NUCL 697 Final Project: Finite element solution of deuterium diffusion in plasma facing components

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May 3rd, 2016

Using a finite element method, calculate the diffusion of Deuterium ions through plasma facing components (Tungsten). Use SRIM to calculate the distribution of incident ions and consider this to be a constant source. Study:
Effect of temperature, that is, diffusion and recombination coefficients, on deuterium recycling.
Explicit/Implicit solution - compare results and time step requirement.

Motivation

Method

We are attempting to solve the diffusion equation, which - with constant diffusion coefficient - can be written as

$$\frac{\partial C\left(\vec{r},\, t\right)}{\partial t} = D\nabla^2 C\left(\vec{r},\, t\right) + S\left(\vec{r},\, t\right)$$

with $C\left(\vec{r},\, t\right)$ the concentration as a function of space ($\vec{r}$) and time (t), D the diffusion coefficient, and $S\left(\vec{r},\, t\right)$ the source term as a function of space and time.

One-Dimensional

With the assumption that the source is constant on the entire plasma facing surface and that the surface can be approximated as infinite compared to the range of diffusion, we can consider the problem to be one dimensional (in depth). We then define our space ($\vec{r}$) as simply the depth variable (x). Then, the diffusion equation can be written as

$$\frac{\partial C\left(x,\, t\right)}{\partial t} = D\frac{\partial^2 C\left(x,\, t\right)}{\partial x^2} + S\left(x,\, t\right)$$

We then can define our boundary and initial conditions needed to solve this.

- By assuming that the plasma is stable, we can assume that the source term will be constant in time. That is:

$$S\left(x,\, t\right) = S\left(x\right)$$

- By assuming that our domain is much larger than the scale of diffusion in the time simulated, we can define the right boundary as a sink. That is:

$$C\left(x = 0.5\,\mu\text{m},\, t\right) = 0$$

- By assuming that the plasma is created instantly at time $t = 0$, we can assume that there is no existing distribution of concentration except for the instantaneous source. That is:

$$C\left(x,\, t = 0\right) = 0 + S\left(x\right)$$

- The left boundary is defined by recombination/desorption of Deuterium. This can be calculated by:

$$\frac{\partial C\left(x = 0\,\mu\text{m},\, t\right)}{\partial x} = -k\left[C\left(x = 0\,\mu\text{m},\, t\right)\right]^2$$

So, we want to solve the equation

$$\begin{aligned}
\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} + S\left(x\right) &\quad \text{on } \Omega \\
C = 0 &\quad \text{on } \Gamma_{right} \\
\frac{\partial C\left(t\right)}{\partial x} = -kC^2 &\quad \text{on } \Gamma_{left} \\
C = S &\quad \text{on } \Omega \text{ at time } t_i = 0
\end{aligned}$$

The residual corresponding to this equation is

$$R\left(\tilde{C}, x\right) \equiv -\frac{\partial \tilde{C}}{\partial t} + D\frac{\partial^2 \tilde{C}}{\partial x^2} + S$$

and thus the weighted residual is

$$\int_0^{x_r} wR\left(\tilde{C}, x\right) dx = \int_0^{x_r} w\left[-\frac{\partial \tilde{C}}{\partial t} + D\frac{\partial^2 \tilde{C}}{\partial x^2} + S\right] dx$$

which, when expanded by integration by parts is

$$\underbrace{-\int_0^{x_r} w\frac{\partial \tilde{C}}{\partial t} dx}_{\text{dissipation term}} + \underbrace{\left[wD\frac{\partial \tilde{C}}{\partial x}\right]_0^{x_r}}_{\text{boundary terms}} - \underbrace{\int_0^{x_r} \frac{\partial w}{\partial x} D\frac{\partial \tilde{C}}{\partial x} dx}_{\text{domain term}} + \underbrace{\int_0^{x_r} wSdx}_{\text{source term}}$$

with linear shape functions and at node j, the residual becomes

$$R_j\left(\tilde{C}\right) \equiv -\int_0^{x_r} w_j\frac{\partial \tilde{C}}{\partial t} + \left[w_jD\frac{\partial \tilde{C}}{\partial x}\right]_0^{x_r} - \int_0^{x_r} \frac{\partial w_j}{\partial x} D\frac{\partial \tilde{C}}{\partial x} dx + \int_0^{x_r} w_jSdx$$

and, because we're using lagrange, w_j is only non-zero over two elements that include j, i.e.

