



# Models of Anti-biofouling Reverse Osmosis Membranes

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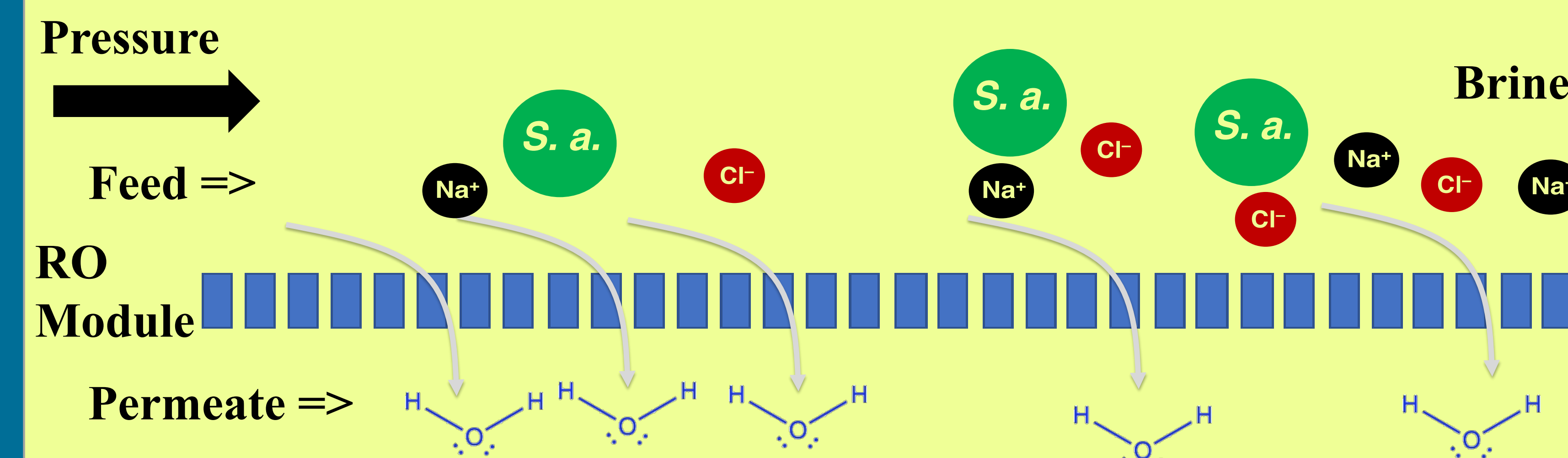
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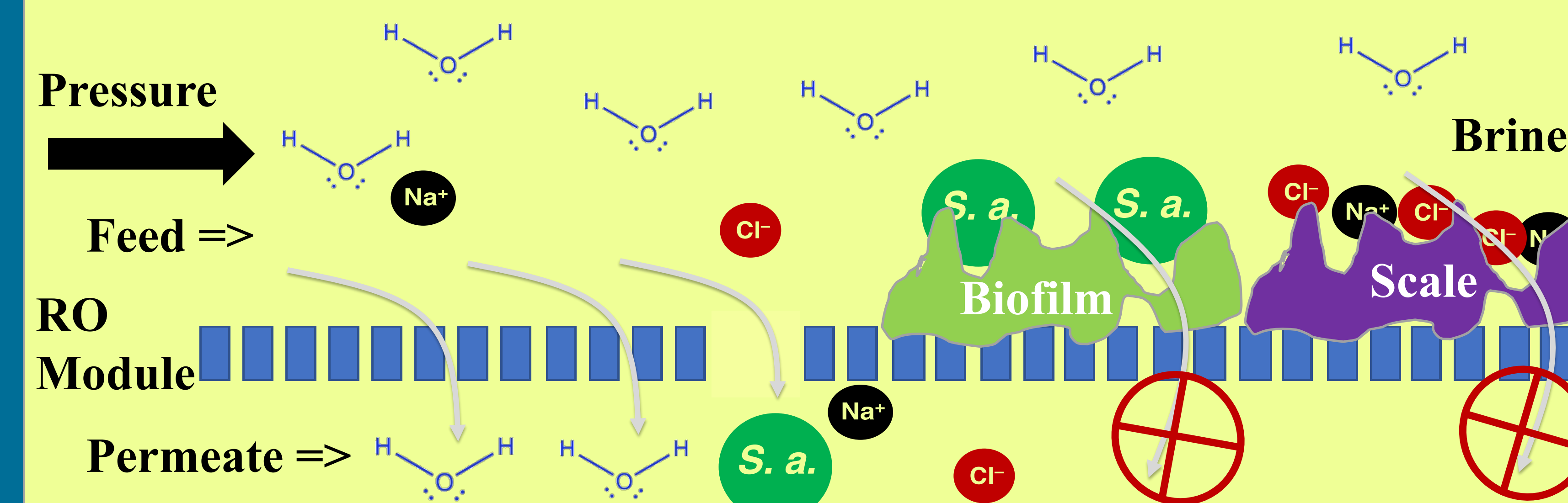


