3

Final Report

A Computational Model of Arsenic Accumulation in Plants

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Background

Heavy metal contamination in soil has significant negative impacts on human health and the environment. The largest poisoning in history is currently taking place in Bangladesh due to people drinking groundwater contaminated with arsenic (Smith). Over 20 million people have been exposed (HRW). The effects of chronic arsenic poisoning include skin lesions and drastic increases in cancer rates. Other heavy metals also contaminate soil and harm the humans and ecosystems they contact.

A variety of soil remediation methods exist (Yao):

- Soil replacement is used on a small scale because it is expensive and does not solve the fundamental problem of having heavy metal in the soil.
- Deep digging is used to spread the contaminant through the soil profile to dilute it.
- Thermal desorption requires heating soils to high temperatures and collecting the heavy metals that desorb from the soil matrix.
- Chemical methods are available to induce leaching of heavy metals at much higher rates than would occur naturally.

These methods are often disruptive, expensive, and can cause more environmental damage than if the heavy metals had been left in the soil in the first place.

Phytoremediation has been proposed as an alternative method to remove heavy metals from the soil. This process consists of cultivating plants which will accumulate contaminants in their tissues and harvesting those tissues to remove the contaminants from the area. Benefits of this technique include ease of implementation, low cost, and limited environmental impact.

Arsenic exists in the soil in ionic forms which are transported into the plant and converted into bound forms (Zhao). The conversion from free arsenic to bound arsenic and the reverse occur via opposing enzymatic reactions (Meharg). Both diffusion and convective transport play an active role in moving free arsenic throughout the plant.

The following computational model attempts to predict the concentration profile of arsenic accumulated by a tall grass plant grown in arsenic contaminated soil. Grass was chosen as the model plant because of its quick growth rate and large biomass density makes it a strong candidate for phytoremediation. The predicted arsenic accumulation can be used to assess the effectiveness of phytoremediation as compared to other methods.

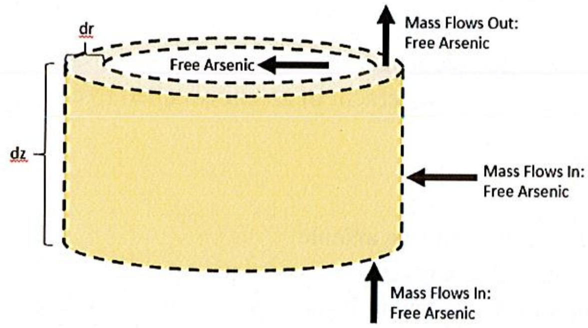


Figure 3: System boundary (dashed line) and mass flows for a differential element of the root. Free arsenic is flowing in the axial and radial directions.

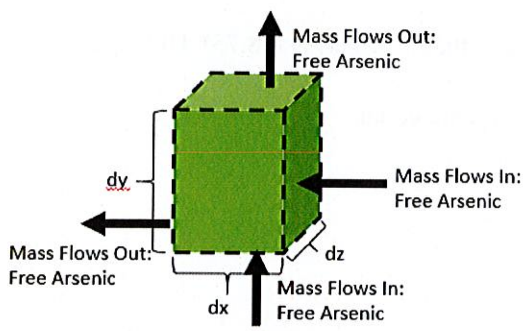


Figure 4: System boundary (dashed line) and mass flows for a differential element of the leaf. Free arsenic is flowing in the x and y dimensions.

The mass balances were combined into a numerical model using the forward finite difference method. The assumptions, derivation, and boundary conditions used to create the model are shown below.

Physical Principles:

- Mass is conserved.
- Fick's Law of Diffusion applies to the movement of free arsenic through the plant.

Biological Principles:

- Convective transport in vascular tissue.
- Reaction to convert free arsenic to bound arsenic via enzymatic reactions.
- Cylindrical geometry of root and rectangular geometry of leaf.

Assumptions:

1. The plant system can be modeled using lumped parameter differential elements.
2. The plant can be described as a root and a leaf with vascular tissue running through both.
3. The root can be described as a cylinder of height d, and radius r.
4. The root is radially symmetric.
5. The leaf can be described as a rectangular prism of given dimensions.
6. The leaf is very thin and can be considered homogenous in that dimension.
7. The leaf has vertical bilateral symmetry.
8. The axial concentration profile of free and bound arsenic in the root is the same as the horizontal profile of arsenic in the leaf at the boundary where the two tissues meet.

Differential Equations that model the system:

General Mass Balance for this model

Accumulation = net Convection + net diffusion + net reaction

For free arsenic in the root

$V*d\,Asf/dt = D((r*d\Theta*dz)*d\,Asf/dr|_{r=r} - (r*d\Theta*dz)*d\,Asf/dr|_{r=r+\Delta r}) + (r*dr*d\Theta)*D(d\,Asf/dz|_{z=z} - d\,Asf/dz|_{z=z+\Delta z}) - V*Vmax*E*Asf/(Km + Asf) + V*0.1Vmax*E*Asb/(Km + Asb) - A*u*(Asf|_{z=z} - Asf|_{z=z+\Delta z})$

Where $V=r*dr*d\Theta*dz$

Using finite difference methodology, this simplifies to

$Asf^{t+\Delta t}_{r,z} = Asf^{t}_{r,z} + \Delta t*D/(r*\Delta r)*[(r+\Delta r/2)*(Asf_{r+\Delta r,z} - Asf_{r,z})/\Delta r - (r-\Delta r/2)*(Asf_{r,z} - Asf_{r-\Delta r,z})/\Delta r]$

$+ \Delta t*D/(\Delta z)^2*(Asf_{r,z+\Delta z} - 2*Asf_{r,z} + Asf_{r,z-\Delta z})$

$- \Delta t*(Vmax*E*Asf^{t}_{r,z}/(Km + Asf^{t}_{r,z}) + 0.1Vmax*E*Asb^{t}_{r,z}/(Km + Asb^{t}_{r,z})$

$+\Delta t*u/\Delta z(-Asf_{r,z} + Asf_{r,z-\Delta z})$

For bound arsenic in the root

$V*dAsb/dt = V*Vmax*E*Asf/(Km + Asf) - V*0.1Vmax*E*Asb/(Km + Asb)$

Where $V=r*dr*d\Theta*dz$

Using finite difference methodology, this simplifies to

$Asb^{t+\Delta t}_{r,z} = \Delta t*(Vmax*E*Asf^{t}_{r,z}/(Km + Asf^{t}_{r,z}) + 0.1Vmax*E*Asb^{t}_{r,z}/(Km + Asb^{t}_{r,z})$

