Modeling of Anabaena colony dynamics

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1 Introduction

Cyanobacteria are a phylum of bacteria which acquire their energy using photosynthesis. They are unicellular organisms (prokaryotes) which exist as filaments, and are able to rpoduce oxygen as an end product. Anabaena is a genus of any such non-dividing cyanobacteria that are able to exhibit nitrogen-fixation (process in which the Earth's atmospheric nitrogen is converted into ammonia or related nitrogenous compounds).

When subjected to conditions of limited nitrogen, the vegetative cells of the organism differentiate into heterocysts, which are specialized nitrogen-fixing cells. These cells are responsible for fixing nitrogen from dinitrogen in the air with the help of the enzyme nitrogenase to provide the cells in the filament with nitrogen for biosynthesis.

In this study, we strive to model and explore the dynamics of Anabaena colonies in the context of heterocyst formation in stressed environments. This is achieved through a series of simulations in MATLAB, which are described below.

2 Procedure and Method

The simulations were conducted progressively; we started off with the simplest scenario and proceeded to more complex settings with the progress of time. A sequential documentation of the simulations follows.

2.1 Single source and sink simulations

We consider a two-dimensional space which has zero concentration of a chemical substance (S). Initially, there is a single agent (source) located at the center of the two-dimensional region that we monitor, that produces a chemical signal. This signal spreads out in all directions by following the diffusion equation.

The parameters for the simulation are:

- A $\equiv$ the initial chemical concentration per active agent
- D $\equiv$ the diffusion coefficient
- $\triangle t \equiv$ the time integration constant (or time discretisation)
- $\triangle x \equiv$ the size of a cell in the simulation space (or space discretization)
- x_{min}, x_{max}, y_{min} and $y_{max} \equiv$ the spatial limits for the simulation space in the x and y-directions
- $t_{total} \equiv$ the total time for which the simulation runs from $t = 0$ in steps of $\triangle t$

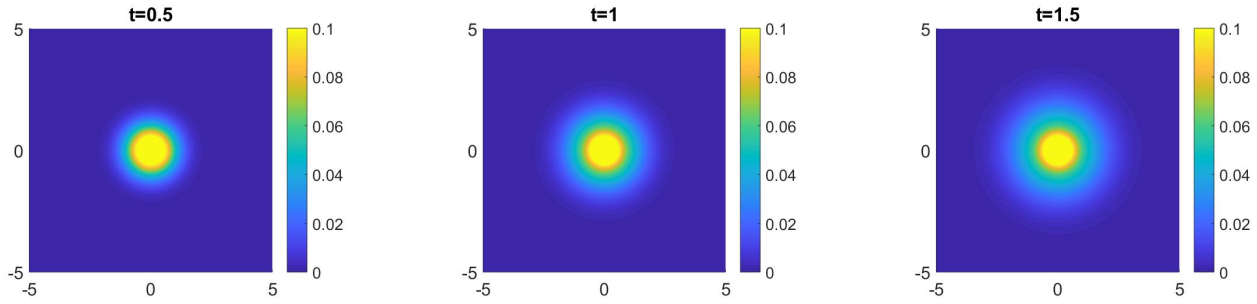
The matlab code (script) skeleton for the simulations is shown below.

```
function y_out = diffusion_test()

%The agent at position (0,0) produces a chemical signal that spreads out following a
%diffusion equation.

%The output of the code is a movie showing the concentration of the
%chemical signal as a function of time in the arena.

% define
A=0.1; %initial chemical concentration per active agent

D=0.5; % diffusion coefficient
delta_t = 0.1; % time integration constant (time discretization)
delta_x = 0.01; % size of a cell in the simulation (space discretization)
B=0; % ignore for now
```

```
SAVE_MOVIE = 1;
t_array=0:delta_t:3.0;
min_x = -5; max_x=5;

source_propagation(A,B,D,t_array,delta_x,min_x,max_x,SAVE_MOVIE);
y_out=0;

end

function source_propagation(A,B,D,t_array,delta_x,min_x,max_x,SAVE_MOVIE)

source_x = 0;
source_y = 0;

[x,y] = meshgrid(min_x:delta_x:max_x,min_x:delta_x:max_x);

if SAVE_MOVIE==1
    fig_densities=figure();
    loops = length(2:length(t_array));
    clear F
    F(loops) = struct('cdata',[],'colormap',[]);
end

for t_i=2:length(t_array)
    t=t_array(t_i);
    c = zeros(size(x));

    curr_t = t;
    curr_c =(A/(curr_t^0.5))*exp(-(((x-source_x).^2)+((y-source_y).^2))./(4*D*curr_t))+B;
    c = c + curr_c;


    if (t_i>1) && SAVE_MOVIE==1
        figure(fig_densities);
        surf(x,y,c,'EdgeColor','none'); view(2); title(['t=',num2str(t)]); xlim([min_x max_x
        daspect([1 1 1]); colorbar; caxis([0 A]); hold on;

        pause(0.001);
        F(t_i-1) = getframe(fig_densities);
        pause(0.001);

        pause(0.1);
    end

end

if SAVE_MOVIE==1
    v = VideoWriter(['A',num2str(A),'B',num2str(A),'D',num2str(A),'test.mp4'],'MPEG-4');
    open(v);
    writeVideo(v,F);
    close(v);
end

end
```

