Peridynamic Model of Corrosion

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Introduction

Corrosion is a result of chemical reactions between a material of interest and it's environment. The chemical products of a corrosion reaction often fuel the reactants leading to a run off process. Corrosion is a general term for any process which degrades a material but we are interested specifically in metals and the electrochemical process. A peridynamic model is implemented to better model the corrosion process
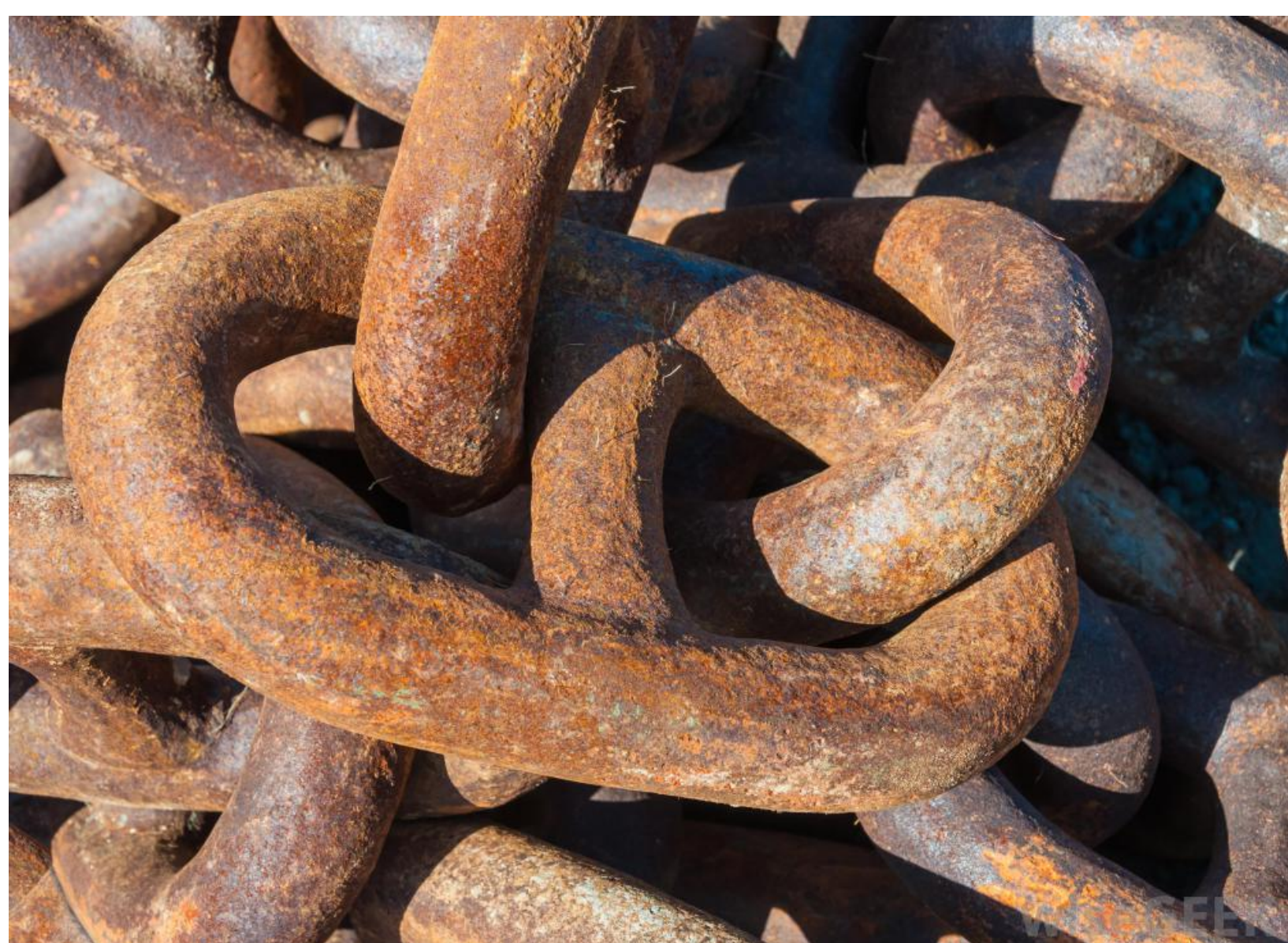

Figure 1: A common form of corrosion is the rust seen on steel

Peridynamics

The standard approach for continuous mechanics depends on the differentiation of a stress tensor σ.

$$\rho \ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t). \quad (1)$$

The stress tensor is a way of mapping normal vectors onto surface forces. Peridynamics models avoid the discontinuity by eliminating the spatial derivatives and instead integrate the bond forced over a region called the horizon, $\mathcal{H}$.