For free arsenic in the leaf

$V*d\,Asf/dt = (dz*dy)*D(d\,Asf/dx|_{x=x+\Delta x} - d\,Asf/dx|_{x=x}) + (dz*dx)*D(d\,Asf/dy|_{y=y} - d\,Asf/dy|_{y=y+\Delta y}) - - V*Vmax*E*Asf/(Km + Asf) + V*0.1Vmax*E*Asb/(Km + Asb) + A*u*(Asf|_{y=y} - Asf|_{y=y+\Delta y})$

Where $V= dx*dy*dz$

Using finite difference methodology, this simplifies to

$Asf^{t+\Delta t}_{x,y} = Asf^{t}_{x,y} + \Delta t/(\Delta x)^2*D*(Asf_{x+\Delta x,y} - 2*Asf_{x,y} + Asf_{x-\Delta x,y}) + \Delta t/(\Delta y)^2*D*(Asf_{x,y+\Delta y} - 2*Asf_{x,y} + Asf_{x,y-\Delta y}) - \Delta t*(Vmax*E*Asf^{t}_{x,y}/(Km + Asf^{t}_{x,y}) + 0.1Vmax*E*Asb^{t}_{x,y}/(Km + Asb^{t}_{x,y}))$

$+ \Delta t*u/\Delta z(-Asf_{x,y} + Asf_{x,y-\Delta y})$

For bound arsenic in the leaf

$V*dAsb/dt = V*Vmax*E*Asf/(Km + Asf) - V*0.1Vmax*E*Asb/(Km + Asb)$

Using finite difference methodology, this simplifies to

$Asb^{t+\Delta t}_{x,y} = Asb^{t}_{x,y} + \Delta t*(Vmax*E*Asf^{t}_{x,y}/(Km + Asf^{t}_{x,y}) - 0.1Vmax*E*Asb^{t}_{x,y}/(Km + Asb^{t}_{x,y})$

Computational Model:

The above finite difference model was implemented in an attached Matlab program titled "Gee_FinalModel.m".

Values used in the calculations are shown below. These values are based on literature sources described in the assumptions section. Note that the plant width and radius is much larger than reasonable in order to prevent stability issues in the model.

```
%Free Arsenic concentration in soil
AsfSoil = 80; %g/m3

%Reaction Rate Constants in plant tissues
Km = 68*10^-6 * 74.92160 *1000; % M*g/mol*L/m3
Kcat = 215 *60 *24 ; % 1/min * min/hr * hr/day
E = 10^-10 * 1000 * 74.92160; % mol/L*1000L/m3*g/mol
Vmax= Kcat*E; % g(m3*day)

%kroot = 0.000001;
%kcortex = 0.000001;
%kleaf = 0.000001;

%Diffusivity Constant for Free Arsenic
Droot = 8.75*10^-10*3600*24 ; %m2/s*s/hr*hr/day
Dcortex= 8.75*10^-10*3600*24 ; %m2/s*s/hr*hr/day
Dleaf = 8.75*10^-10*3600*24 ; %m2/s*s/hr*hr/day

%Convective Transport Velocity
uvascular = 56*10^-5*3600*24 ; %m/s*s/hr*hr/day

dt = 0.0001;
dr = 0.01;
dx = dr;
dz = 0.1;
dh = 0.1;

tinitial= 0;
tmax = 60;


rootRadius=0.5;
rootDepth=.5;
leafWidth=rootRadius;
leafHeight=1;
```

Analysis of Model:

The results above were obtained using parameters (except as noted) based on literature values.

The model provides a reasonable estimate of the concentration profile for arsenic accumulation in plants growing in arsenic contaminated soils. The model shows the gradual diffusion of free arsenic through the root and the rapid transport once it reaches the vascular tissue (right side of pictures). The bound arsenic concentration profile mirrors the free arsenic profile. The high reaction speed prevents speedy flow of the free arsenic and keeps bound and free arsenic at similar concentration levels. The model shows high arsenic concentrations in the vascular tissue due to convection and near the root edges due to proximity of the soil.

An emergent property of the model is higher accumulation of arsenic in the roots as compared to the leaves which matches physical reality.

The bound arsenic exhibits a slight bump at the root edge near ground level that is not observed in the free arsenic. This is most likely a model artifact and is not consistent with a physical understanding of the situation.

The total quantity of arsenic accumulated may be an overestimate. The average arsenic concentration in the plants is usually less than that found in the soil (Porter). Modeling a barrier tissue in the root, such as the cortex may correct this discrepancy.

The model can be improved in the future by:

- Modeling different tissue properties by determining diffusion and reaction rate constants for each tissue. More research must be conducted to determine what these constants may be.
- Modeling the cortex tissue on the outside of the root which would reduce the total amount of arsenic accumulated in the plant.
- Use an implicit model like Crank-Nichelson to avoid the stability issues.
- Correcting the slight aberration in bound arsenic at the ground surface.

7. The concentration of arsenous acid in the soil is 1 mol/m^3.
8. The initial concentration of arsenic in the plant is zero.

Parameters:

t	Time	[s]
r	Radius	[m]
h	Height	[m]
C_p	Concentration of Arsenous Acid in the plant	[mol/m^3]
C_S	Concentration of Arsenous Acid in the soil	[mol/m^3]
J	Molar flux of arsenous acid	[mol/(m^2*s)]
k	Proportionality constant for mass flux	[m/s]

Fundamental relationships:

- Mass is conserved. Since there is no reaction of arsenous acid, moles of arsenous acid are conserved.
- Flux of arsenous acid into the plant can be described by $J_A = k(C_s - C_p)$

Differential Equations that model the system:

$d C_p/dt = J_{in}*pi*r^2/(pi*r^2*h)= h*k(C_s- C_p)$

Calculating the requested parameter:

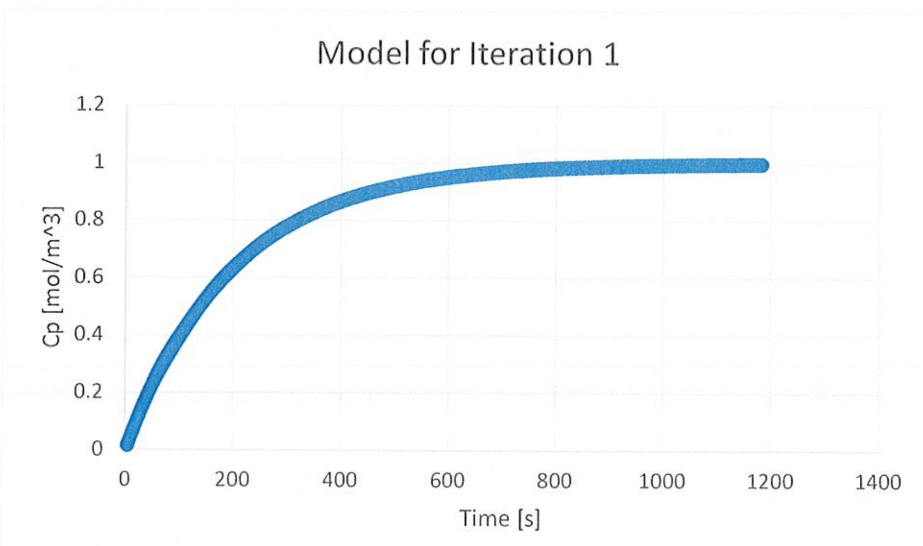
This model can be solved analytically by integration and the result is shown below.

$C_p = -e^{-(hk*t+Co)}+C_s$

A plot of the model is shown below assuming the following conditions

C_s=1 Co = 0 k = 0.005

Since concentration is uniform, this is the concentration profile for the plant.



Iteration 2

Parameter Requested: Concentration profile of arsenic over time in a plant growing in arsenic contaminated soil.

Picture of Situation:

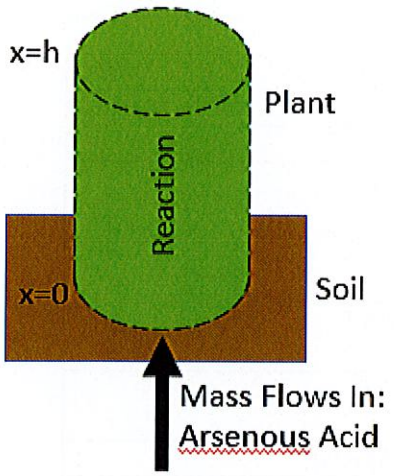


Figure 1: System boundary and mass flows for the entire plant system.

System Definition: The boundary of the plant, shown in a dashed line in the diagram above, is the boundary of the system.

What is crossing the boundaries: Arsenic in the form of arsenous acid is crossing the system boundary at a surface in contact with the soil as shown in Figure 1.

Applicable Principles and theories:

- Mass is conserved.
- Transport of compounds is resisted by boundaries
- The following reaction occurs in the plant

Updated Assumptions:

1. Arsenic acid is immediately sequestered in the plant and does not diffuse.
2. The conversion of arsenous acid to arsenic acid is first order proportional to arsenous acid concentration.
3. The system maintains a constant concentration of hydroxide and water so they do not affect the reaction rates.

Previous Assumptions

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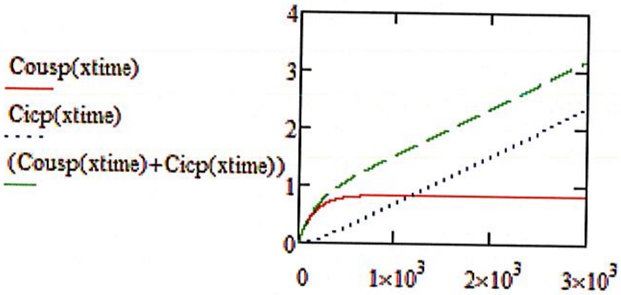


Analysis of Model: The model shows that the concentration of arsenous acid increases by diffusion and reaches steady state when the rate of diffusion equals the rate of removal of arsenous acid by reaction. This steady state concentration is less than the concentration of arsenous acid in the soil. The concentration of arsenic acid increases via reaction and reaches a steady state rate of increase once the concentration of arsenous acid reaches steady state. Thus the concentration of arsenic acid and total arsenic in the plant will be increase continually.

This does not match the physical reality because arsenic can not accumulate infinitely in the plant.

Updated Assumptions:

1. The system can be modeled using a lumped parameter differential element.
2. There is no other forms of arsenic in the plant besides arsenous acid.
3. There is no resistance to movement of arsenous acid into the plant nor within the plant.
4. There is no convective transport of arsenous acid within the plant.
5. The system is homogenous in the radial direction.

Previous Assumptions

6. The plant can be modeled as a cylinder of dimensions r=0.01m and h=1m.
7. The system stays at a constant temperature.
8. The plant does not grow.

Parameters:

t	Time	[s]
r	Radius	[m]
h	Height	[m]
x	Axial Position	[m]
C^t_x	Concentration of Arsenous Acid at time t and position x	[g/m^3]
D	Proportionality constant for mass diffusion	[m^2/s]

Fundamental relationships:

- Mass is conserved.
- Fick's law of diffusion governs the diffusion of arsenous acid into the plant.

Differential Equations that model the system:

Conduct a mass balance on the differential element

$$V*dC/dt = A*D(dC/dx|_{x=x} - dC/dx|_{x=x+\Delta x})$$

Using finite difference methodology, this simplifies to

$$C^{t+\Delta t}_x = C^t_x + D* \Delta t/(\Delta x)^2*(C_{x+\Delta x}-2* C_x+ C_{x-\Delta x})$$

Boundary Conditions

The boundary conditions assumed for the model above are:

- At x=h, dC/dx=0
- At x=0, C = 0.005 g/m^3
- At t=0, C=0 for all x

Calculating the requested parameter:

The above model was implemented in an attached Matlab program titled "Gee_Iteration3.m".
Values used in the calculations were:
D= 0.001 m^2/s
dt = 0.01;

Iteration 4

Parameter Requested: Concentration profile of arsenous acid over time in a plant growing in arsenic contaminated soil.