2.1.1 A single point source

For $A = 0.1$ and $D = 0.5$ with a single point source at (0,0), the figure below shows the spreading of the chemical signal with time t. The three images show the concentration of the chemical at $t = 0.5$, $t = 1.0$ and $t = 1.5$.



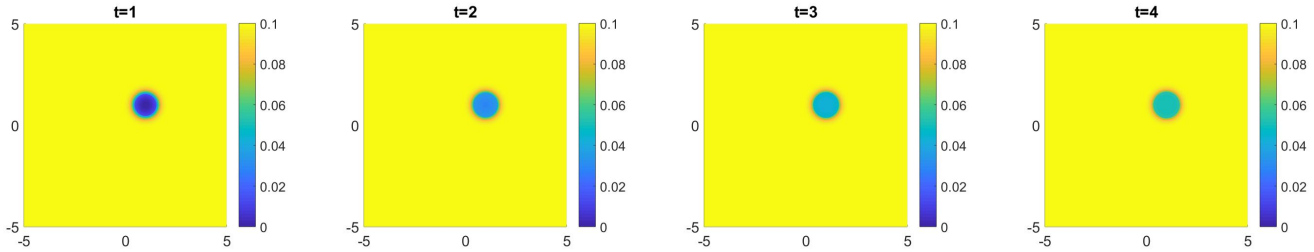
(a) t = 0.5 (b) t = 1.0 (c) t = 1.5

Figure 1: Diffusion from a single point source at (0,0) with A = 0.1 and D = 0.5

2.1.2 A single point sink

When there is a single sink instead of a source, the situation is slightly different. This time, the surrounding has infinite concentration initially, and the chemical diffuses inwards into the sink instead of diffusing outwards from the source.

For $A = 0.1$ and $D = 0.5$ with a single point sink at (1,1), the figure below shows the spreading of the chemical signal with time t. The three images show the concentration of the chemical at $t = 0.5$, $t = 1.0$ and $t = 1.5$.

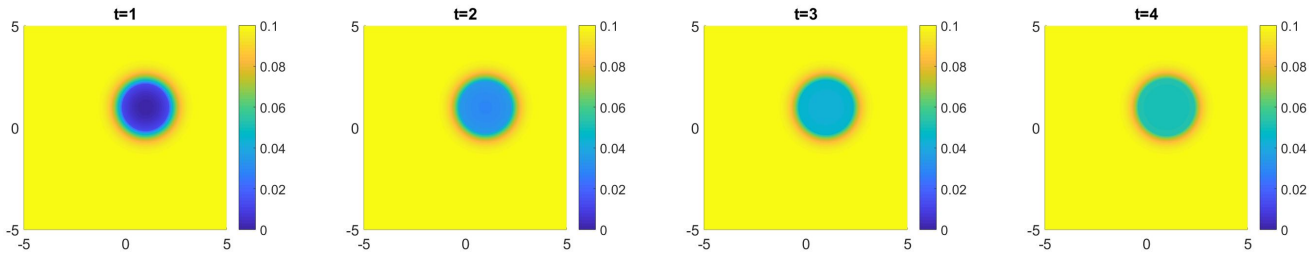


(a) t = 1.0 (b) t = 2.0 (c) t = 3.0 (d) t = 4.0

Figure 2: Diffusion from a single point sink at (1,1) with A = 0.1 and D = 0.5

The gradual change in color in a circle centered at (1,1) shows the inward diffusion of the chemical.

With a larger diffusion coefficient, the size of the circular region where the chemical has diffused into increases, as depicted by the figures below for $D = 2.5$.



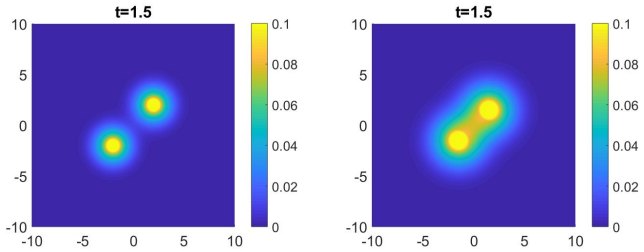
(a) t = 1.0 (b) t = 2.0 (c) t = 3.0 (d) t = 4.0

Figure 3: Diffusion from a single point sink at (1,1) with A = 0.1 and D = 2.5

2.2 Multiple sinks and sources

2.2.1 Two point sources

Instead of a single source or a sink, we now have two or more sinks or two or more sources. The figure below shows the concentration of the surroundings at $t = 1.5$ for two values of the diffusion coefficient, $D = 0.5$ and $D = 1.0$ when we have two sources at (2,2) and (-2,-2).