## Introduction

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

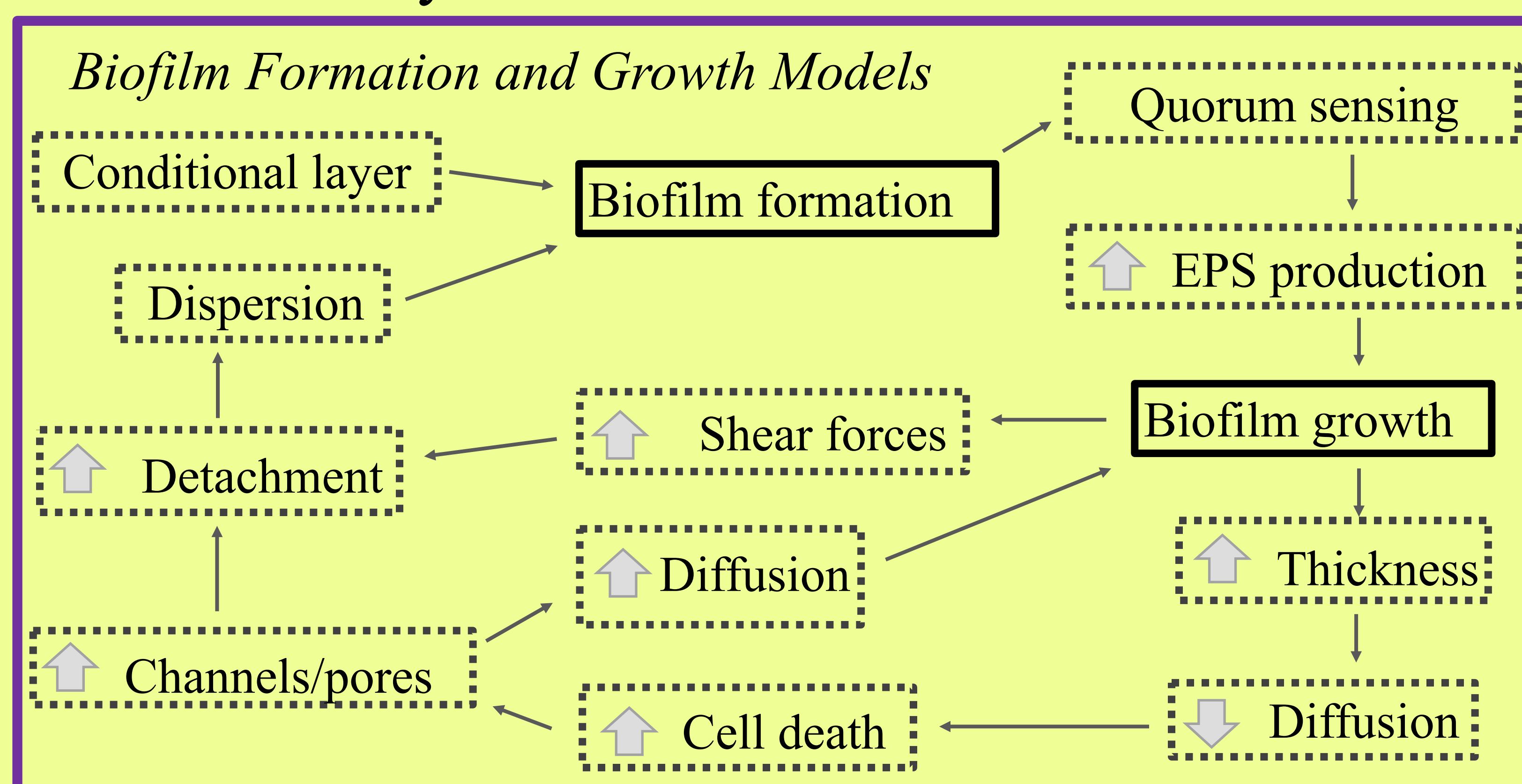


The rejected salt and microorganisms concentrate downstream in the RO