

Supplementary Information

Coarse graining bacteria colonies for modeling critical solute distributions in picoliter bioreactors for bacterial studies on single-cell level

Christoph Westerwalbesloh, Alexander Grünberger,
Wolfgang Wiechert, Dietrich Kohlheyer and Eric von Lieres*

January 23, 2017

Institute of Bio- and Geosciences, IBG-1: Biotechnology,
Forschungszentrum Jülich, Jülich 52425 Germany;
telephone: +49-2461-61-2168; fax: +49-2461-61-3870; e-mail:
e.von.lieres@fz-juelich.de

Table 1: Number of mesh elements

Model	2 Cells	20 Cells	50 Cells	100 Cells	200 Cells
Model 1a	1.3619×10^6	1.3619×10^6	1.3619×10^6	1.3619×10^6	1.3619×10^6
Model 1b	1.3619×10^6	1.3620×10^6	1.3612×10^6	1.3615×10^6	1.3616×10^6
Model 2a	1.3633×10^6	1.3635×10^6	1.3630×10^6	1.3643×10^6	1.3633×10^6
Model 2b	1.3635×10^6	1.3636×10^6	1.3635×10^6	1.3650×10^6	1.3642×10^6
Model 3a	1.5721×10^6	2.9147×10^6	4.3734×10^6	6.8687×10^6	4.7444×10^6
Model 3b	1.5817×10^6	1.7546×10^6	4.4118×10^6	3.1349×10^6	6.4294×10^6

Table 2: Mesh independence for geometry with 100 cells

Model	Elements		Maximum concentration difference in xy-plane at half-chamber height
	Normal mesh	Refined mesh	
Model 1a	1.3619×10^6	6.050076×10^6	4.9×10^{-2} mmol/L
Model 1b	1.3615×10^6	6.052157×10^6	2.1×10^{-3} mmol/L
Model 2a	1.3643×10^6	6.079938×10^6	3.5×10^{-3} mmol/L
Model 2b	1.3650×10^6	6.079938×10^6	3.6×10^{-3} mmol/L
Model 3a	6.8687×10^6	26.281688×10^6	2.7×10^{-3} mmol/L
Model 3b	3.1349×10^6	13.547256×10^6	5.5×10^{-3} mmol/L

