<table>
<thead>
<tr>
<th>Week</th>
<th>Description</th>
<th>Reading Material</th>
</tr>
</thead>
</table>
| 6    | Modeling Temperature Effects on Biological Systems  
  • Effects on chemical reaction rates  
  • Effects on biological activity, general  
  • Effects on developmental processes in plants and other biological organisms  
  • Degree-day models: basis for and use of | Keen & Spain (1992), Ch. 12  
 Handout; degree-days |
Weeks 6 Objectives

1) To review how temperature affects biological and agricultural systems
2) To gain insight into modeling temperature effects on biological and biophysical systems
   a) Continuous processes
   b) Discrete events
Topics on Temperature Effects

- Temperature in the environment
- Heat flow, heat balances
- Temperature control (physical, biological)
- Chemical reactions
- Enzyme activity
- Biological activity
- Developmental processes in biological systems
- Degree-days
Temperature in the Environment

• Affects all biological systems,
• Thus it is usually an important environment variable that changes over time (exceptions?)
• It interacts with other environmental variables
• Measurements of T are normally required
• May be possible to compute T vs. time for certain model uses or times
• May interact with other model components and thus may need to be modeled dynamically as a state variable
Estimating Temperature of the Environment

- Annual variation in daily mean temperature

\[ \bar{T}_{\text{day}}(t) = (\bar{T}_{\text{annual}} + T_{\text{amp}} \cdot \sin[2\pi \frac{(t-t_c)}{365}]) \]
Estimating Temperature of the Environment

- Temperature variations during a day


**Daytime**

\[ T(t) = T_{\text{min}} + (T_{\text{max}} - T_{\text{min}}) \cdot \sin[\pi \frac{(t - 12 + d/2)}{d + 2p}] \]

\[ d = \text{daylength, h} \]
\[ p = \text{time from noon when maximum temperature occurs, h} \]

**Night Time**

\[ T(t) = \frac{T_{\text{min}} - T_{\text{sunset}} \cdot \exp(-n/T_C) + (T_{\text{sunset}} - T_{\text{min}}) \cdot \exp(-(t - t_{\text{sunset}})/T_C)}{1 - \exp(-n/T_C)} \]

\[ n = \text{night length (24-d), h} \]
\[ T_C = \text{nocturnal time coefficient, about 4 h} \]
Temperature during a day

Figure 3.3. The average daily progression of air temperature in the months December, March, June and September in De Bilt, The Netherlands (solid lines). The broken line is the result of Eqns 3.9 and 3.10.
Temperature

• May vary with system dynamics
• May have to model temperature dynamically
Heat Loss and Changes in Temperature

• From Week 3 lectures:

\[ \frac{dT(t)}{dt} = -k[T(t) - T_E] \]

Where:

- \( T(t) \) is temperature of an object, \( ^\circ \text{C} \)
- \( T_E \) is environment temperature, \( ^\circ \text{C} \)
- \( k \) is a heat transfer or cooling constant, with units 1/t
Cooling Simulation, Ex. 1-6

Exact Solution

\[ T(t) = T_E + (T(0) - T_E)e^{-kt} \]

Numerical solution

\[ T(t) = T(t-1) - k[T(t-1) - T_E] \]

For \( t > 0.0 \); initial conditions \( T(0) \)
But, Prior Equations Do Not Show Heat Flow

Starting with heat:

\[ \Delta Q = mc_p \Delta T \]

and

\[ \frac{dQ}{dt} = mc_p \frac{dT}{dt} \]

Where
\[ \Delta Q = \text{change in heat of an object, calories} \]
\[ m = \text{mass of the object, g} \]
\[ c_p = \text{specific heat, a property of the mass, calories g}^{-1} \text{oC}^{-1} \]
\[ T = \text{temperature, } ^\circ\text{C} \]

and heat is the extensive variable that flows from one object to another; temperature is an intensive variable related to the heat content of a body
Written differently

\[ m \cdot c_p \frac{dT(t)}{dt} = -k[T(t) - T_E] \]

or

\[ \frac{dT(t)}{dt} = -\frac{k}{m \cdot c_p} [T(t) - T_E] \]

with, \( k \) = the conduction heat transfer coefficient and now, units of \( k \) are (calories °C\(^{-1}\) time\(^{-1}\))
Set Point Temperature Control

