Agent-Based Modeling of Microbial and Metabolite Interactions in Early Oral Biofilms

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Introduction

The Netherlands: Approximately one-third (33%) of children aged 5 years already have dental caries.

Aim

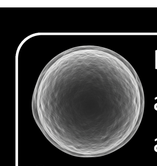
To develop a computational model that simulates oral biofilm formation and enamel demineralization.

Research Questions

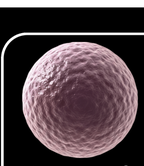
What specific physical and chemical parameters determine the spatial distribution and co-aggregation efficiency of secondary colonizers within a simulated biofilm architecture?

What spatial arrangements of V. parvula relative to S. mutans maximize synergistic growth and biofilm biomass accumulation?

Data Analysis



S. mutans Primary pathogen, produces acid from sugar metabolism and synthesizes EPS



V. parvula Secondary colonizer, ferments lactate to acetate and propionate

Streptococcus *Veillonella*

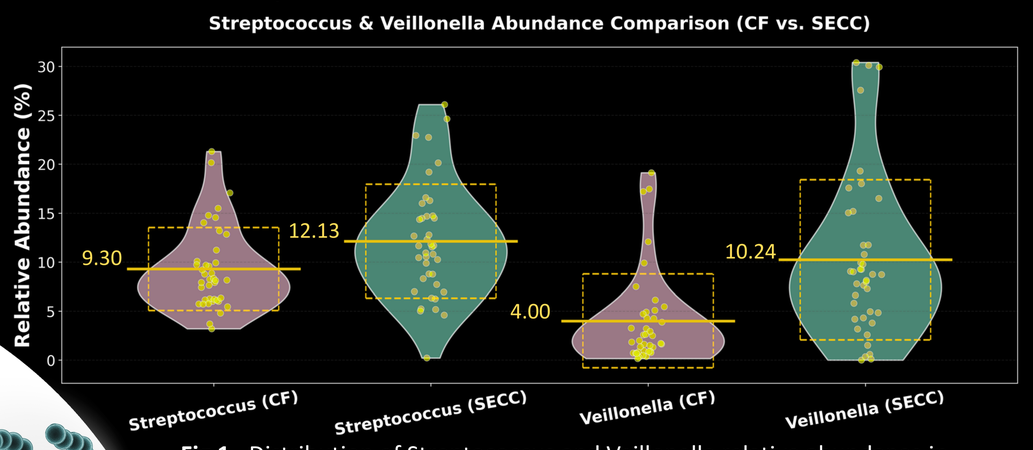
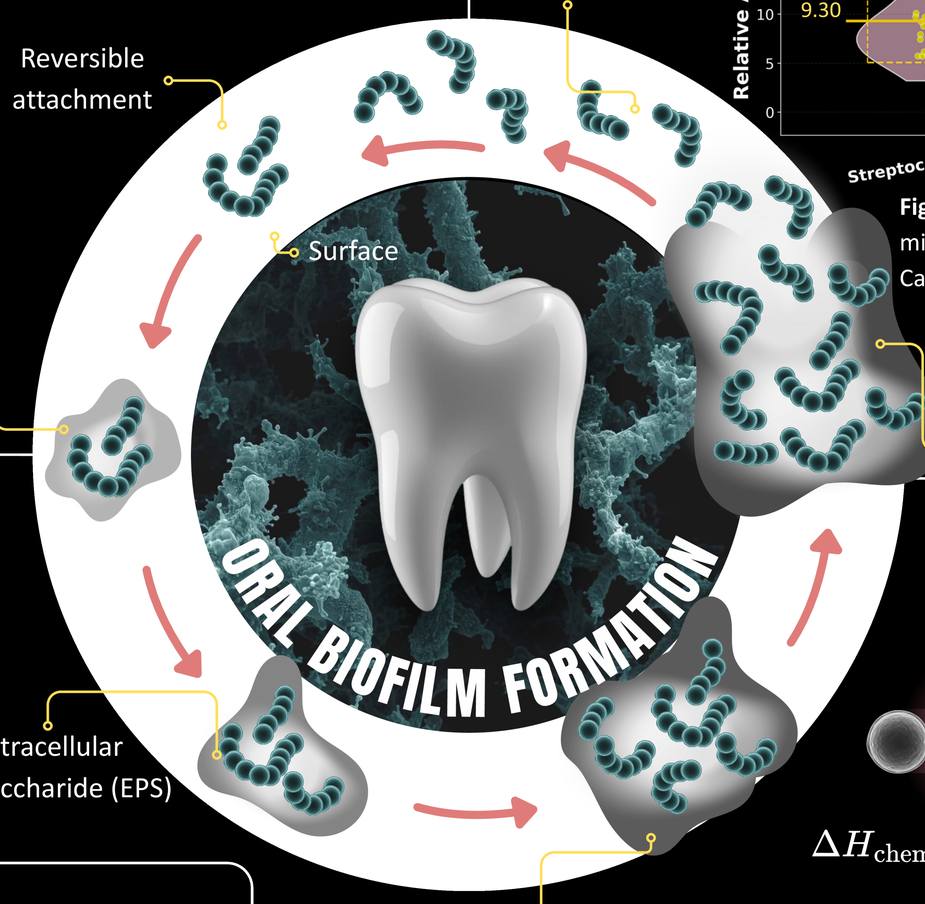