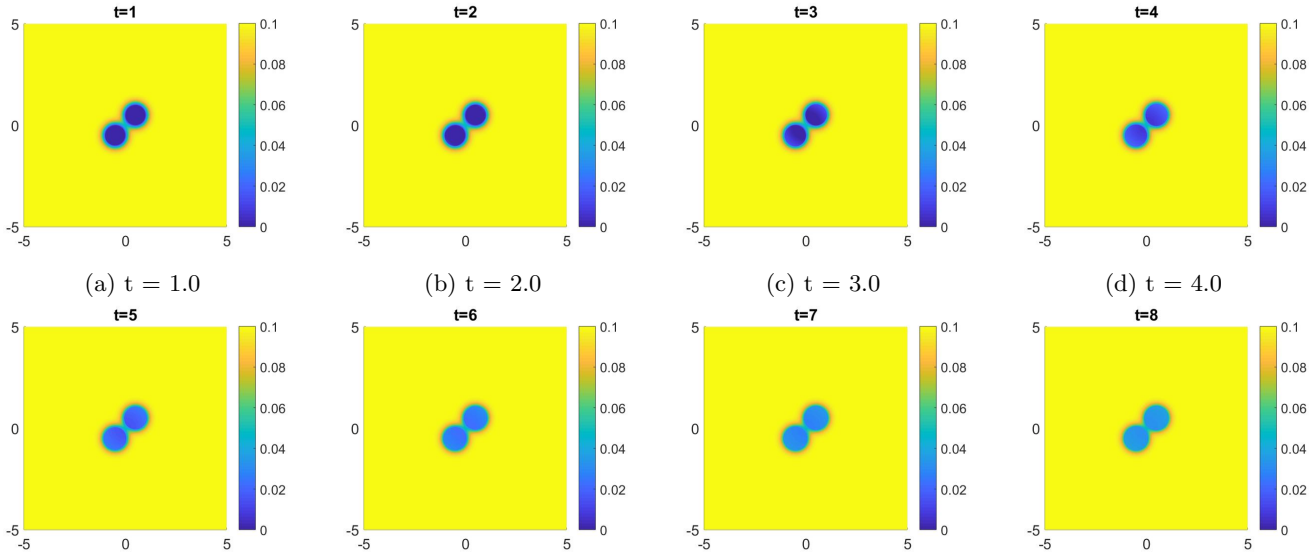
(a) D = 0.5 at t = 1.5 (b) D = 1.9 at t = 1.5

Figure 4: Diffusion from two point sources at (2,2) and (-2,-2) with A = 0.1 and D = 2.5

It is clear that the in region between the two sources, the concentration spreads faster (indicated by the greater intensity of the chemical) due to the fact that the chemical spreads from both the sources in that region.

2.2.2 Two point sinks

If we replace the two sources in the above figure by two sinks, and slightly reduce the distance between them (now they are placed at (1,1) and (-1,-1) keeping the diffusion constant $D = 0.5$, the figures below represent the scenario. Similar to the case with two point sources, the chemical concentration goes down here faster in the region between the two sinks as indicated by the hues in the figure above.



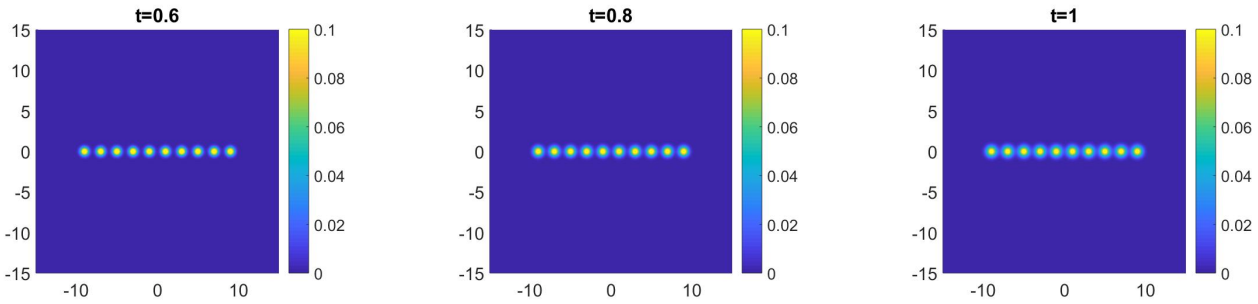
(a) t = 1.0 (b) t = 2.0 (c) t = 3.0 (d) t = 4.0

(e) t = 5.0 (f) t = 6.0 (g) t = 7.0 (h) t = 8.0

Figure 5: Diffusion from a two point sinks at (1,1) and (-1,-1) with A = 0.1 and D = 0.5

