**Model:** The model is a three-component reaction-diffusion system, the variables are the population density of climax bacteria, denoted by , population density of attack bacteria, , and oxygen concentration, . The full model equations are given by

where is the Laplace operator and . This system can be nondimensionalized by defining the scaled variables and and constants and . Rewriting and dropping the \*’s, the nondimensionalized system is

**Boundary Conditions (2-dimensions):** To determine boundary conditions, we consider an open airway lined with mucus. The airway can be represented as a rectangle with periodic boundaries on the left and right side and Neumann and Dirichlet boundary conditions on the top and bottom. Let be the domain. The boundary conditions for the lateral sides are

We consider to be a clogged airway which is open at the top and clogged with mucus at the bottom, so that oxygen is entering from the top but not able to penetrate the mucus at the bottom (1). We also assume that bacteria are neither entering or exiting through the boundary, so the boundary conditions at the top and bottom of are

Top:

Bottom:

where is the constant oxygen flow entering the airway and is a normal vector at the boundary of .

**Initial Conditions (2-dimensions):** Initial conditions for the model are given by

The initial value functions and can be uniform (constant) or spatially dependent. Assuming oxygen concentration decreases from the top of the column, then we can take . Climax and attack bacteria can be initially distributed by choosing constant values for and , or distributed locally using, e.g., Gaussian functions, i.e.,

**Boundary Conditions (1-dimension):** For a one-dimensional domain , we assume constant oxygen inflow on throughout so that and periodic boundaries at and . The BC’s can be written

**Initial Conditions (1-dimension):** Initial conditions for oxygen on are constant, . Initial distributions for *c* and *f* can be either uniform or localized. In the case that they are localized, initial conditions are given by the Gaussian functions

**Initial Parameter Values:** Base parameters are shown in Table 1. Non-dimensionalized parameters are shown in Table 2, using the scaling factors and .

**Table 1:** Base parameter values and descriptions

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | Description | Value | Source |
| *β* | Maximum possible climax growth rate | 20 day-1 | Various |
| *b* | Half-maximum response dose of oxygen | 12.4 *μM* | (2) |
| *n* | Growth rate slope-factor | 1.0 | (2) |
| *dc* | Climax death rate | 0.4 *day-1* | (3) |
| *df* | Attack death rate | 0.4 *day-1* | (3) |
| *q* | Oxygen toxicity coefficient | *μM day-1* | Assumed |
| *k* | Carrying capacity | 109 | Assumed |
| *μ* | Oxygen decay rate | 3.3 x 104 day*-1* | (1, 4) |
| *λ* | In-flow rate of oxygen | 4.4 x 105 *μM* *day-1* | (1, 4) |
| *η* | Climax oxygen consumption rate | 2.0 x 10-7 *day-1* | (5) |
| *Dc* | Climax diffusion rate | 0.001 *cm2 day-1* | Assumed |
| *Df* | Attack diffusion rate | 0.01 *cm2 day-* | Assumed |
| *Dw* | Oxygen diffusion rate | 1.32 *cm2 day-1* | (1) |

**Table 2:** Dimensionless parameter values and expressions

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | Description | Base Value | Expression |
| *β* | Maximum possible climax growth rate | 0.0002 |  |
| *b* | Half-maximum response dose of oxygen | 1 |  |
| *n* | Growth rate slope-factor | 1.0 |  |
| *dc* | Climax death rate | 4.0 x 10-6 |  |
| *df* | Attack death rate | 4.0 x 10-6 |  |
| *q* | Oxygen toxicity coefficient | 2.48 x 10-5 |  |
| *μ* | Oxygen decay rate | 0.3312 |  |
| *λ* | In-flow rate of oxygen | 0.3312 |  |
| *η* | Climax oxygen consumption rate | 0.002 |  |
| *Dc* | Climax diffusion rate | 1.32 x 10-8 |  |
| *Df* | Attack diffusion rate | 1.32 x 10-7 |  |
| *Dw* | Oxygen diffusion rate | 1.32 x 10-5 |  |

**Simulations (1D):** We solved the system of PDEs in one spatial dimension using the Periodic Reaction-Diffusion MATLAB program (6). Figure 1 shows a simulation of the system as heatmaps with time along the horizontal axis and space on the vertical, parameter values for this simulation are shown in Table 3. We used gaussian functions as the initial conditions for *c* and *f*, and the constant value for oxygen. The climax community reached steady-state relatively quickly and drew down oxygen where it was highest in density. The attack community was most prominent slightly off of the climax peak where oxygen was lowest. The initial gaussian function for *f* was centered at versus the climax center at , but over time the attack community was drawn to the lower oxygen environment created by the climax.

**Figure 1:** PDE system solved in one spatial dimension

|  |  |
| --- | --- |
|  |  |
|  | Figure 1: Heatmaps of the climax community (top-left), attack community (top-right), and oxygen (bottom-left). Time is located on the horizontal axis of each figure, and the spatial domain along the vertical. The two bacterial communities were initial distributed according to gaussian functions, oxygen was distributed at the constant value . Periodic boundary conditions are located at ends of the domain, so that , , and . |

**Table 3:** Parameters values used for simulation

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | Value | Parameter | Value |
| *β* | 0.08 | *μ* | 0.01312 |
| *b* | 0.06 | *λ* | 0.01312 |
| *n* | 8.0 | *η* | 1.54 |
| *dc* | 9.0 x 10-7 | *Dc* | 1.32 x 10-8 |
| *df* | 9.0 x 10-7 | *Df* | 1.32 x 10-4 |
| *q* | 4.48 x 10-2 | *Dw* | 1.32 x 10-3 |

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