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Supplementary material to

CHEMICAL ENGINEERING METHODS IN ANALYSES OF 3D CANCER CELL CULTURES: HYDRODYNAMIC AND MASS TRANSPORT CONSIDERATIONS

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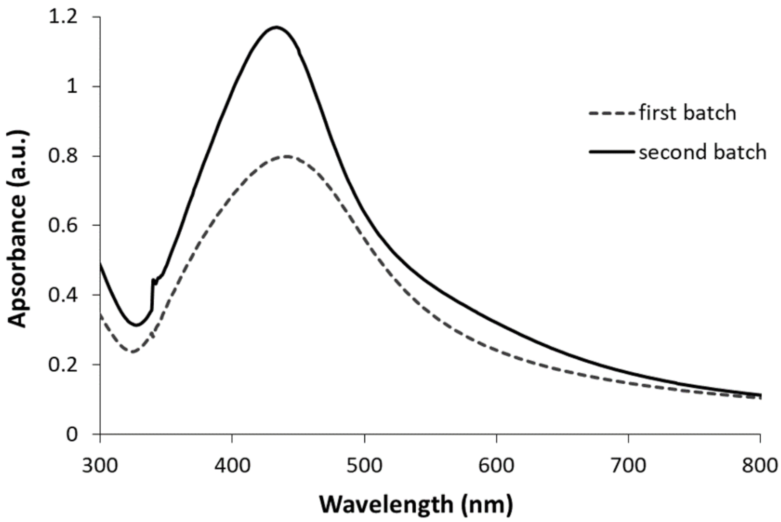

Figure 1S. UV-vis spectra of two batches of Ag/honey/alginate microfibers upon dissolution (data represent average of n=3; standard deviations (≤4%) are omitted from the graph for clarity).

Mathematical modeling of silver release from a packed bed of Ag/honey/alginate microfibers

In this work, the previously applied modeling approach for silver release studies from Ag/alginate microbeads packed in a perfusion bioreactor [1] was adopted for modeling of silver release from a packed bed of Ag/honey/alginate

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microfibers. The microfibers were modeled as a hydrogel cylinder 3 cm in height (as observed experimentally for the bed expansion).

It was assumed that the AgNP oxidation is faster than the mass transport of silver species through the hydrogel so that the change of silver concentration, c_s, in the cylindrical hydrogel over time is described by the diffusion - advection equation in the axial direction, x:

$$\frac{\partial c_s}{\partial t} = D_s\left(\frac{\partial^2 c_s}{\partial x^2}\right) - u\frac{\partial c_s}{\partial x} \tag{1}$$

where D_s is the apparent silver diffusion coefficient (of AgNPs, Ag^+ and formed $AgCl_x^{(x-1)-}$ species) in the alginate hydrogel adopted as 2.1×10^{-15} m^2 s^{-1} [2] and u is the medium velocity through the hydrogel. Silver concentration in the medium, c_{sm}, at each time point is calculated then as:

$$c_{sm} = \frac{V\,(c_{so} - \langle c_s\rangle)}{V_m} \tag{2}$$

where c_{so} is the initial silver concentration in microfibers (2.9×10^{-3} mol dm^{-3} as the average measured concentration), $\langle c_s \rangle$ is the average silver concentration in the hydrogel, V is the hydrogel volume (calculated as 0.49 cm^3 based on the microfiber mass and alginate density of 1020 kg m^{-3} [2]) and V_m is the medium volume (15 cm^3).

Average AgNP concentration in a microfiber $\langle c_s \rangle$ at each time point was calculated by integration:

$$\langle c_s\rangle = \frac{1}{X}\int_0^X c_s(x)\,dx \tag{3}$$

where X is the height of the hydrogel, X=3 cm.

Applied initial conditions were that AgNP concentration in the hydrogel is uniform, while in the medium is equal to zero:

$$t = 0 \qquad c_s = c_o \qquad 0 < x < X$$
$$c_m = 0 \tag{4}$$

The silver concentration in medium was negligible in comparison to that in the hydrogel so that the inlet boundary condition was set as c = 0, while the Neumann boundary condition was set at the outlet boundary:

$$\frac{\partial c_s}{\partial x} = 0 \qquad \text{for} \qquad x = X \tag{5}$$

Equations 1-3 were simultaneously numerically solved, where the second derivative of concentration was solved by using the centered finite difference method, while the first derivative by the backward finite difference method.

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