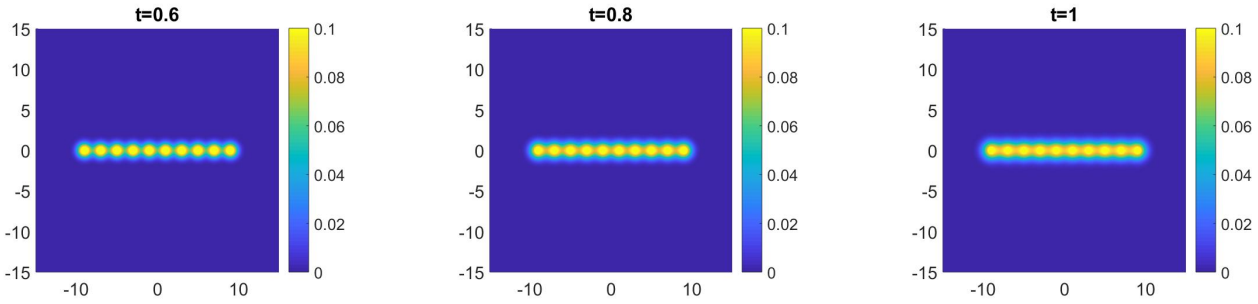
2.2.3 Ten point sources in a linear chain

Increasing the number of sources from 2 to 10 being placed on a single line with each of them 2 units apart, the simulations were run for two values of D given by $D = 0.1$ and $D = 0.3$. The following are the figures representing the simulations.



(a) t = 0.6 (b) t = 2.0 (c) t = 3.0

Figure 6: Diffusion from ten point sources placed on a line 2 units apart with A = 0.1 and D = 0.1



(a) t = 0.6 (b) t = 2.0 (c) t = 3.0

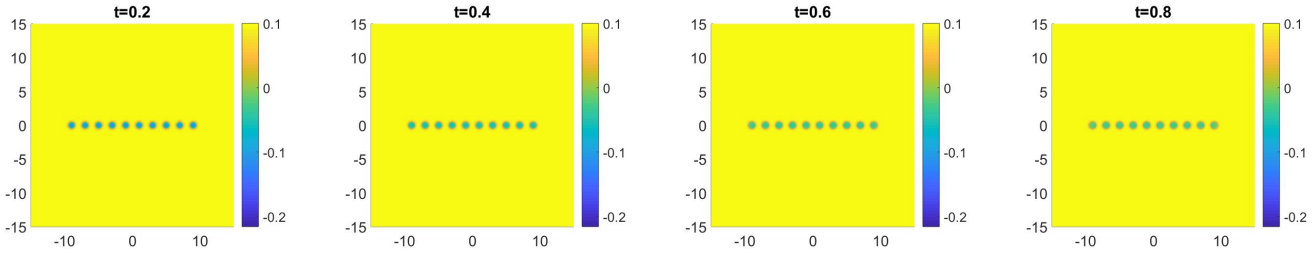
Figure 7: Diffusion from ten point sources placed on a line 2 units apart with A = 0.1 and D = 0.3

As we expected, we note two important observations:

- The rate of diffusion of the chemical is higher in the region between two sources
- With a higher diffusion coefficient, the diffusion rate is also higher, everywhere.

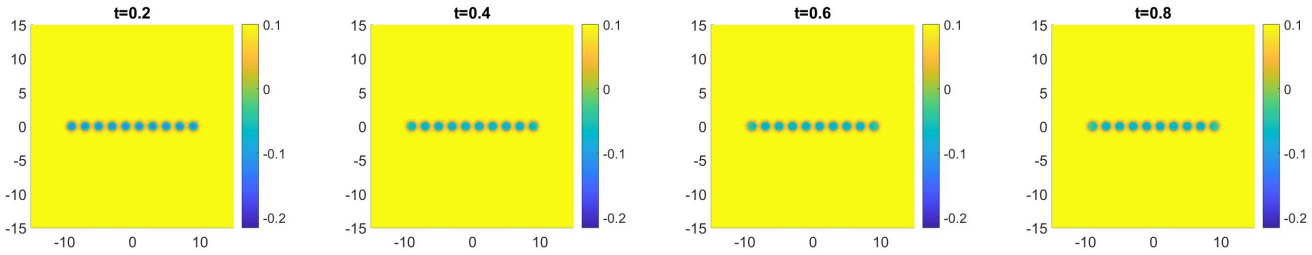
2.2.4 Ten point sinks in a linear chain

Again, if we consider ten sinks instead of the ten sources placed according to the same arrangement as above, but with diffusion coefficients given by $D = 0.5$, $D = 1.0$ and $D = 1.5$, then simulations generate the following figures.



