Supporting information

For: **Mathematical modelling reveals cellular dynamics within tumour spheroids**

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S7 Appendix: Table of parameters Table A contains the default parameter values used in this model (ranges indicate parameters which are altered in different simulations). Where no reference is given, the parameter value has been chosen in order to produce biologically reasonable behaviour. In particular, parameter values were chosen to ensure that spheroids remained compact, exhibited logistic growth patterns characteristic of diffusion-limited spheroid growth and, where possible, were consistent with previous modelling studies. Dimensional values for parameters relating to oxygen thresholds are stated in terms of partial pressures p; following [1] and [2] these can be converted to concentrations ω using Henry's Law $p = \Omega\omega$, with $\Omega = 3.0318 \times 10^7$mmHg kg m^{-3}.

Table A. Parameter values and ranges used for simulations.

Symbol	Parameter	Dimensionless value	Dimensional range	Refs
dt	Timestep	1/120	1/200 - 1/100 (hours)	[3]
R_{Cell}	Radius of a cell	0.5	7 - 12 (μm)	[4]
R_{int}	Radius of interaction	1.5	21 - 36 (μm)	[3]
α	Radius used to determine α-shape	0.5	7 - 12 (μm)	*
ω_∞	Oxygen boundary value	1.0	100 - 150 (mm Hg)	[1, 5]
ω_{h}	Hypoxia threshold	0.1 - 0.7	10 (mm Hg)	[1]
ω_{q}	Quiescence threshold	0.3 - 0.7	30 - 70 (mm Hg)	*
τ	Average cell cycle length	8 - 32	13 - 32 (hours)	[6, 7]
τ_i	Cell cycle duration for cell i	0.75τ- 1.25τ	9.75 - 40 (hours)	*
$\tilde{\tau}$	Average critical hypoxic duration	8 - 16	Assumed (hours)	*
$\tilde{\tau}_i$	Critical hypoxic duration for cell i	$0.75\tilde{\tau}$- $1.25\tilde{\tau}$	Assumed (hours)	*
$\bar{\tau}$	Average necrosis duration	48	Assumed (hours)	*
$\bar{\tau}_i$	Necrosis duration for cell i	$0.75\bar{\tau}$- $1.25\bar{\tau}$	Assumed (hours)	*
ν	Damping coefficient	1	0.4 ($N\,\text{s}^{-1}\text{m}^{-1}$)	[3, 8]
μ	Spring constant	45.0	3 - 50 (μg Cell diameter^{-1} hours^{-2})	[3, 9]
μ_{bead}	Spring constant for microbeads	45.0	3 - 50 (μg Cell diameter^{-1} hours^{-2})	*
λ	Intercellular adhesion scaling coefficient	5.0	Assumed (-)	[3]
s_i	Radius of cell i at equilibrium	R_{Cell}	7 - 12 (μm)	[4]
$s_{i,j}$	Resting spring length between cells i and j	$s_i + s_j$	0 - 24 (μm)	*
D	Random motility coefficient	0.01	Assumed (Cell diameter^2 hours^{-1})	*
κ	Oxygen consumption rate	0.03	20×10^{-18} (mol/(cell s))	[10]
D_ω	Oxygen diffusion coefficient	1	1,750 (μm^2 seconds^{-1})	[10]
β	Surface tension coefficient	5	Assumed (μg hours^{-2})	*

*Estimated to maintain realistic model behaviour.

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