TRANSPORT OF LOGARITHMIC POTENTIALS VERSUS PROCESS DURATION

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Abstract. *The transport of logarithmic potentials provides a dynamical equilibrium that allows obtaining the lasting time estimation of a dynamical process. Bayesian rules are applied as a bridge between logarithmic potentials and the transport equation to obtain the potential associated with the interaction between systems. In this work, a data set from a chemical process is considered to test the method. Then, to enrich the analysis, an actual prediction by dynamical components is perform that illustrates how long every process and the global common process last.*

1 INTRODUCTION

Transport phenomena was considered in the context of social, physical, biological, chemical and engineering processes and was included on the Scopus of several meetings and papers related to problems and methods for modeling complex dynamical systems, [1-10]. In this sense, specific dynamical tools were developed the last decade [1,5]. The goal of this paper is to combine already published scientific results [6,7] together with analytical models [8,9,10] and elementary transport phenomena to validate a Bayesian transport model for obtaining times associated with processes. This Bayesian transport model is developed in this paper and it is applied here to predict the duration of a typical dynamical process. To this end, experimental measurements extracted from a catalyzed chemical reduction [7] together with theoretical tools for modeling complex dynamical systems [9] are considered here to facilitate testing the formulation of how long a biochemical process last. This choice obeys that the experimental measurements provided in [7] register both the global dynamical process between the system and the neighborhood and the influence of every external agent over the system given the fact

every agent has its own dynamical equilibrium [9]. Furthermore, a nonclassical treatment for local dynamics from the catalyzed biochemical reduction was developed and analyzed in [9]. Beyond that work in the recent past, it remains a complementary time estimation carried out today in this paper. For the coming years, it is worth to suspect that a more detailed time estimation of local processes from a special type of social measurements globally obtained such as the lasting time of learning processes, will be available very soon. In fact, the systematic treatment of learning measurements in the context of analytical models based on physical laws, was developed in [10], but not its time estimation which, surely as observed before, it will be a part of the near future after being estimated from a similar theory.

In this paper, the fast access to the measurements of the high efficiency of a strain of *Galactomyces candidus* GZ1 to transform acetophenone (AP) into (*R*)-phenylethanol ((*R*)-1-PE) provided enough material to validate the formulation for obtaining the time the process last. In consequence, here times related to biochemical processes are predicted component by component and globally for the full process.

2 THE BAYESIAN TRANSPORT MODEL

A basal one-dimensional transport equation takes the form

$$\frac{\partial \emptyset}{\partial t} + \frac{\partial q}{\partial x} = 0 \tag{1}$$

, where $\emptyset$ and q are quantities to be physically specified and t and x are time and displacement as usually they are. By choosing $q = -v\emptyset$ and x an arbitrary quantity, then, mass, momentum and energy conservation.

From another perspective, a decreasing x and θ satisfy the following identities along the time, at each time, during the process

$$dt = \frac{dx}{-v} = \frac{rd\theta}{-\omega r} = \frac{d\theta}{-\omega} \tag{2}$$

Here x means displacement and θ means angular displacement. Then, to go on with the steps in order to connect the transport equation (1) with the chain of equalities (2), we have the next equation

$$dt = \frac{d\theta}{-\omega} = \frac{d\theta}{-\sqrt{\omega^2}} = \frac{d\theta}{-\sqrt{\omega^2}} = \frac{d\theta}{-\sqrt{\int_{\theta_0}^{\theta}\left[\frac{\partial(\omega^2)}{\partial\theta}\right]d\theta}} = \frac{d\theta}{-\sqrt{\int_{\theta_0}^{\theta}-\left[\frac{\partial(-\omega^2)}{\partial\theta}\right]d\theta}} \tag{3}$$

If choosing $\emptyset = \omega$ and $q = -\omega^2$, we rewrite the transport equation (1), now in the integral form

$$t = \int_0^t dt = \int_{\theta_0}^{\theta} \frac{d\theta}{-\sqrt{\int_{\theta_0}^{\theta} - \left[\frac{\partial(q = -\omega^2)}{\partial \theta}\right] d\theta}} \tag{4}$$

