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ARTICLE TYPE

Introducing randomness in the analysis of chemical reactions: An analysis based on random differential equations and probability density functions†

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Summary

In this work we consider a particular randomized kinetic model for reaction-deactivation of hydrogen peroxide decomposition. We apply the Random Variable Transformation technique to obtain the first probability density function of the solution stochastic process under general conditions. From the first probability density function, we can obtain fundamental statistical information, such as the mean and the variance of the solution, at every instant time. The transformation considered in the application of the Random Variable Transformation technique is not unique. Then, the first probability density function can take different expressions, although essentially equivalent in terms of computing probabilistic information. To motivate this fact, we consider in our analysis two different mappings. Several numerical examples show the capability of our approach and of the obtained results as well. We show, through simulations, that the choice of the transformation, that permits computing the first probability density function, is a crucial issue regarding the computational time.

KEYWORDS:
Chemical kinetic model, first probability density function, Random Variable Transformation technique, random model

1 | INTRODUCTION

Classically, kinetic equations have been used to describe reaction and deactivation processes in chemistry. Nonlinear differential equations that model these kind of problems depend on two rates, the reaction and deactivation constants. Our analysis is based on a previous contribution [1], where a particular kinetic reaction is considered, the catalysis. Catalysis is a process by which the rate of a chemical reaction is increased. In this process the presence of a substance, called catalyst, accelerates the chemical reaction under study. In reference [1] a particular catalyst is considered, the *catalase*, an enzyme that decomposes hydrogen peroxide to water and oxygen [2]

$$2H_2O_2 \xrightarrow{\text{catalase}} O_2 + H_2O.$$

† Introducing randomness in the analysis of chemical reactions: An analysis based on random differential equations and probability density functions.

[0]**Abbreviations:** IVP, initial value problem; PDF, probability density function; RV, random variable; RVT, Random Variable Transformation technique; SP, stochastic process

This particular chemical reaction can be modeled via the following deterministic initial value problem (IVP)

$$\begin{aligned} \frac{dC_S(t)}{dt} &= -k_R\, C_E(t)\, C_S(t), \quad t > 0, \\ \frac{dC_E(t)}{dt} &= -k_D\, C_E(t)\, C_S(t), \\ C_S(0) &= C_{S_0}, \quad C_E(0) = C_{E_0}, \end{aligned} \tag{1}$$

being, for every time instant t, $C_E(t)$ and $C_S(t)$ the concentration of enzyme and the concentration of hydrogen peroxide, respectively. In IVP (1), k_R and k_D denote the reaction and deactivation rates. After some algebra, and introducing the dimensionless fractional conversion

$$X(t) = (C_{S_0} - C_S(t))/C_{S_0},$$

from the IVP (1) we obtain the following IVP based on a nonlinear differential equation

$$\begin{aligned} \frac{dX(t)}{dt} &= (k_R^* - k_D\, C_{S_0}\, X(t))(1 - X(t)), \quad t > 0, \\ X(0) &= 0, \end{aligned} \tag{2}$$

where $k_R^* = C_{E_0} k_R$. The analysis in this work is based on the IVP (2), whose solution is

$$\begin{cases} X(t) = \dfrac{1 - e^{\left(k_R^* - k_D C_{S_0}\right) t}}{C_{S_0} \frac{k_D}{k_R^*} - e^{\left(k_R^* - k_D C_{S_0}\right) t}} & \text{for } k_D\, C_{S_0} \neq k_R^*, \\ X(t) = 1 - \dfrac{1}{k_R^*\, t + 1} & \text{for } k_D\, C_{S_0} = k_R^*. \end{cases} \tag{3}$$

In practice, the positive parameters, C_{S_0}, k_D and k_R^*, in IVP (2) are usually calculated via experiments, then they have associated a certain measurement error. In addition, there exist some external factors that can affect the system. These facts make more advisable to consider the three aforementioned model parameters as random variables (RVs) rather than deterministic constants. In this contribution, we assume that all the input parameters, $C_{S_0}(\omega)$, $k_D(\omega)$ and $k_R^*(\omega)$, are absolutely continuous RVs defined on a common complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$. For sake of generality, we will consider dependence between the random parameters, being $f_0(C_{S_0}, k_D, k_R^*)$ the joint probability density function (PDF) of the random vector $(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega))$. In this manner, the randomized kinetic model considered in this contribution is a natural randomization of the deterministic one described in IVP (2).

$$\begin{aligned} \frac{dX(t,\omega)}{dt} &= (k_R^*(\omega) - k_D(\omega)\, C_{S_0}(\omega) X(t,\omega))(1 - X(t,\omega)), \quad t > 0, \\ X(0) &= 0. \end{aligned} \tag{4}$$

Therefore, the solution stochastic process (SP) can be directly inferred from (3) as follows

$$X(t,\omega) = \frac{1 - e^{\left(k_R^*(\omega) - k_D(\omega)\, C_{S_0}(\omega)\right) t}}{C_{S_0}(\omega) \frac{k_D(\omega)}{k_R^*(\omega)} - e^{\left(k_R^*(\omega) - k_D(\omega)\, C_{S_0}(\omega)\right) t}}, \qquad \forall \omega \in \Omega, \tag{5}$$

where $\omega \in \Omega$ stands for the sample outcome of the corresponding RV. In the deterministic theory of differential equations, the main goal is the computation of the solution in order to study the behaviour of the dynamical system. In the random framework, as the solution is a SP, the calculation of the main statistical functions (such as the mean and the variance) is also an important objective. If possible, the determination of the 1-PDF, which provides a full probabilistic description of the solution SP, is a more desirable target. In addition, from the 1-PDF the mean and the variance can be calculated from the integration of the 1-PDF. We focus our contribution on the computation of the 1-PDF, $f_1(x,t)$, of $X(t,\omega)$ given in formula (5). With this aim, the Random Variable Transformation (RVT) method will be applied. This technique has been applied by authors in some contributions [3,4]. The RVT method permits to determine the expression of the PDF of a random vector which results from mapping another random vector whose PDF is known. For the sake of completeness, now we state the multidimensional version of the RVT technique that will be extensively applied throughout this paper.