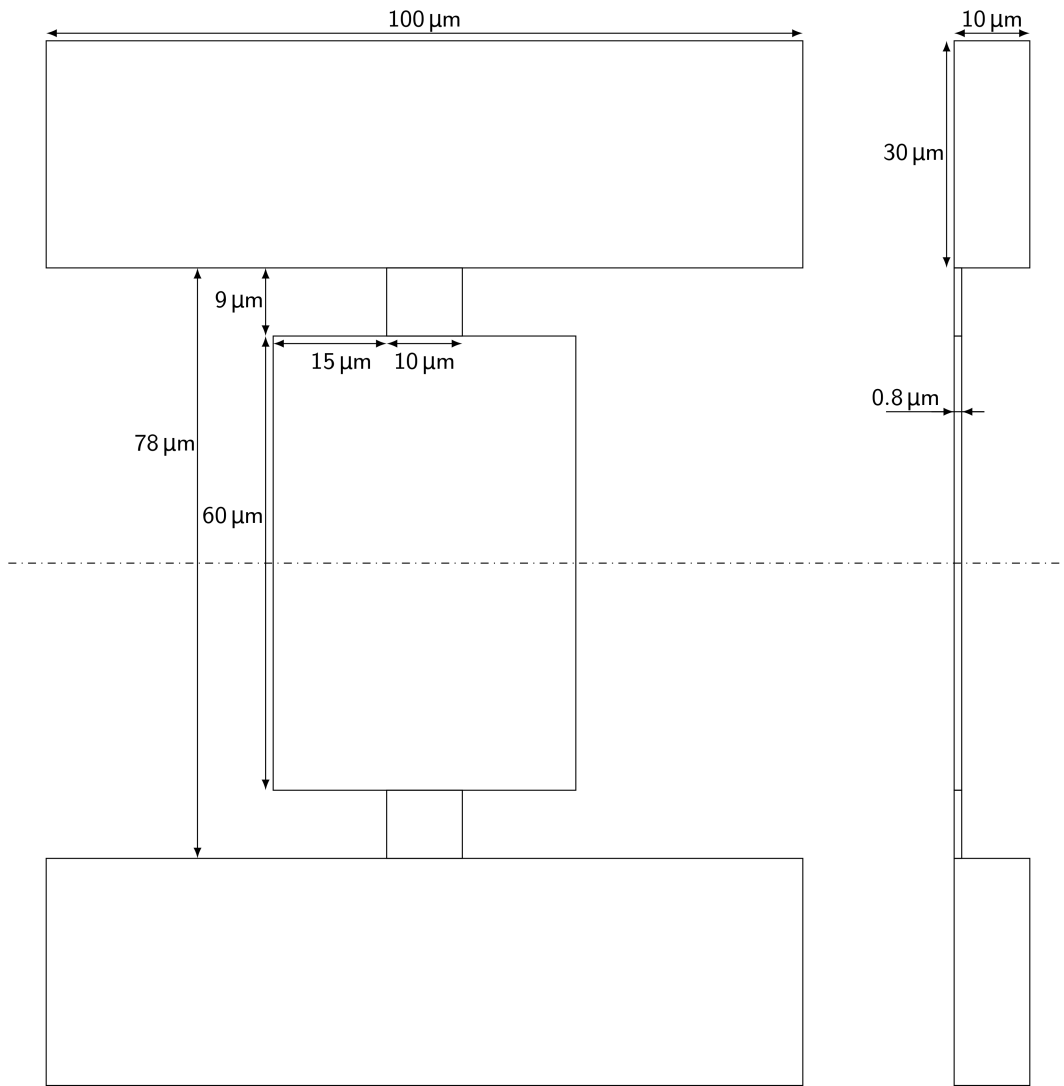


Figure 1: Measurements of the simulated chamber geometry with supply channels.