, where $\omega(t = 0) = 0$, $\omega(t = t) = \omega$, $\theta(t = 0) = \theta_0$, and $\theta(t = t) = \theta$. Since, our goal is to be able to estimate how long a generic process last, at this point we should introduce the type of dynamical equilibrium associated with the flux $q = -\omega^2$. By applying equation (1), now we continue with the fact that we are transporting angular momentum per unit of the inertial moment, $\omega = \frac{I\omega}{I}$. So, we have equation (5), where symbol I represents the inertial moment and U_0 is the highest level of energy of the system. Beyond these observations, the main fact is we have just introduced the hypothesis of logarithmic potential after adopting the expression $U(\theta) = \left(\frac{U_0}{I}\right) ln(\theta)$ in the equilibrium (5).

$$\frac{\partial \omega}{\partial t} + \frac{\partial\left(\left(\frac{U_0}{I}\right) ln(\theta)\right)}{\partial \theta} = 0 \tag{5}$$

By considering $\omega(t = 0) = 0$, $\omega(t = t) = \omega$, $\theta(t = 0) = \theta_0$, and $\theta(t = t) = \theta$ and solving (5) for ω, we obtain

$$\omega = -\sqrt{\frac{2U_0}{I}} ln^{\frac{1}{2}}\left(\frac{\theta_0}{\theta}\right) \tag{6}$$

In consequence, we recognize $\omega^2 = W^2 ln(\frac{\theta_0}{\theta})$, where $W = \sqrt{\frac{2U_0}{I}}$ is a parameter of the problem to be determined from experimental measurements. It is worth to note that the form $\omega^2 = W^2 ln(\frac{\theta_0}{\theta})$ is because we have assumed logarithmic potentials and then we deal with forces that are derived from these potentials. This fact implies we can rewrite equation (4) as the form (5).

$$t = \int_0^t dt = \int_{\theta_0}^{\theta} \frac{d\theta}{-W ln^{\frac{1}{2}}(\frac{\theta_0}{\theta})}, \tag{7}$$

By choosing $t = ln\left(\frac{\theta_0}{\theta}\right)$, we derive from (7) the following expression

$$t = \int_0^t dt = \frac{\theta_0}{W} \int_{\theta_0}^{\theta} t^{-\frac{1}{2}} e^{-t} dt \tag{8}$$

Recalling the definition of the Gamma function and taking $\theta \to 0$, , we obtain

$$T = \int_0^T dt = \frac{\theta_0}{W} \int_0^{\infty} t^{\frac{1}{2}-1} e^{-t} dt = \frac{\theta_0}{W} Gamma\left(\frac{1}{2}\right) = \frac{\theta_0}{W} \sqrt{\pi} \tag{9}$$

Although until this point, we realized we have just provided deterministic paths and meanings for deriving a classical well know result, a clearly defined analytical structure from the transport equation and logarithmic potential becomes powerful after the dimensionless function $ln(\frac{\theta_0}{\theta})$ is able to interact in the context of the Bayesian theories and after W is found and recognized meaningful and decoupled from the rest of the formulation. Note that the frequency $W = \sqrt{\frac{2U_0}{I}}$ is related to the highest energy the system has and note that $ln(\frac{\theta_0}{\theta})$ is bigger than one since $\theta_0 \geq \theta \geq 0$. Then, what follows is a complementary energetic-probabilistic model, which is based on the Bayes theorem. In particular, the neighborhood interacts with the system throughout W, but also the system itself interacts with external agents throughout the Bayesian theory. We call s the number of external agents inside the neighborhood the system is living. Given the case, we may need to avoid such type of external influences and then we adopt $s = 0$. In other words, s will be the number of external agents to the system that are interacting with the system during the process and simultaneously sharing a common neighborhood. It should be noted that, if the external agents and neighborhood help the system to end its process, then the conditional probability grows up and the end of the process will come soon. Otherwise, if the system fights against all odds including external agents in order to end its process, then the conditional probability of the system decreases and, consequently, the end of the process will take place latter. Therefore, the Bayesian complementary model consists of assuming that