Theorem 1. (Multidimensional version, [5, pp. 24–25]). Let $\mathbf{u}(\omega) = (u_1(\omega), \ldots, u_n(\omega))^\top$ and $\mathbf{v}(\omega) = (v_1(\omega), \ldots, v_n(\omega))^\top$ be two n-dimensional absolutely continuous random vectors. Let $\mathbf{r} : \mathbb{R}^n \to \mathbb{R}^n$ be a one-to-one deterministic transformation of $\mathbf{u}$ into $\mathbf{v}$, i.e., $\mathbf{v} = \mathbf{r}(\mathbf{u})$. Assume that $\mathbf{r}$ is continuous in $\mathbf{u}$ and has continuous partial derivatives with respect to $\mathbf{u}$. Then, if $f_{\mathbf{u}}(\mathbf{u})$ denotes the joint probability density function of the random vector $\mathbf{u}(\omega)$, and $\mathbf{s} = \mathbf{r}^{-1} = (s_1(v_1, \ldots, v_n), \ldots, s_n(v_1, \ldots, v_n))^\top$ represents the inverse mapping of $\mathbf{r} = (r_1(u_1, \ldots, u_n), \ldots, r_n(u_1, \ldots, u_n))^\top$, the joint probability density function of vector $\mathbf{v}(\omega)$ is given by

$$f_{\mathbf{v}}(\mathbf{v}) = f_{\mathbf{u}}\left(\mathbf{s}(\mathbf{v})\right) |J_n|\,, \tag{6}$$

where $|J_n|$ is the absolute value of the Jacobian, which is defined by

$$J_n = \det\left(\frac{\partial \mathbf{s}^\top}{\partial \mathbf{v}}\right) = \det\begin{pmatrix} \frac{\partial s_1(v_1,\ldots,v_n)}{\partial v_1} & \cdots & \frac{\partial s_n(v_1,\ldots,v_n)}{\partial v_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial s_1(v_1,\ldots,v_n)}{\partial v_n} & \cdots & \frac{\partial s_n(v_1,\ldots,v_n)}{\partial v_n} \end{pmatrix}. \tag{7}$$

The paper is organized as follows. In Section 2 we calculate the 1-PDF of the solution SP (5). We compute two different expressions for the 1-PDF, by considering two different mappings in the application of the RVT method. We illustrate the capability of the theoretical established results via some numerical examples in Section 3. In these numerical examples we consider a wide range of distributions for the random input parameters. In addition, we show that the mapping considered in the application of the RVT method affects to the computational time to calculate the 1-PDF. Conclusions are drawn in Section 4.

2 | COMPUTING THE 1-PDF OF THE SOLUTION SP $X(t,\omega)$

In this section two expressions for the 1-PDF of the solution SP $X(t,\omega)$ are computed. These formulas are obtained applying the RVT technique, stated in Theorem 1, considering two different mappings.

2.1 | Obtaining the 1-PDF: first mapping

Let $t > 0$ be fixed, we apply the RVT method with the following choice in Theorem 1

$$\begin{aligned} \mathbf{u}(\omega) &= \left(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega)\right)^\top, \\ \mathbf{v}(\omega) &= (v_1(\omega), v_2(\omega), v_3(\omega))^\top, \end{aligned}$$

where, for each $\omega \in \Omega$, the components of $\mathbf{v}$ are defined by the mapping $\mathbf{r} : \mathbb{R}^3 \to \mathbb{R}^3$

$$\begin{aligned} v_1 &= r_1(C_{S_0}, k_D, k_R^*) = \frac{\left(-1 + e^{(C_{S_0}k_D - k_R^*)t}\right) k_R^*}{C_{S_0}k_D\, e^{(C_{S_0}k_D - k_R^*)t} - k_R^*}, \\ v_2 &= r_2(C_{S_0}, k_D, k_R^*) = k_D, \\ v_3 &= r_3(C_{S_0}, k_D, k_R^*) = k_R^*. \end{aligned}$$

The inverse mapping of the transformation $\mathbf{r}$, denoted by $\mathbf{s}$, is calculated isolating parameters C_{S_0}, k_D and k_R^* above

$$\begin{aligned} C_{S_0} &= s_1(v_1, v_2, v_3) = \frac{tv_3 + v_1 W_k\left(\frac{t(-1+v_1)v_3}{v_1}\, e^{\frac{t(-1+v_1)v_3}{v_1}}\right)}{tv_1v_2}, \\ k_D &= s_2(v_1, v_2, v_3) = v_2, \\ k_R^* &= s_3(v_1, v_2, v_3) = v_3, \end{aligned}$$

where $W_k(x)$ denotes the Lambert function, which is a multivalued function, namely the branches of the inverse relation of the function $w\, e^w$ [6]. That is, for each integer k, there is one branch, $W_k(z)$, with the following property: if z and w are any complex numbers, then

$$w\, e^w = z \text{ holds if and only if } w = W_k(z), \text{ for some integer } k.$$