$$\rho \ddot{u}(x,t) = \int_{\mathcal{H}} f(q,x) dV_q + b(x,t). \quad (2)$$

where f us the pairwise bond force density and q is the distance from the point of x to another point within $\mathcal{H}$. [1]
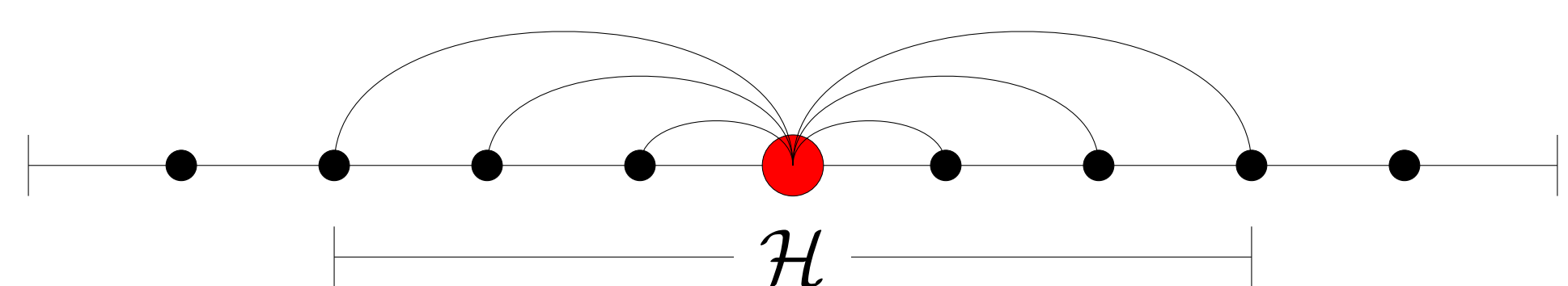

Figure 2: A peridynamic model integrates over a region of influence.

Reaction-Diffusion Model

A simplified 1D model is created to describe the system involving three regions the electrolyte solution Ω_e, the bulk metal Ω_m, and the interaction region Ω_d as seen in Fig.3 .

Figure 3: The 1D model will involve three regions. The electrolyte solution Ω_e, the bulk metal Ω_m, and the interaction region Ω_d

The governing equations for the electrolyte solution with a peridynamic framework would be

$$\dot{C}_j = \int_{\mathcal{H}(\mathbf{x},\delta)} f_j(\mathbf{C},\phi) d\mathbf{y} + \mathcal{J}_j \quad (3)$$

where C_j is a chemical species concentration, f_j is the flux density operator and $\mathcal{J}$ is the reaction term. The flux density operator for a single species, A, would be written as

$$f_{Ak} = \left[D_A(C_A(x_k) - C_A(x_i)) + z_j \frac{FD_A}{2RT}(C_A(x_k) + C_A(x_i))(\phi(x_k) - \phi(x_i)) \right] \mathcal{K}(x_i, x_k)$$

where x_k represents a point that is a distance at most δ aways from the point x_i. The choice of δ is the degree to which our system is non-local.

Electroneutrality

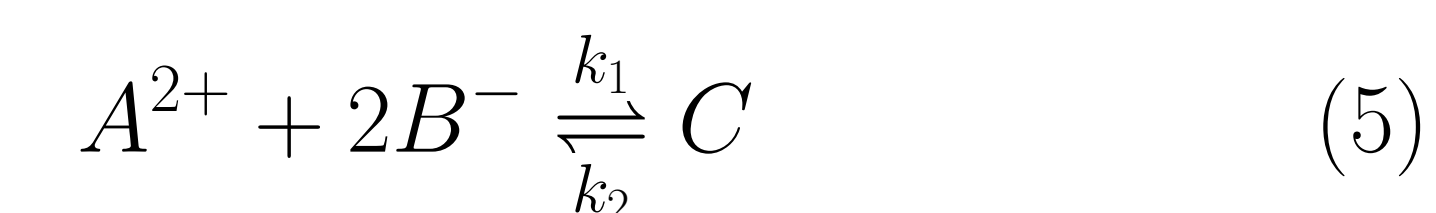Our system will also be subject to an electroneutrality condition

$$\int_{\mathcal{H}(\mathbf{x},\delta)} f_\phi(\mathbf{C},\phi) d\mathbf{y} = 0 \quad (4)$$

with

$$f_\phi = F \sum_{j=1}^{J} z_j f_j$$

Results

To gain insight into the model and run a few test, we will assume relatively simple kinetics:

$$A^{2+} + 2B^- \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C \quad (5)$$

