Optimizing Chlorine Dosing to Control Bacterial Regrowth in Drinking Water Distribution Systems

Using the Adjoint Method

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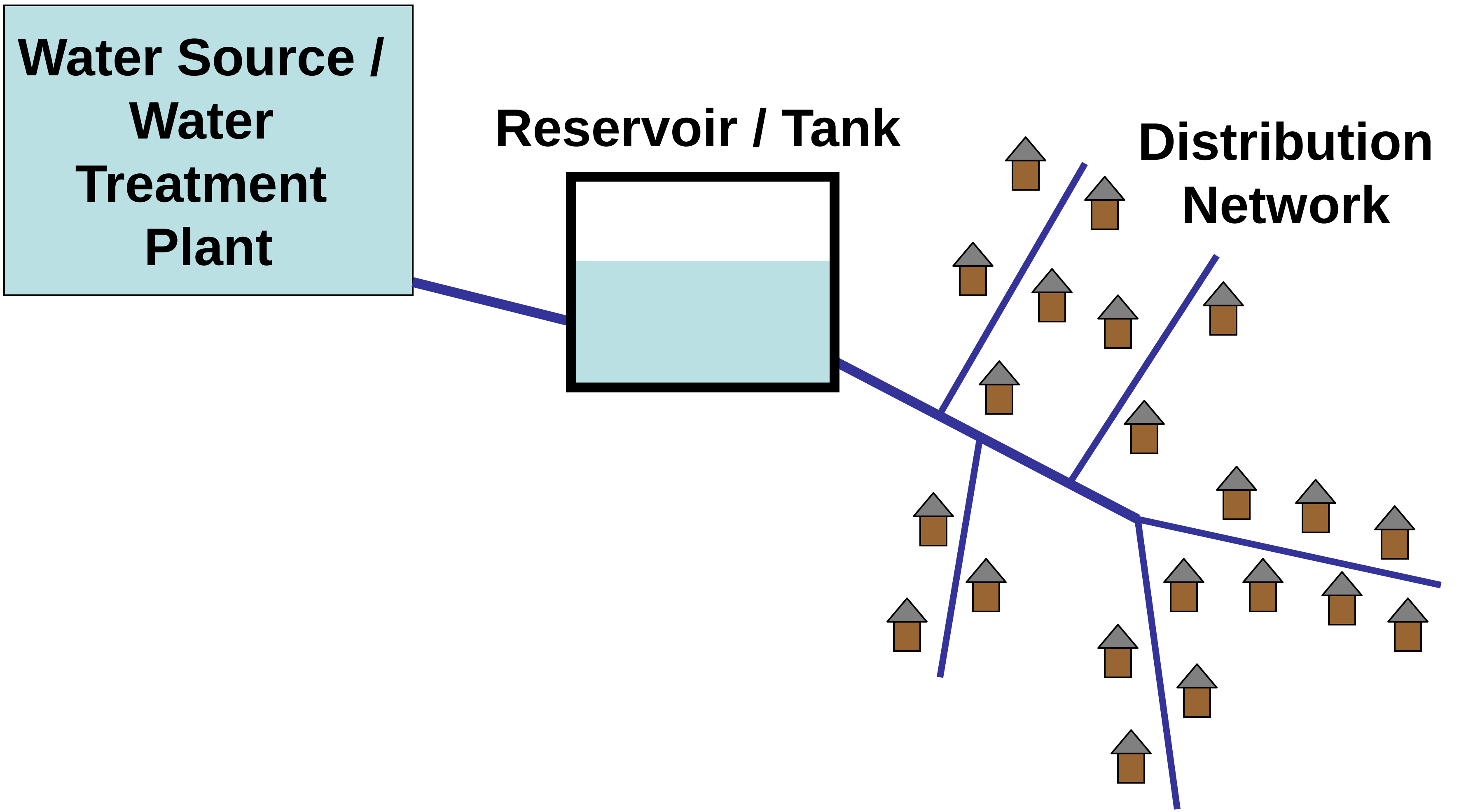
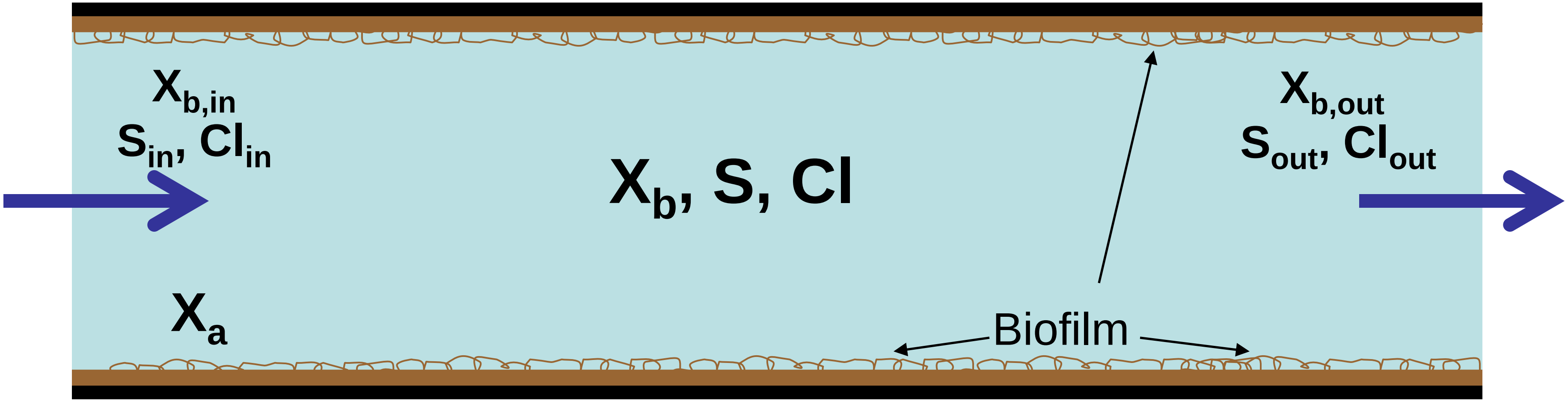
CE 291F/ME236/EE291