W_0 is known as the principal branch, and it gives the principal solution for w in $z = w\, e^w$. In the set of real numbers, two branches W_0 and W_{-1} are sufficient. Then, the system has two solutions, considering $W_0(x)$ and $W_{-1}(x)$, see Figure 1. The Jacobian of the mapping $\mathbf{s}$, for each $k \in \{0, 1\}$ is

$$J_3 = \frac{1}{t(-1+v_1)v_1^2v_2}\left(v_1 - \frac{v_1 + t(-1+v_1)v_3}{1 + W_k\left(\frac{t(-1+v_1)v_3}{v_1}\, e^{\frac{t(-1+v_1)v_3}{v_1}}\right)}\right).$$

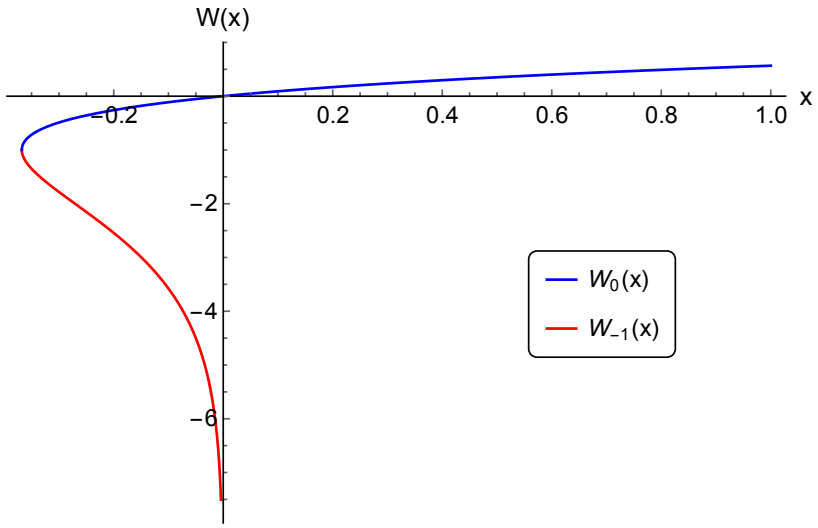

FIGURE 1 Lambert function in the set of real numbers. Red line: $W_{-1}(x)$. Blue line $W_0(x)$.

Therefore, applying RVT method, the PDF of the random vector $\mathbf{v}(\omega)$ is obtained in terms of the joint PDF, $f_0(C_{S_0}, k_D, k_R)$, of the random input parameters $\left(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega)\right)$

$$f_{\mathbf{v}}(v_1,v_2,v_3) = f_0\left(\frac{tv_3 + v_1 W_k\left(\frac{e^{\frac{t(-1+v_1)v_3}{v_1}}}{v_1}\right)}{tv_1v_2}, v_2, v_3\right)\left|\frac{1}{t(-1+v_1)v_1^2v_2}\left(v_1 - \frac{v_1 + t(-1+v_1)v_3}{1+W_k\left(\frac{e^{\frac{t(-1+v_1)v_3}{v_1}}}{v_1}\right)}\right)\right|.$$

Marginalizing with respect to $v_2(\omega) = k_D(\omega)$ and $v_3(\omega) = k_R^*(\omega)$, and taking $t > 0$ arbitrary, we obtain the 1-PDF of the solution SP $X(t,\omega)$, which depends on $k \in \{0,1\}$,

$$f^1_{1,k}(x,t) = \int_0^{+\infty}\int_0^{+\infty} f_0\left(\frac{tk_R^* + xW_k\left(\frac{e^{\frac{t(-1+x)k_R^*}{x}}}{x}\right)}{t\,x\,k_D}, k_D, k_R^*\right)\left|\frac{1}{t(-1+x)x^2k_D}\left(x - \frac{x + t(-1+x)k_R^*}{1+W_k\left(\frac{e^{\frac{t(-1+x)k_R^*}{x}}}{x}\right)}\right)\right| \mathrm{d}k_D\,\mathrm{d}k_R^*. \tag{8}$$

As we have previously indicated, the density function obtained depends on k, then the 1-PDF $f^1_1(x,t)$ shall be split into two pieces, $f^1_{1,0}(x,t)$ and $f^1_{1,-1}(x,t)$, corresponding to the contribution of W_0 and W_{-1}, respectively. Then, the complete 1-PDF must be expressed by

$$f^1_1(x,t) = f^1_{1,0}(x,t) + f^1_{1,-1}(x,t). \tag{9}$$

Notice that for each $t > 0$, $f^1_{1,0}(x,t)$ and $f^1_{1,-1}(x,t)$ are not separately PDF.

2.2 | Obtaining the 1-PDF: second mapping

Given the complexity of the expression of the 1-PDF obtained in Eq. (8) and Eq. (9), in this subsection, we consider a different mapping. The chosen transformation it is more complex than the previous one, but we obtain a simpler formula for the 1-PDF of the solution SP. Let $t > 0$ be fixed, we apply Theorem 1 with

$$\mathbf{u}(\omega) = \left(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega)\right)^\top,$$
$$\mathbf{v}(\omega) = \left(v_1(\omega), v_2(\omega), v_3(\omega)\right)^\top.$$

