Modeling Temperature in Compost

Blerta and Marc and others! :-)

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Abstract

Making compost relies on microbial processes to break organic matter down...

Introduction

Any references would be greatly appreciated.

I would like to craft this next week, so we can both agree on its content before Spring break.

Problem Statement

Composting is a process. In spite of our appreciation of the decomposition process, the breakdown of organic matter from "raw waste" into "mature compost" may rely on numerous indicators that signify maturity. But determining what maturity means is far from deterministic.

Many uses of compost require a mature product that prevents nutrients present in the soil from being tied up (immobilized). Therefore, mature compost is important because it will not adversely affect plant development due to reduced oxygen or nitrogen availability and/or the presence of phytotoxic compounds.

However, immature compost products can be used beneficially. For example, conventional growers may apply unstable compost to increase soil organic matter. They may not intend to plant for several weeks, or may not be concerned about a small amount of nitrogen immobilization from unstable compost. In general, immature compost is used to build organic matter content in depleted soils.

Why is Compost Maturity Important?

Stability and maturity are terms often used to characterize compost, yet compost specialists have varying opinions about what these terms mean.

The term "stable" typically refers to a compost that is not undergoing rapid decomposition and whose nutrients are slowly released into the soil. Stability is important in determining the potential impact of the compost material on nitrogen availability in soil or growth

media. Stable compost consumes little nitrogen and oxygen and generates little CO_2 or heat. Unstable, active compost demands nitrogen when applied to soil and growth media.

Composts that cause nitrogen deficiency can be detrimental to plant growth, even causing death to plants in some cases. If stored improperly and left unaerated, unstable compost can become anaerobic and generate nuisance odors. Maturity is the degree or level of completeness of the composting process. For mature compost, raw starting materials (feedstocks) have been sufficiently decomposed to produce a stable product. In contrast, immature compost may contain one or more compounds that inhibit plant growth, may contain viable weed seeds, or have other undesirable characteristics, such as odor.

Compost Laboratory Analysis Maturity cannot be described by a single property, but can be measured by two or more chemical and biological properties. The California Compost Quality Council (CCQC) has developed a numerical âĂIJMaturity IndexâĂİ that uses standard laboratory test methods to rate compost maturity.

CCQC Maturity Index

The CCQC Maturity Index uses a sampleâĂŹs organic carbon-to-nitrogen ratio as an initial pass/fail screening. A compost sample must have C:N ratio equal to or less than 25:1 to be considered mature enough for further testing. If a compost sample passes this initial screening, it is then subjected to two sets of tests.

Tests from group A measure whether adequate decomposition has occurred by measuring carbon dioxide release or oxygen use. Tests from group B directly measure the level of potentially phytotoxic compounds, like ammonia, in a compost sample. Or alternatively, they indirectly assess whether a compost sample has phytotoxic compounds present by measuring seed germination and/or plant growth.

Length of the Composting Process

State of California Regulations (Title 14, California Code of Regulations, Division 7, Chapter 3.1, section 17868.3, Pathogen Reduction) requires compost producers to adhere to a process to reduce pathogens (PFRP).

For example, in regard to static pile or windrow composting, the regulations require compost sampling to verify an internal temperature of 55 degrees centigrade for 15 days, and be turned a minimum of five times. These requirements will ensure that pathogens and weed seeds are killed.

https://solvita.com/compost/

Farm Context

The Pomona Farm relies on simply indicators to assess maturity.

Materials and Methods

Materials

Three compost piles... at various stages of decomposition and monitoring over the semester...

- 8 (I have four, but we should get more!) tid-bit temperature loggers http://www.onsetcomp.com/products/data-loggers/ua-001-64

Session Outcomes

1. Describe Advection Mathematically
2. Analyze 1-dimensional movement using advection equations
3. Describe Diffuions mathematically
4. Analyze 1-dimensional movement using Fick's law.
5. Two dimensional analysis of advention

Theory of Temperature Diffusion

According to Wikipedia, advection can be described as as "velocity vector" and the del operator.

Blerta, I sure wish I knew where these terms came from!

$$\mathbf{u} \cdot \nabla = u_x \frac{\partial}{\partial x} + u_y \frac{\partial}{\partial y} + u_z \frac{\partial}{\partial z}. \tag{1}$$

where $u = (u_x, u_y, u_z)$ is the velocity field, and ∇ is the del operator (note that Cartesian coordinates are used here).

The rest of the equation is... ???

Apparently, solving this equation is a nightmare! So, we will come up with an alternative way to predict concentration gradients...

Diffusion versus Advection

Fick's first law relates the diffusive flux to the concentration under the assumption of steady state. It postulates that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative), or in simplistic terms the concept that a solute will move from a region of high concentration to a region of low concentration across a concentration gradient. In one (spatial) dimension, the law is:

$$J = -D\frac{\partial \varphi}{\partial x} \tag{2}$$

where

J is the "diffusion flux," of which the dimension is amount of substance per unit area per unit time, so it is expressed in such units as $mol \cdot m^2 \cdot s^1$. J measures the amount of substance that will flow through a unit area during a unit time interval.