$$w_j = \begin{cases} 0, & \text{for } x < x_{j-1} \\ \frac{x - x_{j-1}}{x_j - x_{j-1}}, & \text{for } x_{j-1} \leq x \leq x_j \\ \frac{x_{j+1} - x}{x_{j+1} - x_j} & \text{for } x_j < x \leq x_{j+1} \\ 0, & \text{for } x > x_{j+1} \end{cases}$$

and its derivative is

$$\frac{\partial w_j}{\partial x} = \begin{cases} 0, & \text{for } x < x_{j-1} \\ \frac{1}{x_j - x_{j-1}}, & \text{for } x_{j-1} \leq x \leq x_j \\ \frac{-1}{x_{j+1} - x_j}, & \text{for } x_j < x \leq x_{j+1} \\ 0, & \text{for } x > x_{j+1} \end{cases}$$

so

$$\int_0^{x_r} \frac{\partial w_j}{\partial x} D\frac{\partial \tilde{C}}{\partial x} dx = \int_{x_{j-1}}^{x_{j+1}} \frac{\partial w_j}{\partial x} D\frac{\partial \tilde{C}}{\partial x} dx = \frac{1}{x_j - x_{j-1}} \int_{x_{j-1}}^{x_j} D\frac{\partial \tilde{C}}{\partial x} dx - \frac{1}{x_{j+1} - x_j} \int_{x_j}^{x_{j+1}} D\frac{\partial \tilde{C}}{\partial x} dx$$

Now, using the lagrange approximation to the real solution C and taking the derivative, we get

$$\frac{\partial \tilde{C}}{\partial x} = \sum_{i=1}^{N+1} C_i \frac{\partial w_i}{\partial x}$$

and again noting that the only contributions for lagrange elements come for the nodes including j, we can reduce this sum to two terms:

$$\frac{\partial \tilde{C}}{\partial x} = \begin{cases} C_{j-1}\frac{\partial w_{j-1}}{\partial x} + C_j\frac{\partial w_j}{\partial x} = \frac{C_j - C_{j-1}}{x_j - x_{j-1}}, & \text{for } i = j-1 \\ C_j\frac{\partial w_j}{\partial x} + C_{j+1}\frac{\partial w_{j+1}}{\partial x} = \frac{C_{j+1} - C_j}{x_{j+1} - x_j}, & \text{for } i = j \end{cases}$$

so the integral becomes

$$\int_0^{x_r} \frac{\partial w_j}{\partial x} D \frac{\partial \tilde{C}}{\partial x} dx = \frac{C_j - C_{j-1}}{\left(x_j - x_{j-1}\right)^2} \int_{x_{j-1}}^{x_j} D dx - \frac{C_{j+1} - C_j}{\left(x_{j+1} - x_j\right)^2} \int_{x_j}^{x_{j+1}} D dx$$

and with constant D

$$\int_0^{x_r} \frac{\partial w_j}{\partial x} D \frac{\partial \tilde{C}}{\partial x} dx = D \frac{C_j - C_{j-1}}{\left(x_j - x_{j-1}\right)^2} - D \frac{C_{j+1} - C_j}{\left(x_{j+1} - x_j\right)^2}$$

We can expand that equation into a matrix by adding matrices for each node j. A quick example shows the pattern, for 5 nodes j

$$I_{\substack{\text{stiffness}\\\text{terms}}} = \begin{cases} D\frac{C_1 - C_0}{\Delta x_0^2} - D\frac{C_2 - C_1}{\Delta x_1^2} & \text{for node 1} \\ D\frac{C_2 - C_1}{\Delta x_1^2} - D\frac{C_3 - C_2}{\Delta x_2^2} & \text{for node 2} \\ D\frac{C_3 - C_2}{\Delta x_2^2} - D\frac{C_4 - C_3}{\Delta x_3^2} & \text{for node 3} \\ D\frac{C_4 - C_3}{\Delta x_3^2} - D\frac{C_5 - C_4}{\Delta x_4^2} & \text{for node 4} \\ D\frac{C_5 - C_4}{\Delta x_4^2} - D\frac{C_6 - C_5}{\Delta x_5^2} & \text{for node 5} \end{cases}$$