module into the brine solution.



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

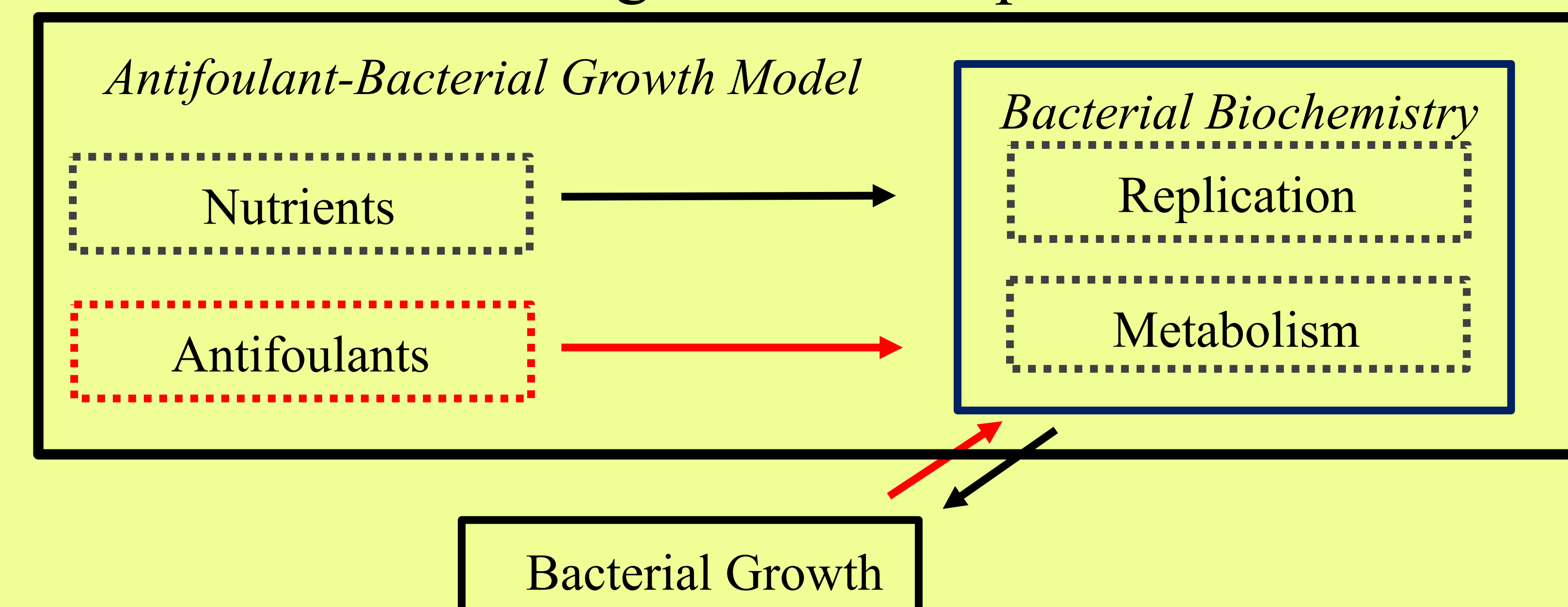
## Biofilm Physical Characteristics and Interactions