Heater (on/off)

\[ h = 0 \text{ if } T > T_{set} + \text{tol} \]

\[ h_{\text{max}} \text{ if } T < T_{set} - \text{tol} \]

\[
\frac{dT(t)}{dt} = \frac{h}{m \cdot c_p} - \frac{k}{m \cdot c_p} [T(t) - T_E]
\]
Proportional Temperature Control

Proportional control (lags in sensing temperature & heater output)

\[ h = h_{\text{max}} (T_c - T_s) \text{ if } T_s < T_c \]

otherwise, \( h = 0 \)

\( T_s \) = temperature of sensor

\( T_c \) = control or desired temperature

\[
\frac{dT(t)}{dt} = \frac{h}{m \cdot c_p} - \frac{k}{m \cdot c_p} [T(t) - T_E] - \frac{k_s}{m_s \cdot c_{sp}} [T(t) - T_s(t)]
\]

\[
\frac{dT_s(t)}{dt} = \frac{k_s}{m_s \cdot c_{sp}} [T(t) - T_s(t)]
\]
Implications

- Simple examples show lags in temperature control
- Both demonstrate very simple forms of feedback control
- Biological control systems are similar
  - Feedback control of body temperature
  - Usually, more like proportional control such that internal heat production, for example, varies in response to a biological setpoint or range
  - Lags also exist between a state and output from the biological control system (sensing, metabolism, muscle response, etc.)
  - What are other examples of biological control systems?
Temperature and Chemical Reactions

- Arrhenius equation
- $Q_{10}$ approach
- Also used directly in some enzyme-substrate reactions
Arrhenius Equation

Consider the equation:

\[
\frac{dS}{dt} = f_i - k(T) \cdot S
\]

where

- \( f_i \) = flow rate of S into reaction
- \( K(T) \) = rate constant, dependent on temperature
Arrhenius Equation

- Assumes that substrate (S) must reach an activated state ($E_a$) for the reaction to occur.
- The faster that S reaches the activation state, the faster the reaction rate.

See Thornley and Johnson (Chapter 5).
Arrhenius Equation

\[ A = \text{a constant} \]
\[ E_a = \text{Energy of activation} \]
\[ R = \text{gas constant} \]
\[ T = \text{Absolute Temperature, } 0\,\text{K} \]

\[ k = A \exp\left(-\frac{E_a}{RT}\right) \]

\[ \frac{dS}{dt} = f_i - k(T) \cdot S \]

\( \frac{E_a}{R} \) typically in range of 5,000 to 15,000 K
**Q\textsubscript{10} Approximation**

- \( Q\textsubscript{10} \) is the factor at which the rate constant, \( k \), increases for a temperature increment of 10 \(^{0}\)K
- Empirical, based on observations
- Also 3 parameters to estimate

\[ k = k_r Q_{10}^{[(T-T_r)/10]} \]
Conceptual Pools of Enzymes

Fig. 3.6. Control enzyme states: active and low- and high-temperature inactive. The transition rates between states $\mu_i$ are assumed to have a mean rate described by the exponential distribution.
Enzyme Reactions

- Have optimal temperature range
- Enzymes assumed to be in inactive state (denatured), initial active state, and activated state (Ea), depending on temperature
Enzyme Reaction Rate

\[ k(T) = \frac{A \exp(-E_a / RT)}{1 + \exp(\Delta S / R - \Delta H / RT)} \]

\( \Delta H = \) enthalpy of reaction
\( \Delta S = \) entropy of reaction
Others same as in Arrhenius equation
Enzyme Reaction Rates vs. Temperature

Fig. 5.7. Rate constant $k$ for the case when equilibrium between two species, one active and the other inactive, is assumed (eqn (5.3d)): (a) $A = 3.2 \times 10^{12}$, $E_a/R = 7.5 \times 10^3$ K, $\Delta S/R = 48$, and $\Delta H/R = 15 \times 10^3$ K; (b) $A = 1.3 \times 10^{23}$, $E_a/R = 15 \times 10^3$ K, $\Delta S/R = 81$, and $\Delta H/R = 25 \times 10^3$ K. The parameter values have been chosen so that $k$ is a maximum at $T = 310$ K and takes the value 50 at the maximum.
Enzyme Reaction Rates vs. Temperature

