# Decomposition Rate as an Emergent Property of Optimal Microbial Foraging

Glenn Ledder[1] Stefano Manzoni[2]

[1]Department of Mathematics
University of Nebraska-Lincoln
gledder@unl.edu

[2]Department of Physical Geography and Bolin Centre for Climate Research
Stockholm University

November 10, 2022

S.M. created the model and solved a special case.[1]
G.L. found the full analytical solution.

[1]A rare example of my inheriting a model and not needing to change it.

# Overview

- Decomposition kinetics are fundamental for quantifying carbon and nutrient cycling in terrestrial and aquatic ecosystems.
- Our aim is to develop a theory that can predict rates of microbial decomposition and subsequent growth...
    - based on the assumption that natural selection has led to microbial communities that optimize their growth

# Fundamental Assumptions

- The initial amount of $C_0$ units of substrate is decomposed in some unknown time $T_f$.
- Substrate "C" is decreased by abiotic decomposition $\gamma C$ as well as microbial uptake $U$.
  - This means that very low uptake will not be optimal.
- Microbial growth $G(U)$ is a saturating function of "C" uptake.
  - This means that very high uptake will not be optimal.
- Microbial population is constant because of population dynamics (an oversimplification that makes the problem tractable).
- A fraction $0 \leq \mu \leq 1$ of the biomass of dead microbes is returned to the substrate pool.

# The Dynamical System

$$\frac{dC}{dT} = -\gamma C - U + \mu G(U), \qquad C(0) = C_0, \quad C(T_f) = 0.$$

$$G(U) = \alpha \frac{U - \rho}{\beta + U} < \frac{\alpha}{\beta} U, \qquad \frac{\alpha}{\beta} < 1.$$

- The function $U$ and time $T_f$ are chosen to optimize the total microbial growth.

Scaling and Dimensionless Parameters (WLOG $\beta = 1$):

$$t = \gamma T, \quad c = \frac{\gamma}{\beta} C, \quad u = \frac{U}{\beta}, \quad g = \frac{G}{\alpha}.$$

$$\tau = \gamma T_f, \quad c_0 = \frac{\gamma}{\beta} C_0, \quad p = \frac{\rho}{\beta} < 1, \quad m = \frac{\alpha \mu}{\beta} < 1.$$

# The Math Problem

Choose the function $u(t)$ and time $\tau$ to maximize the total growth

$$J = \int_0^\tau g(u)\,dt,$$

where

$$\frac{dc}{dt} = -c - u + mg(u), \qquad c(0) = c_0, \quad c(\tau) = 0,$$

and

$$g(u) = \frac{u - p}{1 + u}.$$

# Goals and Method

1. Find the optimal decomposition rate $u(t)$ and time $t_f$.
2. If possible, obtain formulas for $u$ and $g$ in terms of $c$ rather than $t$.
   - Microorganisms might be able to measure the state of their environment, but not the time, and they cannot record history.
3. Determine how the system behavior depends on the parameters $\gamma$, $C_0$, $\rho$, and $\mu$.

- This is an optimal control problem. Such problems can be solved using Pontryagin's Maximum Principle (or nonlinear optimization methods with a large vector of unknowns).

# Pontryagin's Maximum Principle (indeterminate end time)

For the problem of maximizing $J(u) = \int_0^\tau g(u)\,dt$ with dynamic variable $x' = f(x,u)$, $x(0) = x_0$, and $x(\tau) = x_\tau$ and with $\tau$ unspecified, formulate the Hamiltonian

$$H(x,u,\lambda) = g(u) + \lambda f(x,u).$$

If $u$ maximizes $J$, then

1. $u$ maximizes $H$;
2. $\frac{d\lambda}{dt} = -\frac{\partial H}{\partial x}$;
3. $H(\tau) = 0$.

- $H(\tau) = 0$ provides a terminal condition for the $\lambda$ equation.
- We can solve the system in backward time $s = \tau - t$.
- The extra condition for $c$ (initial in $t$, terminal in $s$) will determine $\tau$.

