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Instituto Universitario
de Matemática Multidisciplinar

MODELLING FOR ENGINEERING & HUMAN BEHAVIOUR 2020

July 8-10, 2020

Edited by

R. Company, J.C. Cortés,
L. Jódar and E. López-Navarro



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Statistical solution of a second-order chemical reaction

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1 Introduction

In Reference [1] different and interesting differential equations with applications are considered. In this contribution, motivated by one of the models described in [1], we focus our analysis in how to model a chemical reaction by a differential equation and how to obtain the main statistical information of the solution stochastic process.

A chemical reaction is a process that leads to the chemical transformation of one set of chemical substances to another. In particular, a second-order chemical reaction is a chemical reaction that depends on the concentrations of one-second order reactant or two first-order reactants. That is, let $[A]$ and $[B]$ be the concentrations of two reactants. Given a constant k , usual examples of second-order chemical reactions are:

- $\nu = k[A]^2$, one reactant is consumed at a rate proportional to the square of the reactant's concentration.
- $\nu = k[A][B]$, both reactants are consumed linearly over time.

Where ν denotes the reaction rate and it measures how fast the reactants are consumed. We focus this study in the second type of chemical reaction established below. We start from two reactants A and B which will be consumed linearly. Let $X(t)$ be the number of grams of chemical C formed after the second-order chemical reaction in a time instant t . Suppose that we have a grams of chemical A and b grams of chemical B and the compound is formed by M and N parts of A and B , respectively. Then, the number of grams of chemicals A and B remaining at time t are:

$$A(t) = a - \frac{M}{M+N}X(t), \quad B(t) = b - \frac{N}{M+N}X(t).$$

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Therefore, by the law of mass, the reaction rate is proportional to the product of the amounts of A and B remaining at time t , i.e., $\nu \propto A(t)B(t)$. As the derivative of $X(t)$, $X'(t)$, is the exchange rate of the quantity of chemical C , then

$$X'(t) \propto \left(a - \frac{M}{M+N}X(t)\right) \left(b - \frac{N}{M+N}X(t)\right). \quad (1)$$

Reordering expression (1) and introducing a constant of proportionality $k > 0$, we obtain the following second-order differential equation

$$X'(t) = k(\alpha - X(t))(\beta - X(t)), \quad (2)$$

being $\alpha = a(M+N)/N$ and $\beta = b(M+N)/N$. Clearly $X(0) = 0$, thus the solution of equation (2) with initial condition $X(0) = 0$ is established

$$X(t) = \frac{(1 - e^{(\beta-\alpha)kt}) \alpha \beta}{(\alpha - \beta e^{(\beta-\alpha)kt})}. \quad (3)$$

In practice, parameters α and β are fixed at the beginning of the experiment, therefore they have an associated inherent error. In addition, the constant of proportionality k must be obtained from experimental data, thus it contains a certain measurement error. In order to capture this uncertainty, it is more advisable to consider k , α and β as random variables instead of a deterministic constants. Therefore, the randomized initial value problem is

$$\begin{cases} X'(t, \omega) &= k(\omega)(\alpha(\omega) - X(t, \omega))(\beta(\omega) - X(t, \omega)), \\ X(0) &= 0, \end{cases} \quad (4)$$

where $k(\omega)$, $\alpha(\omega)$ and $\beta(\omega)$ are assumed to be absolutely continuous random variables defined in a common complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$, with a known joint probability density function, $f_0(k, \alpha, \beta)$, defined on a positive region. The solution of (4) can be obtained directly from the deterministic, given in (3), by randomizing all the parameters

$$X(t, \omega) = \frac{(1 - e^{(\beta(\omega)-\alpha(\omega))k(\omega)t}) \alpha(\omega) \beta(\omega)}{(\alpha(\omega) - \beta(\omega) e^{(\beta(\omega)-\alpha(\omega))k(\omega)t})}. \quad (5)$$

Therefore, taking into account the randomness, the solution of the initial value problem (4) is a stochastic process.

2 Computing the first probability density function

In this section, we apply the Random Variable Transformation method (see Reference [2]) to obtain the first probability density function of the solution stochastic process $X(t, \omega)$ defined in (5). Fixing $t > 0$, we apply RVT method with the following choice:

$$\begin{aligned} \mathbf{U}(\omega) &= (k(\omega), \alpha(\omega), \beta(\omega))^\top, \quad \mathbf{V}(\omega) = (V_1(\omega), V_2(\omega), V_3(\omega))^\top, \\ \mathbf{g} : \mathbb{R}^3 &\rightarrow \mathbb{R}^3, \quad \mathbf{g}(k, \alpha, \beta) = (g_1(k, \alpha, \beta), g_2(k, \alpha, \beta), g_3(k, \alpha, \beta))^\top, \end{aligned}$$

being

$$\begin{aligned} v_1 &= g_1(k, \alpha, \beta) = X(t) = \frac{(1 - e^{(\beta-\alpha)kt})\alpha\beta}{(\alpha - \beta e^{(\beta-\alpha)kt})}, \\ v_2 &= g_2(k, \alpha, \beta) = \alpha, \\ v_3 &= g_3(k, \alpha, \beta) = \beta. \end{aligned}$$