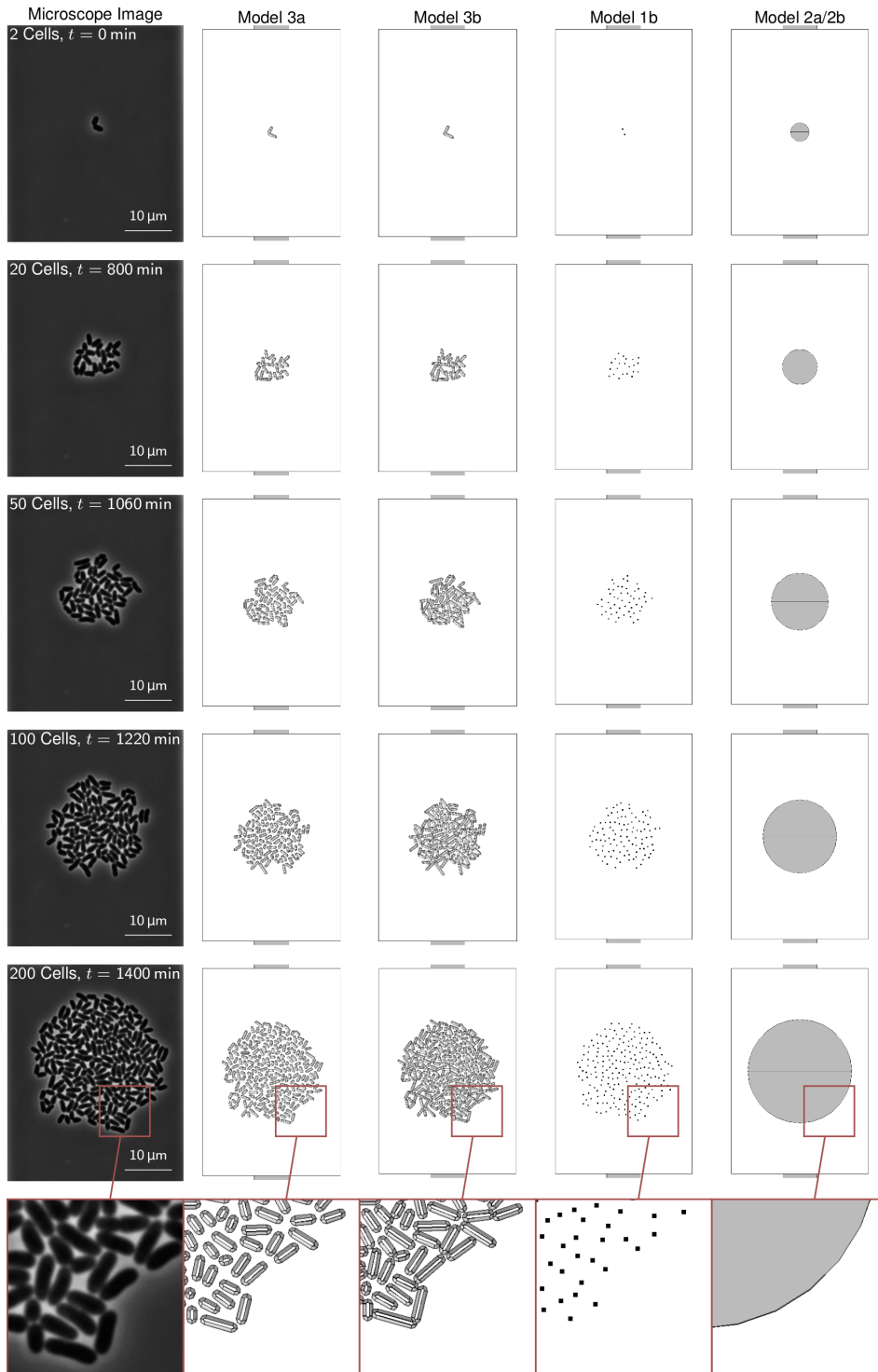
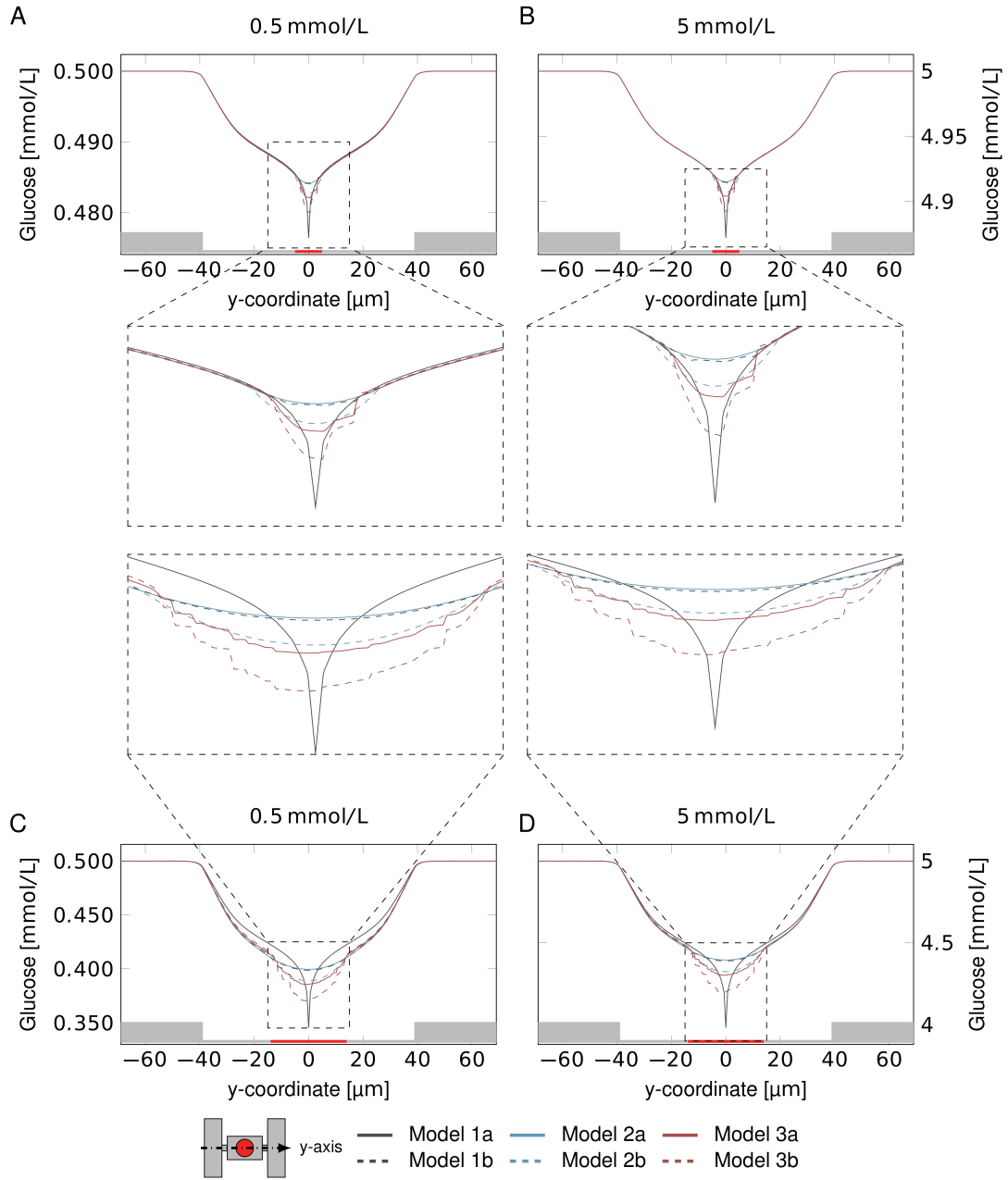