Quorum sensing<sup>1</sup>  
Biofilm Growth Model<sup>2</sup>  
Digital Biofilm Model<sup>3</sup>  
Individual-based Algorithm<sup>4</sup>

Descriptive models

## Biofouling model Compartments



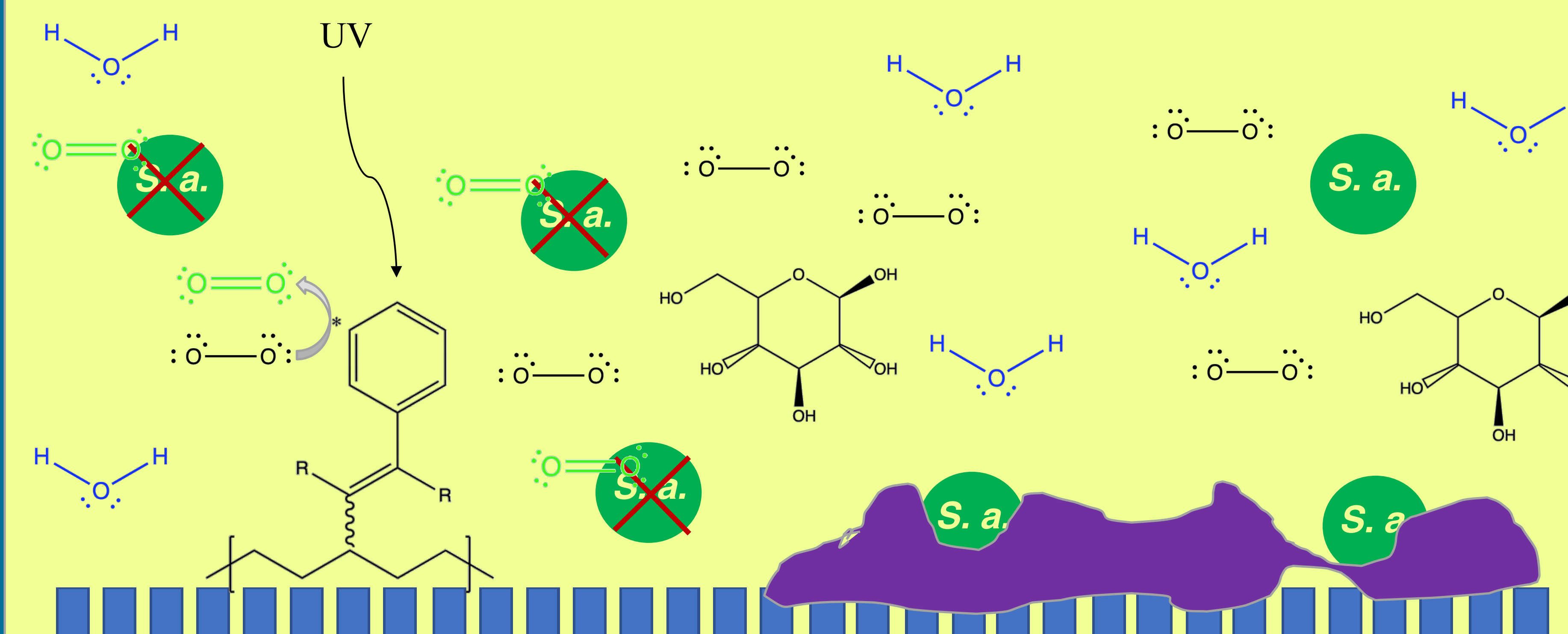
Descriptive models

Michaelis-Menten-Monod kinetics  
Molecular Dynamics<sup>5</sup>  
Whole Cell Model<sup>6</sup>

## Research Goal and Intention

**Essential Challenge:** Develop a mesoscale simulation of biofilm growth and biochemistry. The simulation may guide the identification and development of efficacious antifoulants and anti-biofouling RO systems that prevent and/or treat membrane biofouling.