# Optimality Condition Details

$$H(c, u, \lambda) = g(u) + \lambda[-c - u + mg(u)].$$

1. Maximum $u$ will be at an interior point, so
$$0 = \frac{\partial H}{\partial u} = g' + \lambda(-1 + mg')$$
2. $$\frac{d\lambda}{dt} = \lambda$$
3. $$g_\tau + \lambda_\tau(-u_\tau + mg_\tau) = 0$$

# The Problem to Solve

- Auxiliary function in reverse time:

$$\frac{d\lambda}{ds} = -\lambda, \qquad \lambda(0) = \lambda_\tau, \qquad s \equiv \tau - t. \tag{1}$$

- Dynamical system in reverse time:

$$\frac{dc}{ds} - c = u - mg(u), \qquad c(0) = 0, \quad c(\tau) = c_0. \tag{2}$$

- Optimality condition and constitutive relations:

$$g' = \frac{\lambda}{1 + m\lambda}, \quad g = \frac{u - p}{1 + u}, \quad g' = \frac{1 + p}{(1 + u)^2}. \tag{3}$$

- Optimality boundary condition:

$$g_\tau + \lambda_\tau(-u_\tau + mg_\tau). \tag{4}$$

# Solution Plan

1. Use the algebraic relations to get $u_\tau$ and $\lambda_\tau$.
2. Solve the reverse time IVP for $\lambda$.
3. Use the algebraic relations to get $g'$, $u$, and $g$.
4. Solve the reverse time IVP for $c$.
5. Write $u$ and $g$ in terms of $c$ if possible.
6. Use $c(\tau) = c_0$ to get $\tau$.

# Important Results from First 3 Steps

Let $\bar{u} = 1 + u$, $\bar{p} = 1 + p$, etc.

$$\bar{u}_\tau = \bar{p} + \sqrt{p\bar{p}}.$$

$$\bar{u}^2 = \left(\bar{u}_\tau^2 - m\bar{p}\right) e^s + m\bar{p}$$

$$g = 1 - \frac{\bar{p}}{\bar{u}}$$

Then

$$\frac{dc}{ds} - c = u - mg = \bar{u} - (1 + m) + \frac{m\bar{p}}{\bar{u}}$$

# Solving the Dynamical System Equation

1. Differentiate
$$\bar{u}^2 = \left(\bar{u}_\tau^2 - m\bar{p}\right) e^s + m\bar{p}$$
to get
$$\frac{d\bar{u}}{ds} = \frac{\bar{u}^2 - m\bar{p}}{2\bar{u}}$$

2. Use $dc/ds = dc/d\bar{u} \cdot d\bar{u}/ds$ to get
$$\left(\bar{u}^2 - m\bar{p}\right) \frac{dc}{d\bar{u}} - 2\bar{u}c = 2\bar{u}^2 - 2(1+m)\bar{u} + 2m\bar{p}.$$

3. Solve the $c(\bar{u})$ problem to get the surprisingly simple solution
$$c = \frac{\bar{u}^2}{\bar{p}} - 2\bar{u} + 1.$$

4. Invert the result to get $u$ as a function of $c$.

# Summary of Solutions

- $u$ and $c$ as functions of $t$:

$$\bar{u} = \sqrt{\left(\bar{u}_0^2 - m\bar{p}\right) e^{-t} + m\bar{p}}, \quad \bar{u}_0 = \bar{p} + \sqrt{\bar{p}(c_0 + p)} \tag{5}$$

$$u = \bar{u} - 1, \qquad c = \frac{\bar{u}^2}{\bar{p}} - 2\bar{u} + 1. \tag{6}$$

- $u$ and $g$ as functions of $c$:

$$u = p + \sqrt{(1+p)(c+p)}, \quad g = \frac{\sqrt{c+p}}{\sqrt{1+p} + \sqrt{c+p}} \tag{7}$$

- Terminal time:

$$e^{\tau} = \frac{\left(\sqrt{1+p} + \sqrt{c_0 + p}\right)^2 - m}{\left(\sqrt{1+p} + \sqrt{p}\right)^2 - m} \tag{8}$$