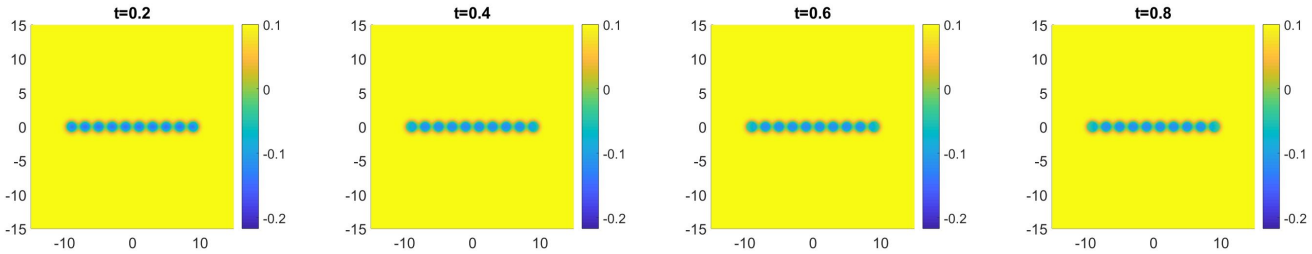
(a) t = 0.2 (b) t = 0.4 (c) t = 0.6 (d) t = 0.8

Figure 8: Diffusion from ten point sinks placed on a line 2 units apart with A = 0.1 and D = 0.5



(a) t = 0.2 (b) t = 0.4 (c) t = 0.6 (d) t = 0.8

Figure 9: Diffusion from ten point sinks placed on a line 2 units apart with A = 0.1 and D = 1.0



(a) t = 0.2 (b) t = 0.4 (c) t = 0.6 (d) t = 0.8

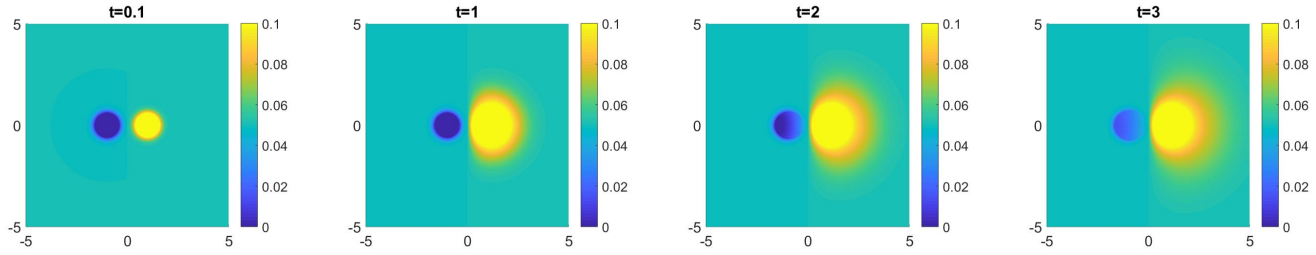
Figure 10: Diffusion from ten point sinks placed on a line 2 units apart with A = 0.1 and D = 1.5

2.3 Sinks and sources together

How does the scenario change when there are sinks and sources in the same simulation? This has been investigated in this section.

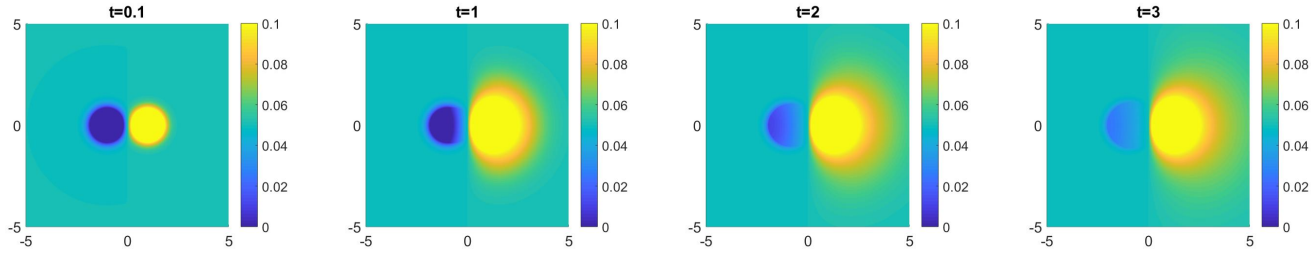
2.3.1 A single point source and a point sink

We started with the simplest case when there is a single point source and a single point sink. Let them placed at (1,0) and (-1,0) respectively, and let the the concentration of the surrounding region be at a level that is exactly midway between the highest and lowest concentrations possible. We simulate the diffusion of a chemical substance for this scenario, and figures below show the concentrations at time t for $D = 0.5$, $D = 1.0$ and $D = 1.5$. Since the rate of diffusion was slow enough to not reveal drastic changes in the surrounding concentrations over small time scales, screenshots were taken between larger time intervals.