Figure 2: Different model geometries in comparison to the respective microscope images. Model 1a is not shown.



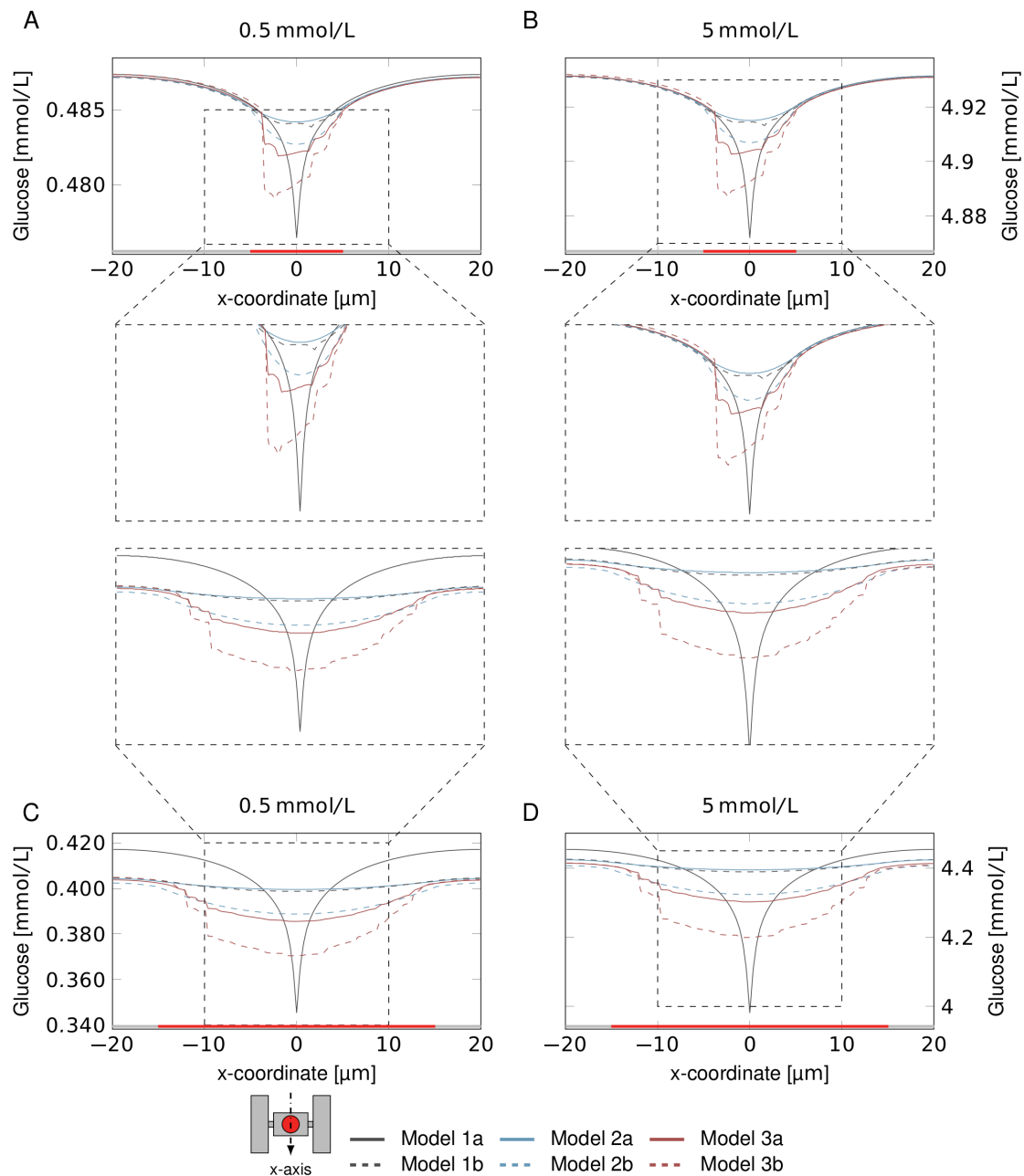


Figure 4: Nutrient distribution within microcolonies based on simulations with different coarse graining concepts. The graphs and respective zoom-outs show the glucose concentration along the x-axis through the center of the chamber/colony