STOCHASTIC SIMULATION OF CHEMICAL REACTION BY
DIGITAL COMPUTER, I. THE MODEL

T. Sipos, 1 J. Tóth, 2 and P. Erdi 1
1. Danube Oil Company Computer Center,
2. Institute of Medical Chemistry, Semmelweis
University Medical School, Budapest
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A stochastic model of complex chemical reactions is outlined. A discrete
Markov process corresponds to the complex chemical reaction in the model
i.e. the concentrations of the components are discrete quantities. The dif-
f erences between the stochastic and deterministic models are discussed.

INTRODUCTION

Both deterministic and stochastic models are known to describe complex chem-
ic reactions phenomenologically. The stochastic model of complex chemical reac-
tions has been developed essentially by Rényi [1].

In the first part of this paper an extension of the stochastic model is presented.
This model provides a framework for as many elementary reactions of as many
components as desired under practically general conditions.

It should be pointed out that the stochastic model is more natural than the de-
terministic one.

As the solutions for possible models of even relatively less complex reactions
cannot be presented in a closed form, which is also true for the deterministic model,
one has to use approximate solutions or simulations. In fact we intend to show how
to turn from the model described here to another permitting direct simulation experi-
ment.
In the second part of the paper the computer realization of the model will be reported with some particular examples to prove that simulation experiments can be performed without the usual simplifying assumption of reaction kinetics.

A more detailed comparison of the deterministic and stochastic models, a full presentation of the program and an exhaustive list of references are given elsewhere [2].

II. THE STOCHASTIC MODEL

Let us take a vessel (e.g. a test tube, a reactor, a living organism, etc.) containing the components \( K_i \) in quantities \( \xi_i(t) \) \( (i = 1, 2, \ldots, k) \) at moment \( t \). The system may be open or isolated, changes in pressure, temperature and volume are disregarded.

We suppose that only reactions involving one or two components (so called unicomponent and bicomponent reactions, \( 2 \)) take place, i.e.

\[
\begin{align*}
K_p & \xrightarrow{\alpha_{p,q}} \sum_{i=1}^{k} A_{1,p_i} K_i; p = 1, 2, \ldots; e_p = 1, 2, \ldots \ E_p; \\
K_r + K_s & \xrightarrow{\beta_{q,f}} \sum_{i=1}^{k} B_{1,q_i} K_i; q = 1, 2, \ldots; f_q = 1, 2, \ldots \ F_q; \\
q & = Z(r,s)
\end{align*}
\]

where \( \alpha_{p,q} \) and \( \beta_{q,f} \) correspond to the reaction rate constants \([1]\) and \( A_{1,p_i} \) and \( B_{1,q_i} \) are stoichiometric coefficients, i.e. non-negative integers,

\( P \) is the number of components on the left-hand side of the unicomponent reactions,