1) the amount of time (in the appropriate units) that any interacting system needs for lasting the process is one over the probability of the system for being able to finish the same process. This fact is independent of the helpful (or not helpful) interactions the system can have with external agents inside the neighborhood.
2) The Bayes theorem is valid. The external agents to the system that affect the lasting time of the process change the probability of the system to reach the end of the same process. Such probability reduction or amplification obeys the Bayes theorem, which then implies that the external agents can reduce or enlarge the lasting time of the process.
3) All agents together with the system have the same intensity, size or importance during the process.

What was explained in 1), 2) and 3) can be formulated as follows

$$w = W \frac{ln\left(\frac{\theta_0}{\theta}\right)}{ln\left(\frac{\theta_1}{\theta}\right) \dots ln\left(\frac{\theta_s}{\theta}\right)} = W \frac{P(\theta_1) \dots P(\theta_s)}{P(\theta_0)} = W \left[ln\left(\frac{\theta_0}{\theta}\right)\right]^{1-s} \tag{10}$$

Since we know who is w, we solve from equations (4) and (10)

$$t = \int_0^t dt = \int_{\theta_0}^{\theta} \frac{d\theta}{-W\sqrt{\left[ln\left(\frac{\theta_0}{\theta}\right)\right]^{1-s}}} = \int_{\theta_0}^{\theta} \frac{d\theta}{-W\left[ln\left(\frac{\theta_0}{\theta}\right)\right]^{1-\frac{(s+1)}{2}}} \tag{11}$$

From (11) and considering $\theta \to 0$

$$T = = \frac{\theta_0}{W} \int_0^\infty t^{\frac{(s+1)}{2}-1} e^{-t} dt \tag{12}$$

Finally, by applying the definition of the gamma function, we have

$$T = \frac{\theta_0.}{\omega} \; Gamma \left(\frac{s+1}{2}\right) \tag{13}$$

The model of interactions between the system, the neighborhood and external agents obeys the Bayes theorem. The applicability of (13) is guaranteed after detailed measurements are obtained trustily and systematically along the time. This fact allows somebody to better know how much do helpers, or friends, or enemies, or partners, or problems, or economic issues or just political tendencies, inside the global structure given by the set system-neighborhood-external agents affect the lasting time of the process. Expression (13) helps in understanding the mechanism that increases the waiting time while a dynamical system is developing a process in the context of physical interactions.

3   THE VALIDATION TEST FOR THE PREDICTIONS

In this section, both the treatment and interpretation of experimental measurements and the application of recently developed dynamical models are combined for testing predictions related to times of involved process and sub-process. Then, we choose a three-component chemical process provided by [7]. For simplicity, let us rename every interactive component of the process, by using capital letters **AP**, **(*R*)-1-PE** and **GZ1** according to **Table 1.** A typical design of the analysis of the experimental data can be as follows: the system (one of the components), the external agents (the other two or more components) and the neighborhood (the medium, which is the support having for instance aerobic conditions).

**Table 2**: Components of the dynamical process

AP	:	acetophenone
(*R*)-1-PE	:	phenylethanol
GZ1	:	*Galactomyces candidus*

In order to compute and verify how long this biochemical process last and to examine the dynamics of AP (acetophenone) reduction to (*R*)-1-PE (phenylethanol) by the biocatalyst *Galactomyces candidus* GZ1, let us also consider **Table 2,** where quantities associated with strong dynamical interactions between components are detailed over time.

