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The measurement problem on classical diffusion process: inverse method on stochastic processes

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Abstract

In a high number of diffusive systems, measures are processed to calculate material parameters such as diffusion coefficients, or to verify the accuracy of mathematical models. However, the precision of the parameter determination or of the model relevance depends on the location of the measure itself. The aim of this paper is first to analyse, for a mono-dimensional system, the precision of the measure in relation with its location by an inverse problem algorithm and secondly to examine the physical meaning of the results.

Statistical mechanic considerations show that, passing over a time–distance criterion, measurement becomes uncertain whatever the initial conditions. The criterion proves that this chaotic mode is related to the production of anti-entropy at a mesoscopique scale that is in violation to quantum theory about measurement.

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1. Parabolic differential equations

The parabolic differential equations (PDEs) are ruled by the general following expression:

$$\frac{\partial \mathbf{u}}{\partial t} - \sum_{i,j} \frac{\partial}{\partial x_i} a_{i,j} \frac{\partial}{\partial x_j} \mathbf{u} = f(\mathbf{x}, t) \quad (1)$$

where $(\mathbf{x}, t) \in \Omega \times \mathbb{R}_+$, Ω an open set of \mathbb{R}^n . These equations characterise a high number of transport phenomena met in materials science such as atom-vacancy transport, Ohm law. . . [1,2]. Diffusion processes can be derived from probabilistic considerations meaning that diffusion laws are stochastic in nature. Asymptotic considerations will lead to the suppression of this stochastic aspect in order to obtain deterministic equation (1). In other terms microscopic fluctuations are “removed” (by averaging) to formulate the macroscopic system. However we might wonder what are the mathematical properties of the solutions given by Eq. (1) when noisy measures of \mathbf{u} are carried out on the system (\mathbf{x}, t) to estimate the physical parameters $a_{i,j}$. The second question is to know weather the stochastic aspects of the microscopic system emerge.

2. Properties of the mono-dimensional diffusion equation

We shall limit this paper to the study of the simple mono-dimensional Fick equation that reduces Eq. (1) to

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$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2} \quad (2)$$

where $C(x, t)$ is the concentration of the diffusion species, at depth x , after a diffusion time t and D is the diffusion coefficient considered independent of composition. The application of the boundary conditions to Eq. (2): $C(0, 0) = C_0 \delta_0$ and $\Omega =] - \infty, +\infty[$, corresponding to a sandwich of particles that diffuse in an infinite media leads to the well-known solution:

$$C(x, t, C_0, D) = \frac{C_0}{2\sqrt{\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad (3)$$

This solution is a Gaussian probability density function (PDF), at a multiplying constant factor, with zero mean and $\sigma(t) = \sqrt{2Dt}$ standard deviation. According to the properties of the Gaussian PDF, 68% of the diffused mass belong to the interval $[-\sigma(t), \sigma(t)]$, 95% in $[-2\sigma(t), 2\sigma(t)] \dots$. This clearly means that the value $\Psi(P)\sigma(t)$ with

$$\int_{-\Psi(P)}^{\Psi(P)} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx = P \quad (4)$$

can be seen as a mean diffusion front length and therefore $L(P) = \Psi(P)\sqrt{2Dt}$ is a characteristic length of the diffusion process. The question that arises is how to choose $L(P)$, i.e. P to obtain the most relevant characteristic length?

3. Characterisation of the relevance of the measure by an inverse method

The main problem is to find the depth x (and $-x$ since the concentration profile is symmetrical versus $x = 0$) where information on the diffusion process is the most relevant. The expression “*x position is more relevant*” is mathematically formulated and studied by the inverse problem methodology. Concentration that theoretically obeys Eq. (2), measured at the position x with an experimental noise that follows a Gaussian PDF $B(t, x)$ is given by

$$C_M(x, t, C_0, D) = C(x, t, C_0, D) + B(t, x) \quad (5)$$

We postulate that the best position x is the position that allows us to determine the diffusion coefficient D of Eq. (2) with utmost precision. Given a measure at the position x noted $C_M(x, t, C_0, D)$ that follows Eq. (5), a L^2 norm $N(x, T, C_0, D)$ is defined as

$$N(x, T, C_0, D) = \int_{t=0}^T (C_M(x, t, C_0, D) - C(x, t, C_0, D))^2 dt \quad (6)$$

where T is the time scale at which the diffusion is observed.