Where A, B, and C are chemical species, such as aluminum, sodium or oxygen [2][3]. In Fig. 1 we can see that the concentrations are fixed on the boundaries to satisfy equilibrium. Reaction rates $k_1 = 0.01$ and $k_2 = 0.03$ were chosen.
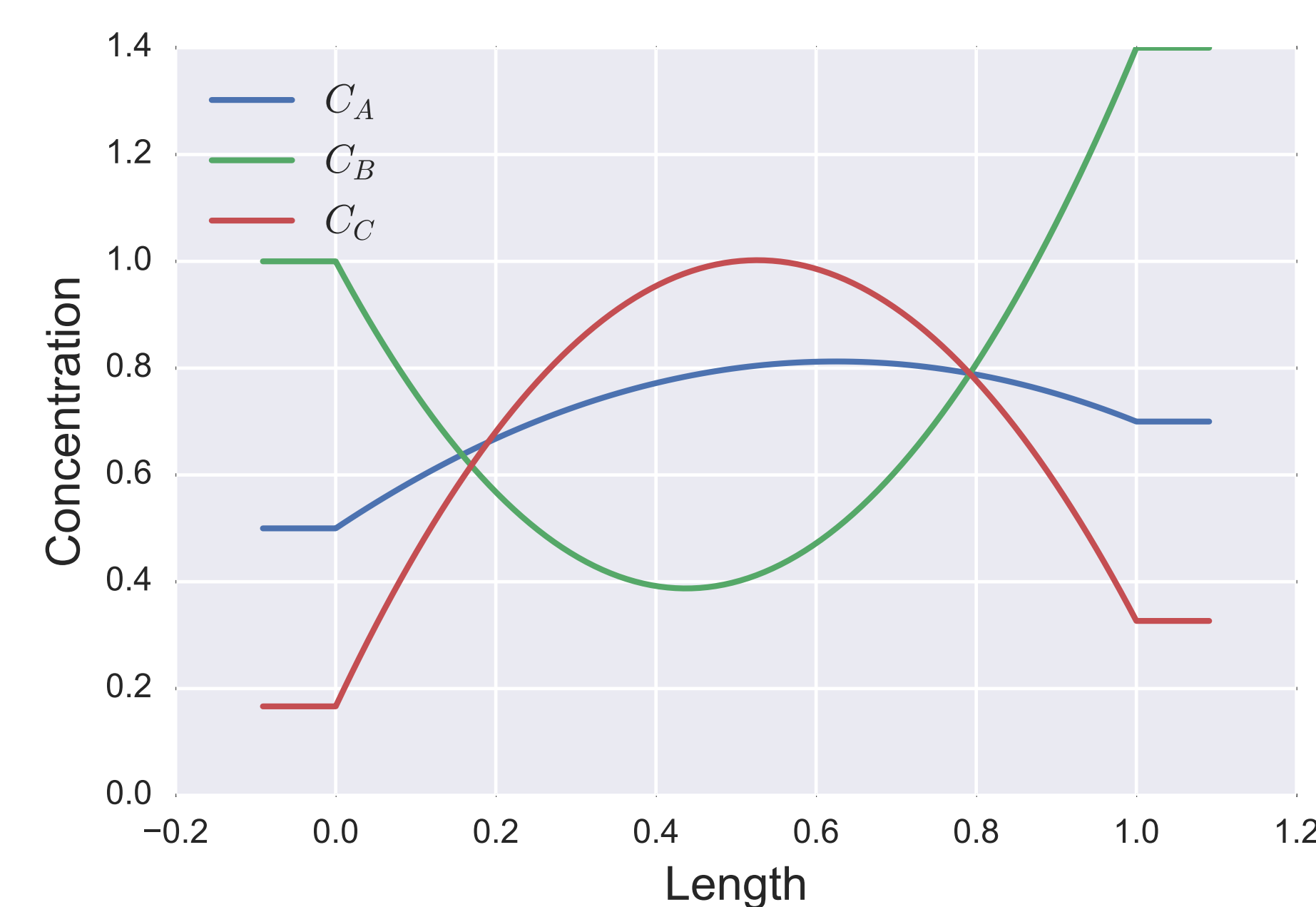