Isolating k , α and β , the inverse mapping $\mathbf{h} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is

$$\begin{aligned} k &= h_1(v_1, v_2, v_3) = \frac{\ln\left(\frac{(v_1-v_2)v_3}{v_2(v_1-v_3)}\right)}{t(v_2 - v_3)}, \\ \alpha &= h_2(v_1, v_2, v_3) = v_2, \\ \beta &= h_3(v_1, v_2, v_3) = v_3. \end{aligned}$$

The Jacobian of the inverse mapping \mathbf{h} is

$$J = \frac{1}{t(v_1 - v_2)(v_1 - v_3)} \neq 0.$$

Thus, the joint PDF of the random vector $\mathbf{V}(\omega)$ is

$$f_{\mathbf{V}}(v_1, v_2, v_3) = f\left(\frac{\ln\left(\frac{(v_1-v_2)v_3}{v_2(v_1-v_3)}\right)}{t(v_2 - v_3)}, v_2, v_3\right) \left| \frac{1}{t(v_1 - v_2)(v_1 - v_3)} \right|.$$

Marginalizing with respect to the random variables $V_2(\omega) = \alpha(\omega)$ and $V_3(\omega) = \beta(\omega)$, and considering $t > 0$ arbitrary, the first probability density function of the solution stochastic process $X(t, \omega)$ is determined

$$\boxed{f_1(x, t) = \iint_{\mathbb{R}^+} f_0\left(\frac{\ln\left(\frac{(x-\alpha)\beta}{\alpha(x-\beta)}\right)}{t(\alpha - \beta)}, \alpha, \beta\right) \left| \frac{1}{t(x - \alpha)(x - \beta)} \right| d\alpha d\beta.} \quad (6)$$

3 Numerical example

In this example, we consider that the random parameters $k(\omega)$, $\alpha(\omega)$ and $\beta(\omega)$ are independent random variables with the following distributions:

- $k(\omega)$ follows a Gamma distribution with parameters 3 and 5, i.e., $k(\omega) \sim \text{Ga}(3; 5)$.
- $\alpha(\omega)$ is a truncated Gaussian distribution with mean 1 and standard deviation 0.01, i.e., $\alpha(\omega) \sim N_T(1, 0.01)$, with $T = (0, \infty)$.
- $\beta(\omega)$ follows an Uniform distribution in the interval $[0.4, 0.5]$, i.e., $\beta(\omega) \sim U([0.4, 0.5])$.

Thus, the joint probability density function can be calculated as the product of the marginals

$$f_0(k, \alpha, \beta) = f_k(k)f_\alpha(\alpha)f_\beta(\beta),$$

being $f_k(k)$, $f_\alpha(\alpha)$ and $f_\beta(\beta)$ the probability density functions of $k(\omega)$, $\alpha(\omega)$ and $\beta(\omega)$, respectively. The choice of that probabilistic distributions has been considered taking into account

the positiveness of the parameters. Furthermore, we know the expression for each probability density function:

$$f_k(k) = \begin{cases} \frac{1}{250} e^{-k/5} k^2 & k > 0, \\ 0 & \text{Otherwise.} \end{cases} \quad f_\alpha(\alpha) = \begin{cases} 39.8942 e^{-5000(1-\alpha)^2} & \alpha > 0, \\ 0 & \text{Otherwise.} \end{cases}$$

$$f_\beta(\beta) = \begin{cases} 10 & 0.4 \leq \beta \leq 0.5, \\ 0 & \text{Otherwise.} \end{cases}$$

In Figure 1 we have plotted the first probability density function of the solution stochastic process given in expression (6) in the time interval $[0, 0.5]$. We observe that when the time increases the number of grams (or quantity) of the chemical C also increases. This augment is more pronounced in the early stages, after that it tends to stabilize (approximately with 4 grams of component C). The behaviour of the first probability density function can be also