## Modeled Biofilm Growth amidst an Antifoulant



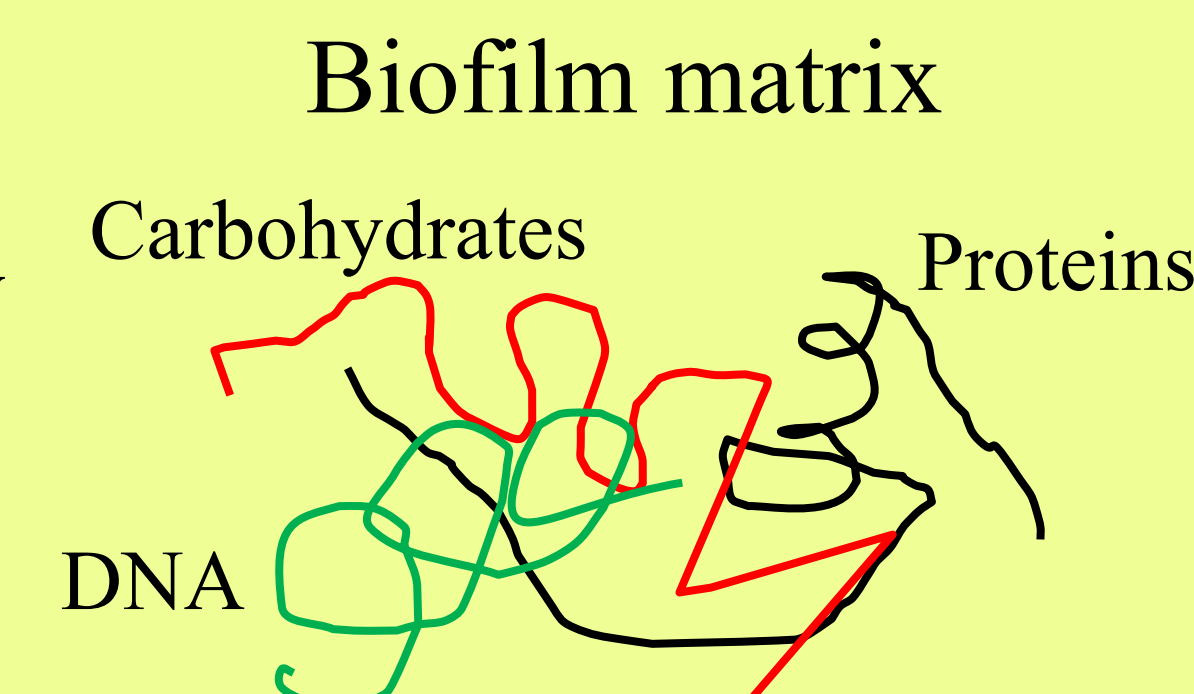
*Staphylococcus aureus* (*S. a.*) is an archetype bacterium for biofilm establishment. Singlet oxygen is potent non-selective antifoulant<sup>7</sup> that is created when a type II photosensitizer<sup>8</sup> excites dissolved oxygen into the singlet state.