Picture of Situation:

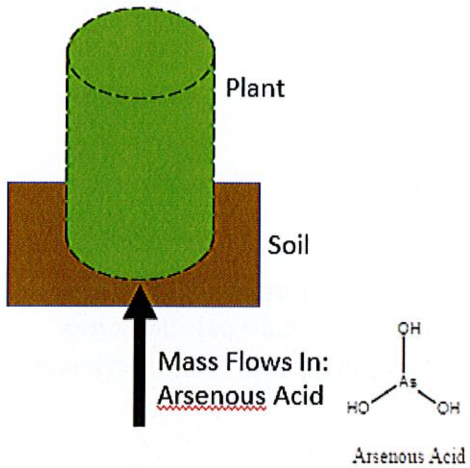


Figure 1: System boundary (dashed line) and mass flow for the entire plant system.

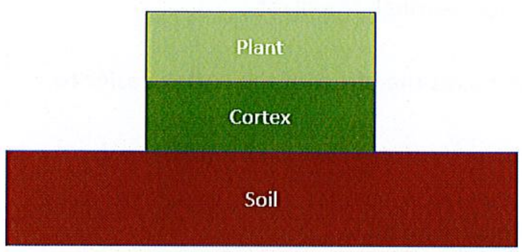


Figure 2. Close depiction of the soil-plant interface. The cortex is an external layer of plant material that resists movement of materials from the soil into the plant.

System Definition: The boundary of the plant, shown in a dashed line in the diagram above, is the boundary of the system. However, thinking about the system in terms of a differential element is useful in the modeling process and the differential element system is shown below with the boundary being the dashed line around the differential element.

Differential Equations that model the system:
Conduct a mass balance on the differential element

$V*dC/dt = A*D(dC/dx|_{x=x} - dC/dx|_{x=x+\Delta x})$

Using finite difference methodology, this simplifies to

$C^{t+\Delta t}_{x} = C^{t}_{x} + D* \Delta t /(\Delta x)^2*(C_{x+\Delta x}-2* C_x+ C_{x-\Delta x})$

Boundary Conditions
The boundary conditions assumed for the model above are:

- At x=h, dC/dx=0
- At x=0, C = 0.005 g/m^3
- At t=0, C=0 for all x

Calculating the requested parameter:
The above model was implemented in an attached Matlab program titled "Gee_Iteration4.m".
Values used in the calculations were:
D = 0.000005 m^2/s for 0<x<0.01 and D=0.001 m^2/s for x>=0.01.
dt = 0.0005;
dx = 0.001;
tinitial= 0;
xinitial= 0;
tmax = 100;
xmax = 1;

The plot below shows the concentration profile of arsenic in the plant at ten evenly spaced time points from t=initial to t=tmax.

Iteration 5

Parameter Requested: Concentration profile of arsenic over time in a plant growing in arsenic contaminated soil.

Picture of Situation:

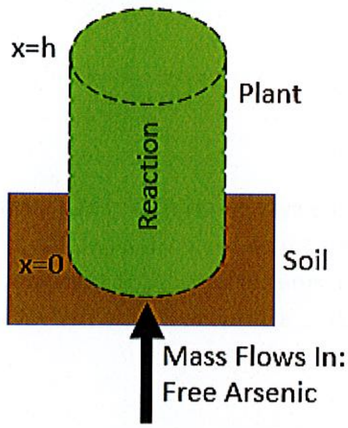


Figure 1: System boundary (dashed line) and mass flow for the entire plant system.

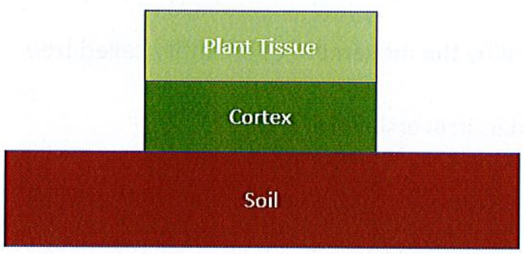


Figure 2. Close depiction of the soil-plant interface. The cortex is an external layer of plant material that resists movement of materials from the soil into the plant.

$$As_f \rightarrow As_b$$

Figure 3. Reaction of free arsenic (As_f) to bound arsenic (As_b). This reaction occurs in the plant tissue that is not the cortex.

System Definition: The boundary of the plant, shown in a dashed line in Figure 1 above, is the boundary of the system. However, thinking about the system in terms of a differential element is useful in the modeling process and the differential element system is shown in Figure 4 with the boundary being the dashed line around the differential element.

x	Axial Position	[m]
C^t_x	Concentration at time t and position x	[g/m^3]
D	Proportionality constant for mass diffusion	[m^2/s]
A	Area	[m^2]
V	Volume	[m^3]
Asf	Free arsenic concentration	[g/m^3]
Asb	Bound arsenic concentration	[g/m^3]
k	Reaction Rate constant (first order)	[1/s]

Differential Equations that model the system:

Conduct a component mass balance on the differential element

For free arsenic

$V*d\ Asf/dt = A*D(\ d\ Asf/dx|_{x=x} - d\ Asf/dx|_{x=x+\Delta x}) - V*k*Asf$

Using finite difference methodology, this simplifies to

$Asf^{t+\Delta t}_x = Asf^t_x + \Delta t/(\Delta x)^2*D*(\ Asf_{x+\Delta x}-2*\ Asf_x + Asf_{x-\Delta x}) - k*\ \Delta t*Asf^t_x$

For bound arsenic

$V*dAsb/dt = V*k*Asf$

Using finite difference methodology, this simplifies to

$Asb^{t+\Delta t}_x = Asb^t_x + k*\ \Delta t*Asf^t_x$

Boundary Conditions

The boundary conditions assumed for the model above are:

- At x=0, Asf = 0.005 g/m^3
- At t=0, Asf=0 g/m^3 for all x
- At x=h, dAsf/dx=0

- At t=0 Asb = 0 g/m^3 for all x

Calculating the requested parameter:

The above finite difference model was implemented in an attached Matlab program titled "Gee_Iteration5.m". Values used in the calculations were:

D = 0.000001 m^2/s for 0<x<0.01 and D=0.001 m^2/s for x>=0.01.

```
kp = 0.000001; %Reaction Rate Constant in plant tissues
kc = 0; %Reaction Rate Constant in cortex
Dp= 0.001; %Mass Diffusivity constant of the plant
Dc= 0.0000005; %Mass Diffusivity constant of the cortex
dt = 0.0005;
dx = 0.001;
```