in mmol/L for the colony with 20 cells (A, B) and 200 cells (C, D) and two medium glucose concentrations of 0.5 mmol/L (A,C) and 5 mmol/L (B,D).

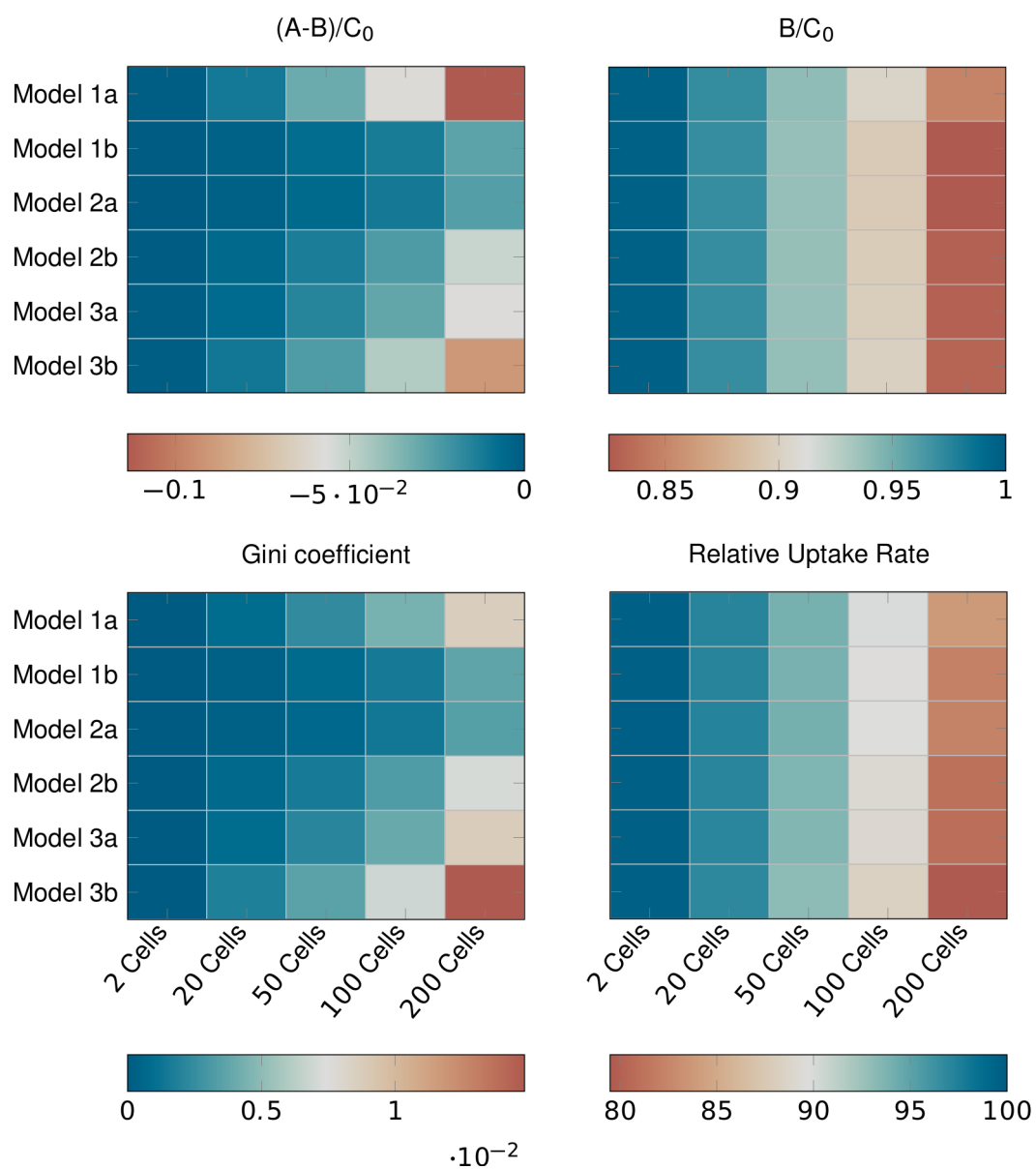


Figure 5: The concentrations B and A – B normalized to C, the Gini coefficient and the average relative uptake rate for each model and colony size and the nutrient concentration of 0.5 mmol/L.