D is the diffusion coefficient or diffusivity. Its dimension is area per unit time, so typical units for expressing it would be m^2/s. φ (for ideal mixtures) is the concentration, of which the dimension is amount of substance per unit volume. It might be expressed in units of mol/m^3. x is position, the dimension of which is length. It might thus be expressed in the unit m.

What is diffusion?

Why is diffusion important?

What do we know about diffusion? In free solution and in the absence of any interactions with other macromolecules, the diffusion process is controlled by the size of the macromolecule as described by the Stokes-Einstein relation:

$$D_0 = \frac{k_B T}{6\pi\nu R_H} \tag{3}$$

where k_B is Boltzmann's constant, T the temperature in Kelvin, ν the solvent viscosity, and R_H the hydrodynamic radius.

Steady-state versus ??

What are current areas of research concerning diffusion and environmental issues?

Modeling with R

One Dimensional Diffusion

Steady-state solution of 2-D PDEs

To develop our models, we will use the **rootSolve** Package. For this portion of our work, we will rely on the `steady.2D()` function that can solve steady-state, 2-dimensional problems.

(4)

a substance C is consumed at a quadratic rate (r dot C2), while dispersing in X- and Y-direction. At certain positions (x,y) the substance is produced (rate p).

The model is solved on a square (100*100) grid. There are zero-flux boundary conditions at the 4 boundaries.

The term Dx . . . ,

i.e. it is the negative of the ux gradient, where the ux is due to diffusion. In the numerical approximation fo the ux, the concentration gradient is approximated as the subtraction of two matrices, with the columns or rows shifted (e.g. Conc[2:n,]-Conc[1:(n-1),]).

The flux gradient is then also approximated by subtracting entire matrices (e.g. Flux[2:(n+1),]-Flux[1:(n),]). This is very fast. The zero-flux at the boundaries is imposed by binding a column or row with o-s.

```
library(rootSolve)
diffusion2D <- function(t,conc,par){
Conc <- matrix(nr=n,nc=n,data=conc) # vector to 2-D matrix
dConc <- -r*Conc*Conc # consumption
BND <- rep(1,n) # boundary concentration

# constant production in certain cells
dConc[ii]<- dConc[ii]+ p

#diffusion in X-direction; boundaries=imposed concentration

Flux <- -Dx * rbind(rep(0,n),(Conc[2:n,]-Conc[1:(n-1),]),rep(0,n))/dx
dConc <- dConc - (Flux[2:(n+1),]-Flux[1:n,])/dx

#diffusion in Y-direction
Flux <- -Dy * cbind(rep(0,n),(Conc[,2:n]-Conc[,1:(n-1)]),rep(0,n))/dy
dConc <- dConc - (Flux[,2:(n+1)]-Flux[,1:n])/dy
```

```
return(list(as.vector(dConc)))
}
```

After specifying the values of the parameters, 10 cells on the 2-D grid where there will be substance produced are randomly selected (ii).

Figure 5: Steady-state solution of the nonlinear 2-Dimensional model

```
# parameters
dy <- dx <- 1 # grid size
Dy <- Dx <- 1.5 # diffusion coeff, X- and Y-direction
r <- 0.01 # 2-nd-order consumption rate (/time)
p <- 20 # 0-th order production rate (CONC/t)
n <- 100
# 10 random cells where substance is produced at rate p
ii <- trunc(cbind(runif(10)*n+1,runif(10)*n+1))
```

The steady-state is found using function steady.2D. It takes as arguments a.o. the dimensionality of the problem (dimens) and lrw=1000000, the length of the work array needed by the solver. If this value is set too small, the solver will return with the size needed. It takes about 0.5 second to solve this 10000 state variable model.

```
Conc0 <- matrix(nr=n,nc=n,10.)
# print(system.time(
# not working yet...

ST3 <- steady.2D(Conc0,func=diffusion2D,parms=NULL,pos=TRUE,dimens=c(n,n), lrw=1000000,atol=1e-10,rtol=1e-
```

The S3 image method is used to generate the steady-state plot.