You can then place this in matrix form

$$I_{\substack{\text{stiffness}\\\text{terms}}} = D \begin{bmatrix} \left(\frac{1}{\Delta x_0^2} + \frac{1}{\Delta x_1^2}\right) & -\frac{1}{\Delta x_1^2} & & & \\ -\frac{1}{\Delta x_1^2} & \left(\frac{1}{\Delta x_1^2} + \frac{1}{\Delta x_2^2}\right) & -\frac{1}{\Delta x_2^2} & & \\ & -\frac{1}{\Delta x_2^2} & \left(\frac{1}{\Delta x_2^2} + \frac{1}{\Delta x_3^2}\right) & -\frac{1}{\Delta x_3^2} & \\ & & -\frac{1}{\Delta x_3^2} & \left(\frac{1}{\Delta x_3^2} + \frac{1}{\Delta x_4^2}\right) & -\frac{1}{\Delta x_4^2} \\ & & & -\frac{1}{\Delta x_4^2} & \left(\frac{1}{\Delta x_4^2} + \frac{1}{\Delta x_5^2}\right) \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{bmatrix}$$

So, we move on to converting the source term to a matrix. Using our weighting function w_j, we get

$$\int_0^{x_r} w_j S dx = \int_{x_{j-1}}^{x_j} \frac{x - x_{j-1}}{x_j - x_{j-1}} S dx - \int_{x_j}^{x_{j+1}} \frac{x_{j+1} - x}{x_{j+1} - x_j} S dx$$

and since S is a function of x and an interpolated function, we cannot exactly integrate it. Thus, we will use midpoint rule to integrate.

$$\begin{aligned} \int_{x_{j-1}}^{x_j} \frac{x - x_{j-1}}{x_j - x_{j-1}} S dx - \int_{x_j}^{x_{j+1}} \frac{x_{j+1} - x}{x_{j+1} - x_j} S dx &\approx \Delta x_{j-1} \left(\frac{\frac{x_j - x_{j-1}}{2}}{x_j - x_{j-1}}\right) S\left(\frac{x_j + x_{j-1}}{2}\right) - \Delta x_j \left(\frac{\frac{x_{j+1} - x_j}{2}}{x_{j+1} - x_j}\right) S\left(\frac{x_{j+1} + x_j}{2}\right) \\ &\approx \frac{\Delta x_{j-1}}{2} S\left(\frac{x_j + x_{j-1}}{2}\right) - \frac{\Delta x_j}{2} S\left(\frac{x_{j+1} + x_j}{2}\right) \end{aligned}$$

Again using the five element case to determine a pattern, we have

$$I_{\substack{\text{source}\\\text{terms}}} = \begin{cases} \frac{\Delta x_0}{2} S\left(\frac{x_1 + x_0}{2}\right) - \frac{\Delta x_1}{2} S\left(\frac{x_2 + x_1}{2}\right) & \text{for node 1} \\ \frac{\Delta x_1}{2} S\left(\frac{x_2 + x_1}{2}\right) - \frac{\Delta x_2}{2} S\left(\frac{x_3 + x_2}{2}\right) & \text{for node 2} \\ \frac{\Delta x_2}{2} S\left(\frac{x_3 + x_2}{2}\right) - \frac{\Delta x_3}{2} S\left(\frac{x_4 + x_3}{2}\right) & \text{for node 3} \\ \frac{\Delta x_3}{2} S\left(\frac{x_4 + x_3}{2}\right) - \frac{\Delta x_4}{2} S\left(\frac{x_5 + x_4}{2}\right) & \text{for node 4} \\ \frac{\Delta x_4}{2} S\left(\frac{x_5 + x_4}{2}\right) - \frac{\Delta x_5}{2} S\left(\frac{x_6 + x_5}{2}\right) & \text{for node 5} \end{cases}$$

which can be easily written as a vector. So, checking in on our overall equation, we have

$$R_j\left(\tilde{C}\right) \equiv -\int_0^{x_r} w_j \frac{\partial \tilde{C}}{\partial t} + \left[w_j D \frac{\partial \tilde{C}}{\partial x}\right]_0^{x_r} - \cancelto{I_{\substack{\text{stiffness}\\\text{terms}}}}{\int_0^{x_r} \frac{\partial w_j}{\partial x} D \frac{\partial \tilde{C}}{\partial x} dx} + \cancelto{I_{\substack{\text{source}\\\text{terms}}}}{\int_0^{x_r} w_j S dx}$$