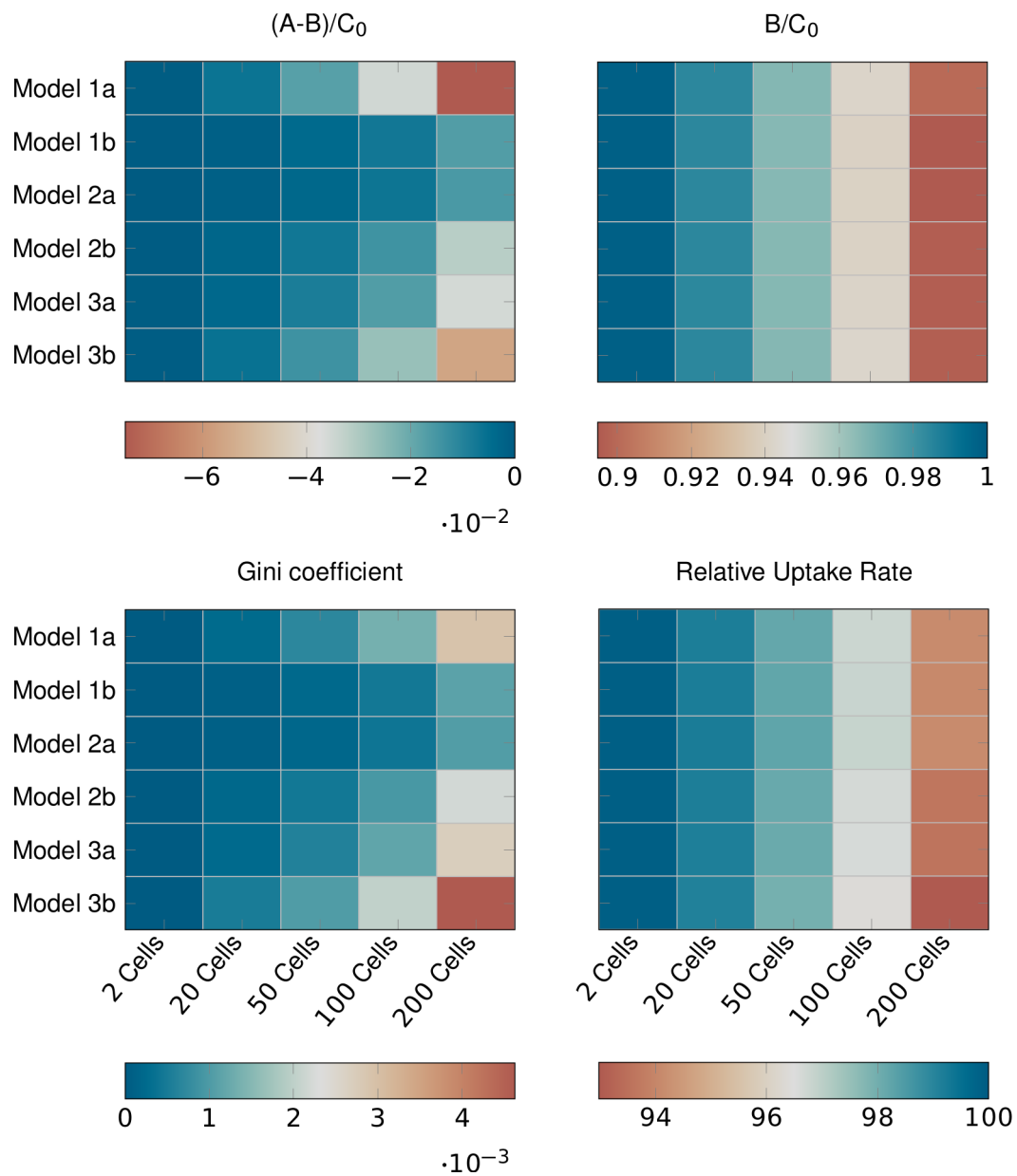


Figure 6: The concentrations B and A – B normalized to C, the Gini coefficient and the average relative uptake rate for each model and colony size and the nutrient concentration of 5 mmol/L.