Drinking Water System



Pipe as a Reactor



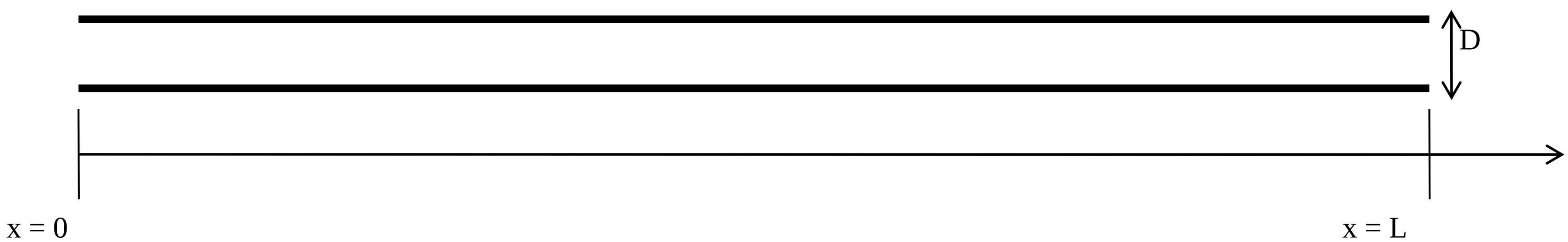
X_b = Bacterial Concentration in Bulk Water

X_a = Attached Bacteria Concentration

S = Substrate Concentration (bacteria food)

Cl = Chlorine Concentration (inhibits bacterial growth)

Regrowth Model



Accum.	Advection	Diffusion	Growth	Decay
$\frac{\partial X_b}{\partial t} =$	$-v\frac{\partial X_b}{\partial x}$	$+D_d\frac{\partial^2 X_b}{\partial x^2}$	$+\mu_b X_b + \frac{k_{\det} X_a v}{R_h}$	$-k_d X_b - k_{dep} X_b$
$\frac{\partial X_a}{\partial t} =$			$+\mu_a X_a + k_{dep} X_b R_h$	$-k_d X_a - k_{\det} X_a v$
$\frac{\partial S}{\partial t} =$	$-v\frac{\partial S}{\partial x}$	$+D_d\frac{\partial^2 S}{\partial x^2}$		$-\left(\frac{1}{Y_g \beta}\right)\left(\frac{\mu_a X_a}{R_h} + \mu_b X_b\right)$
$\frac{\partial Cl}{\partial t} =$	$-v\frac{\partial Cl}{\partial x}$	$+D_d\frac{\partial^2 Cl}{\partial x^2}$		$-k_b Cl - \frac{k_w}{R_h}$