Parameters must be estimated (4) from data [A, Ea/R, ΔH/R, ΔS/R]

*Fig. 5.1. Temperature response of the specific growth rate of *Escherichia coli* (adapted from the data of Ingraham (1958)). The curve has been drawn by eye.*
Estimation of Enzyme Parameters

Other Equations for Temperature Effects on Biological Systems

\[ k_T = k_{\text{max}} U^x \exp(xV) \]

\[ U = \frac{T_{\text{max}} - T}{T_{\text{max}} - T_{\text{opt}}} \]

\[ V = \frac{T - T_{\text{opt}}}{T_{\text{max}} - T_{\text{opt}}} \]

\[ x = \frac{W^2 (1 + \sqrt{1 + 40/W})^2}{400} \]

\[ W = (Q_{10} - 1)(T_{\text{max}} - T_{\text{opt}}) \]

O’Neill et al. (1972)

Keen and Spain, pp193-4
Other Equations for Temperature Effects on Biological Systems

Logan (1988)

\[ k_T = k_1 \left( \frac{\tau_1^2}{\tau_1 + k_2} - \exp(-\tau_2) \right) \]

with

\[ \tau_1 = (T - T_{\text{min}}) \]

\[ \tau_2 = \frac{T_{\text{max}} - T_{\text{min}}}{T_{\text{max}} - T_{\text{opt}}} \]

Keen and Spain, pp193-4
Temperature Effects on Enzyme-Mediated Reactions

Figure 12.3. Curves showing simulation results of response of enzymes to different temperatures.
Discussion

• Arrhenius
• $Q_{10}$
• Enzyme, biological reactions
• Practical implications
  – Parameter estimation
  – Normalization
  – Implementation
Temperature and Development

• Temperature has major influence on developmental processes of plants, insects, other organisms
• Duration of time between egg and pupae in insects may vary between 8 and 40 days, depending on temperature
• Similarly, duration of time from planting to emergence, time from emergence to 1st flower, time needed to complete its lifecycle to maturity, etc. depend strongly on temperature
Experiments to Measure Development

Typically, temperature treatments, each having a constant temperature
Time measured until a particular development stage (duration)

Fig. 3.2. Boll weevil egg to adult emergence times in flowerbuds for various constant temperature experiments as compared with the best-fit exponential curve. (Experimental data are from Isely 1932.)
Development Rates Computed as Reciprocal of Duration

Development "rate" is the inverse of days required to complete a phase

\[ k_d(T) = \frac{1}{\text{Dur}(T)} \]

Units are \((1/\text{time})\)

Fig. 5.12. Temperature summation rule: \(k_d\) is the developmental rate, \(T\) is the temperature, and \(T_c\) is a temperature threshold. The line drawn represents a linear approximation to development (cf. eqns (5.7j) and (5.7n)). The data points (●) denote the germination rate of mustard seed (the reciprocal of the time for 50 per cent germination) and are derived from Simon et al. (1976).
Modeling Development

If temperature varies with time, one can integrate development rate (which is dependent on temperature) until cumulative development is equal to 1.0.

The general relationship for computing a development index, $h_{ij}$ is:

$$h_{ij} = \int_{t_i}^{t_j} k_d \cdot dt$$

$h_{ij}$ = index of progress along the development pathway from i to j.

The length of the phase is $t_i - t_j$, also referred to as Developmental time.

$h_{ij}$ starts at 0.0 at $t_i$ and progresses until 1.0 at $t_j$ when stage j occurs.
Another way to write this equation is:

\[
\frac{dh_{ij}}{dt} = k_d
\]

Where \( k_d \) is a function of Temperature (or \( k_d(T) \), and \( T \) may vary with time (then \( k_d = k_d(T(t)) \)). This is in the same form as our rate equations, and can be solved using Euler. This will be shown later on, with a \( \Delta t = 1 \).