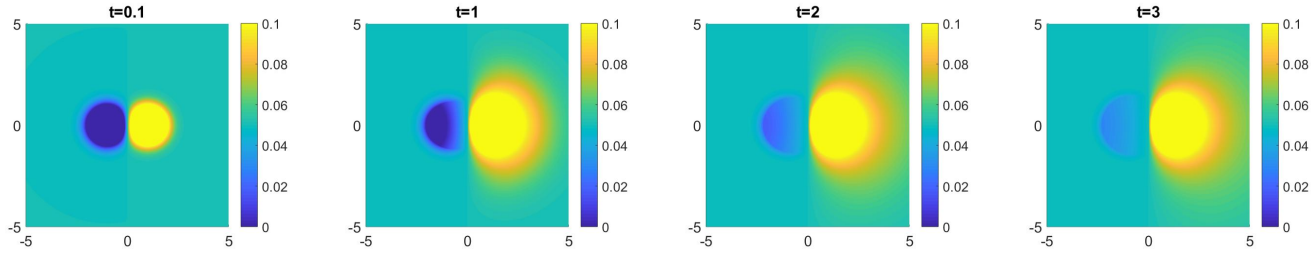
(a) t = 0.1 (b) t = 1.0 (c) t = 2.0 (d) t = 3.0

Figure 11: Diffusion from a point source and a point sink at (1,0) and (-1,0) respectively with A = 0.1 and D = 0.5



(a) t = 0.1 (b) t = 1.0 (c) t = 2.0 (d) t = 3.0

Figure 12: Diffusion from a point source and a point sink at (1,0) and (-1,0) respectively with A = 0.1 and D = 1.0

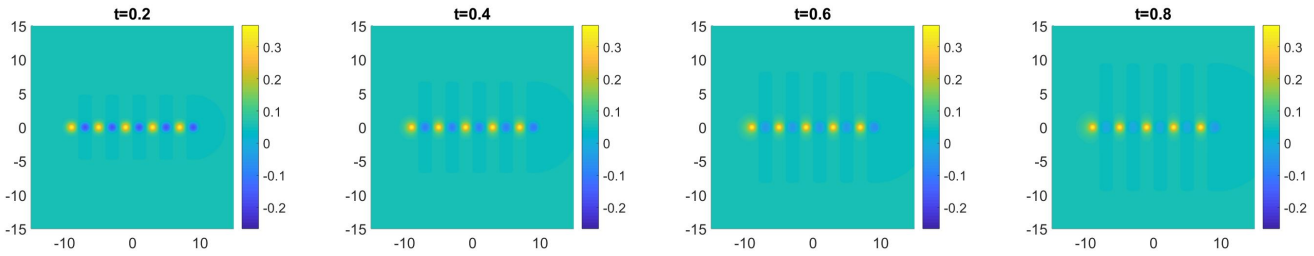


(a) t = 0.1 (b) t = 1.0 (c) t = 2.0 (d) t = 3.0

Figure 13: Diffusion from a point source and a point sink at (1,0) and (-1,0) respectively with A = 0.1 and D = 1.5

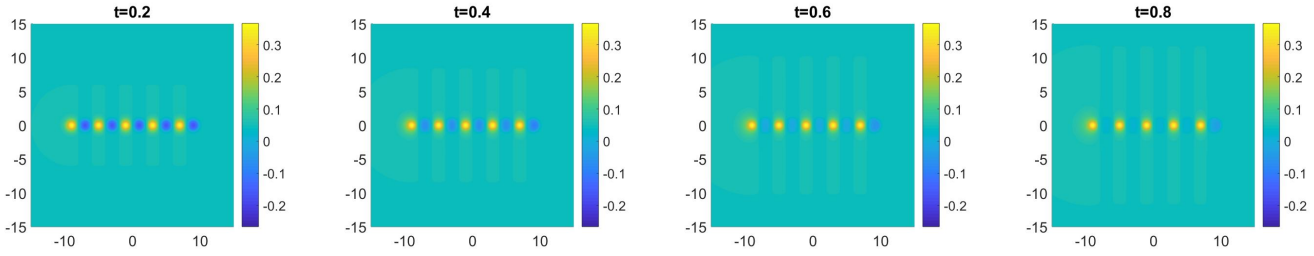
2.3.2 Alternating chain of point sources and sinks

In the next step, a series of ten 10 alternating sources and sinks were placed on a line next to each other 2 units apart with sources at (-9,0), (-5, 0), (-1, 0), (3, 0) and (7, 0) and sinks at (-7, 0), (-3, 0), (1, 0) and (5, 0). The simulations were run for $D = 0.8$ and $D = 1.2$. The figures have been shown below.