Figure 4: Initial concentration profiles

After our simulation has been run we see that the concentrations fall into an equilibrium state throughout the solution as seem in Fig. 5. The program has been written to handle multiple reaction and chemical species allowing for more complex chemistry to be modeled.
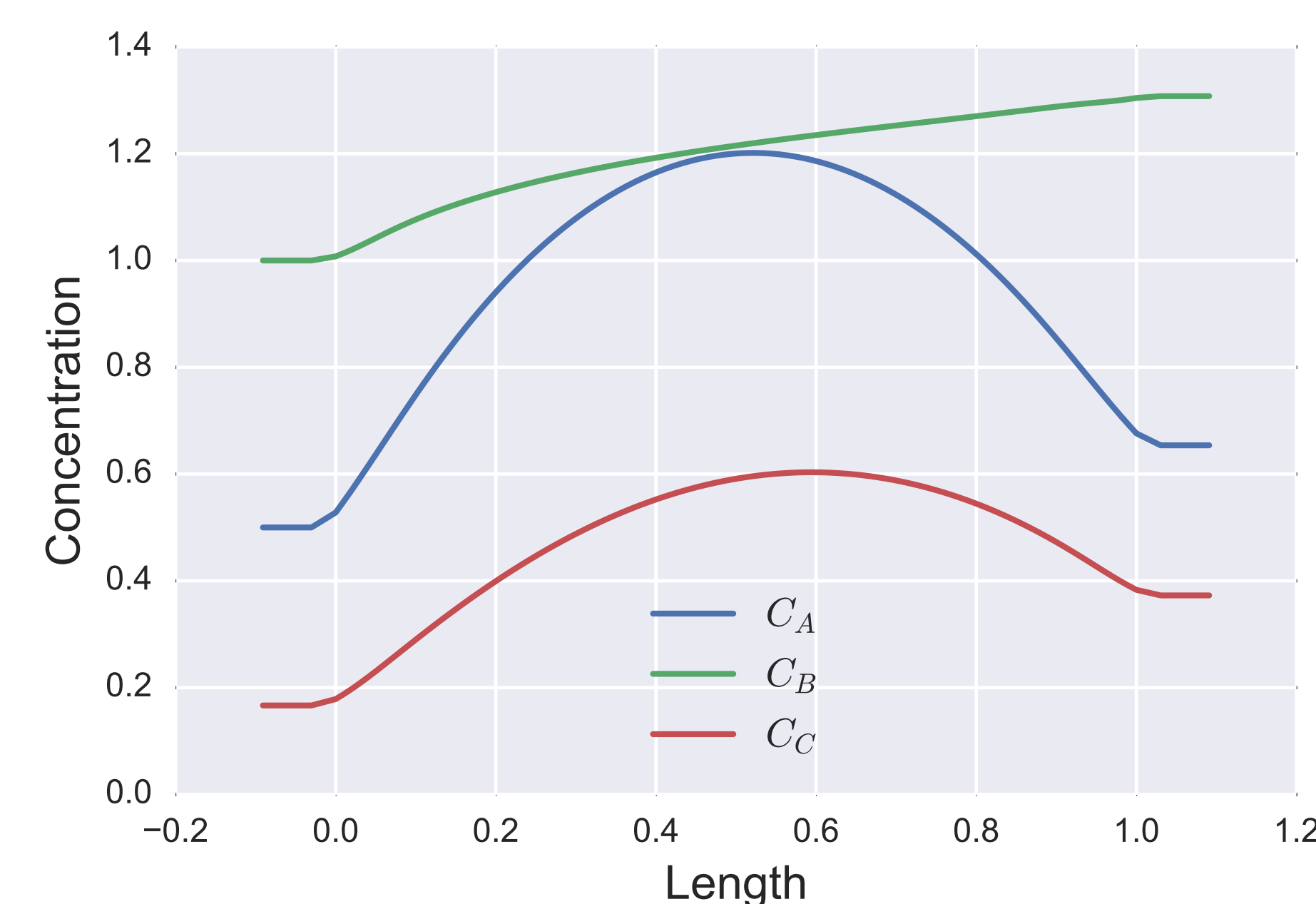

Figure 5: Final concentration profiles.

Conclusion

A peridynamic model was made that to model the corrosion process. The liquid solution was modeled using a homogeneous reaction-diffusion model subject to electroneutrality constraints. Initial test of a peridynamic model was implemented in one dimension. The program to model this behavior was written to be scalable to account for multiple species and multiple reactions.

Future Work

The work presented is part of an on going research project. Future work includes:

- Implementing a peridynamic model of the solid phase to measure structural failure.
- Scaling up our model to higher dimensions.
- Modeling more complex chemistry with more reactions and chemical species.

References

[1] S.A. Silling. "Reformulation of elasticity theory for discontinuities and long-range forces". In: *Journal of the Mechanics and Physics of Solids* 48.1 (2000), pp. 175–209.

[2] L.C. Abodi et al. "Modeling localized aluminum alloy corrosion in chloride solutions under non-equilibrium conditions: Steps toward understanding pitting initiation". In: *Electrochimica Acta* 63 (2012), pp. 169–178.

[3] Olga Guseva et al. "Modelling of anodic dissolution of pure aluminium in sodium chloride". In: *Electrochimica Acta* 54.19 (2009), pp. 4514–4524.

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