Table 2: Conversion percentages of the AP, (R)-1-PE and (S)-1-PE over time

Time (Hs)	[AP]	[(R)-1-PE]	[(S)-1-PE]
1	79,53	1,11	19,36
2	73,6	2,75	23,62
4	68,81	6,21	29,61
5	64,33	8,50	27,17
7	63,8	12,41	23,79
8	63,88	14,97	21,15
9	71,21	17,03	11,8
10	73,27	19,51	7,20
11	72,61	23,21	4,14
12	69,71	27,54	2,74
15	37,11	62,79	0,10
18	17,62	82,38	0,10
21	3,80	96,10	0,10
24	0,10	99,90	0,10
31	0,01	99,99	0,01
39	0,01	99,99	0,01

The experimental results are shown in **Table 2** and visualized in **Figure 1**
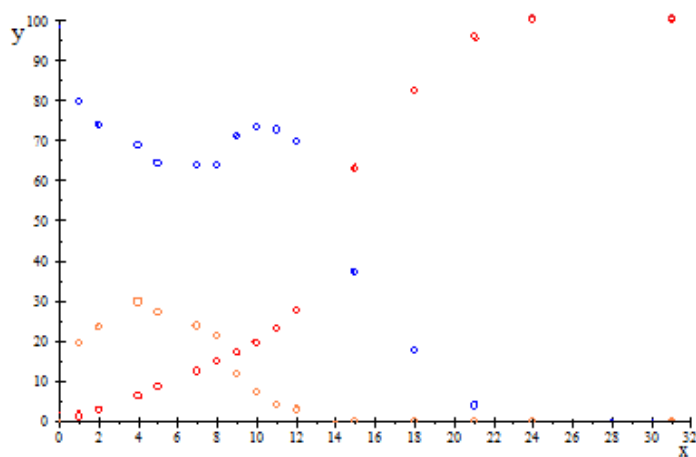
Figure 2: Experimental results: Evolution of the reduction reaction of AP = o to (R)-1-PE = o catalyzed by (S)-

1-PE = o along the time. The vertical axis is conversion, while the horizontal one is time measured in hours.

The conversions percentages of AP to (*R*)-1-PE catalyzed by (*S*)-1-phenylethanol ((*S*)-1-PE) over time are illustrated in **Figure 3** by distributed dots. The Law of Mass conservation is held during the process, which is a common assumption in chemical processes.

As mentioned earlier, a kinetic study of AP reduction to (*R*)-1-PE promoted by a strain of *Galactomyces candidus* GZ1 was reported in [7] and a mechanistic interpretation was proposed through a qualitative interpretation of reaction profiles. So, with permission, it follows the next paragraph extracted from [7] related to the precise description of the reduction process.

'It can be observed in **Figure 4**, the AP (o blue) concentration percentage decreased to 64% (representing approximately a 36% conversion to the products) after 5–7 hours of reaction. From this moment, the percentage of AP began to increase again until reaching a maximum of 73% (27% conversion) approximately 10 hours from the start of the reaction, before falling again until it reached practically zero concentration (24 hours of reaction). The appearance of the products was directly related to the variation of AP. As shown in **Figure 5**, the component (*S*)-1-PE (o orange) formed more rapidly than the component (*R*)-1-PE (o red), with 19% of the component (*S*)-1-PE being formed during the first hour of reaction, while only 1% of (R)-1-PE was observed at this time. The maximum concentration for (*S*)-1-PE was reached approximately after 4–5 hours of reaction, and from this point onwards its conversion percentage began to decrease and reached zero approximately 15 hours after starting the reaction. It should be noted that when (*S*)-1-PE reached the conversion percentage maximum, this situation coincided with the beginning of the increase in the percentage of AP observed in the reaction medium, which may indicate that *S* enantiomer was oxidized and gave rise to the formation of AP. In parallel, this percentage of (*R*)-1-PE formation continued to increase over time, but at varying speeds. At 11 hours of reaction (where there was a marked decrease in the percentage of (*S*)-1-PE, the system seemed to accelerate towards the accumulation of (*R*)-1-PE, which coincided with the beginning of a second decrease in the percentage of AP. In fact, as can be observed from the first 15 hours of reaction, the formation of (*R*)-1- PE was essentially due to a reduction in AP, with the formation percentage of (*R*)-1-PE reaching a maximum, at approximately 24 hours of reaction, when both AP and (*S*)-1-PE had disappeared completely'.