Eq. (6) cannot be transformed into a linear equation and will only be computed via non-linear optimisation procedure. In this procedure, the regression coefficients are estimated by searching the values of D that minimises the residual variance (sum of squared residuals) around the best fitting line. Any deviation of an observed score from a predicted one signifies a lack of accuracy of our prediction, meaning that position x is not optimal. When this function reaches its minimum, then an estimation of D noted $D_M(x, T)$ is obtained, which corresponds to the measure at position x for a final diffusion time T . Non-linear estimation is processed by a very efficient algorithm (quasi-Newton) that approximates the second-order derivatives of the loss function to guide the search for the minimum.

The best position, x_{opt} , is the one that minimises the variation of $D_M(x, T)$ characterised by the standard deviation $\sigma_D(x, T)$. To estimate this standard deviation, n measures are carried out, which allows us to calculate n values of $D_M(x, T)$ and then the estimation of $\sigma_D(x, T)$ is noted $\sigma_D^n(x, T)$:

$$x_{\text{opt}}(T) = \min\{\sigma_D(x, T), x \in X\} \quad (7)$$

where X is the length of observation of the diffusion process.

Let us now analyse more precisely the influence of the x position on the error made in the determination of the $D_M(x, T)$ values. At $x = 0$, the concentration $C(0, t, C_0, D)$ will always be maximal whatever the diffusion time t . Theoretically, the diffusion problem given by Eq. (2) contains only one parameter and only one measure at position x is required to determine $D_M(x, T)$. Then it becomes logical to think that information on the diffusion equation will be more relevant at $x = 0$. To verify the accuracy of Eq. (3) to represent the physical process, measurements at different x values are needed. However, we might wonder about the influence of positions when $x > 0$ on the $D_M(x, T)$ precision. Precision depends on the final diffusion time T : the higher T , the better the precision on $D_M(x, T)$. Indeed, when increasing time,

the diffusion process enlarges the Gaussian shape of the diffusion profile given by Eq. (3). As a consequence, Eq. (6) is estimated on a wider range of data and the $D_M(x, T)$ variance diminishes. However, for T we can admit that precision will decrease with x as the concentration decreases. As the decrease rate is not known, simulations are required.

Theorem 1. Under the Gauss Markov hypothesis [3], $D_M(x, t)$ follows a Gaussian law. As a consequence, the standard deviation $\sigma_D(x, t)$ becomes the best estimator of the dispersion of the $D_M(x, t)$ values.

We shall illustrate this fact by a Monte Carlo simulation. We retain the following values $D = 1$, $T = 1$, $B(t, x)$ follows a Gaussian law with zero mean and 0.0001 standard deviation (noted $B(t, x) = 0.0001$), $C_0 = 100$, $x \in X$ where

$$X = \{0, 0.5\sqrt{2DT}, \dots, 2\sqrt{2DT}, 2.5\sqrt{2DT}\} = \{0, 0.5\sqrt{2}, \dots, 2\sqrt{2}, 2.5\sqrt{2}\} \quad \text{and} \quad n = 10^5$$

Fig. 1 represents the variation of the concentration with and without noise at time $T = 1$, $T = 2$ and $T = 4$, and Fig. 2 the $D_M(x, T)$ histograms with different x values.

Three remarks have to be made:

- (i) The analysis of variance is proceeded to test if Gaussian mean $D_M(x, t) \forall x \in X$, is equal to unity (the real value is $D = 1$). The Fischer test gives the critical value $p = 0.8$ meaning that all mean values equal the real unknown diffusion coefficient $D = 1$ whatever the x position: no bias is introduced by our inverse method.

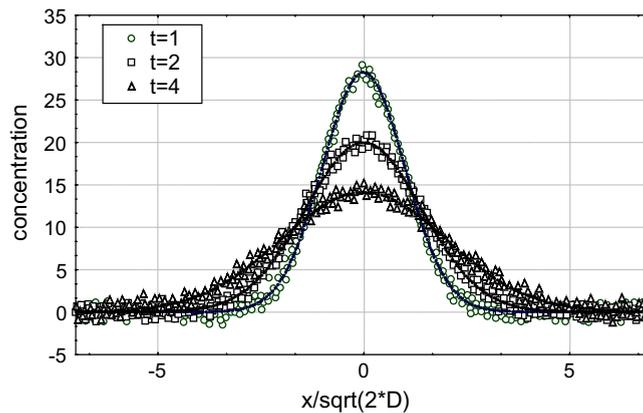


Fig. 1. Concentration profile with (standard deviation of the noise: 1) and without noise (lines) for three different diffusion times ($t = 1, 2, 4$).