How would \( k_d \) vary with Temperature? How would Temperature vary with time?
From figure 5.12 in Thornley and Johnson,

\[ k_d = \text{slope} \times (T - T_B) \]

where \( T \) units are \( ^0K \) and slope units are \( 1/(^0C-t) \)

or

\[ k_d = 0.0588 \times (T-3.0) \]

If \( T \) is \( ^0C \)

**Plant and crop modelling**

**Fig. 5.12.** Temperature summation rule: \( k_d \) is the developmental rate, \( T \) is the temperature, and \( T_c \) is a temperature threshold. The line drawn represents a linear approximation to development (cf. eqns (5.7j) and (5.7n)). The data points (○) denote the germination rate of mustard seed (the reciprocal of the time for 50 per cent germination) and are derived from Simon et al. (1976).
Modeling Germination

\[ h_{ij} = \int_{t_i}^{t_j} k_d \cdot dt \]

or in our example:

\[ h_{ij} = \int_0^{t_j} [0.0588 \cdot (T - T_B)] dt \]

Fig. 5.12. Temperature summation rule: \( k_d \) is the developmental rate, \( T \) is the temperature, and \( T_c \) is a temperature threshold. The line drawn represents a linear approximation to development (cf. eqns (5.7j) and (5.7n)). The data points (●) denote the germination rate of mustard seed (the reciprocal of the time for 50 per cent germination) and are derived from Simon et al. (1976).
Modeling Germination

\[ h_{ij} = \int_{0}^{t_j} [0.0588 \cdot (T - T_B)] dt \]

which can be approximated via Euler:

\[ h_{ij} = \sum_{0}^{t_j} [0.0588 \cdot (T - 3)] \cdot \Delta t \]

When the summation \((h_{ij}) = 1.0\), germination occurs.

\(T_B = \) base temperature, \(^0K\) or \(^0C\)
Modeling Germination

- The 0.0588 can be moved outside the summation sign (it is constant),
- And if \( \Delta t = 1 \), then we can re-write the equation as:

\[
\frac{h_{ij}}{0.0588} = \sum_{o}^{t_j} (T - 3) \cdot 1
\]

- When \( h_{ij} = 1 \), germination occurs, and at this time, the left side of the equation above is \((1/0.0588) = 17.0\)
- Note that units of the left side of the equation are in \(^0C\)-time; if time is in days, units are \(^0C\)-days
Modeling Development Using Degree-Days

The previous equation can be generalized to show the widely-used degree-day model

\[ DD = \sum_{o}^{t_j} (T - T_B) \]

Where DD = degree days
and the summation is carried out until a Threshold is reached
When the threshold is reached (on day \( t_j \)), development is complete and the germination (or other event) occurs on that day

In the example above, the threshold would be 17.0
Degree Days

- Check units on DD, what are they?
- What are the assumptions of this method?
- Can it be further generalized?
- How can you compute the parameters needed to use DD to model time to first flower, time to germination, time to maturity, time between egg and larvae, ???
Modeling Development

\[ h_{ij} = \int_{t_i}^{t_j} k_d \cdot dt \]

What if \( k_d \) is not linear? We have seen how enzyme kinetics depend on temperature, and the internal biological reactions that lead to development are enzyme reactions.
What if $k_d$ is not linear? In many models, $k_d$ is approximated by a piecewise linear function:

$$h_{ij} = \int_{t_i}^{t_j} k_d \cdot dt$$

**Fig. 3.3.** Degree-day rate function with temperature thresholds of 12 and 35°C.
Development in Varying Temperature Environments

- Assumption is that development continues at the temperature it experiences, with no lags, memory effect, etc.
- Choice of using daily average vs. hourly temperatures will affect results
Discussion

• Temperature in the environment
• Heat flow, heat balances
• Temperature control (physical, biological)
• Chemical reactions
• Enzyme activity
• Biological activity
• Developmental processes in biological systems
• Degree-days
Homework Set 4  
ABE 5646  
Due on February 19, 2010  

1. Work camel body temperature simulation problem 12-3 in Keen & Spain, pp. 187-188  

2. Work problem 12-4 in Keen & Spain on enzyme-catalyzed reactions, p. 191  

3. Use the O’Neill temperature function with the following parameters:  
   \[ Q_{10} = 2.1 \quad T_{\text{max}} = 40 \]  
   \[ T_{\text{opt}} = 28 \quad k_{\text{max}} = 0.025 \text{ (units of d}^{-1}) \]  

   a. Plot rate \( (k_T) \) vs. Temperature \( (T) \) over the range of 0 to 40 °C.  
   b. Assume that we want to use a linear approximation to this function for temperatures below 30 °C, what are the slope and intercept values?  
   c. Explain how you could use this approximation with a degree-day model. What would the threshold be for development?
Questions?