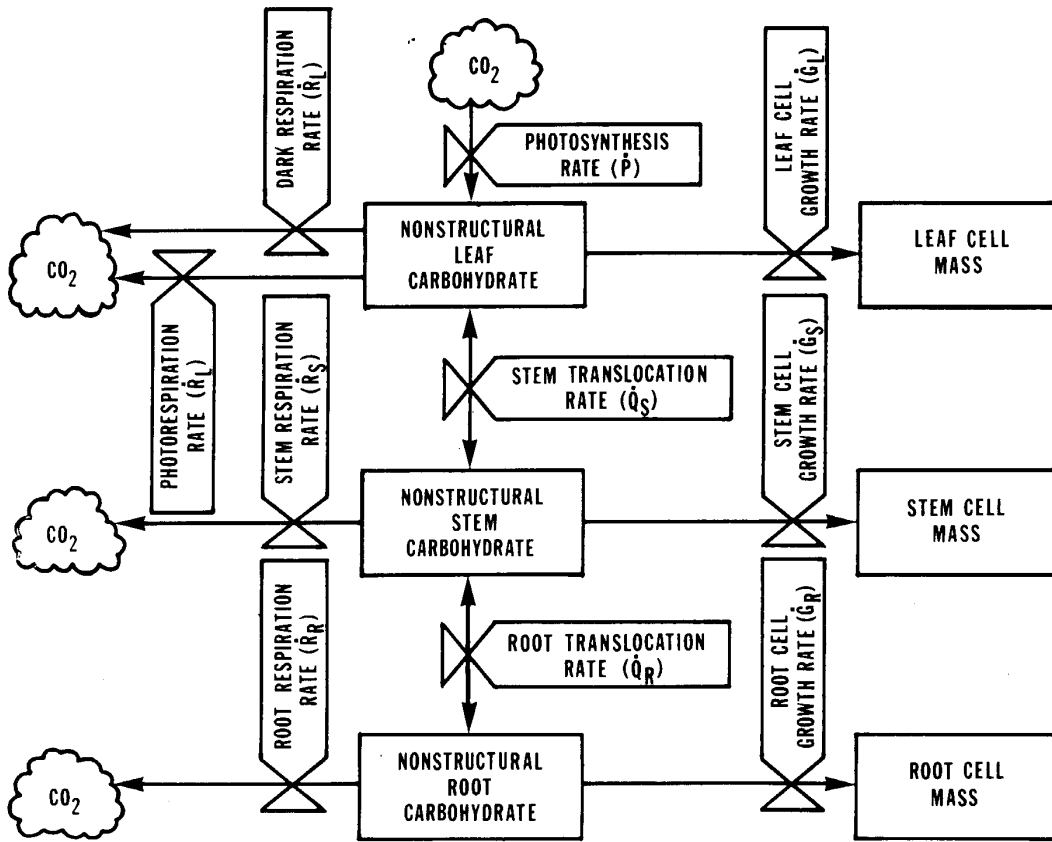


Figure 8. Conceptual framework for SIMED, a crop growth model for alfalfa.

Photosynthesis:

$$\dot{P}_i = 0.1 W_L \frac{I}{1.8} P(M_L) P(A_L) P(C_L) \quad (22)$$

Leaf Respiration:

$$\dot{R}_{Li} = 0.002 W_L R_L (C_L) [R_L(M_L) 2^{(T_a-25)/10} + \frac{I}{1.8} 3^{(T_a-25)/10}] \quad (23)$$

Leaf Cell Growth:

$$\dot{G}_{Li} = 0.0083 W_L G_L (T_a) G_L(C_L) G_L(M_L) G_L(H) G_L(V_A) \quad (24)$$

Translocation Between Leaf and Stem:

$$\dot{Q}_{si} = 0.031 W_L Q_s (T_a) Q_s (C_{SL}) Q_s (V_A) \quad (25)$$

SIMED does not include a factor for soil moisture. Moisture limitation is dealt with using a vapor pressure factor. The developers of SIMED argue that leaf processes slow when the atmospheric vapor pressure deficit (concept learned in Chapter 2) is above 1.5 kPa. Atmospheric vapor pressure can be calculated from weather station data, whereas soil moisture is a much more difficult parameter to calculate.

The students are not assigned a simulation of one of the crop growth models. They are given a simple model and asked to simulate nitrogen accumulation in Helleberr leaf tissue using different rates of nitrogen application in irrigation water.

Chapter 7

As previously mentioned, modeling of plant growth is dependent, in large degree, on the accuracy of the soil moisture parameter. Chapter 7 deals with soil moisture and plant water use. Development of this chapter is not complete at this writing. It will introduce the Land and Water Engineering students to concepts that will be more fully developed in subsequent coursework.

SUMMARY

A Biological Systems Engineering curriculum at Virginia Tech has evolved from a traditional Agricultural Engineering curriculum. Two limited specializations are offered: Land and Water Resource Engineering and Biological Engineering.

One of the courses designated as a core course for both specializations is “Simulation of Biological Systems.” This course is taught during the spring semester of the junior year. Students learn the mathematical techniques used to simulate the drying of biological material, growth of microorganisms, and growth of plants.

Each problem begins with a derivation of the relevant differential equations. Principles learned in thermodynamics and fluid mechanics (both prerequisites) are applied to biological systems. The students write FORTRAN programs or use the Advanced Continuous Simulation Language (ACSL) software for their assignments. Other software (word processors, EXCEL, TK Solver, etc.) is available to the students and used at their discretion.

Mathematics is a tool that greatly aids our understanding of biological systems. Programming is a tool that greatly aids our understanding of mathematics. The assignments are organized to progressively teach the key concepts. Certain guidance for the layout of the programs is given, often in the form of an example program. Teaching programming skills is not the objective. Programming reinforces understanding of the mathematics which reinforces understanding of the concept.

Considering the “business” of our engineering curriculums, most students need to hear a concept several times before it is really becoming a part of their thinking. Applying the same techniques (and notation) to several different kinds of problems within the framework of a single course aids this process.

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