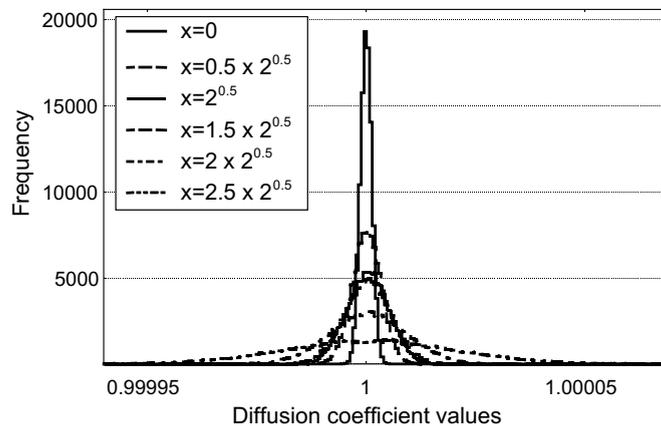


Fig. 2. Variation of the diffusion coefficient estimation for different sensor locations.

- (ii) For all histograms Shapiro–Wilk tests show that $D_M(x, T)$ Gaussian PDF are never rejected at the critical value $p = 0.4$ which illustrates Theorem 1.
- (iii) As the Gaussian PDF is never rejected, standard deviation is the best estimator of the $D_M(x, t)$ dispersion. Histograms in Fig. 2 show that dispersion increases with depth x . Over the critical value $x = \sqrt{2DT}$ ($x = 2^{0.5}$, $T = 1, D = 1$) dispersion seems to increase more rapidly with x .

We then analyse the influence of both the noise $B(t, x)$ and the depth x on the dispersion by plotting in Fig. 3 $\sigma_D^{n=10000}(x, T)$ versus x for four noises $B(t, x) \in \{1.10^{-4}, 2.10^{-4}, 8.10^{-4}, 1610^{-4}\}$ and four values of T , $T \in \{1, 4, 8, 16\}$. The following remarks can be made:

- (i) Precision always decreases as x increases.
- (ii) All curves present an inflexion point noted \hat{x} .
- (iii) Precision decreases with increasing noise, but the noise amplitude leaves the position of \hat{x} unchanged for a given diffusion time.
- (iv) The inflexion point, \hat{x} , increases with the diffusion time leaving $\sigma_D(\hat{x}, T)$ unchanged for a given diffusion time T .

As the diffusion front follows the law $\Psi(P)\sigma(t)$ (cf. Eq. (4)), the x depth may be normalised by $\tilde{x} = x/\sqrt{2DT}$ to obtain a characteristic curve. In the same way, according to the usual laws of the regression statistics [3], we can admit that $\sigma_D(x, T) \propto \sqrt{\text{var}[B(t, x)]}$, then standard deviations are normalised by $\tilde{\sigma}_D(x, T) = \sigma_D(x, T)/\sqrt{\text{var}[B(t, x)]}$.

$\tilde{\sigma}_D^{n=10000}(\tilde{x}, T)$ is plotted in Fig. 4 versus \tilde{x} : the reduced curves presented in Fig. 3 superpose very well, proving that our normalisation is correct. As can be observed, there is an inflexion point \hat{x} where derivative is null: $\partial^2 \tilde{\sigma}_D(x, T)/\partial \tilde{x}^2 = 0$. This point is characteristic: for lower values the precision will decrease lower and lower $\partial^2 \tilde{\sigma}_D(x, T)/\partial \tilde{x}^2 < 0$ and for $x > \hat{x}$ the error will rise exponentially ($\partial^2 \tilde{\sigma}_D(x, T)/\partial \tilde{x}^2 > 0$). This clearly means that \hat{x} is a pivot point after which the information on D coefficient will decrease dramatically. The most surprising and interesting result is that this point is independent of the noise amplitude. When small perturbations are introduced in the measure of the diffusion process, it will grow with the same kinetic movement leading to a loss in information, i.e. the knowledge of the physical parameter. In Chaos theory, this point is a bifurcation after which non-deterministic chaos emerges. To determine precisely the \hat{x} co-ordinate, an iterative algorithm is implemented. As could be observed in Fig. 3, the finite number of simulations, n , involves a noise on the $\sigma_D^n(\Psi(P)\sqrt{2Dt}, T)$ determination which does not allow us to determine \hat{x} precisely. At first a cubic weighted splines fitting curve is used to interpolate the data. Secondly, this fitting curve is differentiated giving a confidence interval for \hat{x} . Thirdly, we double the n value and calculate $\sigma_D^{2n}(\Psi(P)\sqrt{2Dt}, T)$ until all simulated values are statistically different (thanks to a Levene test). Then a new restricted interval X^1 , $\hat{x} \in X^1 \subset X$, is built and so on. This techniques allows us to find the value:

$$\hat{x} = 1.0001_{\pm 0.0001} \sqrt{2Dt} \cong \sqrt{2Dt}$$

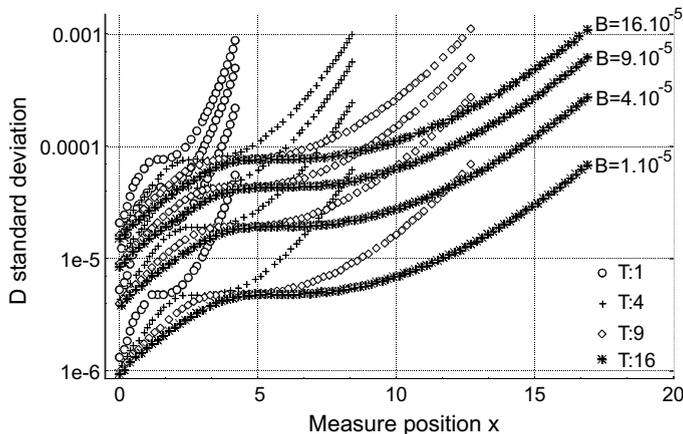


Fig. 3. Values of $\tilde{\sigma}_D(x, T)$ versus measured depth x for four Gaussian noises B and four values of diffusion time T .

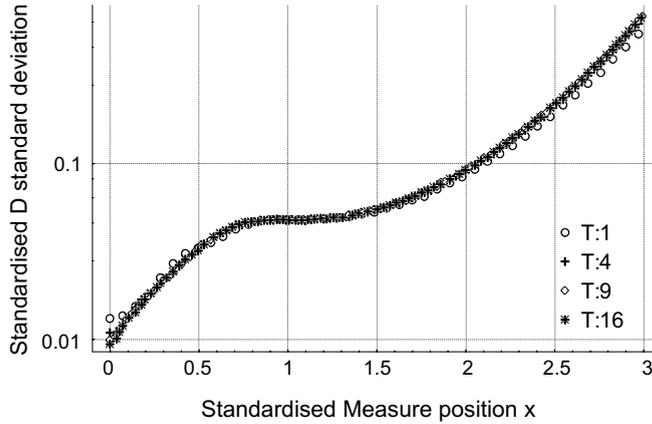


Fig. 4. Normalisation of Fig. 3; values of $\bar{\sigma}_D(x, T)$ versus the standardised measure depth \bar{x} for four Gaussian noises B and four values of diffusion time T .

4. Physical interpretation of the threshold \hat{x}

We have proved that a complex macroscopic diffusive system (probability to find particles) can be partitioned into a summation of elementary Gaussian distributions taken at the scale Δx [5].

To find a physical interpretation for the threshold \hat{x} , we suppose that all systems are governed by Eq. (2). This equation could be seen as modelling the diffusion in all the media and therefore is an intrinsic physical property of the system.