Fig 1. Distribution of Streptococcus and Veillonella relative abundance in microbial samples from Caries Free (CF, pink violins) and Severe Early Childhood Caries (SECC, Viridian violins) cohorts.

CF Caries Free

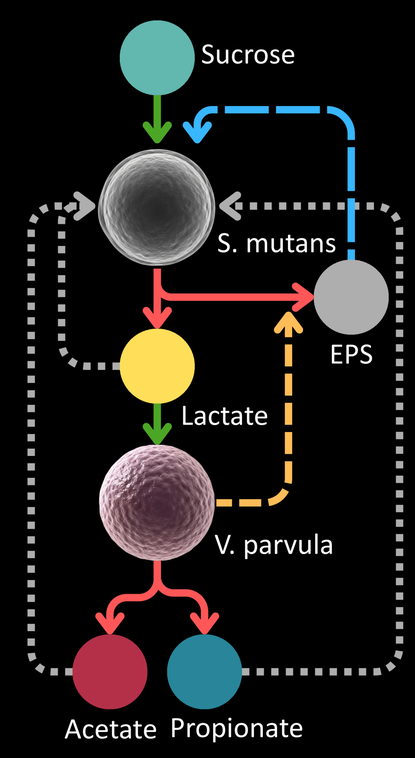
SECC Severe Early childhood caries

Individual samples
Mean
±1 SD



Model

METABOLIC NETWORK



consumes
produces
inhibits
enhances
protects

Primary source for *S. mutans*
Sucrose

Primary source for *V. parvula* stronger acid produced by *S. mutans*
Lactate

Weaker acids produced by *V. parvula*
Acetate

Weaker acids produced by *V. parvula*
Propionate

Equations

Cellular Potts Model (CPM)

