

***In silico* modelling to differentiate the contribution of sugar frequency  
versus total amount in driving biofilm dysbiosis in dental caries**

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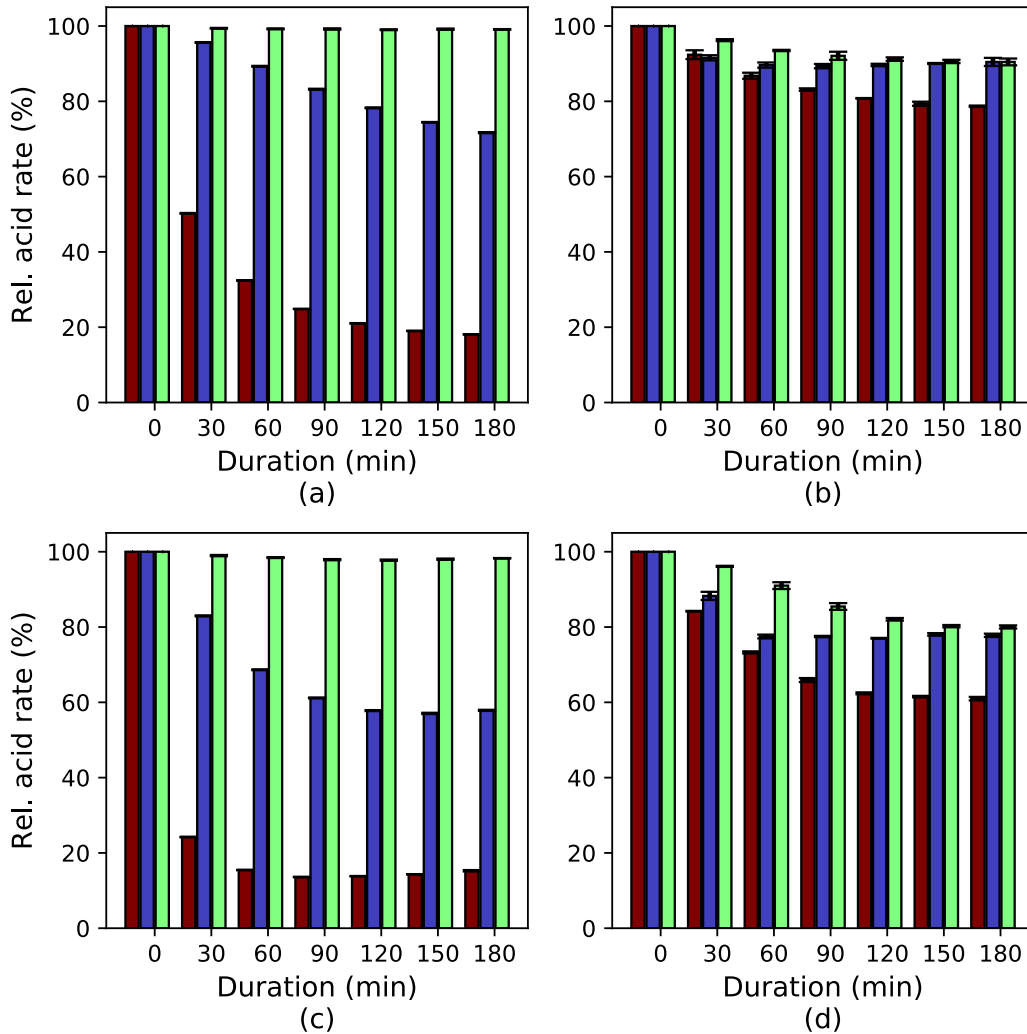
**Page 2: Supplementary Table S1:** Summary of the dispersed phases in the model.

**Page 3: Supplementary Figure S1:** Calibration assays for the adaptation parameters in the model.

**Page 4: Supplementary Videos S1 and S2:** Videos for the same parameters as Fig. 1(a) and Fig. 1(b) in the main text. Video files provided separately.

| <b>Label</b> | <b>Meaning</b>      | <b>Spatial<br/>varying?</b> | <b>Boundary conditions</b>  |
|--------------|---------------------|-----------------------------|---|
| [intakeGl]   | Glucose intake      | Yes                         | Given value at air-saliva interface.<br>No flux through enamel surface. |
| [acid]       | Lactic acid         | Yes                         | Zero at air-saliva interface.<br>No flux through enamel surface.        |
| [polyGl]     | Polyglucose storage | No                          | n/a   |

**Supplementary Table S1:** The dispersed phases included in the model, with boundary conditions for those that vary spatially.



**Supplementary Figure S1:** The relative drop in acid production rate on recovery of pH=7 after the pH was lowered to one of pH=4 (dark red bars), pH=5 (blue bars) or pH=6 (light green bars) for the specified duration, for mono-species systems of particles of type NA in the left panes (a,c), or A on the right panes (b,d). The adaptation rates were  $M_A = M_{NA} = 10^{-2}h^{-1}$  for the top panes (a,b) and  $M_A = M_{NA} = 3 \times 10^{-2}h^{-1}$  for the bottom panes (c,d).

**Supplementary Video S1:** 60 days biofilm evolution for an intake of 10 g/L/d and 6 glucose pulses per day, the same parameters as Fig. 1(a). Green spheres denote particles of type NA, and red spheres those of type A. The blue background is calibrated to the concentration of acid, with the maximum shown in the upper bar (note that this is the concentration prior to the disassociation calculation).

**Supplementary Video S2:** Same as Supplementary Video 1, but with double the total amount of glucose intake, *i.e.* 20 g/L/d, the same parameters as Fig. 1(b).