For each $\omega \in \Omega$, we define the mapping $\mathbf{r} : \mathbb{R}^3 \to \mathbb{R}^3$

$$\begin{aligned} v_1 &= r_1(C_{S_0}, k_D, k_R^*) = \frac{\left(-1 + e^{(C_{S_0} k_D - k_R^*)t}\right) k_R^*}{C_{S_0} k_D \, e^{(C_{S_0} k_D - k_R^*)t} - k_R^*}, \\ v_2 &= r_2(C_{S_0}, k_D, k_R^*) = C_{S_0} k_D - k_R^*, \\ v_3 &= r_3(C_{S_0}, k_D, k_R^*) = k_D. \end{aligned}$$

The inverse mapping of the transformation $\mathbf{r}$, denoted by $\mathbf{s}$, and the Jacobian are given by

$$\begin{aligned} C_{S_0} &= s_1(v_1, v_2, v_3) = -\frac{(-1 + e^{tv_2} + v_1)\, v_2}{(-1 + e^{tv_2})\,(-1 + v_1) v_3}, \\ k_D &= s_2(v_1, v_2, v_3) = v_3, \\ k_R^* &= s_3(v_1, v_2, v_3) = -\frac{e^{tv_2}\, v_1 v_2}{(-1 + e^{tv_2})\,(-1 + v_1)}, \end{aligned}$$

$$J_3 = -\frac{e^{tv_2}\, v_2}{(-1 + e^{tv_2})\,(-1 + v_1)^2 v_3}.$$

Applying RVT method, Theorem (1), we obtain the joint PDF of the random vector $(v_1(\omega), v_2(\omega), v_3(\omega))$ in terms of $f_0(C_{S_0}, k_D, k_R)$, which is assumed known,

$$f_{\mathbf{v}}(v_1, v_2, v_3) = f_0\left(-\frac{\left(-1 + e^{tv_2} + v_1\right) v_2}{(-1 + e^{tv_2})\,(-1 + v_1) v_3}, v_3, -\frac{e^{tv_2}\, v_1 v_2}{(-1 + e^{tv_2})\,(-1 + v_1)}\right) \left| -\frac{e^{tv_2}\, v_2}{(-1 + e^{tv_2})\,(-1 + v_1)^2 v_3} \right|.$$

Finally, as we are interested in computing the PDF of $v_1(\omega) = X(t, \omega)$, we take the marginal with respect to $v_2(\omega)$ and $v_3(\omega)$, and taking $t > 0$ arbitrary, we obtain the 1-PDF of the solution SP $X(t, \omega)$

$$f_1^2(x, t) = \int_{-\infty}^{+\infty} \int_{0}^{+\infty} f_0\left(-\frac{\left(-1 + e^{ta} + x\right) a}{(-1 + e^{ta})\,(-1 + x) k_D}, k_D, -\frac{e^{ta}\, x\, a}{(-1 + e^{ta})\,(-1 + x)}\right) \left| \frac{e^{ta}\, a}{(-1 + e^{ta})\,(-1 + x)^2 k_D} \right| \mathrm{d}k_D \, \mathrm{d}a. \tag{10}$$

3 | NUMERICAL EXAMPLES

In this section, we show two examples where the theoretical results obtained in Section 2 are applied. In the first example statistical independence between the RVs is assumed, thus the joint PDF of the random vector $(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega))$ can be written as the product of the marginals

$$f_0(C_{S_0}, k_D, k_R^*) = f_{C_{S_0}}(C_{S_0}) f_{k_D}(k_D) f_{k_R^*}(k_R^*).$$

In the second example, we assume dependent RVs with a Gaussian distribution. In both examples we compute the 1-PDF of the solution SP, $X(t, \omega)$, the mean and the variance with the both mappings indicated in Section 2. The mean and the variance are fundamental statistical functions that can be directly calculated from the 1-PDF. Let $f_1(x, t)$ be a given 1-PDF of a SP, $X(t, \omega)$, the mean and the variance in every time instant t are defined by

$$\begin{aligned} \mu_X(t) &= \mathbb{E}\left[X(t, \omega)\right] = \int_{\mathbb{R}} x\, f_1(x, t) \mathrm{d}x, \\ \sigma_X^2(t) &= \mathbb{E}\left[X(t, \omega)^2\right] - \mathbb{E}\left[X(t, \omega)\right]^2 = \int_{\mathbb{R}} x^2\, f_1(x, t) \mathrm{d}x - \mu_X(t). \end{aligned} \tag{11}$$

In both examples we show how the chosen transformation significantly affects the computational time needed to calculate the 1-PDF.

3.1 | Numerical Example 1. Independent RVs

We consider the randomized kinetic model described in (4) and we chose the following independent probability distributions for the input parameters

- $C_{S_0}(\omega)$ has a truncated Gaussian distribution with mean 0.01 and standard deviation 0.005 on the interval $T = [0, 0.015]$, i.e., $C_{S_0}(\omega) \sim N_T(0.01, 0.005)$. This selection is motived by the previous contribution [1], where the deterministic kinetic model is constructed under the condition $0 < C_{S_0} < 0.015$.
- $k_D(\omega)$ has a Gamma distribution with parameters 20 and 15, i.e., $k_D(\omega) \sim G(20, 15)$.
- $k_R^*(\omega)$ follows a Beta distribution with parameters 15 and 20, i.e., $k_R^*(\omega) \sim B(15, 20)$.