Also, as mentioned previously, a nonclassical dynamical study was carried out in [9] for obtaining the local dynamic of the components (products) of a complex system during a biochemical process (namely a catalyzed reduction process). So, it follows the next dynamical formulation extracted from [9], which is related to the precise description of kinetical velocities of the catalyzed reduction process.

After a physical analysis from measurements it had found in [9] three dynamical equations, which can be summarized in the form of a first order differential system, where X_R, X_{AP} and X_S are the concentration of the involved products.

$$\begin{pmatrix} \dot{X}_R \\ \dot{X}_{AP} \\ \dot{X}_S \end{pmatrix} = \begin{pmatrix} -\alpha_R & 0 & 0 \\ 0 & -\alpha_{AP} & -\alpha_S \\ 0 & 0 & -\alpha_S \end{pmatrix} \begin{pmatrix} X_R \\ X_{AP} \\ X_S \end{pmatrix} \tag{14}$$

The companion system (14) has its matrix, which has components defined in (15). These

components are variable coefficients (kinetic velocities) for $t < 14$. It should be noted that only α_R is a constant coefficient inside the matrix under the condition $t < 14$, while the other two coefficients are variable. Furthermore, the variable coefficients α_{AP} and α_S under the restriction $t < 14$ are the derivatives of two functions g and f, respectively.

$$\begin{pmatrix} \alpha_R \\ \alpha_{AP} \\ \alpha_S \end{pmatrix} = \begin{pmatrix} h'(t) \\ g'(t) \\ f'(t) \end{pmatrix} = \begin{pmatrix} 0.22 \\ g'(t) \\ f'(t) \end{pmatrix} \tag{15}$$

So, there exists three functions defined in (16) that drives the evolution of the companion matrix over time

$$\begin{pmatrix} h(t) \\ g(t) \\ f(t) \end{pmatrix} = \begin{pmatrix} 0.22.t \\ -e^{ln(2)} + e^{-0.25(t-14)} + e^{-f(t)+ln\left(\frac{8}{5}\right)} \\ ln\left(\frac{X_S}{80}\right) \end{pmatrix} + \begin{pmatrix} h(t_0) \\ g(t_0) \\ f(t_0) \end{pmatrix} \tag{16}$$

The functions h(t), g(t) and f(t) are derived from the computations carried out in obtaining the normalized form of the solution, while its derivatives provide the kinetic velocities for (R)-1-PE, AP and (S)-1-PE, respectively. From **Table 2**, we can read the initial conditions to determine the problem. Default values of $h(t_0) = g(t_0) = f(t_0) = 0$ was taken. So, the solution of the system (14) for $t < 14$ is

$$\begin{pmatrix} X_R \\ X_{AP} \\ X_S \end{pmatrix} = 50 \begin{pmatrix} e^{0.22(t-14)} \\ e^{-g(t)} \\ e^{-f(t)+ln\left(\frac{8}{5}\right)} \end{pmatrix} \tag{17}$$

In the first half of the total time interval, the kinetic velocities for the (R)-1-PE product is 0.22. This value can be seen explicitly in the formulation. **Table 3** shows that AP and (S)-1-PE have a variable kinetic velocity. It also let us know how $f'(t)$ can be obtained over time. Furthermore, **Table 3** allows us to know $h'(t)$, $g'(t)$, $f'(t)$, the kinetic velocities for the three products

Table 3: Kinetic velocities over time for the AP, (R)-1-PE and (S)-1-PE over time

