Modeling the Sustainable Electrosynthesis of Adiponitrile

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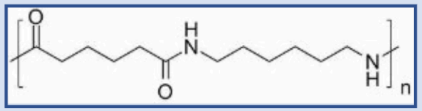
Introduction

- Adiponitrile (ADN): chemical intermediate used in the production of Nylon 66 (textiles and plastics).
- Produced through an organic electrosynthesis process that can be powered by renewable energy sources.
  - Low energy conversion efficiency & selectivity.
- **Goal**: Build a computational model of a flow reactor that can simulate the electrosynthesis of ADN.

Nylon



Methods

- Matlab Functions:
  - *ode15s*–– solves nonlinear differential equations.

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[t,C_dt] = ode15s(@f_dt,tspan,C);
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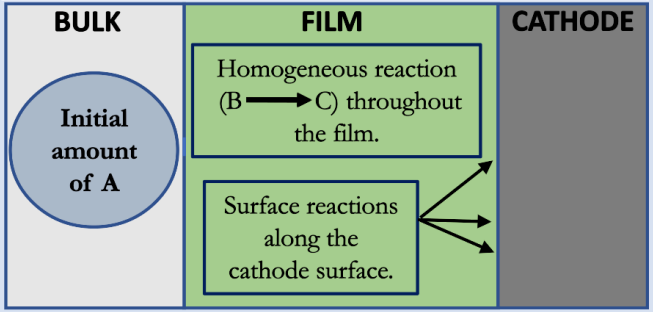
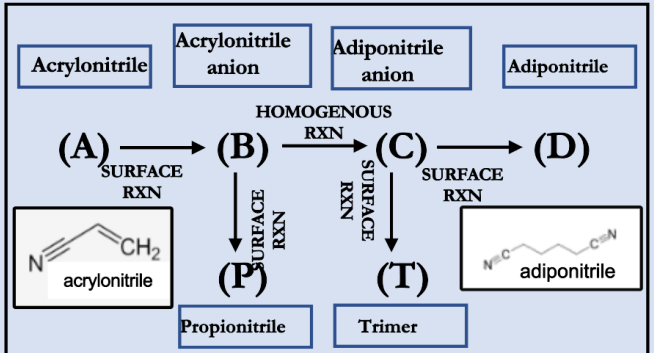
- Finite Difference Method––helps convert nonlinear differential equations to a linear system.
- Simplified Nernst-Planck equation.

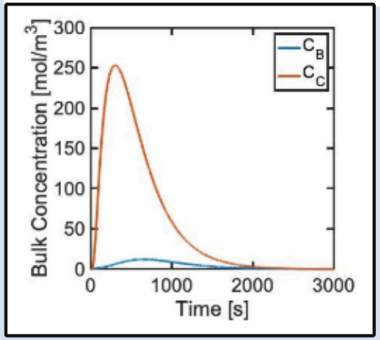
$$\frac{dC_i}{dt} = D_i \frac{d^2C_i}{dx^2} - r_i$$

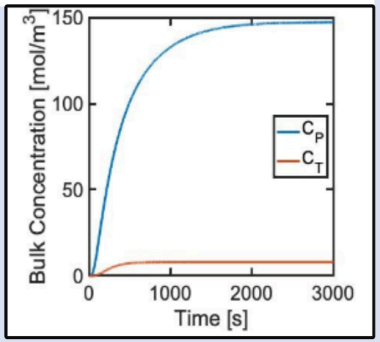
Inside the Flow Reactor

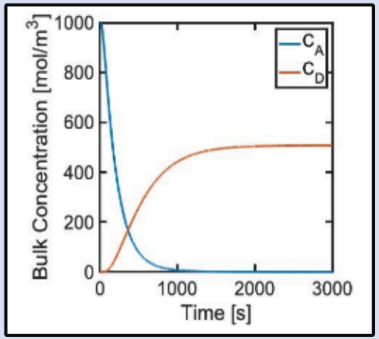


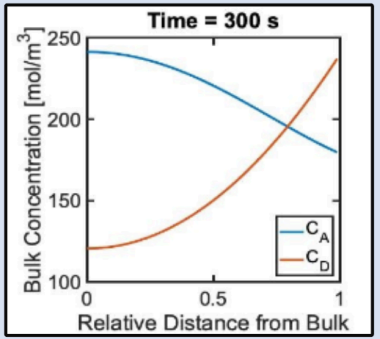


Results & Conclusions









References

1. Daniela E. Blanco, Aaliyah Z. Dookhith, Miguel A. Modestino. *Enhancing selectivity and efficiency in the electrochemical synthesis of adiponitrile.* Reaction Chemistry and Engineering, January 2019.

2. Piyachat Suwanvaipattana, Sunun Limtrakul, Terdthai Vatanatham, P.A. Ramachandran. *Modeling of electro-organic synthesis to facilitate cleaner chemical manufacturing: Adiponitrile production.* Journal of Cleaner Production, September 8, 2016.