We have chosen the distributions of the RVs $k_D(\omega)$ and $k_R^*(\omega)$ taking into account only the positiveness restriction of both parameters. All the computations have been carried out using the Mathematica® software. We have calculated the 1-PDF of the solution SP, $X(t,\omega)$, with the both mapping, $f_1^1(x,t)$ and $f_1^2(x,t)$ for different time instants $t \in \{0.1, 0.2, \ldots, 1\}$. In Figure 2 we observe that the 1-PDF is *practically* the same in both cases. Although theoretically $f_1^1(x,t)$ and $f_1^2(x,t)$ match, due to numerical errors they slightly differ. We use the L^1-norm to measure, for each t fixed, this difference

$$e_t = \int_{\mathbb{R}} |f_1^1(x,t) - f_1^2(x,t)| \mathrm{d}x. \tag{12}$$

In Table 1 we collect the values of this norm at different time instants. On the other hand, in Figure 2 we observe that both the mean and the variability of the distribution increase over the time. This behaviour is in agreement with the expectation and the variance plotted in Figure 3. The computational time needed for the calculation of the 1-PDFs, for each time instant, is shown in Figure 4. We observe that the computational time is approximately 26 times greater for the first mapping than for the second one, given the complexity of the expression of the 1-PDF obtained in equations 8 and 9 compared with the formula obtained in (10). Notice that, for the calculation of the involved integrals we have used the command **NIntegrate** and the "QuasiMonteCarloMethod" with "MaxPoints→200 000", implemented in Mathematica®.

t	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
e_t	0.023889	0.025619	0.017179	0.016514	0.017891	0.012177	0.019279	0.013842	0.017829	0.017866

TABLE 1 Difference between the 1-PDFs, $f_1^1(x,t)$ and $f_1^2(x,t)$, for different time instants $t \in \{0.1, 0.2, \ldots, 1\}$. This difference has been measured via the L^1-norm defined in (12). Numerical Example 3.1.

3.2 | Numerical Example 2. Dependent RVs

In contrast to Example 3.1, in this numerical example we consider that $C_{S_0}(\omega)$, $k_D(\omega)$ and $k_R^*(\omega)$ are dependent random variables. We assume that the random vector $(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega))$ has a truncated Gaussian distribution on the region $T = [0, 0.015] \times [0, 1] \times [290, 310]$, $(C_{S_0}(\omega), k_D(\omega), k_R^*(\omega)) \sim N_T(\mu, \Sigma)$, being μ and Σ the mean and the variance-covariance matrix, respectively, given by

$$\mu = \begin{pmatrix} 0.01 \\ 0.5 \\ 300 \end{pmatrix}, \qquad \Sigma = \frac{1}{200} \begin{pmatrix} 1 & 2 & 1 \\ 2 & 10 & 1.4 \\ 1 & 1.4 & 200 \end{pmatrix}.$$

In Figure 5 the 1-PDFs of the solution SP, $X(t,\omega)$, for each mapping, have been plotted. This graphical representation has been done for different time instants $t \in \{0.1, 0.2, \ldots, 1\}$. We observe that, as in the previous example, both 1-PDF *practically* match, being the longer the time, the greater the expectation and the variability. As in Example 3.1, to highlight the numerical differences in the calculation of both 1-PDFs, $f_1^1(x,t)$ and $f_1^2(x,t)$, in Table 2 we show the values of the L^1-norm given in (12) at different time instants $t \in \{0.1, 0.2, \ldots, 1\}$. In this case, the differences are smaller perhaps because of the probabilistic dependence assumed for model parameters. The behaviour agrees with the expectation and the variance represented in Figure 6. The computational time needed for the calculation of the 1-PDFs, for each time instant, is shown in Figure 7. In this case, the computational time, in seconds, to compute the 1-PDF with the first mapping is also approximately 26 times greater than with the second mapping considered in Section 2. To calculate the integrals in formulas (8) and (10), we also have used the command **NIntegrate** and the "QuasiMonteCarloMethod" with "MaxPoints→200 000", implemented in Mathematica® software.

t	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
e_t	0.000668	0.000574	0.000391	0.000504	0.000566	0.000395	0.000367	0.000276	0.000433	0.000417

TABLE 2 Difference between the 1-PDFs $f_1^1(x,t)$ and $f_1^2(x,t)$ for different time instants $t \in \{0.1, 0.2, \ldots, 1\}$, this error has been calculated from formula (12). Numerical Example 3.2.