Time (Hs)	Kinetic Velocities		
	α_{AP}	α_S	α_R
1	0,056	2,330	0,22
2	-0,077	0,199	0,22
4	-0,034	0,113	0,22
5	-0,067	-0,086	0,22
7	-0,004	-0,066	0,22
8	0,001	-0,118	0,22
9	0,109	-0,583	0,22

10	0,028	-0,494	0,22
11	-0,009	-0,553	0,22
12	-0,041	-0,413	0,22
15	-0,210	-1,103	0,22
18	-0,248	0	0,11
21	-0,511	0	0,03
24	-1,212	0	0,01
31	-0,329	-0,329	0,002
39	0	0	0,0002

As soon as the first half of the period ends, a new stage starts. Then, for the second fourteen hours the dynamic becomes simpler than before. The solution, Eq. (8), for $t > 14$ is

$$\begin{pmatrix} X_R \\ X_{AP} \\ X_S \end{pmatrix} = \begin{pmatrix} 100 - 50e^{-0.33(x-14)} \\ 50e^{-0.33(x-14)} \\ 0 \end{pmatrix} \tag{18}$$

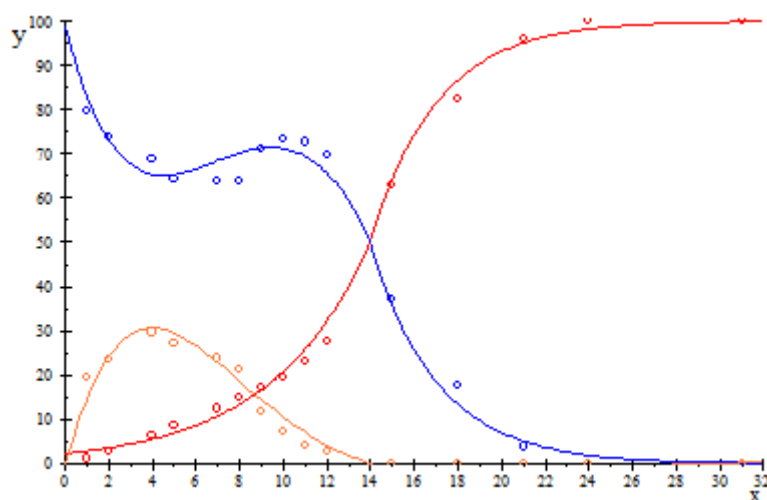The theoretical and experimental results are in **Figure 2**.

Figure 2: Non classical analytical results: Evolution of the reduction reaction of AP = o to (*R*)-1-PE = o catalyzed by (*S*)-1-PE = o along the time. The vertical axis is conversion, while the horizontal one is time measured in hours

As it can be seen in **Figure 2**, there is a good agreement between analytical non classical predictions and experimental measurements. Thus, the proposed analytical model predicts the full chemical products evolution. So, it fits measurements through analytical predictions

obtained from first order differential systems with variable coefficients, straightforwardly. This treatment for obtaining kinetic velocities can be considered nonclassical [9]. Beyond these results, what follows is the global time estimation that allows us to know how long the process last. The golden standard for the global (W) and local (w) frequency analysis is the expression derived from (10). Thus, the same occurs between the temporal step between measurements and the global time the total process last.

$$w = W \frac{ln\left(\frac{\theta_0}{\theta}\right)}{ln\left(\frac{\theta_1}{\theta}\right)...ln\left(\frac{\theta_s}{\theta}\right)} = \frac{2\pi}{t} = \frac{2\pi}{T} \frac{ln\left(\frac{\theta_0}{\theta}\right)}{ln\left(\frac{\theta_1}{\theta}\right)...ln\left(\frac{\theta_s}{\theta}\right)} \tag{19}$$

Also, testing expression (19) guarantee that every derived formulation for time estimation in this paper works as it should do it for solving dynamical problems.