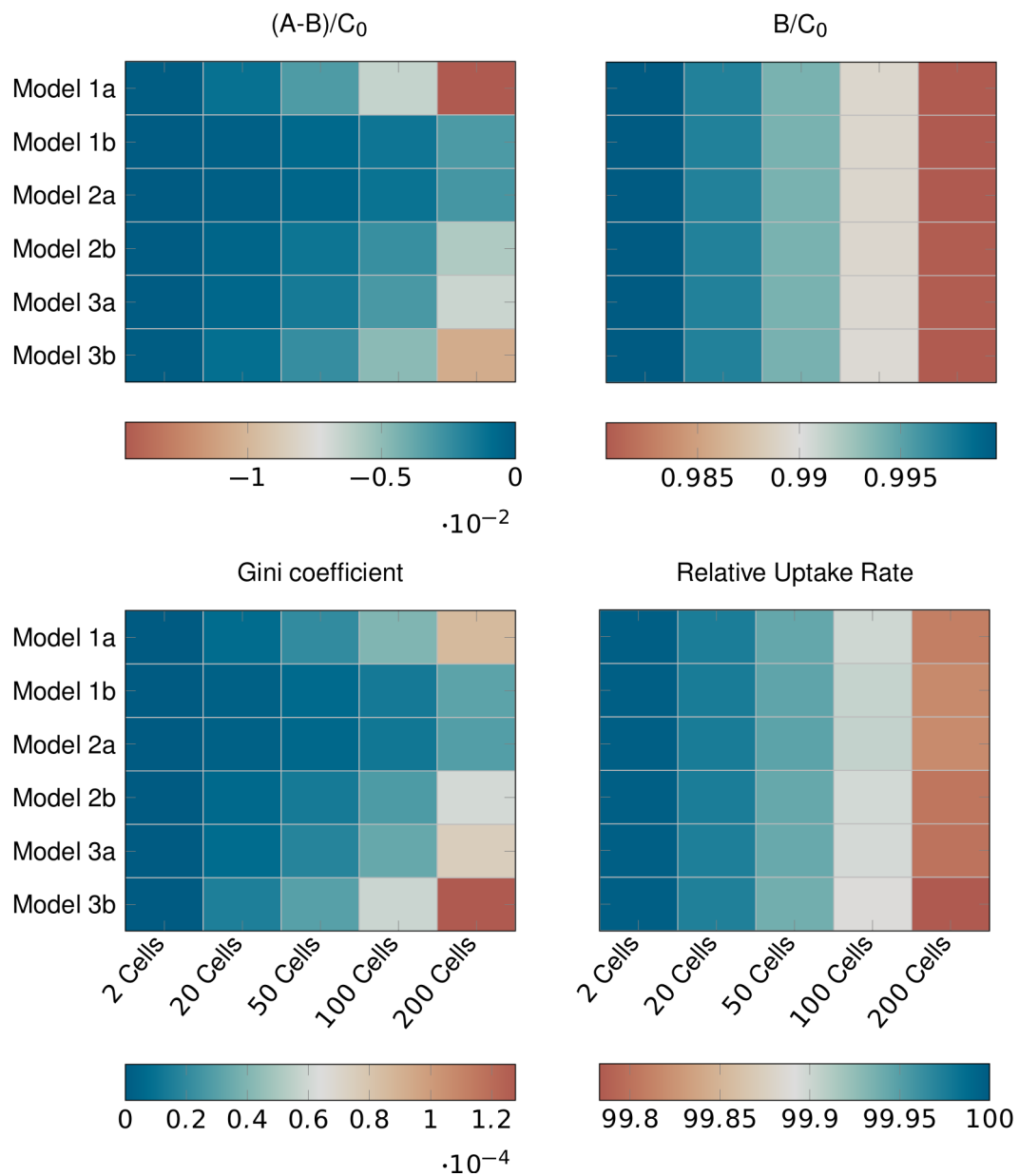


Figure 7: The concentrations B and A – B normalized to C, the Gini coefficient and the average relative uptake rate for each model and colony size and the nutrient concentration of 50 mmol/L.