Contribution ID : **76** Type : **not specified**

Simulation of cell morphology using models derived from cell features and components

Simulation of cell populations can be carried out by using parameters obtained from experimental cell cultures producing cells defined in terms of position, size or growth state. However representation of cell shape is desirable in order to better visualise the results as well as predicting interactions with the culture substrate or between bordering cells. Here we describe a procedure for prediction and visualisation of cell shape according to cell parameters such as volume, attachment status, growth conditions, movement and interaction with other cells. Cells are simulated as "2.5-dimensional" objects, where a relatively detailed two-dimensional footprint is complemented by a volume-dependent thickness to provide the third dimension. Detached cells are modelled as simple spheres freely floating in the medium, but as they become attached, they spread and flatten on the substrate, modifying height and surface, according to a cell specific index that numerically describes the spreading degree. After spreading, cells assume their final morphology (i.e. circular, polygonal or star-shaped), that is modelled by using a polygonal representation where contours are described by vertices connected by Bezier curves. This process causes cells to redistribute their internal volume into a different shape which requires a in larger membrane surface, modelled as an internal membrane reservoir which can quickly bring new membrane to the surface. To take movement into account, changes in morphology, normally observed in cultured cells when they move and possibly interact with each other, are obtained modifying the previously defined shape by updating the entire set of vertices and curves following changes in position and formation of contacts between touching cells. The system was integrated within SimulCell, an in silico simulation tool developed in-house, where each cell is an independent agent able to interact with the surrounding cells and the external environment. Visualisation techniques, similar to sample staining in fluorescence microscopy, were also introduced to visually highlight structural and molecular aspects of individual cells as well as time-dependent differences.

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