To test (19) let us consider first the interval $(0 < t < 14)$, where the system has the AP component catalyzed by GZ1. It means $s = 1$.

$$T(s = 1) = \frac{\theta_{0.}}{W(s = 1)} \, Gamma\left(\frac{1+1}{2}\right) = \frac{\theta_{0.}}{W} \tag{20}$$

Them from the physical evaluation it is known the complete evolution of **[(*R*)-1-PE]** for the interval $(14 < t < 32)$ as it can be seen in **Figure 2**. In this interval $s = 0$ So, we find

$$T(s = 0) = \frac{\theta_{0.}}{W(s = 0)} \, Gamma\left(\frac{0+1}{2}\right) = \frac{\theta_{0.}}{W} \sqrt{\pi} \tag{21}$$

Now, since $\theta_{0.}$ is always the same in both intervals, from expressions (21) and (22) it can be derived

$$\frac{T(s = 1)}{T(s = 0)} = \frac{W(s = 0)}{W(s = 1)} \frac{1}{\sqrt{\pi}} = \frac{0.33}{0.22} \frac{1}{\sqrt{\pi}} = \frac{3}{2} \frac{1}{\sqrt{\pi}} = 0.84628 \tag{21}$$

Now, since $s = 1$ implies $Gamma\left(\frac{1+1}{2}\right) = 1$, and given the first interval $T(s = 1) = 14$, it follows $T(s = 0) = 14\left(\frac{3}{2}\right)\left(\frac{1}{\sqrt{\pi}}\right) = 14\left(\frac{3}{2}\right)(0.84628) = 17.772$ and then

$$T[(s = 0) \cup (s = 1)] = T(s = 0) + T(s = 1) = 14 + 17.772 = 31.772 \approx 32 \tag{22}$$

Given $T[(s = 1) \cup (s = 2)] \approx 32$, since the experimental design is available from the beginning of the measurements and knowing the **[(*R*)-1-PE]** experimental behavior, the expression (18) allows us to recognize $W(s = 0) = 0.33$, while expression (17) shows $W(s = 1) = 0.22$ So, it is estimated

$$W[(s = 0) \cup (s = 1)] = \left(\frac{18}{32}\right) W(s = 0) + \left(\frac{14}{32}\right) W(s = 1) = 0.28188 \approx 0.28 \tag{23}$$

Finally, it follows the global parameter of the whole process

$$\theta_0 = \ln\left(\frac{T[(s = 0) \cup (s = 1)]}{W[(s = 0) \cup W(s = 1)]}\right) = ln\left(\frac{32}{0.28}\right) \approx 4.74 \tag{24}$$

As it can be seen, results are in total agreement between analytical predictions and experimental measurements.

4   CONCLUSIONS

- The transport equation was applied to obtain an integral powerful format of itself were the energy related global frequency W was discovered and isolated in term of the global parameters of the system.
- The integral form of the transport equation was applied for transporting angular momentum in order to find an operational expression for a cumulative angular frequency w which depends on both the global frequency W and the logarithmic potentials.
- Logarithmic potentials were related to probabilities and connected to conditional probabilities throughout the Bayes theorem
- The operational cumulative angular frequency w was adapted from the Bayesian theory to include the interactions between the system and some external agents that could affect the lasting time of the process the system is carrying on.
- The interaction between the system, the neighborhood and the external agents are all modeled into the cumulative angular frequency w throughout W, ln(to/t) and s, respectively
- Logarithmic potentials, the global frequency, the cumulative angular frequency, the integral form of the transport equation and the Bayes theorem allow to find the lasting time of a dynamical process.
- Selective computations for local dynamics provide the lasting time associated with every component that is interacting in the common process.
- Scientific experimental results from the evolution of the reduction reaction of component AP to component (R)-1-PE catalyzed by component GZ1 were considered for the validation of the formulation that was developed in this paper.
- Temporal subintervals with physical insight were found and computed
- A global parameter for the whole process was found
- Future developments should include step by step computations for obtaining kinetical velocities from this new perspective and to avoid higher computations.

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