## Model Limitations

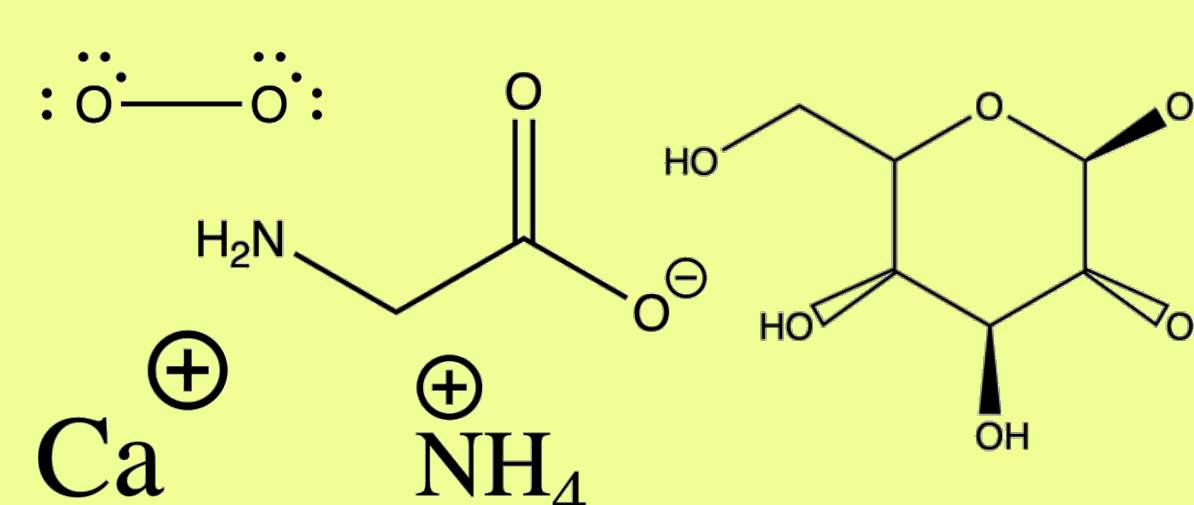
The Whole Cell model comprehensively models the one of the smallest bacteria, *Mycoplasma genitalium* (*M. g.*), which is substantially less complex than *S. a.*

	<i>M. g.</i>	<i>S. a.</i>
Genome size	580 kb	2.8 Mb
Genes	525 genes	2600 genes

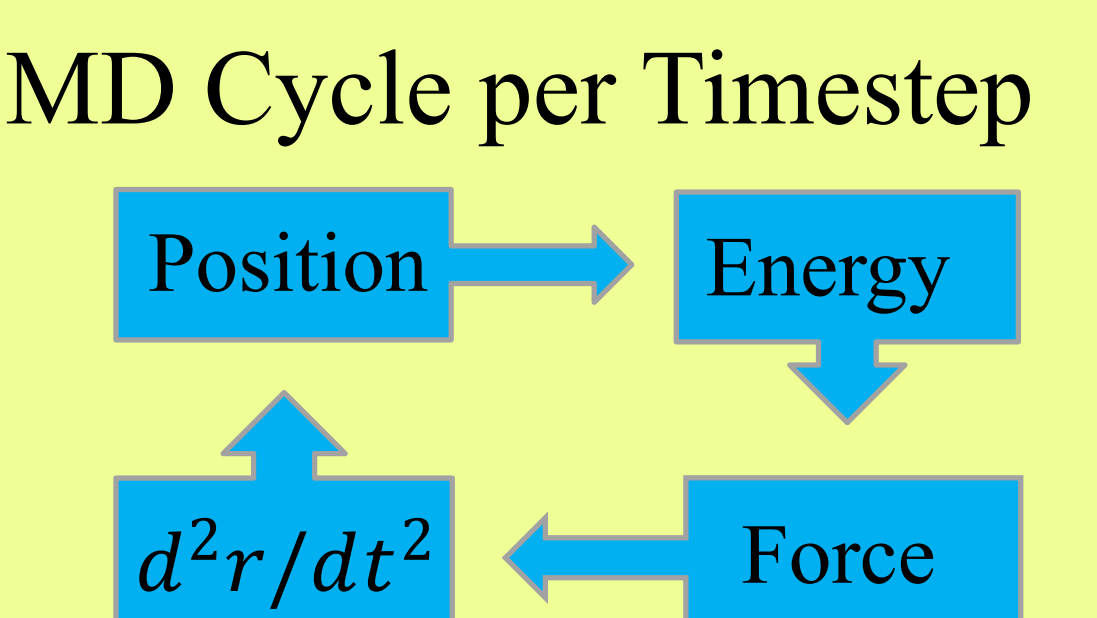
The biofilm structure is assumed to only consist of protein, water, and cells.



Monod kinetics assumes that a only single nutrient, amongst the numerous, is limiting the colonial growth.