Diffusion Derivation

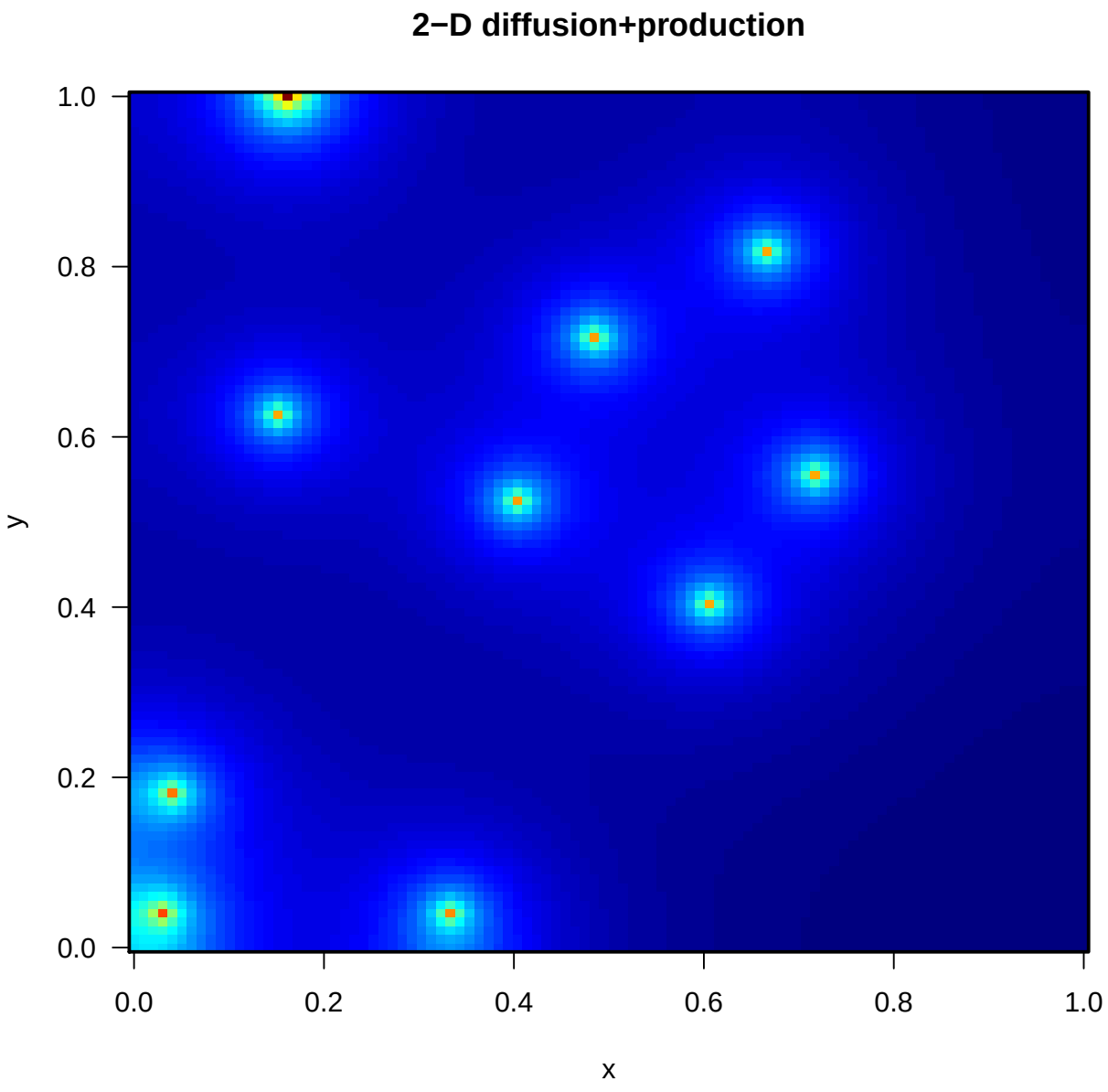
a.) From 9.3, Special Case 2, we know that if $A(x,t) = \bar{A}(x) \neq 0$ (if area does not change with time), then the equation can be written as

$$\frac{\partial c(x,t)}{\partial t} = -\frac{1}{\bar{A}(x)}\frac{\partial}{\partial x}[J(x,t)\bar{A}(x)] \pm \sigma(x,t) \tag{5}$$

We now need to find an equation for $\bar{A}(x)$. Since arc length equals radius times angle, we get

$$\bar{A}(r) = \theta r h \tag{6}$$

```
image(ST3,main="2-D diffusion+production", xlab="x", ylab="y", las=1)
```



where θ is the angle of the arc, r is radial distance, and h is height of the section. Therefore we get the equation

$$\frac{\partial c(r,t)}{\partial t} = -\frac{1}{\theta r h}\frac{\partial}{\partial r}[J(r,t)\theta r h] \pm \sigma(r,t) \tag{7}$$