Which means we have to determine the boundary and the time derivative, still. The time derivative can be written at each node as

$$\int_0^{x_r} w_j \frac{\partial \tilde{C}}{\partial t} dx = \int_{x_{j-1}}^{x_j} \frac{x - x_{j-1}}{\Delta x_{j-1}} \frac{\partial \tilde{C}}{\partial t} dx - \int_{x_j}^{x_{j+1}} \frac{x_{j+1} - x}{\Delta x_j} \frac{\partial \tilde{C}}{\partial t} dx$$

And, using only an euler step for the time step, we have

$$\frac{\partial \tilde{C}}{\partial t} = \frac{\tilde{C}_k - \tilde{C}_{k-1}}{\Delta t}$$

where k is the time step. Therefore, we have

$$\begin{aligned}
\int_0^{x_r} w_j \frac{\partial \tilde{C}}{\partial t} dx &= \int_{x_{j-1}}^{x_j} \frac{x - x_{j-1}}{\Delta x_{j-1}} \frac{\tilde{C}_{k,j} - \tilde{C}_{k-1,j}}{\Delta t} dx - \int_{x_j}^{x_{j+1}} \frac{x_{j+1} - x}{\Delta x_j} \frac{\tilde{C}_{k,j} - \tilde{C}_{k-1,j}}{\Delta t} dx \\
&= \frac{\tilde{C}_{k,j} - \tilde{C}_{k-1,j}}{\Delta t} \cancelto{1}{\int_{x_{j-1}}^{x_j} \frac{x - x_{j-1}}{\Delta x_{j-1}} dx} - \frac{\tilde{C}_{k,j} - \tilde{C}_{k-1,j}}{\Delta t} \cancelto{-1}{\int_{x_j}^{x_{j+1}} \frac{x_{j+1} - x}{\Delta x_j} dx} \\
&= 2 \frac{\tilde{C}_{k,j} - \tilde{C}_{k-1,j}}{\Delta t}
\end{aligned}$$

and using the five element example, we have

$$I_{\substack{\text{dissipation}\\\text{terms}}} = \begin{cases} 2\frac{C_{k,1} - C_{k-1,1}}{\Delta t} & \text{for node 1} \\ 2\frac{C_{k,2} - C_{k-1,2}}{\Delta t} & \text{for node 2} \\ 2\frac{C_{k,3} - C_{k-1,3}}{\Delta t} & \text{for node 3} \\ 2\frac{C_{k,4} - C_{k-1,4}}{\Delta t} & \text{for node 4} \\ 2\frac{C_{k,5} - C_{k-1,5}}{\Delta t} & \text{for node 5} \end{cases}$$

which can be written as a matrix such as

$$\mathbb{M} = \begin{bmatrix} \frac{2}{\Delta t} & & & & \\ & \frac{2}{\Delta t} & & & \\ & & \frac{2}{\Delta t} & & \\ & & & \frac{2}{\Delta t} & \\ & & & & \frac{2}{\Delta t} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{bmatrix} - \begin{bmatrix} \frac{2}{\Delta t} & & & & \\ & \frac{2}{\Delta t} & & & \\ & & \frac{2}{\Delta t} & & \\ & & & \frac{2}{\Delta t} & \\ & & & & \frac{2}{\Delta t} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{bmatrix}_{k-1}$$

From our original equation, we only have the boundary terms to replace, i.e.

$$R_j\left(\tilde{C}\right) \equiv -\cancelto{I_{\substack{\text{dissipation}\\\text{terms}}}}{\int_0^{x_r} w_j \frac{\partial \tilde{C}}{\partial t}} + \left[w_j D \frac{\partial \tilde{C}}{\partial x} \right]_0^{x_r} - \cancelto{I_{\substack{\text{stiffness}\\\text{terms}}}}{\int_0^{x_r} \frac{\partial w_j}{\partial x} D \frac{\partial \tilde{C}}{\partial x} dx} + \cancelto{I_{\substack{\text{source}\\\text{terms}}}}{\int_0^{x_r} w_j S dx}$$