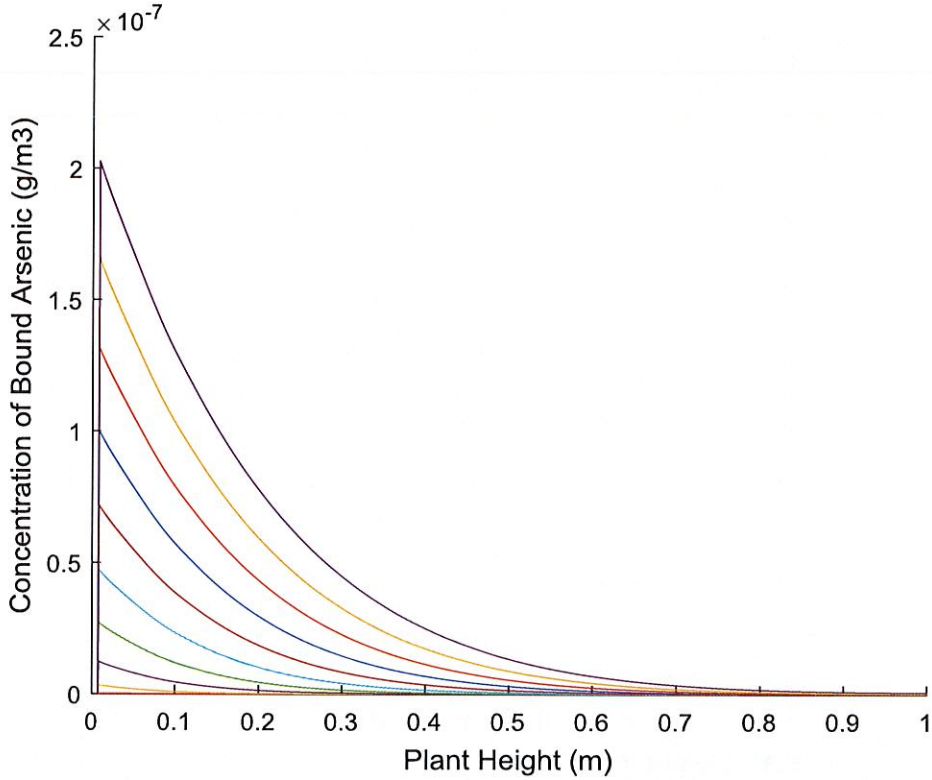


Figure 6. Concentration of bound arsenic in the plant at regularly spaced time points. Note the cortex preventing accumulation of bound arsenic from 0<x<0.01 m.

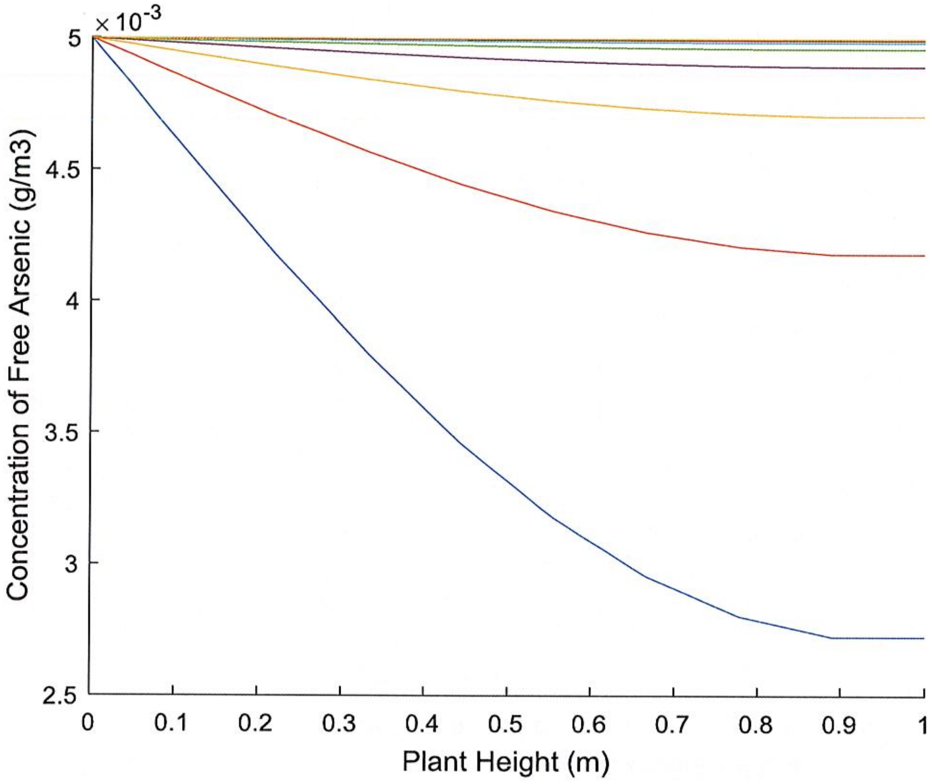


Figure 8. Concentration of free arsenic in the plant. Notice how the concentration reaches a steady state throughout the plant at long times.

