Fouling and Biofilm Growth Models towards Anti-fouling Desalination Membranes

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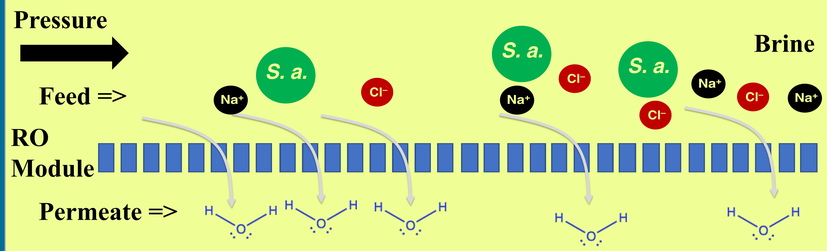
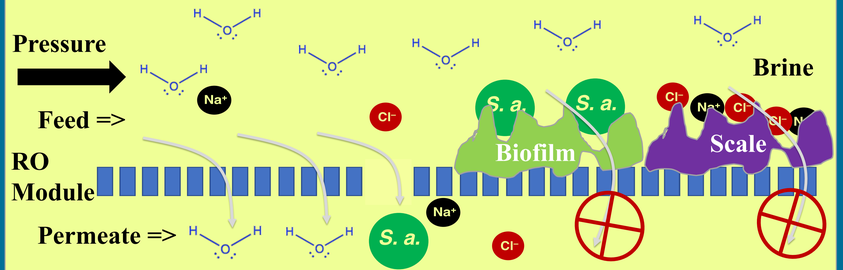
Introduction

Reverse osmosis (RO) membranes reject salt and microorganisms from pressurized flows of feed water.

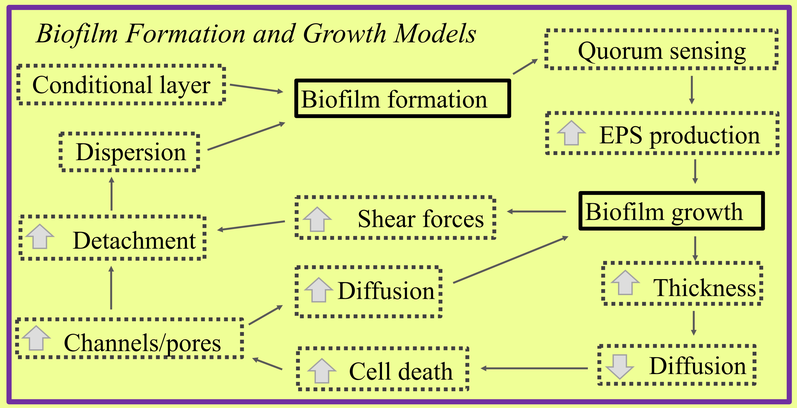


The rejected salt and microorganisms concentrate downstream in the RO module into the brine solution.



Biofilms and scale from brine clog membrane pores and/or degrades the membrane, both of which impedes RO functionality.

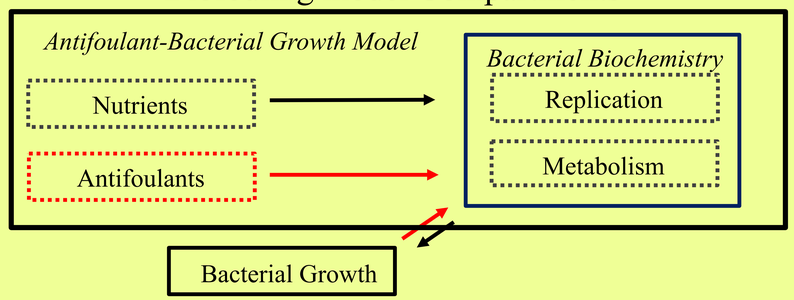
Biofilm Physical Characteristics and Interactions



Descriptive models

- Quorum sensing[1]
- Biofilm Growth Model[2]
- Digital Biofilm Model[3]
- Individual-based Algorithm[4]

Biofouling model Compartments



Descriptive models

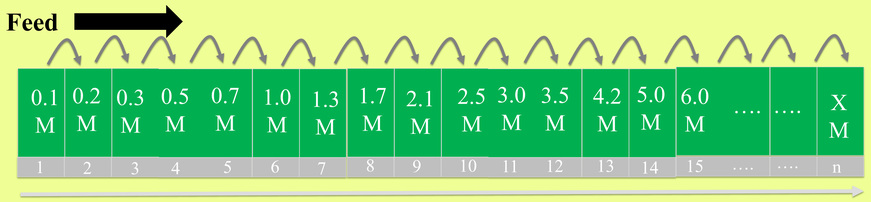
- Michaelis-Menten-Monod kinetics
- Molecular Dynamics[5]
- Whole Cell Model[6]

Research Goal and Intention

Essential Challenge: Expand models of mesoscale systems biology and desalination reactive transport to simulate the biofouling and scaling processes of desalination, respectively, which may guide the development of anti-biofouling and anti-scaling RO systems.

PHREEQC Reactive Transport Geochemical Simulations

PHREEQC[7] is a geochemical C-based coding language that can program simulations of pH-REdox-EQuilibrium interactions and transport phenomena. The reactive transport process simulates iterative reactions as feed progresses through a desalination module. The RO membrane is discretized into an arbitrary quantity of cells **n**, which progressively dehydrate with each simulated shift to an arbitrary concentration **x.**



The Pitzer model predicated calculations of activity in the simulations, since the Pitzer model[8] is ideal for solutions of 1-6M ionic strength like desalination brine.

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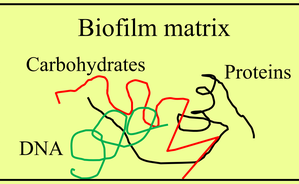
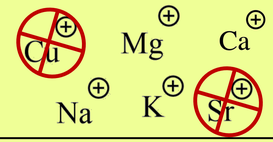
Model Limitations

The Whole Cell model comprehensively models the one of the smallest bacteria: *Mycoplasma genitalium* (*M. g.*).

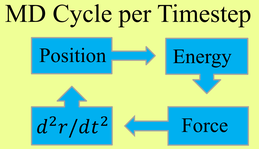
The biofilm structure is assumed to only consist of protein, water, and alive and dead cells.



The Pitzer model is limited by the breadth of chemical species for which thermodynamic data exists.

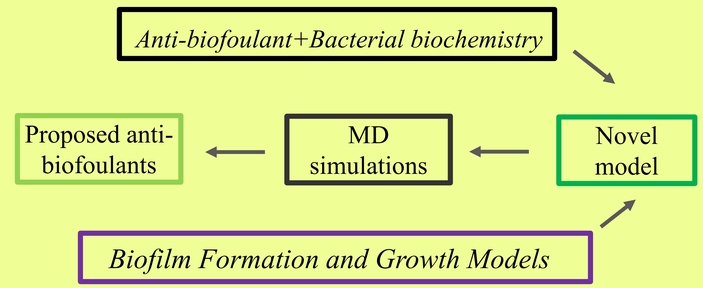


MD simulations require small timesteps to maintain accuracy, which encumbers computational time and therefore simulation replication.

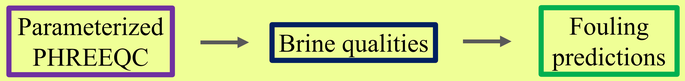


Summary and Future Directions

Biofouling and Biofilm Models Schematic



Brine and Scaling Simulation Schematic



The Biofouling model will screen potential anti-biofoulants and may support fundamental biofilm investigations. The PHREEQC simulations of scaling will identify ideal feed water sources.

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