So, finally, our boundary terms can be defined by

$$I_{\substack{\text{boundary}\\\text{terms}}} = \left[w_j D \frac{\partial \tilde{C}}{\partial x} \right]_0^{x_r} = \begin{cases} D\left(-k\tilde{C}_1^2\right) & \text{for node 1} \\ D\cancelto{0}{\frac{\tilde{C}_{J+1} - \tilde{C}_J}{\Delta x_J}} & \text{for node } J \end{cases}$$

which can be written in a vector quite simply. So now we've finished all terms in our equation, and we can write the residual as

$$R_j\left(\tilde{C}\right) = -I_{\substack{\text{dissipation}\\\text{terms}}} + I_{\substack{\text{boundary}\\\text{terms}}} - I_{\substack{\text{stiffness}\\\text{terms}}} + I_{\substack{\text{source}\\\text{terms}}}$$

which can be written as a matrix as

$$R\left(\vec{C}\right) = \underbrace{\begin{bmatrix} \frac{2}{\Delta t} & & & & \\ & \frac{2}{\Delta t} & & & \\ & & \frac{2}{\Delta t} & & \\ & & & \frac{2}{\Delta t} & \\ & & & & \frac{2}{\Delta t} \end{bmatrix}}_{\mathbb{M}} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{bmatrix} - \underbrace{\begin{bmatrix} \frac{2}{\Delta t} & & & & \\ & \frac{2}{\Delta t} & & & \\ & & \frac{2}{\Delta t} & & \\ & & & \frac{2}{\Delta t} & \\ & & & & \frac{2}{\Delta t} \end{bmatrix}}_{\mathbb{M}_{k-1}} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{bmatrix}_{k-1} + \underbrace{\begin{bmatrix} -DkC_1^2 \\ 0 \\ 0 \\ 0 \\ -\frac{DC_5}{\Delta x_5} \end{bmatrix}}_{\vec{l}} -$$

$$\underbrace{D \begin{bmatrix} \left(\frac{1}{\Delta x_0^2} + \frac{1}{\Delta x_1^2}\right) & -\frac{1}{\Delta x_1^2} & & & \\ -\frac{1}{\Delta x_1^2} & \left(\frac{1}{\Delta x_1^2} + \frac{1}{\Delta x_2^2}\right) & -\frac{1}{\Delta x_2^2} & & \\ & -\frac{1}{\Delta x_2^2} & \left(\frac{1}{\Delta x_2^2} + \frac{1}{\Delta x_3^2}\right) & -\frac{1}{\Delta x_3^2} & \\ & & -\frac{1}{\Delta x_3^2} & \left(\frac{1}{\Delta x_3^2} + \frac{1}{\Delta x_4^2}\right) & -\frac{1}{\Delta x_4^2} \\ & & & -\frac{1}{\Delta x_4^2} & \left(\frac{1}{\Delta x_4^2} + \frac{1}{\Delta x_5^2}\right) \end{bmatrix}}_{\mathbb{K}} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{bmatrix}$$

$$+ \underbrace{\begin{bmatrix} \frac{\Delta x_0}{2} S\left(\frac{x_1+x_0}{2}\right) - \frac{\Delta x_1}{2} S\left(\frac{x_2+x_1}{2}\right) \\ \frac{\Delta x_1}{2} S\left(\frac{x_2+x_1}{2}\right) - \frac{\Delta x_2}{2} S\left(\frac{x_3+x_2}{2}\right) \\ \frac{\Delta x_2}{2} S\left(\frac{x_3+x_2}{2}\right) - \frac{\Delta x_3}{2} S\left(\frac{x_4+x_3}{2}\right) \\ \frac{\Delta x_3}{2} S\left(\frac{x_4+x_3}{2}\right) - \frac{\Delta x_4}{2} S\left(\frac{x_5+x_4}{2}\right) \\ \frac{\Delta x_4}{2} S\left(\frac{x_5+x_4}{2}\right) - \frac{\Delta x_5}{2} S\left(\frac{x_6+x_5}{2}\right) \end{bmatrix}}_{\vec{S}}$$

So we have the matrix equation

$$\begin{aligned} 0 &= -\mathbb{M}\vec{C} + \mathbb{M}_{k-1}\vec{C}_{k-1} + \vec{l} - \mathbb{K}\vec{C} + \vec{S} \\ &= -\underbrace{(\mathbb{M} + \mathbb{K})}_{\mathbb{A}}\underbrace{\vec{C}}_{\vec{x}} + \underbrace{\left(\mathbb{M}_{k-1}\vec{C}_{k-1} + \vec{l} + \vec{S}\right)}_{\vec{b}} \end{aligned}$$