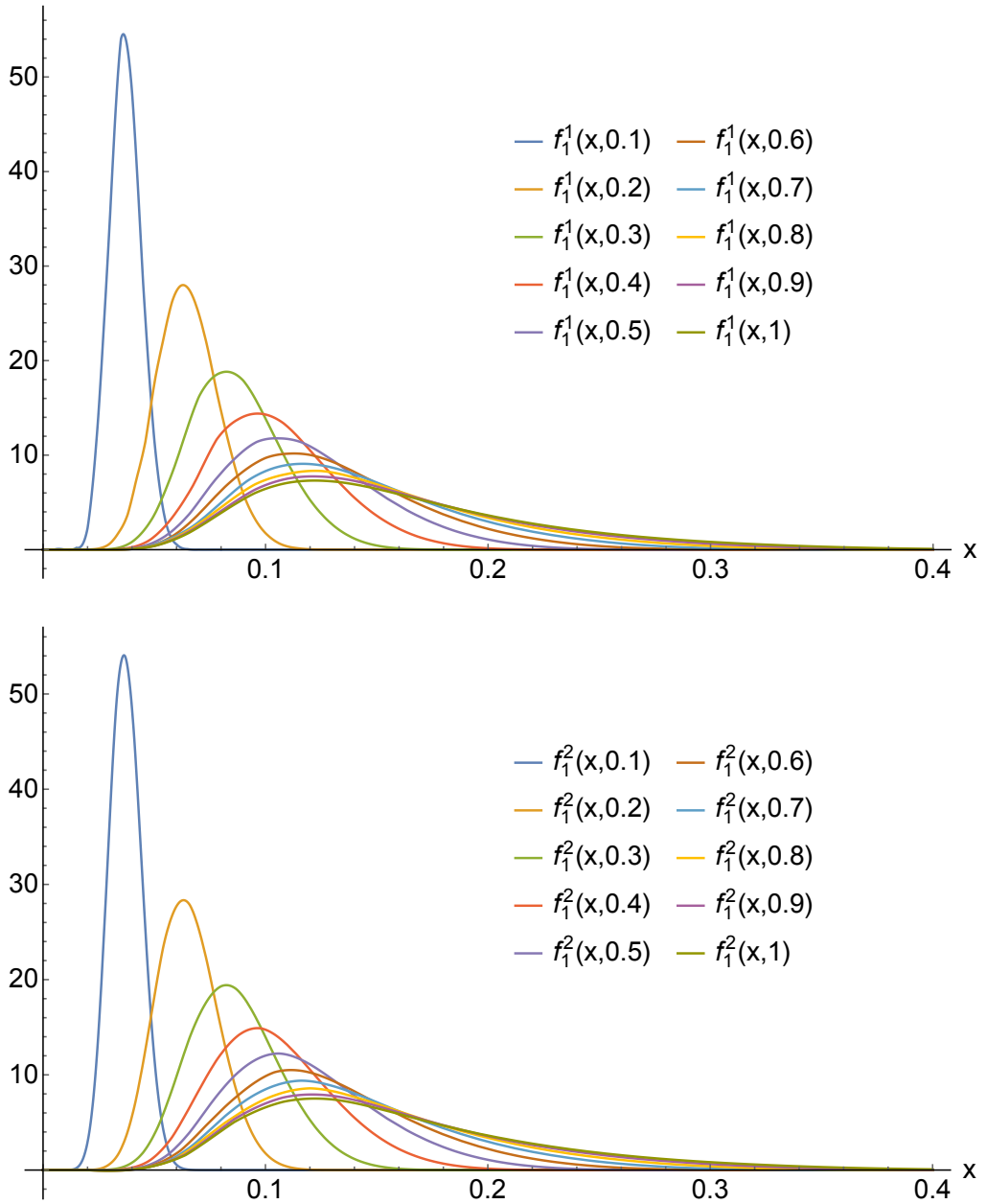

FIGURE 2 1-PDF of the solution SP, $X(t,\omega)$ for different time instants $t \in \{0.1, 0.2, \ldots, 1\}$. Top: 1-PDF calculated from expressions (8) and (9) (First mapping); Bottom: 1-PDF calculated from expression (10) (Second mapping). Numerical Example 3.1

4 | CONCLUSIONS

In this paper we have obtained a full probabilistic description of the solution stochastic process of a particular randomized kinetic model. The analysis have been done via the computation of the first probability density function of the solution stochastic process. We have obtained two equivalent expressions for the first probability density function. With this aim we have applied the random variable transformation technique to two different mappings. Despite both representations of the first probability density functions are valid, the computations reveal that there are significant differences regarding the computational time required to carry out calculations from both expressions. Therefore, the choice of the mapping required to apply the Random Variable Transformation technique to compute the first probability density function is a key point to save computational time in the mathematical expressions where the first probability density function is involved.

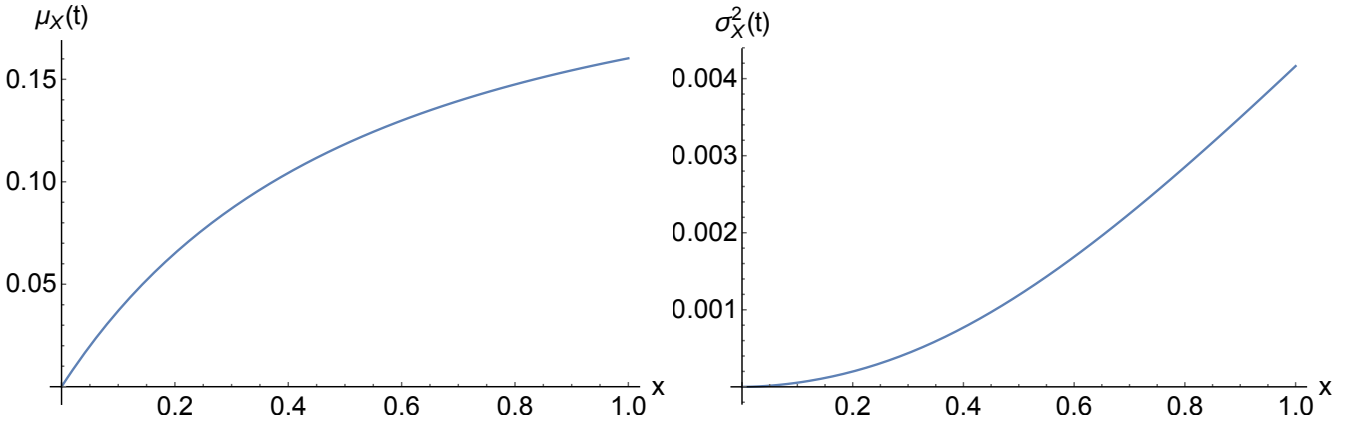

FIGURE 3 Expectation (left), $\mu_X(t)$, and variance (right), $\sigma^2_X(t)$, of the solution SP, $X(t,\omega)$, in the time interval $[0,1]$. Numerical Example 3.1