Source: Zhang et al, 2004

Parameters, Boundary Conditions

$$\mu_{b/a} = \begin{cases} \mu_{\max,b/a}\left(\dfrac{S}{S+K_s}\right)\exp\left(-\dfrac{Cl_2 - Cl_{2,t,b/a}}{Cl_{2,c}}\right)\exp\left(-\left(\dfrac{T_{opt}-T}{T_{opt}-T_i}\right)^2\right) & \text{when } Cl_2 > Cl_{2,t,b/a} \\ \mu_{\max,b/a}\left(\dfrac{S}{S+K_s}\right)\exp\left(-\left(\dfrac{T_{opt}-T}{T_{opt}-T_i}\right)^2\right) & \text{when } Cl_2 \le Cl_{2,t,b/a} \end{cases}$$

v = velocity

(Determined by hydraulic model, Assumed constant)

Boundary Conditions

$S(x = 0, t) = S_{in}$

$X_b(x = 0, t) = X_{b,in}$

$Cl_2(x=0, t) = Cl_{2,in}$ (Control)

Initial Conditions

$Cl_2(x, t = 0) = 0$

$S(x, t = 0) = 0$

$X_b(x, t = 0) = 0$

$X_a(x, t = 0) = 0$

Source: Zhang et al, 2004

Project Objective

- Control: $Cl_2(x=0, t) = Cl_{2,in}$
- To Minimize:
  - X_b (bacterial regrowth)
  - Cost of chlorination
- Use: Adjoint Method

Model of the Problem

Define the operator * such that:

$$\begin{bmatrix} a_1 \\ b_1 \\ c_1 \\ d_1 \end{bmatrix} * \begin{bmatrix} a_2 \\ b_2 \\ c_2 \\ d_2 \end{bmatrix} = \begin{bmatrix} a_1 a_2 \\ b_1 b_2 \\ c_1 c_2 \\ d_1 d_2 \end{bmatrix}$$

Governor PDE:

$$\partial_t Z(x,t) = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} * \left(-v \partial_x Z(x,t) + D_d \partial_{xx} Z(x,t) \right) + P[Z(x,t)] - \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{k_w}{R_h} \end{bmatrix}$$

Where P(Z) is a growth and decay function R4 → R4:

$$P(Z) = \begin{bmatrix} (\mu_b - k_d - k_{dep}) X_b + \left(\frac{k_{\det} v}{R_h} \right) X_a \\ \left(k_{dep} R_h \right) X_b + \left(\mu_a - k_d - k_{\det} v \right) X_a \\ -\left(\frac{\mu_a}{Y_g \beta R_h} \right) X_b - \left(\frac{\mu_b}{Y_g \beta} \right) X_a \\ \left(-k_b \right) Cl \end{bmatrix}$$

$$Z(x,t) = \begin{bmatrix} X_b(x,t) \\ X_a(x,t) \\ S(x,t) \\ Cl(x,t) \end{bmatrix}$$

Objective Function:

$$\min J(\theta(t)) = \int_0^L \int_0^T \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} * Z(x,t)\,dt\,dx + K \int_0^T \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} * Z(x=0,t)\,dt \quad ,$$

and K = a constant representing the cost of chlorine addition relative to the cost of bacterial re-growth.

Control:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} * Z(x,t) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ Cl_{in}(t) = \theta \end{bmatrix}$$

Linearize Objective Function, PDE, Boundary Conditions, Initial Conditions and Control

$$Z = \overline{Z} + \tilde{Z}; \quad P(Z) = P(\overline{Z}) + \frac{\partial P}{\partial Z}\tilde{Z} = P(\overline{Z}) + (\partial_z P)\tilde{Z}$$

$$\partial_t \overline{Z} + \partial_t \tilde{Z} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} * \left[-v(\partial_x \overline{Z} + \partial_x \tilde{Z}) + D_d (\partial_{xx} \overline{Z} + \partial_{xx} \tilde{Z}) \right] + P(\overline{Z}) + (\partial_z P)\tilde{Z} - \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{k_w}{R_h} \end{bmatrix}$$

$$\text{Subtract : } \left\{ \partial_t \overline{Z} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} * \left(-v\partial_x \overline{Z} + D_d \partial_{xx} \overline{Z} \right) + P(\overline{Z}) - \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{k_w}{R_h} \end{bmatrix} \right\}$$