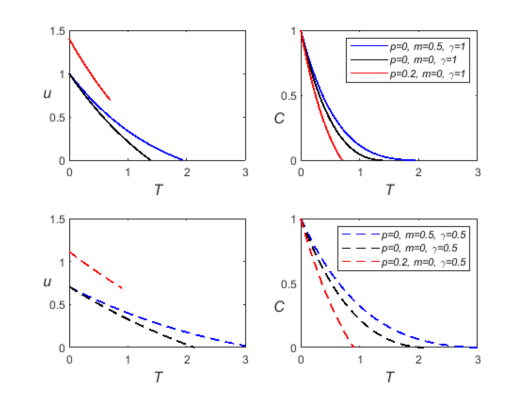
# Questions for the Model

1. How do **the time history of uptake** $u$ **and "C" content** $C$ depend on the maintenance loss $p$, recycling ratio $m$, and abiotic decomposition rate $\gamma$?

2. How do **the total time** $T_f$ **and the efficiency** $J/C_0$ depend on the amount of substrate, and how are these dependencies modified by the values of $p$, $m$, and $\gamma$?

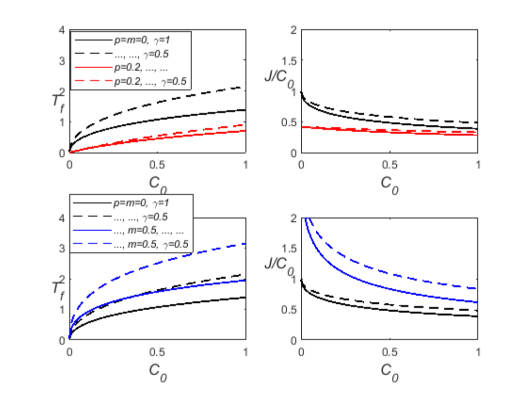
3. What would the microorganisms need to "know" or "measure" to implement the optimal strategy (**how to determine** $u$ **without knowing** $t$)?

# Time History of $u$ and $C$



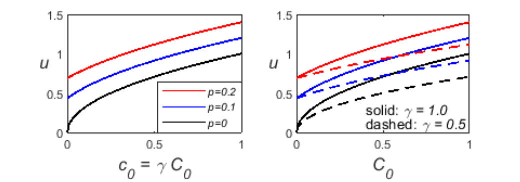

- Larger $p$ increases uptake and speeds decomposition.
- Larger $m$ increases uptake but slows decomposition.
- Smaller $\gamma$ makes the decomposition less intense and slower.

# Decomposition Time $T_F$ and Growth Efficiency $J/c_0$




- Larger $p$ speeds decomposition and reduces efficiency.
- Smaller $\gamma$ allows for slower decomposition to increase efficiency.
- Larger $m$ slows decomposition and 'increases' efficiency.

# What Would Implementation Require?




- The microorganisms would need to "know" their own semisaturation constant $\beta$ & maintenance cost $\rho$ ($p = \rho/\beta$).
  - "Knowing" $\beta$ and $\rho$ means being selected for a combination of $\beta$, $\rho$, $u$ that is optimal over some biologically feasible domain for $\beta$ and $\rho$.
- They would need to measure the abiotic decomposition rate $\gamma C$ or measure the substrate content $C$ and "know" $\gamma$.
  - "Knowing" $\gamma$ means living in an environment where $\gamma$ changes only slowly.

# A Different Formulation of the Biological Problem

- How sure are we that the microbes optimize their growth for a given amount of substrate?
- Maybe instead they optimize their net growth rate, which would favor faster decomposition?

New Problem:
Choose the function $u(t)$ and time $\tau$ to maximize the mean growth rate

$$J = \frac{1}{\tau} \int_0^\tau g(u)\, dt,$$

where

$$\frac{dc}{dt} = -c - u + mg(u), \quad c(0) = c_0, \quad c(\tau) = 0, \quad g(u) = \frac{u - p}{1 + u}.$$