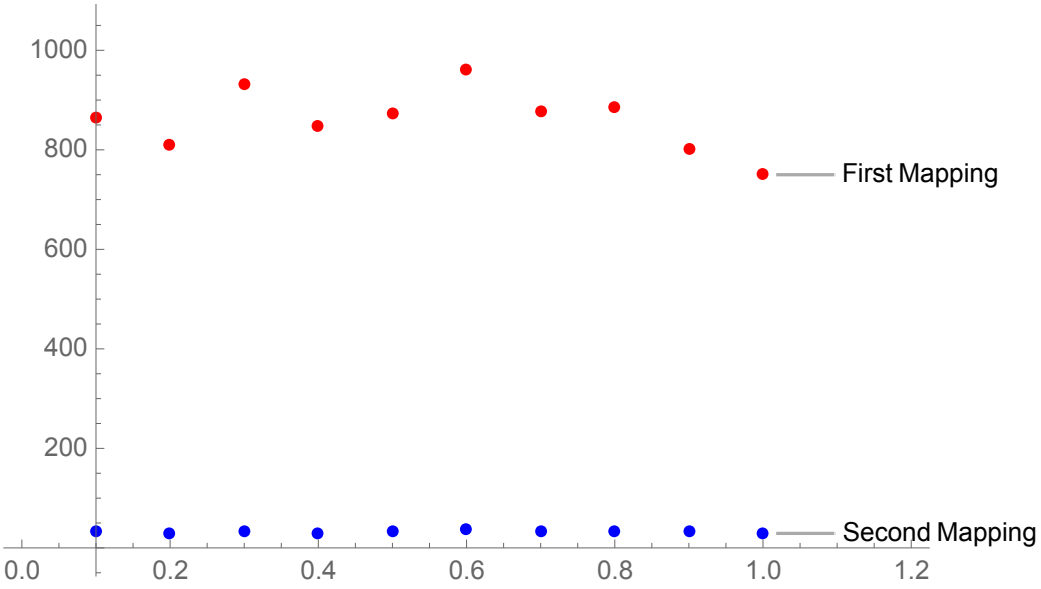

FIGURE 4 Computational time (in seconds) needed for the calculation of the 1-PDFs, first mapping in red colour and second mapping in blue colour, for every time instant $t \in \{0.1, 0.2, \ldots, 1\}$. Numerical Example 3.1

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Removed by authors for review process

Author contributions

All authors contributed equally to this work.

Conflict of interest

The authors declare no potential conflict of interests.