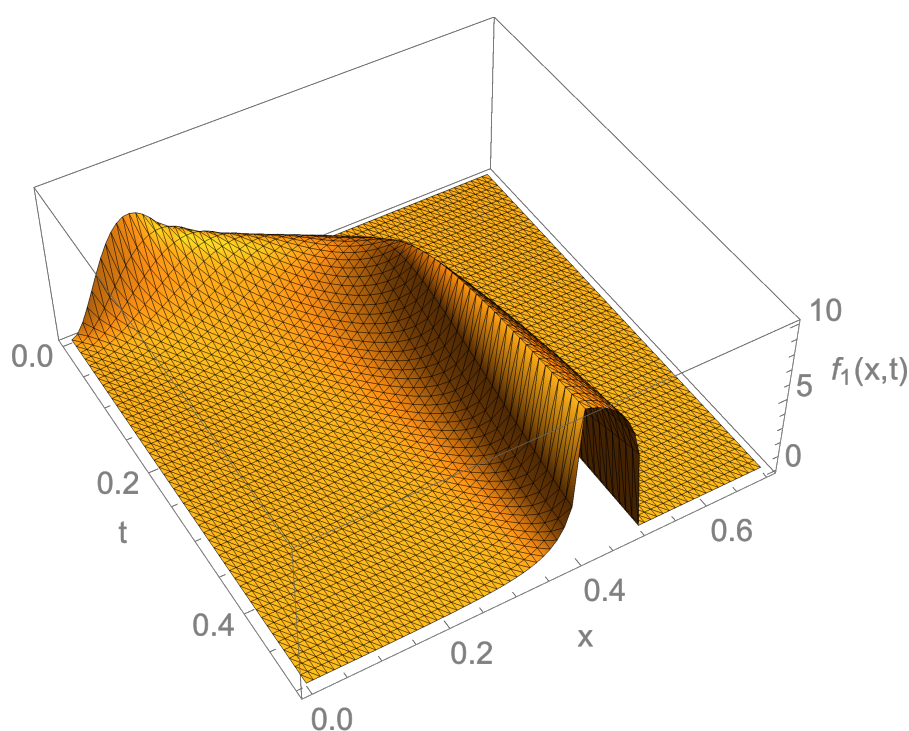


Figure 1: First probability density function, given in (6), of the solution stochastic process, $X(t, \omega)$, in the time interval $[0, 0.5]$.

observed in Figure 2 where the contour plot is represented. We observe also that for larger times the variability tends to vanish. Both graphical representation are in agreement with Figure 3 where the mean and the mean plus/minus a standard deviation is plotted. The mean increase at the first moments and then it stabilizes while the variability also increases but it tends to vanish when the time passes.

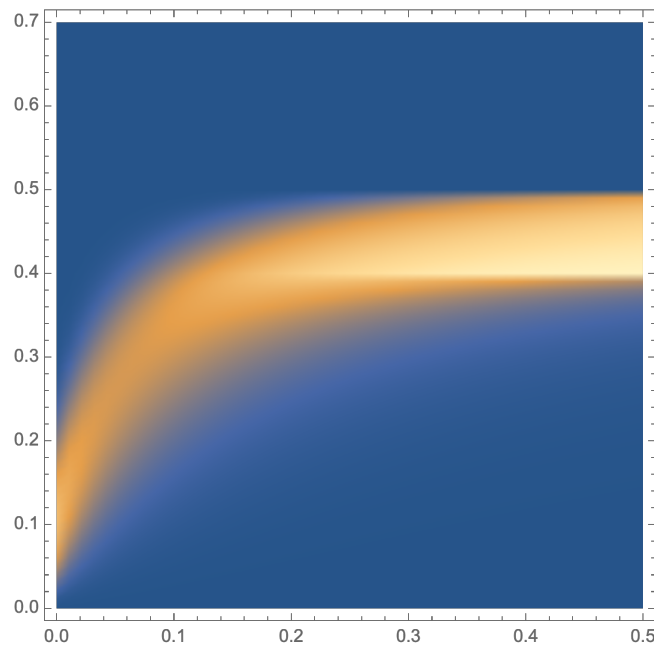


Figure 2: Contour plot of the first probability density function, $f_1(x, t)$, of the solution stochastic process, $X(t, \omega)$, in the time interval $[0, 0.5]$.

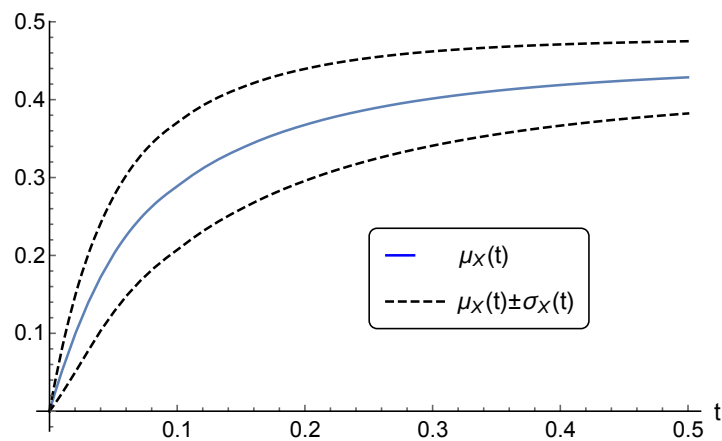


Figure 3: Mean (blue line) and mean plus/minus one standard deviation (black dashed line) of the solution stochastic process, $X(t, \omega)$, in the time interval $[0, 0.5]$.

4 Conclusions

In this work, the first probability density function of a general chemical reaction has been determined. The computation has been carried out by applying the Random Variable Transformation technique. This technique allows us to obtain the joint probability density function of a given random whose comes from mapping another random vector which distribution is assumed known. A numerical example has been performed in order to show the capability of the theoretical result established.

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