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Size Optimization of Microfluidic Polymerase Chain Reaction Devices Using COMSOL

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Abstract : The invention and development of the Polymerase Chain Reaction (PCR) technology have revolutionised molecular biology and molecular diagnostics. There is an urgent need to optimise their performance of those devices while reducing the total construction and operation costs. The present study proposes a CFD-enabled optimisation methodology for continuous flow (CF) PCR devices with serpentine-channel structure, which enables the trade-offs between competing objectives of DNA amplification efficiency and pressure drop to be explored. This is achieved by using a surrogate-enabled optimisation approach accounting for the geometrical features of a CF μPCR device by performing a series of simulations at a relatively small number of Design of Experiments (DoE) points, with the use of COMSOL Multiphysics 5.4. The values of the objectives are extracted from the CFD solutions, and response surfaces created using the polyharmonic splines and neural networks. After creating the respective response surfaces, genetic algorithm, and a multi-level coordinate search optimisation function are used to locate the optimum design parameters. Both optimisation methods produced similar results for both the neural network and the polyharmonic spline response surfaces. The results indicate that there is the possibility of improving the DNA efficiency by ~2% in one PCR cycle when doubling the width of the microchannel to 400 μm while maintaining the height at the value of the original design (50μm). Moreover, the increase in the width of the serpentine microchannel is combined with a decrease in its total length in order to obtain the same residence times in all the simulations, resulting in a smaller total substrate volume (32.94% decrease). A multi-objective optimisation is also performed with the use of a Pareto Front plot. Such knowledge will enable designers to maximise the amount of DNA amplified or to minimise the time taken throughout thermal cycling in such devices.

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