(a) t = 0.2 (b) t = 0.4 (c) t = 0.6 (d) t = 0.8

Figure 14: Diffusion from a series of 10 points sources and sinks with A = 0.1 and D = 0.8



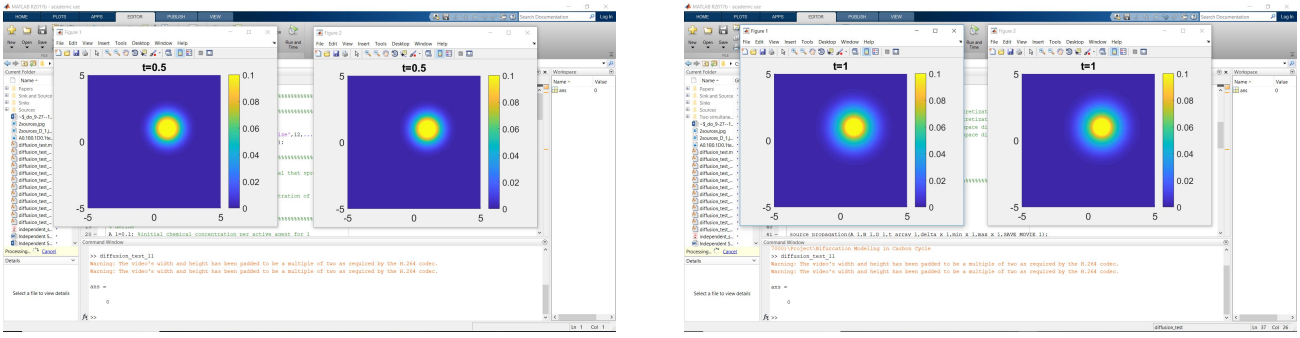
(a) t = 0.2 (b) t = 0.4 (c) t = 0.6 (d) t = 0.8

Figure 15: Diffusion from a series of 10 points sources and sinks with A = 0.1 and D = 1.2

2.4 Simultaneous simulations

In this section, we explored the possibility of conducting two independent but simultaneous simulations involving sources and sinks. This mimics the situation in which there is a point that acts as a source for one substance and a sink for a second substance, while the second point acts as a sink for the first substance and a source for the second substance.

For this, we tried to simulate the spreading of a chemical from two point sources, one in each simulation with identical values of A and D, and independent of each other. The figures below show the simulations when they run initially, on two different windows. These windows were later combined to display both the simulations together using the subplot function in MATLAB.



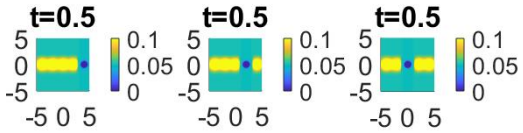
(a) t = 0.2 (b) t = 0.4

Figure 16: Simultaneous Diffusion from two separate point sources with A = 0.1 and D = 0.5 for both

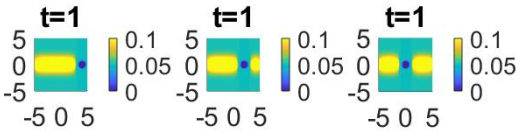
Now we explore simultaneous simulations with 4 point sources and one point sink where the position of the sink changes in each simulation. In the first simulation, there are point sources at (-4,0), (-2,0), (0,0) and (2,0) and a point sink at (4,0). In the second simulation, the point sink replaces the point source at (2,0) and vice-versa. In the third simulation, the point sink replaces the point source at (0,0) and vice-versa. The other two simulations (where the point sink replaces the sources at (-2,0) and (-4,0)) were not conducted in since they were structurally symmetric in nature to the first two simulations.

The first figure below shows the simulations for $A_1 = A_2 = A_3 = 0.1$, and $D_1 = D_2 = D_3 = 0.5$. In the second figure, the values of the diffusion coefficient are $D_1 = 0.5$, $D_2 = 0.7$ and $D_3 = 0.9$, while in the third figure $D_1 = 0.9$, $D_2 = 0.7$ and $D_3 = 0.5$. The values of D_1 and D_3 were interchanged from the second and third figures below to examine the effect of the difference between a sink being enclosed between an equal number of sources and a sink being placed at the end of a series of sources.

It is to be noted that for all the simulations from here onward, the value of $\triangle x \equiv$ the size of a cell in the simulation space (or space discretization) was changed from 0.01 to 0.1.