Let us now consider three adjacent cells x_1, x_2, x_3 we call PDE cells, distant from $\sqrt{2Dt} = \Delta x$. Fig. 5 represents the Gaussian concentration when $\sqrt{2Dt} = \Delta x$. Each elementary cell diffuses on the adjacent intervals (a probability calculus shows that 24% of the mass is diffused on adjacent cells). If we consider particles from the cell x_2 , no particle of the adjacent PDE cells x_1 or x_3 are present at $t = 0$, and then the x_2 particles will diffuse into the cells x_1, x_3 with respect to time. Let us now formulate the configuration entropy of the particles on each PDE cell x_1, x_3 . Entropy is null at the onset (no particle) and increases thanks to diffusion. Let now introduce the mathematical formalism of entropy evaluation. Based on the statistical thermodynamics [4], the cell PDE will be divided into k microsystems with δx length, ($\Delta x = k\delta x, k \gg 1$) called the sub-PDE cells. On each sub-PDE cell, we will calculate the probability for a particle of the adjacent cell to be present. The time dependant probability of the presence of particles localised on an interval of length δx , ($\delta x \ll \Delta x$) localised on x in the PDE cell ($x \in [\Delta x/2, \dots, \Delta x/2]$) is given by

$$P(x, t, \Delta x, \delta x) = \operatorname{erf}\left(\frac{\Delta x - x + \delta x}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{\Delta x - x}{\sqrt{4Dt}}\right) \tag{8}$$

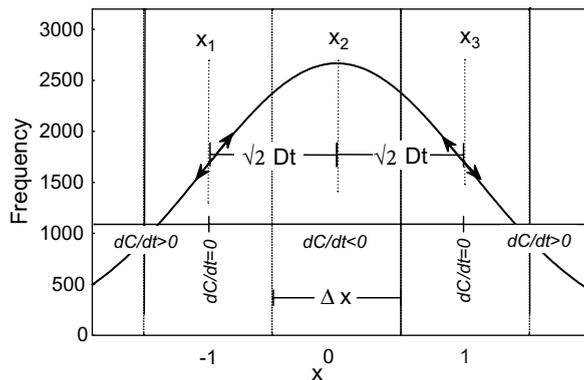


Fig. 5. Concentration profiles when $\sqrt{2Dt} = \Delta x$.

Then the configuration entropy on each sub-PDE cell is given by

$$\Delta S(x, t, \Delta x, \delta x) = -RP(x, t, \Delta x, \delta x) \log P(x, t, \Delta x, \delta x) \tag{9}$$

where R is the gas constant.

Thanks to the entropy additivity, entropy in a PDE cell is

$$\Delta S(t, \Delta x, k) = -R \sum_{i=-k/2+1}^{k/2} \left(\left[\operatorname{erf} \left(\frac{\Delta x(1 - \frac{i-1}{k})}{\sqrt{4Dt}} \right) - \operatorname{erf} \left(\frac{\Delta x(1 - \frac{i}{k})}{\sqrt{4Dt}} \right) \right] \log \left[\operatorname{erf} \left(\frac{\Delta x(1 - \frac{i-1}{k})}{\sqrt{4Dt}} \right) - \operatorname{erf} \left(\frac{\Delta x(1 - \frac{i}{k})}{\sqrt{4Dt}} \right) \right] \right) \tag{10}$$

And finally, the cell entropy is obtained when $\delta x \rightarrow 0$ meaning that $k \rightarrow \infty$: $\Delta S(t, \Delta x) = \lim_{k \rightarrow \infty} \Delta S(t, \Delta x, k)$.

Theorem 2

$$\partial \Delta S(t, \Delta x) / \partial x < 0 \quad \text{if } \Delta x > \sqrt{2Dt}, \quad t > 0: \quad \text{Anti - entropyproduction} \tag{11}$$

$$\partial \Delta S(t, \Delta x) / \partial x = 0 \quad \text{if } \Delta x = \sqrt{2Dt}, \quad t > 0: \quad \text{Spatio - temporalequilibriumstate} \tag{12}$$

$$\partial \Delta S(t, \Delta x) / \partial x > 0 \quad \text{if } \Delta x < \sqrt{2Dt}, \quad t > 0: \quad \text{Entropyproduction} \tag{13}$$

We shall now estimate the entropy of the cell x_2 shown in Fig. 5 by the numerical estimation of Eq. (10) for the configuration $k = 30, D = 1, \Delta x = 1, T = 10$. Fig. 6 represents the entropy variation of cell x_1 (or x_3) versus the value of the measured position. As can be observed, entropy increases up to the value of $\xi = 2Dt/(\Delta x)^2 = 1$, while it decreases when $\xi > 1$.