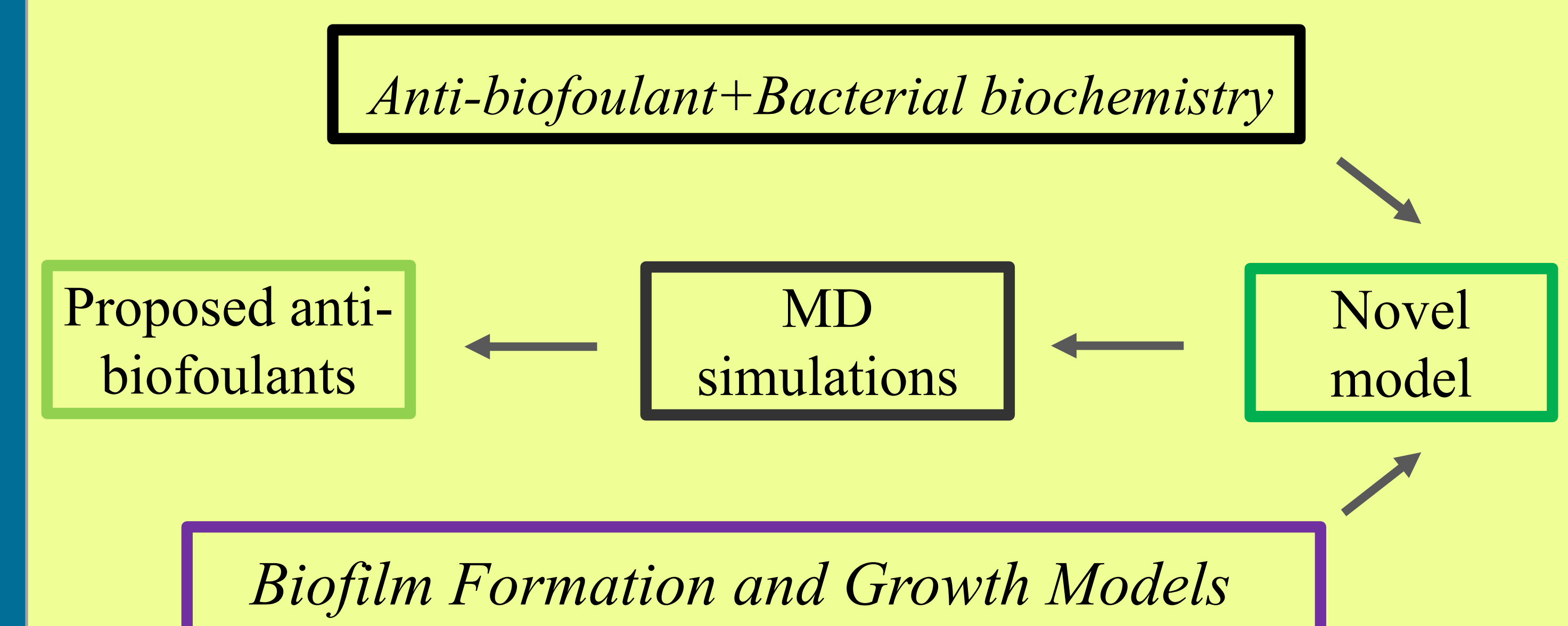


Accurate MD simulations require small timesteps, which increases computational and therefore lessens reproducibility.



## Summary and Future Directions

### Biofouling and Biofilm Simulations Schematic



The Biofouling model will screen potential anti-biofoulants and may support fundamental investigations of biofilm characteristics.

The simulation will be validated with experimental research in our lab and comparable literature to refine the model assumptions and simulation accuracy.

A GUI for the simulation will be devised to facilitate usability.

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2. *Math. Comput. Model.* **2001**, 33, 299–319

3. *PLoS One* **2016**, 11, 1–16  
4. *Microbiology* **1998**, 144, 3275–3287

5. *J. Chem. Phys.* **2017**, 146, 150901-1,16  
6. *Cell* **2012**, 150, 389–401

7. *Environ. Sci. Technol.* **2012**, 46, 12098–12104  
8. *Photochem. Photobiol.* **2017**, 93, 912–919