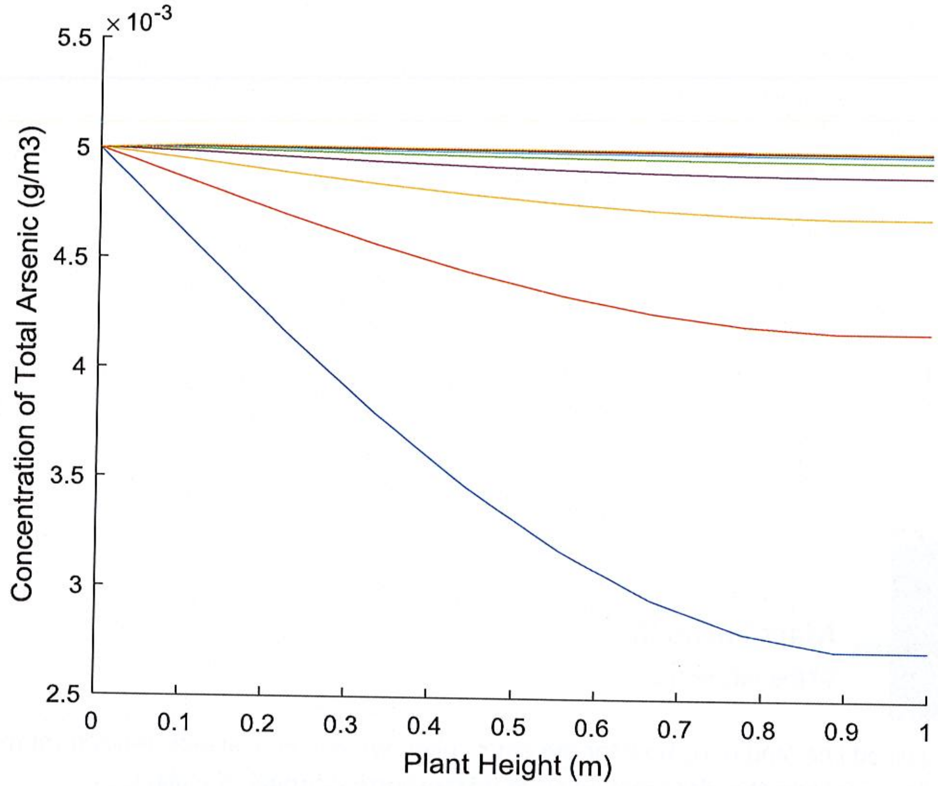


Figure 10. Total concentration of arsenic at long time frames. Notice how the diffusion reaches a steady state and further increases in arsenic concentration are caused by the reaction from free arsenic to bound arsenic.

Analysis of Model:

The model shows that for early time points, the diffusion of free arsenic is the determining factor in total arsenic concentration.

At longer time points, the concentration of free arsenic reaches steady state at the environmental concentration. The total arsenic continues to increase as the free arsenic is reacted to bound arsenic.

As time approaches infinity, the total arsenic concentration will increase as free arsenic is continuously reacted to bound arsenic.

This demonstrates how a plant can become enriched for arsenic relative to the soil concentration.

At all time points, the effect of the cortex can be seen.

The model can be improved by more accurately representing the reaction of free arsenic to bound arsenic and the chemical nature of these two species.

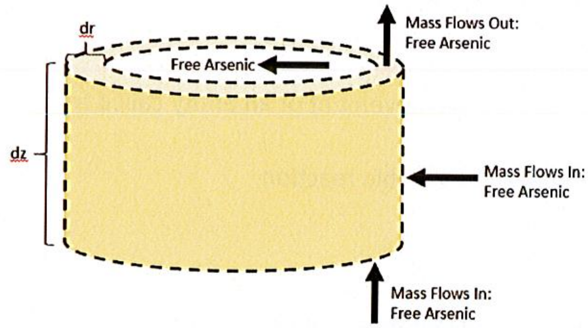


Figure 4: System boundary and mass flows for a differential element of the root. Free arsenic is flowing in the axial and radial directions.

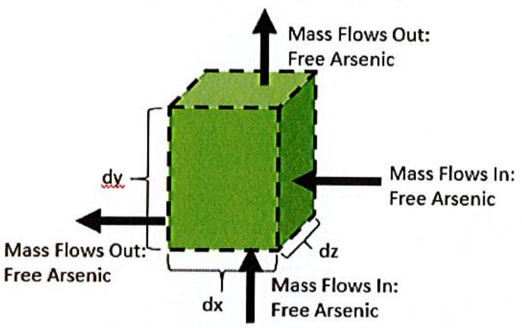


Figure 5: System boundary and mass flows for a differential element of the leaf. Free arsenic is flowing in the x and y dimensions.

What is crossing the boundaries: Arsenic in the form of free arsenic is crossing the system boundary at a surface of the root in contact with the soil as shown in Figure 1. As shown in Figure 2, the arsenic must pass the cortex before entering the rest of the root. For the root differential element, free arsenic is flowing across all surfaces as shown in Figure 4, but is not flowing in the angular direction. For the leaf differential element, free arsenic is flowing across the system boundary in the x and y dimension as shown in Figure 5. The reaction of free arsenic to bound arsenic occurs in the plant tissues. Bound arsenic does not move.

Applicable Principles and theories:

- Mass is conserved.
- Fick's Law of Diffusion applies to the movement of free arsenic through the plant.

Updated Assumptions:

1. The plant can be described as a root and a leaf.
2. The root can be described as a cylinder of height d, and radius r.
3. The root is radially symmetric.
4. The leaf can be described as a rectangular prism of given dimensions.
5. The leaf is very thin so it can be considered homogenous in that dimension.
6. The leaf has vertical bilateral symmetry.
7. The axial concentration profile of free and bound arsenic in the root is the same as the horizontal profile of arsenic in the leaf at the boundary where the two tissues meet.

Using finite difference methodology, this simplifies to
$Asf^{t+\Delta t}_{x,y} = Asf^{t}_{r,z} +$

$\Delta t*D/(r*\Delta r)*[(r+\Delta r/2)*(Asf_{r+\Delta r,z} - Asf_{r,z})/\Delta r - (r-\Delta r/2)*(Asf_{r,z} - Asf_{r-\Delta r,z})/\Delta r] +$

$\Delta t*D/(\Delta z)^2*(Asf_{r,z+\Delta z} - 2*Asf_{r,z} + Asf_{r,z-\Delta z}) - k*\Delta t*Asf^{t}_{r,z}$

For bound arsenic in the root
V*dAsb/dt = V*k*Asf
Where V=r*dr*dΘ*dz

Using finite difference methodology, this simplifies to
$Asb^{t+\Delta t}_{r,z} = Asb^{t}_{r,z} + k*\Delta t*Asf^{t}_{r,z}$

For free arsenic in the leaf
$V*d\,Asf/dt = (dz*dy)*D(d\,Asf/dx|_{x=x+\Delta x} - d\,Asf/dx|_{x=x}) + (dz*dx)*D(d\,Asf/dy|_{y=y} - d\,Asf/dy|_{y=y+\Delta y}) - V*k*Asf$
Where V= dx*dy*dz

Using finite difference methodology, this simplifies to
$Asf^{t+\Delta t}_{x,y} = Asf^{t}_{x,y} + \Delta t/(\Delta x)^2*D*(Asf_{x+\Delta x,y} - 2*Asf_{x,y} + Asf_{x-\Delta x,y}) + \Delta t/(\Delta y)^2*D*(Asf_{x,y+\Delta y} - 2*Asf_{x,y} + Asf_{x,y-\Delta y}) - k*\Delta t*Asf^{t}_{x,y}$

