Computerized Simulation and Experimental Analysis for Efficient Polymerase Chain Reaction*

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Polymerase chain reaction (PCR) is a useful biochemical operation not only in biological application but also in DNA computing. It can be used for *in vitro* selective amplification of nucleic acids, which makes PCR a useful tool for signal amplification and detection. Recently, modified forms of PCR such as exclusive PCR, whiplash PCR, DNA shuffling, and PNA-mediated PCR were suggested as DNA computing operators. In spite of its usefulness, PCR has significant limits. It falls into a plateau phase after an initial exponential phase and subsequent quasi-linear phases.

In this work, we focus on the cause of plateau phenomenon and the improvement of the PCR efficiency. We investigate the effect of possible limiting components during the PCR process, such as *Taq* polymerase, primer pairs, and dNTPs, by real-time monitoring of the amplification profile experimentally. The mathematical model in our previous work [1] was extended and modified [2]. Simulations were performed to investigate the complex mechanism of the reaction, such as the efficiency at each PCR step and the effective enzyme concentration within cycle progress which are hard to investigate experimentally.

The results show that the PCR plateau is caused by the decrease of effective polymerase concentration due to heat inactivation and product accumulation. Addition of PCR components could increase the amount of final product, but the PCR process still reached a plateau phase after some time. Simulation results suggest that the main contribution to plateau forming is the renaturation of templates before competitive annealing reaction and decrease of effective enzyme concentration by non-specific binding of polymerase to double-stranded DNA. The detailed model in our simulation and experimental results will be presented at the poster session.

References

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