Let us now interpret these results. We shall consider Δx the range of accessible measurements. We have shown that the physical system can be measured with acceptable errors if $\Delta x < \sqrt{2Dt} = \Delta x_c$ meaning from Eq. (13) that the entropy of the system should increase. Suppose that the cell measurement Δx is set. To process a measure at position $x = \Delta x + \delta x$, the observation scale must be increased by δx which will change the system's entropy according to Theorem 2. Physically speaking the variation of entropy can be interpreted as a disorder introduced by the operator while measuring. Then from Eq. (13), a measurement increases entropy if $\Delta x < \Delta x_c$ (low measure uncertainty) and decreases entropy if $\Delta x > \Delta x_c$ (high measure uncertainty). In the quantum measurement, Entropy (i.e. the Von Neumann entropy) is defined by the number of wave functions compatible with the same macrostate [6]. According to Landau and Lifshitz [7,8], the foundation of the second law lie in the process of quantum measurement [9] that was reformulated by Srivastava et al. [10] by an increase of the Von Neumann entropy as a consequence of the Von Neumann projective measurement. By means of measurement theory in the field of modern physics, Conrad [11] proved that a measure must increase the entropy of the system due to a randomisation of the phase factor. This was confirmed by Kirby [12] using the Conrad 'theory who calculate the density matrix of a coupled biota-environment systems. As consequence, if $\Delta x > \Delta x_c$ Entropy will diminish that is a violation of quantum theory about measurement. Considering the example of the double slit diffraction, the measurement process (closure of one of the slits) diminishes the diffusion gradients produced by the incident beam and increases the entropy of the entire system. Then the distribution of positions and moment corresponds to a situation of higher entropy that is perfectly similar to our diffusion problems. However

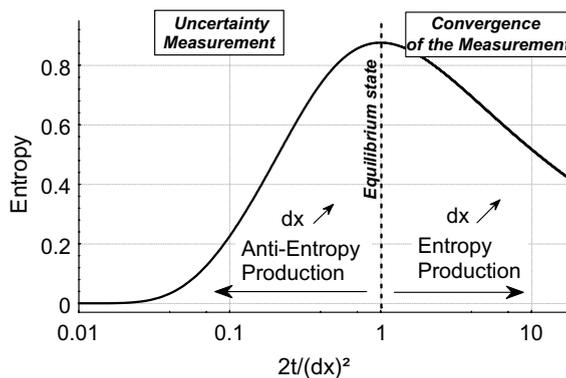


Fig. 6. Evolution of the configuration entropy of cells versus the criteria $2t/(\Delta x)^2$.

Conrad proves [13] that decorrelation is associated with increasing entropy, whereas recorelation is associated with decreasing entropy. The correlation–decorrelation process is associated with the observation scale. The smaller the scale ($\Delta x < \Delta x_c$), the more important the contribution to decorrelation. Besides the larger the scale ($\Delta x > \Delta x_c$) the more important the contribution to recorelation, i.e. anti-entropy production [14]. More interestingly, the fact that Δx_c does not depend on the value of the noise added to the system is consistent with the theory of Conrad according to the anti-entropy process does not depend on the atypical conditions. Penrose [15] described this correlation as a quantum coherence and Kirby [12] by unifying the Conrad adaptability theory [16] with quantum entropies proves that the measure destroy the quantum coherence and increases the entropy. When $\Delta x > \Delta x_c$, the ground state of the universe is inherently unstable if we are in the anti-entropy production. Conrad used the self-affine structure of the Cantorian space-time proposed by El Naschie [17–19] to show that such a space provides an infinite source of information for the recorelation process that underlies anti-entropy production [11]. El Naschie proved that the exact spatial localisation of a microspacial point is fundamentally undecidable due to the geometrical structure of such a space [20]. As a consequence, in the anti-entropy production process, the localisation ($\Delta x > \Delta x_c$) becomes undecidable and then all measures will be intrinsically uncertain.

5. Conclusions

By means of an inverse procedure carried out on stochastic equation, we have shown that for sandwich problems, the diffusion coefficient must be estimated by measuring the concentration for a depth x as near the source as possible. If the sensor is located far from this source, the precision in the measurement depends on both the diffusion time t and on depth x . If $x \geq \sqrt{2Dt}$ the error on the determination of the physical parameters will increase exponentially with depth x and could be related to a decrease in entropy despite the second principle of thermodynamics. These results are consistent with the theory of Conrad on anti-entropy production.

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