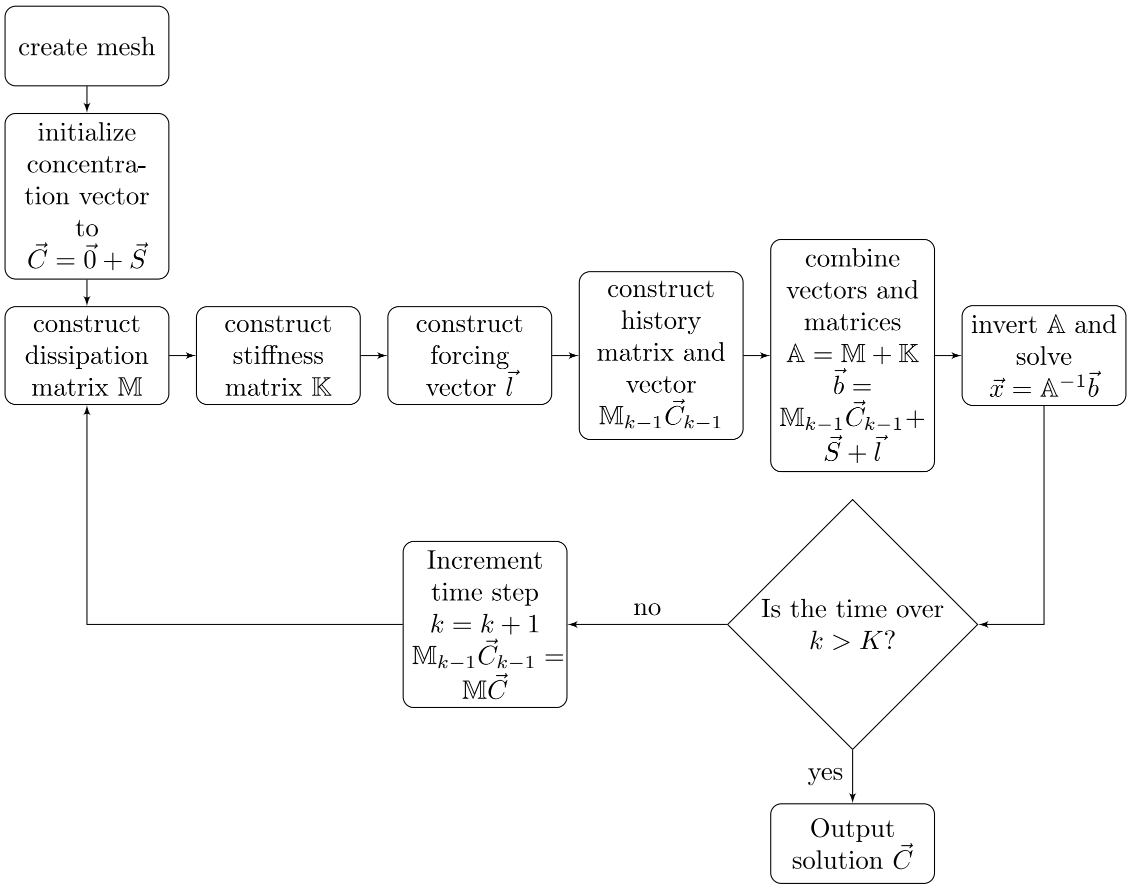
so we can simplify this to

$$\mathbb{A}\vec{x} = \vec{b}$$

which can be solved with

$$\vec{x} = \mathbb{A}^{-1}\vec{b}$$

at each time step.


create mesh
initialize concentration vector to $\vec{C} = \vec{0} + \vec{S}$
construct dissipation matrix $\mathbb{M}$
construct stiffness matrix $\mathbb{K}$
construct forcing vector $\vec{l}$
construct history matrix and vector $\mathbb{M}_{k-1}\vec{C}_{k-1}$
combine vectors and matrices $\mathbb{A} = \mathbb{M} + \mathbb{K}$ $\vec{b} = \mathbb{M}_{k-1}\vec{C}_{k-1} + \vec{S} + \vec{l}$
invert $\mathbb{A}$ and solve $\vec{x} = \mathbb{A}^{-1}\vec{b}$
Is the time over $k > K$?
no
Increment time step $k = k + 1$ $\mathbb{M}_{k-1}\vec{C}_{k-1} = \mathbb{M}\vec{C}$
yes
Output solution $\vec{C}$