PDE becomes: $$\partial_t \tilde{Z} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} * \left(-v\partial_x \tilde{Z} + D_d \partial_{xx} \tilde{Z} \right) + (\partial_z P)\tilde{Z}$$

Boundary Conditions:

$$\begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} * Z(x=0,t) = \begin{bmatrix} X_{b,in} \\ 0 \\ S_{in} \\ 0 \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} * \tilde{Z}(x=0,t) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Initial Conditions:

$$Z(x,t=0) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \Rightarrow \quad \tilde{Z}(x,t=0) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Control:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} * \tilde{Z}(x,t) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \tilde{C}l_{in}(t) = \theta \end{bmatrix}$$

Objective Function:

$$\tilde{J} = \int_0^L \int_0^T \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} * \tilde{Z}(x,t)\,dt\,dx + K \int_0^T \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} * \tilde{Z}(x=0,t)\,dt$$

Add PDE multiplied by an arbitrary function λ to the perturbation of the objective function

$$0 = -\partial_t \tilde{Z} + \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} * \left(-v\partial_x \tilde{Z} + D_d \partial_{xx} \tilde{Z} \right) + (\partial_z P)\tilde{Z}$$

$$\tilde{J} = \int_0^L \int_0^T \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} * \tilde{Z}(x,t)\,dt\,dx + K \int_0^T \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} * \tilde{Z}(x=0,t)\,dt$$

$$+ \int_{x=0}^{L} \int_{t=0}^{T} \lambda(x,t) * \left\{ -\partial_t \tilde{Z} + \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} * \left(-v\partial_x \tilde{Z} + D_d \partial_{xx} \tilde{Z} \right) + (\partial_z P)\tilde{Z} \right\} dt\,dx$$

Where $\lambda(x,t) = \begin{bmatrix} \lambda_1(x,t) \\ \lambda_2(x,t) \\ \lambda_3(x,t) \\ \lambda_4(x,t) \end{bmatrix}$

$$\tilde{J} = \int_0^L \int_0^T \begin{bmatrix}1\\0\\0\\0\end{bmatrix} * \tilde{Z}(x,t)dtdx + K\int_0^T \begin{bmatrix}0\\0\\0\\1\end{bmatrix} * \tilde{Z}(x=0,t)dt + \int_{x=0}^{L} \int_{t=0}^{T} -\lambda * \partial_t \tilde{Z}dtdx$$

$$+ \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \int_{x=0}^{L} \int_{t=0}^{T} -v\lambda * \partial_x \tilde{Z}dtdx + \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \int_{x=0}^{L} \int_{t=0}^{T} D_d \lambda * \partial_{xx} \tilde{Z}dtdx + \int_{x=0}^{L} \int_{t=0}^{T} \lambda * (\partial_z P)\tilde{Z}dtdx$$

Integrating by parts:

$$\tilde{J} = \int_0^L \int_0^T \begin{bmatrix}1\\0\\0\\0\end{bmatrix} * \tilde{Z}(x,t)dtdx + K\int_0^T \begin{bmatrix}0\\0\\0\\1\end{bmatrix} * \tilde{Z}(x=0,t)dt - \int_{x=o}^{L} \left[\lambda * \tilde{Z}\right]_{t=o}^{T} dt + \int_{x=0}^{L} \int_{t=0}^{T} \tilde{Z} * \partial_t \lambda dtdx$$

$$+ v\begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \left\{ - \int_{t=o}^{T} \left[\lambda * \tilde{Z}\right]_{x=o}^{L} dx + \int_{x=0}^{L} \int_{t=0}^{T} \tilde{Z} * \partial_x \lambda dtdx \right\} + D_d \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \left\{ \int_{t=0}^{T} \left[\lambda * \partial_x \tilde{Z}\right]_{x=o}^{L} dt - \int_{t=0}^{T} \left[\tilde{Z} * \partial_x \lambda\right]_{x=o}^{L} dt + \int_{x=0}^{L} \int_{t=0}^{T} \tilde{Z} * \partial_{xx} \lambda dtdx \right\}$$