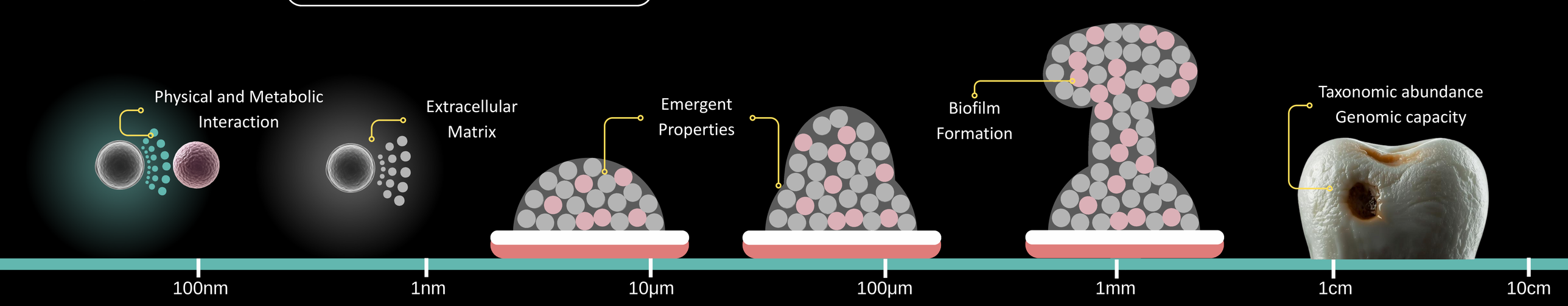
$$\Delta H_{\text{chemotaxis}} = -\mu(C_j - C_i) \quad H_{\text{volume}} = \sum_{\sigma} \lambda_{\sigma}(v_{\sigma} - V_{\sigma})^2$$

Growth Function

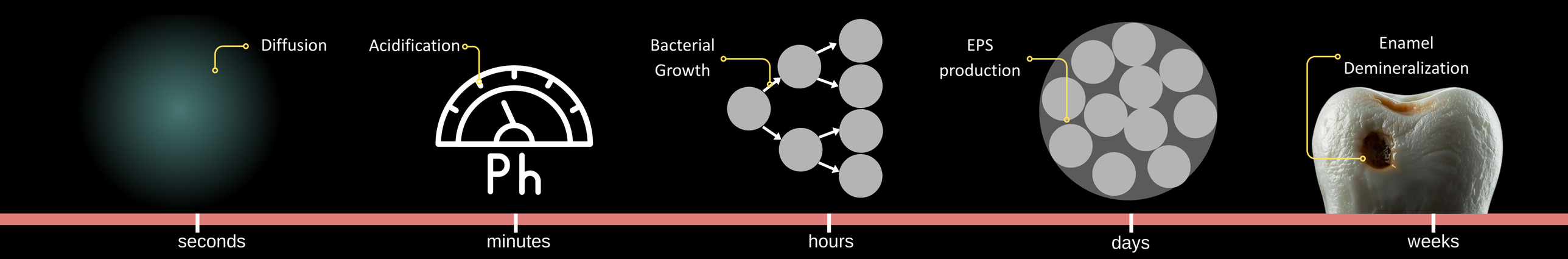
$$\frac{dSM}{dt} = \underbrace{\mu_{\max,SM} \frac{Su}{K^{Su}_{S,SM} + Su} \cdot SM}_{\text{Growth}} \cdot \underbrace{\Phi(La, Ac, Pr)}_{\text{Inhibition}} - \underbrace{d_1 SM}_{\text{Death}}$$

Reaction-Diffusion Equation

$$\frac{\partial La}{\partial t} = \underbrace{D_{La}\nabla^2 La}_{\text{Diffusion}} + \underbrace{Y_{La/Su}}_{\text{Yield}} \cdot \underbrace{\frac{V^{Su}_{\max,SM} \cdot Su}{K^{Su}_{M,SM} + Su} \cdot SM}_{\text{Production}} - \underbrace{\frac{V^{La}_{\max,VP} \cdot La}{K^{La}_{M,VP} + La} \cdot VP}_{\text{Consumption}} - \underbrace{\delta_{La} La}_{\text{Decay}}$$



SPATIAL SCALE



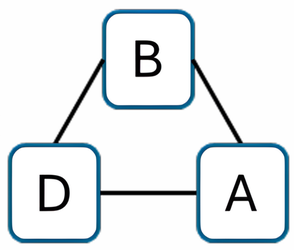
TEMPORAL SCALE

UvA

MetaHealth
HEALTHY WEIGHT AND HEALTHY TEETH FOR CHILDREN

NWO

Computational Science



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