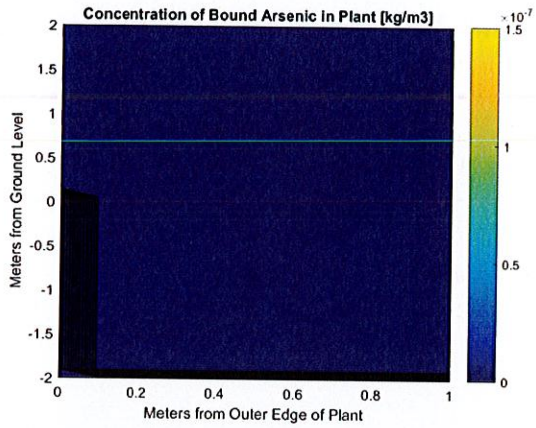
For bound arsenic in the leaf
V*dAsb/dt = V*k*Asf

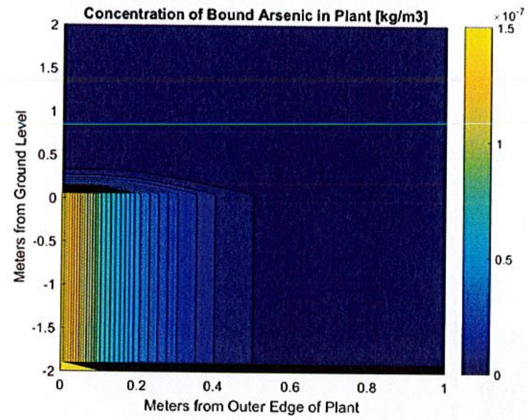
Using finite difference methodology, this simplifies to
$Asb^{t+\Delta t}_{x,y} = Asb^{t}_{x,y} + k*\Delta t*Asf^{t}_{x,y}$

Boundary Conditions
For the root:
- At z=0, Asf = soil concentration
- At z=d, Asf = leaf concentration
- At r=0, Asf = soil concentration
- At r=R, dAsf/dx=0
- At t=0, Asf = 0 g/m^3

For the leaf
- At y=0, Asf = Asf(root surface)
- At y=h, dAsf/dx=0
- At x=0, dAsf/dx=0
- At x=w, dAsf/dx=0
- At t=0, Asf = 0 g/m^3

Calculating the requested parameter:





The bound arsenic mirrors the free arsenic concentration.

Analysis of Model:

This model accurately portrays the physical processes of two dimensional diffusion and a first order reaction.

The model also depicts the differences in leaf and root tissues with respect to arsenic concentration.

The model shows that radial diffusion is much more important to the arsenic profile due to the geometry of the plant.

Several biological aspects are not represented in the model including cortex tissue, convective transport through capillaries, and enzymatic reactions. Also, the plant dimensions are unrealistic.

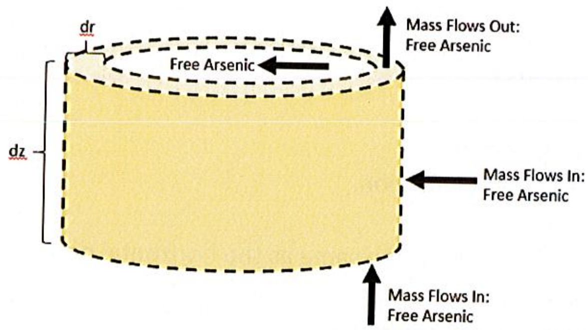


Figure 4: System boundary and mass flows for a differential element of the root. Free arsenic is flowing in the axial and radial directions.

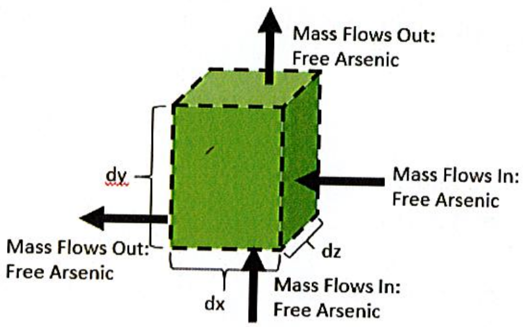


Figure 5: System boundary and mass flows for a differential element of the leaf. Free arsenic is flowing in the x and y dimensions.

What is crossing the boundaries: Arsenic in the form of free arsenic is crossing the system boundary at a surface of the root in contact with the soil as shown in Figure 1. As shown in Figure 2, the arsenic must pass the cortex before entering the rest of the root. For the root differential element, free arsenic is flowing across all surfaces as shown in Figure 4, but is not flowing in the angular direction. For the leaf differential element, free arsenic is flowing across the system boundary in the x and y dimension as shown in Figure 5. The reaction of free arsenic to bound arsenic occurs in the plant tissues. Bound arsenic does not move.

Physical Principles and theories:

- Mass is conserved.
- Fick's Law of Diffusion applies to the movement of free arsenic through the plant.

Biological Principles

- Difference of diffusion properties in cortex, root, leaf, and vascular tissue.
- Convective transport in vascular tissue.
- Reaction to convert free arsenic to bound arsenic.
- Cylindrical geometry of root and rectangular geometry of leaf.

Updated Assumptions:

1. The inner 10% of the plant is a vascular tissue that moves free arsenic by convection in the vertical direction.

Differential Equations that model the system:

Mass balances will be conducted on a root differential element and a leaf differential element. Important phenomena are diffusion, reaction and conduction.