$$+ \int_{x=0}^{L} \int_{t=0}^{T} \lambda * (\partial_z P)\tilde{Z}dtdx$$

Separating:

$$\tilde{J} = K\int_0^T \begin{bmatrix}0\\0\\0\\1\end{bmatrix} * \tilde{Z}(x=0,t)dt - \int_{x=o}^{L} \left[\lambda * \tilde{Z}\right]_{t=o}^{T} dt - v\begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \int_{t=o}^{T} \left[\lambda * \tilde{Z}\right]_{x=o}^{L} dx + D_d \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \left\{ \int_{t=0}^{T} \left[\lambda * \partial_x \tilde{Z}\right]_{x=o}^{L} dt - \int_{t=0}^{T} \left[\tilde{Z} * \partial_x \lambda\right]_{x=o}^{L} dt \right\} + \tilde{Z} * \int_{x=0}^{L} \int_{t=0}^{T} \left\{ \begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \partial_t \lambda + \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * [v\partial_x \lambda + D_d \partial_{xx} \lambda] + \lambda * (\partial_z P) \right\} dtdx$$

Thus:

$$\tilde{J} = K\int_0^T \begin{bmatrix}0\\0\\0\\1\end{bmatrix} * \tilde{Z}(x=0,t)dt - \int_{x=o}^{L} \left[\lambda * \tilde{Z}\right]_{t=o}^{T} dt$$

$$-v\begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \int_{t=o}^{T} \left[\lambda * \tilde{Z}\right]_{x=o}^{L} dx + D_d \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * \left\{ \int_{t=0}^{T} \left[\lambda * \partial_x \tilde{Z}\right]_{x=o}^{L} dt - \int_{t=0}^{T} \left[\tilde{Z} * \partial_x \lambda\right]_{x=o}^{L} dt \right\}$$

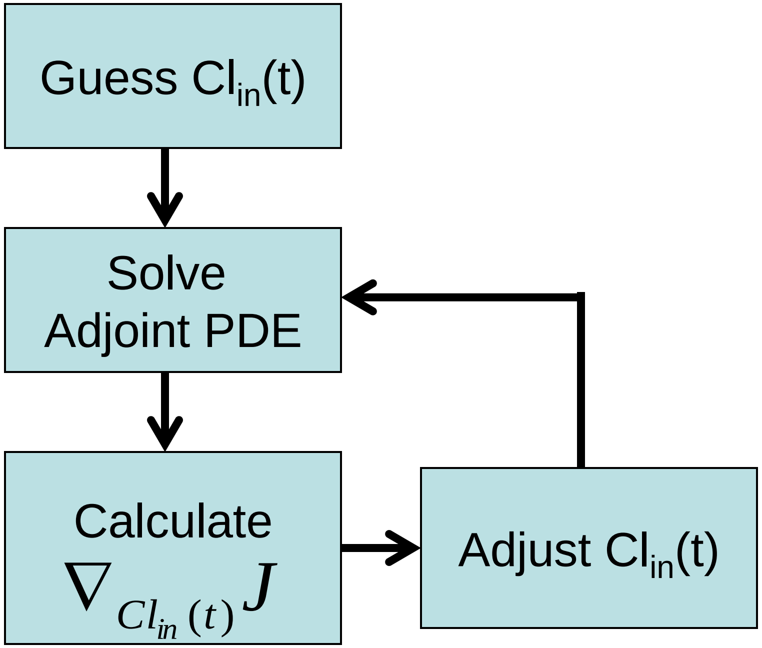
If λ is chosen such that:

$$\begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \partial_t \lambda + \begin{bmatrix}1\\0\\1\\1\end{bmatrix} * [v\partial_x \lambda + D_d \partial_{xx} \lambda] + \lambda * (\partial_z P) = 0$$

Future Work

- This semester:
  - Put $\tilde{J}$ into a solvable form
  - Use $\tilde{J} = \left\langle \nabla_{Cl_{in}(t)} J \mid \tilde{C}l_{in}(t) \right\rangle$ to calculate $\nabla_{Cl_{in}(t)} J$

- Develop code to:



Potential Expansions

- Intermittent pipeflow
  - Common in developing countries
  - $v(t)$ varying with time
- Networks of multiple pipes