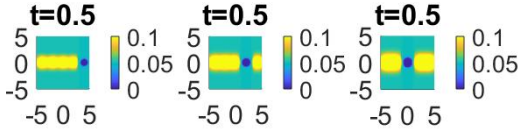


(a) t = 0.5

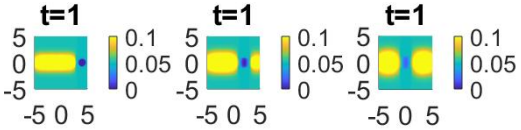


(b) t = 1.0

Figure 17: Three simultaneous simulations for four sources and a single sink with the location of the sink differing in each simulation, and $A_1 = A_2 = A_3 = 0.1$, and $D_1 = D_2 = D_3 = 0.5$

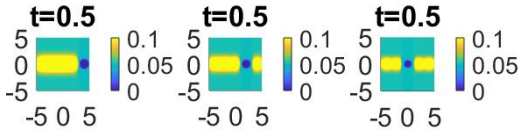


(a) t = 0.5

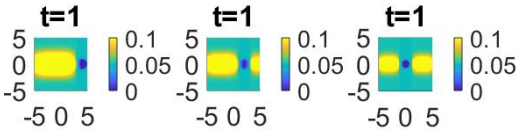


(b) t = 1.0

Figure 18: Three simultaneous simulations for four sources and a single sink with the location of the sink differing in each simulation, and $A_1 = A_2 = A_3 = 0.1$, and $D_1 = 0.5$, $D_2 = 0.7$ and $D_3 = 0.9$

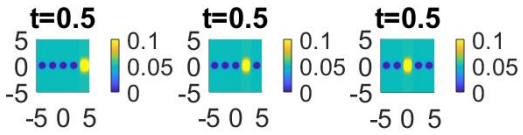


(a) t = 0.5

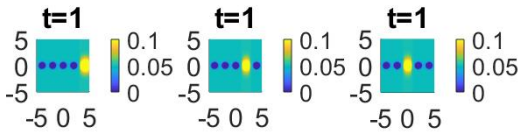


(b) t = 1.0

Figure 19: Three simultaneous simulations for four sources and a single sink with the location of the sink differing in each simulation, and $A_1 = A_2 = A_3 = 0.1$, and $D_1 = 0.9$, $D_2 = 0.7$ and $D_3 = 0.5$

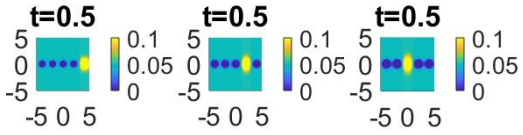


(a) t = 0.5

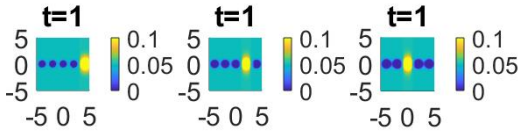


(b) t = 1.0

Figure 20: Three simultaneous simulations for four sinks and a single source with the location of the source differing in each simulation, and $A_1 = A_2 = A_3 = 0.1$, and $D_1 = D_2 = D_3 = 0.5$

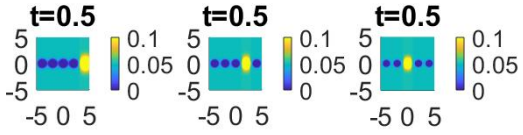


(a) t = 0.5

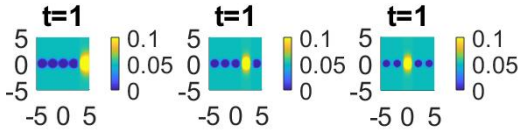


(b) t = 1.0

Figure 21: Three simultaneous simulations for four sinks and a single source with the location of the source differing in each simulation, and $A_1 = A_2 = A_3 = 0.1$, and $D_1 = 0.5$, $D_2 = 0.7$ and $D_3 = 0.9$



(a) t = 0.5



(b) t = 1.0

Figure 22: Three simultaneous simulations for four sinks and a single source with the location of the source differing in each simulation, and $A_1 = A_2 = A_3 = 0.1$, and $D_1 = 0.9$, $D_2 = 0.7$ and $D_3 = 0.5$

It is evident from the figures above that as the value of the diffusion coefficient D_i increases, the concentrations in the region surrounding both the sources and the sinks increase faster. In the following three figures, the simulations

shown above were done (with the same set of parameters), but with one source and four sinks instead of one sink and four sources.

3 Results and Conclusions

In summary, a systematic modeling of Anabaena colony dynamics was conducted starting with diffusion from a single point source and a single point sink, and two points sources and two point sinks. We moved on to the diffusion of the substances from a linear chain of point sources, and point sinks. Then we included a point source and a point sink in the same simulation. This was advanced to explore the effects of a linear chain of alternating point sources and point sinks.

We then tried to see if we can setup a scenario where a point acts as a sink and a source for different substances. To do this, we first tried to run two simulations independently at the same time, showing a point which acts a source for one substance and a sink for the other.

Finally we progressed to a five point system - where each point could be a sink or a source for a substance. In the first situation, there were four sources and one sink, and the location of the sink was altered in each simulation to mimic a different substance. In the second situation, there were four sinks instead and a single source, and the location of the source was altered in each simulation to mimic a different substance.

4 Notes

The matlab scripts for the simulations can be found at (https://github.com/basakrajarshi/Anabaena-Modeling), which is the authors github repository for the project.

5 References

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