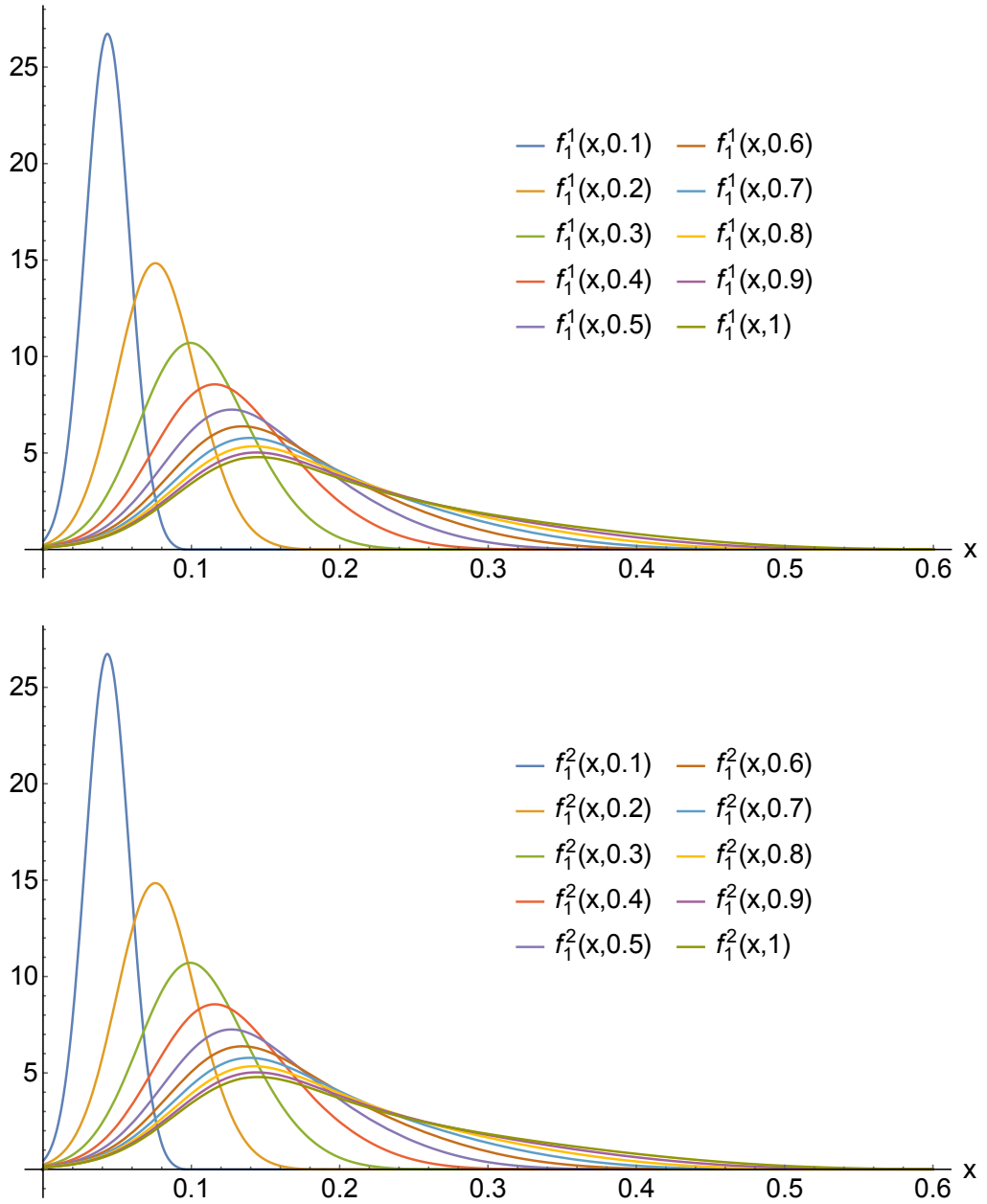

FIGURE 5 1-PDF of the solution SP, $X(t,\omega)$, for different time instants $t \in \{0.1, 0.2, \ldots, 1\}$. Top: 1-PDF calculated from expressions (8) and (9) (First mapping); Bottom: 1-PDF calculated from expression (10) (Second mapping). Numerical Example 3.2

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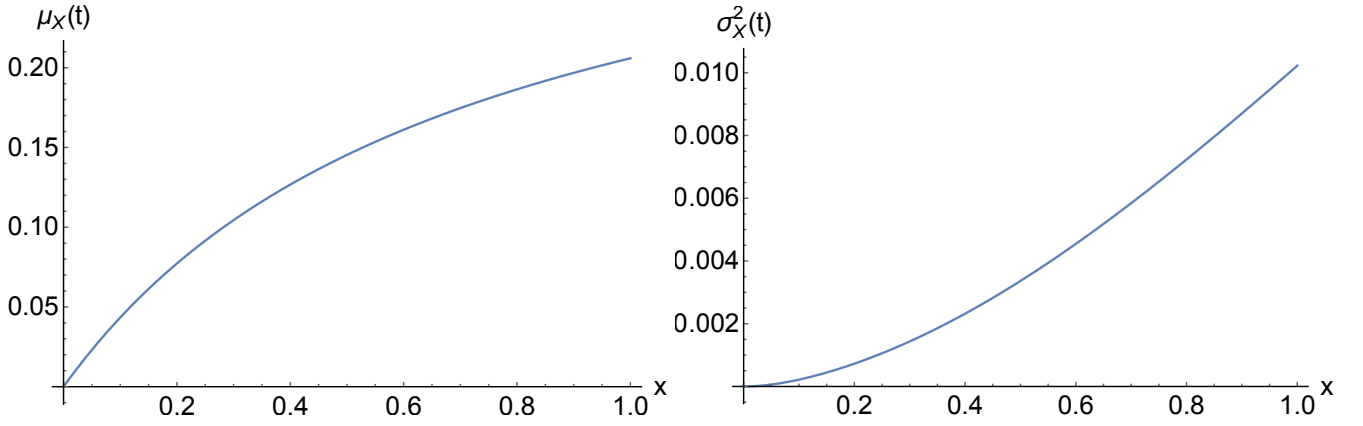

FIGURE 6 Expectation (left), $\mu_X(t)$, and variance (right), $\sigma_X^2(t)$, of the solution SP, $X(t,\omega)$, in the time interval $[0,1]$. Numerical Example 3.2

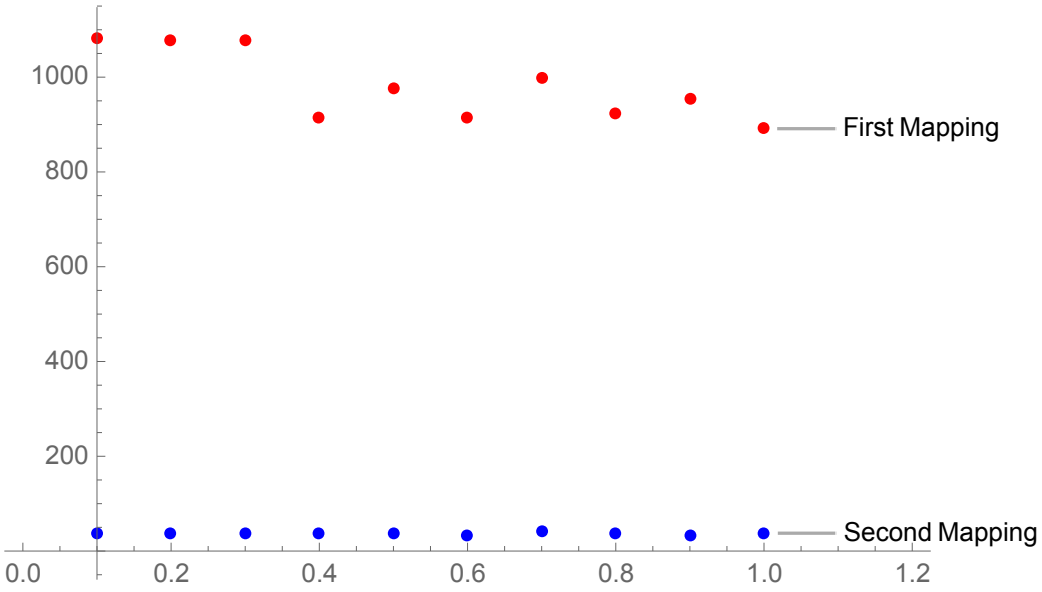

FIGURE 7 Computational time (in seconds) needed for the calculation of the 1-PDFs, first mapping in red colour and second mapping in blue colour, for every time instant $t \in \{0.1, 0.2, \ldots, 1\}$. Numerical Example 3.2

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