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Hardware architecture for superoxide production in CKDu initiation

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Simulation of molecular mechanisms of a disease is important in drug discovery and treatments of the disease. There are many difficulties in performing extensive biological experiments to investigate of a disease with living organisms or even with cell lines because of high cost, the requirement of expensive instrumentation and expertise knowledge. Further, there are lots of ethical and legal limitations for doing these experiments. Modeling these processes using mathematical modeling and simulating them with latest technologies would accompany to further investigate the disease condition while finding and testing new drugs by bypassing limitations. In recent past, usage of hardware simulations for the biological system modeling has become more frequent due to high speed solving capacity of hardware compared to much time consuming process of simulation using software. Field Programmable Gate Array is a semiconductor device designed to build reconfigurable digital circuits and has been used more frequently for simulation and acceleration purposes these days. In this work, we propose a hardware architecture utilizing Field Programmable Gate Array for superoxide production in initiation of Chronic Kidney Disease of uncertain etiology with heavy metal exposure which is one of the identified etiological factors of the disease. Since oxidative stress is identified as main mediator of heavy metal induced renal injury in the disease, mechanisms for increase of oxidative stress is further explored. To that end, the increase of reactive oxygen species initiated first with superoxide generation is identified as a leading cause for increase of oxidative stress. Therefore, the superoxide increment was mathematically expressed using kinetic laws. Ordinary differential equations based mathematical expression is used to describe the variation of superoxide concentration with time in cells. The ordinary differential equations are then can be converted into the hardware description language code which could run on Field Programmable Gate Array. In this conversion, Register Transfer Level design of the superoxide increment process was created based on the mathematical expression as the initial step before the implementation on Field Programmable Gate Array. In the circuit, input signals are the main variables considered in the mathematical model and adders, sub tractors, multipliers, and dividers are the algebraic representations. The constant parameter values are included in the algebraic representation. The rate of the reaction is the final output of this reconfigurable architecture. In addition to acceleration, Field Programmable Gate Array has advantages as optimization and initiating system-on-chip implementations. Accuracy of simulation can be confirmed by observing the experiment data patterns.

Keywords: CKDu, Superoxide, Mathematical modeling, FPGA

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