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Monte Carlo modeling of the formation of branched tube structures from cellular aggregates

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Monte Carlo method has been used previously for modeling the fusion of cellular aggregates to produce capillary-like structures and hollow tubes from cell aggregates consisting of smooth muscle cells and endothelial cells. Here we have extended these modeling efforts to branched tubular structures built of cellular aggregates in the presence of two types of biocompatible gels. A MATLAB script was created to generate a construct of simulated cell aggregates resembling a branched tube. All of the simulated cells and gel particles were placed on a uniform 3D lattice. The main tube consisted of layers of spherical cell aggregates arranged in circles and stacked on top of each other in a close-packed arrangement. All the aggregates were composed of 30% endothelial cells and 70% smooth muscle cells, randomly distributed, with the exception of a set of three cells adjacent to any branch. These aggregates were filled to 83% of their radius with gel. Branches were attached at a site of three gel-filled aggregates, and the aggregates comprising the branch had a radius between 165% and 185% of that of the aggregates in the main tube; these aggregates were gel-filled to approximately 80% of their radius, with the remaining cells distributed as described above. The lumen of the main tube was filled with the same type of gel as in the centers of the aggregates, and the remainder of the environment was filled with a second type of gel. The structure was then subjected to Monte Carlo simulation for fifty-thousand steps. The final equilibrium structure (when simulated with the proper parameters) strongly resembles a branched blood vessel: the cell aggregates fused, and the smooth muscle cells migrated to the outside of the main tube and branch, while the endothelial cells migrated to the interior of the tube and branch. In addition, the lumen of the branch and main tube were contiguous. The results of these simulations are currently being used to guide the construction of such structures through in vitro experiments.