Chapter 12
Toward Biomolecular Computers Using Reaction–Diffusion Dynamics

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ABSTRACT
This article investigates a possibility of constructing massively parallel computing systems using molecular electronics technology. By employing the specificity of biological molecules, such as enzymes, new integrated circuit architectures that are free from interconnection problems could be constructed. To clarify the proposed concept, we present a functional model of an artificial catalyst device called an enzyme transistor. In this article, we develop artificial catalyst devices as basic building blocks for molecular computing integrated circuits, and explore the possibility of a new computing paradigm using reaction-diffusion dynamics induced by collective behavior of artificial catalyst devices.

INTRODUCTION
The purpose of this article is to discuss the possibility of constructing massively parallel computing architectures using molecular electronics technology. By employing the specificity of biological catalysts, such as enzymes, new circuit/system integration could be realized. Recently, we have presented a model of molecular computing using
artificial catalyst networks (Aoki et al., 1998; Hiratsuka et al., 1999, 1999a). We have shown that artificial catalysts having activity control function, such as enzyme transistors (Aoki et al., 1998), can realize various analog/digital computing circuits as molecular reaction networks.

Currently, we are interested in creating new information processing functions, which are essentially different from those of conventional electronic systems, using artificial catalyst devices (Hiratsuka et al., 1999, 1999a). An important feature of molecular information processing is its massive parallelism based on reaction-diffusion molecular dynamics in a continuous signal transfer/processing medium. Our current project aims

i. To develop artificial catalyst devices as basic building blocks for molecular computing integrated circuits, and

ii. To explore the possibility of a new computing paradigm using reaction-diffusion dynamics induced by collective behavior of artificial catalyst devices.

TOWARD WIRE-FREE SYSTEM INTEGRATION

A Model of Enzyme Transistors

An enzyme transistor presented here is a molecular device based on activity-controlled enzyme reactions. Figure 1(a) schematically illustrates an effector-controlled enzyme reaction. An enzyme $E$ catalyzes the reaction that converts its substrate $S$ into the corresponding product $P$. The catalytic activity of the enzyme is regulated by the specific effector $C$. We assume that the enzyme transistor is an artificial catalyst whose activity is controlled by some effector.

Figure 1(b) shows the model of an enzyme transistor, where $C$, $S$, $P$, and $J$ represent the concentrations of the effector, substrate, product, and the substrate flux (the rate of substrate supply), respectively. The catalytic activity of the enzyme transistor varies in response to the concentration of the effector $C$. We assume that the rate constant $k_1$ of the enzymatic reaction, which is a measure of catalytic efficiency, is expressed as a function of the effector concentration $C$, and is denoted by $k_1(C)$. In general, $k_1(C)$ is assumed to have a sigmoid characteristic which has a steep slope near the operating-point concentration $C_0$, as illustrated in Figure 1(c). (These types of characteristics are widely found in living systems.)

By coupling multiple enzyme transistors, we can construct an artificial network of biochemical...