Since θ and h are constants, we can factor them out to get

$$\frac{\partial c(r,t)}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}[J(r,t)r] \pm \sigma(r,t) \tag{8}$$

b) Extending the principle applied in part (a), we first need to find $\bar{A}(R)$. Since θ is small, we can approximate cross sectional area by taking horizontal arc length times vertical arc length. Therefore we get the equation

$$\bar{A}(R) = \theta_1\theta_2 R^2 \tag{9}$$

where θ_1 is the horizontal angle of the arc, θ_2 is the vertical angle of the arc, and R is radial distance. Combining this with equation (1) from above, we get

$$\frac{\partial c(R,t)}{\partial t} = -\frac{1}{\theta_1\theta_2 R^2}\frac{\partial}{\partial R}[J(R,t)\theta_1\theta_2 R^2] \pm \sigma(R,t) \tag{10}$$

Since θ_1 and θ_2 are constants, we can simplify the equation as such:

$$\frac{\partial c(R,t)}{\partial t} = -\frac{1}{R^2}\frac{\partial}{\partial R}[J(R,t)R^2] \pm \sigma(R,t) \tag{11}$$

c) Part A: In order to obtain the equations in 9.5, we apply Fick's law:

$$J = -\mathcal{D}\nabla c \tag{12}$$

In this case, we use the one-dimensional version:

$$J = -\mathcal{D}\frac{\partial c}{\partial x} \tag{13}$$

Applying this to equation (4), we get

$$\frac{\partial c(r,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}[\mathcal{D}\frac{\partial c}{\partial r}r] \pm \sigma(r,t) \tag{14}$$

Simplifying, and assuming that no particles are created or eliminated at the source, we get:

$$\frac{\partial c(r,t)}{\partial t} = \frac{\mathcal{D}}{r}\frac{\partial}{\partial r}(\frac{\partial c}{\partial r}r) \tag{15}$$

Part B: Once again, we apply Fick's law in one dimension to get

$$\frac{\partial c(R,t)}{\partial t} = \frac{1}{R^2}\frac{\partial}{\partial R}[\mathcal{D}\frac{\partial c}{\partial R}R^2] \pm \sigma(R,t) \tag{16}$$

We again simplify, assuming no particles are created or destroyed at the source.

$$\frac{\partial c(R,t)}{\partial t} = \frac{\mathcal{D}}{R^2}\frac{\partial}{\partial R}(\frac{\partial c}{\partial R}R^2) \tag{17}$$

Chang 1997 Key Points

Data

- Size of halos measured with a ruler over constant time intervals
- Experiment repeated three times to calculate average values used in model

Methodology

- Mathematical model formed using Fick's law
- c(r,t) = lipase concentration as a function of time and radial distance
- Used regression analysis to fit hindered diffusion coefficients and threshold values of lipase concentration as parameters. The finite difference method outlined in Constantinides, 1987 was used specifically.
- Amount of lipase in plate at each time calculated by numerical integration. The total amount of lipase varied by 2.5%, confirming the appropriateness of the mathematical model used.

Discretization

Fick's second law of molecular diffusion, expressed in cylindrical coordinates.

$$\begin{aligned}\frac{\partial C}{\partial t} &= D\Delta^2 C \\ &= D(\frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial r^2})\end{aligned}$$

Initial conditions:

$$\begin{cases} C = C_0 & \text{for } R_w < r < R_r \\ C = 0 & \text{for } r < R_w \ \& \ R_r < r \end{cases} \tag{18}$$

where D is the effective hindered diffusion coefficient, C_0 is the feed enzyme concentration, R_w is the radius of the well, and R_r is the outer radius of the absorption ring. The lipase concentration as a function of time and radial distance can be solved using the finite difference method.

$$\frac{1}{\Delta t}(C_{i,j+1} - C_{i,j}) = [\frac{1}{i\Delta r}\frac{D}{2\Delta r}(C_{i+1,j} - C_{i-1,j}) + \frac{D}{\Delta r^2}(C_{i+1,j} - 2C_{i,j} + C_{i-1,j})] \tag{19}$$

$$\frac{1}{\Delta t}C_{i,j+1} = \frac{1}{\Delta t}C_{i,j} - \frac{2D}{\Delta r^2}C_{i,j} + \frac{D}{2i\Delta r^2}(C_{i+1,j} - C_{i-1,j}) + \frac{D}{\Delta r^2}(C_{i+1,j} + C_{i-1,j}) \tag{20}$$

$$C_{i,j+1} = (1 - \frac{2D\Delta t}{\Delta r^2})C_{i,j} + \frac{D\Delta t}{\Delta r^2}[(\frac{1}{2i} + 1)C_{i+1,j} - (\frac{1}{2i} - 1)C_{i-1,j}] \tag{21}$$

For convergence, to hold:

$$\frac{D\Delta t}{\Delta r^2} \leq \frac{1}{2} \tag{22}$$

Lastly, the amount of lipase can be calculated using

$$A = \int_{R_w}^{R_r} 2\pi r l C(r)\, dr \tag{23}$$

where A is the total amount of lipase in terms of enzyme activity, R_w and R_h are the radius of well and halo, respectively, $C(r)$ is the concentration at the radial distance of r, and l is the thickness of agar plate.