For free arsenic in the root

$V*d\ Asf/dt = D((r*d\Theta*dz)*d\ Asf/dr|_{r=r} - (r*d\Theta*dz)*d\ Asf/dr|_{r=r+\Delta r}) +(r*dr*d\Theta)*D(d\ Asf/dz|_{z=z} - d\ Asf/dz|_{z=z+\Delta z}) - V*k*Asf - A*u*(Asf|_{z=z} - Asf|_{z=z+\Delta z})$

Where $V=r*dr*d\Theta*dz$

Using finite difference methodology, this simplifies to

$Asf^{t+\Delta t}_{x,y} = Asf^{t}_{r,z} +$

$\Delta t*D /(r*\Delta r)* [(r+ \Delta r/2)*(Asf_{r+\Delta r,z} - Asf_{r,z})/ \Delta r - (r - \Delta r/2)*(Asf_{r,z} - Asf_{r-\Delta r,z})/ \Delta r] +$

$\Delta t*D /(\Delta z)^2* (Asf_{r,z+\Delta z} -2* Asf_{r,z}+ Asf_{r,z-\Delta z}) - k* \Delta t*Asf^{t}_{r,z} +$

$\Delta t*u/ \Delta z (-Asf_{r,z}+ Asf_{r,z-\Delta z})$

For bound arsenic in the root

$V*dAsb/dt = V*k*Asf$

Where $V=r*dr*d\Theta*dz$

Using finite difference methodology, this simplifies to

$Asb^{t+\Delta t}_{r,z} = Asb^{t}_{r,z} + k* \Delta t*Asf^{t}_{r,z}$

For free arsenic in the leaf

$V*d\ Asf/dt = (dz*dy)*D(d\ Asf/dx|_{x=x+\Delta x} - d\ Asf/dx|_{x=x}) +(dz*dx)*D(d\ Asf/dy|_{y=y} - d\ Asf/dy|_{y=y+\Delta y}) - V*k*Asf + A*u*(Asf|_{y=y} - Asf|_{y=y+\Delta y})$

Where $V= dx*dy*dz$

Using finite difference methodology, this simplifies to

$Asf^{t+\Delta t}_{x,y} = Asf^{t}_{x,y} + \Delta t /(\Delta x)^2*D*(Asf_{x+\Delta x,y}-2* Asf_{x,y}+ Asf_{x-\Delta x,y}) + \Delta t /(\Delta y)^2*D*(Asf_{x,y+\Delta y} -2* Asf_{x,y}+ Asf_{x,y-\Delta y}) - k* \Delta t*Asf^{t}_{x,y} + \Delta t*u/ \Delta z (-Asf_{x,y}+ Asf_{x,y-\Delta y})$

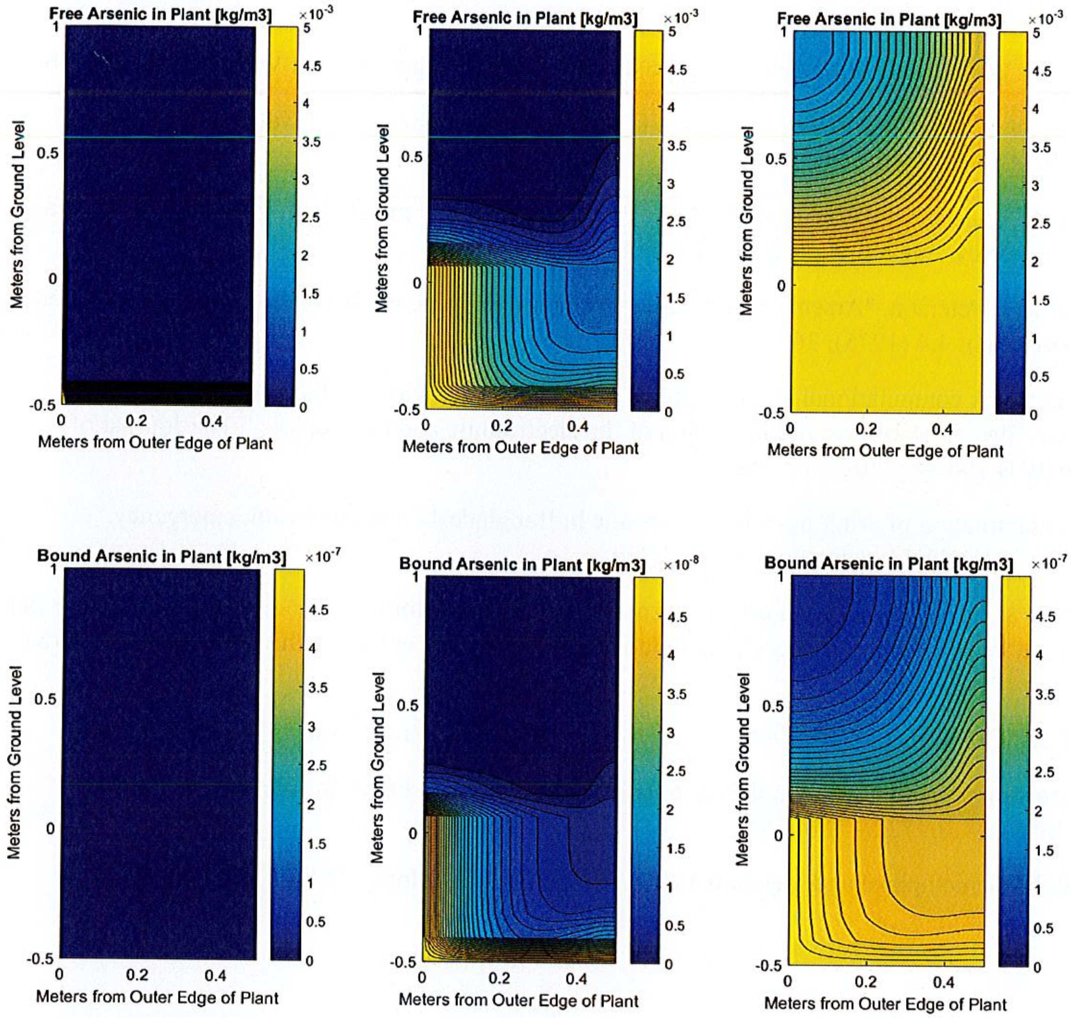
For bound arsenic in the leaf

$V*dAsb/dt = V*k*Asf$

Using finite difference methodology, this simplifies to

$Asb^{t+\Delta t}_{x,y} = Asb^{t}_{x,y} + k* \Delta t*Asf^{t}_{x,y}$

Boundary Conditions



Analysis of Model:

This model shows no values which are unreasonable except the time scale at which the process occurs.

Key observations from the model are:

- Concentration of arsenic is much higher in the roots than in the leaves.
- Concentration of arsenic in the roots is almost uniform at long times.
- Diffusion control of mass flow at short times and convective control of mass flow at long times once the arsenic reaches the vascular tissue.

Limitations of the model are:

- Failure to show behavior of cortex tissue.
- Reaction is unidirectional.
- Bound arsenic does not contribute significantly to the total arsenic concentration.