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▶ To cite this version:

Nadia Rosero, John Jairo Martinez Molina, Matteo Corno. Modeling of gas exchange dynamics using cycle-ergometer tests. MATHMOD 2018- 9th Vienna International Conference on Mathematical Modelling, Feb 2018, Vienne, Austria. hal-01737743

HAL Id: hal-01737743

https://hal.science/hal-01737743

Submitted on 19 Mar 2018

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Modeling of gas exchange dynamics using cycle-ergometer tests

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Abstract: This paper presents a novel discrete-time linear parameter-varying model for gas exchange dynamics during cycling. This model is intended to be used for enhancing the control design process of electrical assistance in bicycles. The mathematical model relates the oxygen consumption and carbon dioxide production to the developed power at the pedal level. The proposed model is also able to predict the excess of CO_2 while high intensity workout is performed. This has been possible by using a time-varying parameter which is scheduled according to the difference between the masses per unit time of O_2 and CO_2 . An illustration of the proposed methodology for identification and validation of the model is also presented in this paper. The model parameters for a given individual, were obtained by using measured data of cycle-ergometer tests from two different cycling scenarios.

Keywords: Physiological models, gas exchange dynamics, bicycles.

1. INTRODUCTION

The increased promotion of electrical bicycles as an accessible and friendly-environmental transport has opened new researches in the electrical-assistance control area. Nowadays, the comprehension of the cyclist-bicycle set as a whole system, has conducted scientific efforts for understanding physiological processes from an engineering point of view.

Human physiology can be regarded as a complex machine which transforms chemical energy (oxygen and nutrients) into mechanical energy. This approach has been used long time ago (Hill and Lupton, 1923). Chemical reactions between oxygen and substrates within the human physiology are in the first level of the energetic chain. In the literature, several static models have been proposed, for example works by (Olds et al., 1993) and (Martin et al., 1998). Nevertheless, due to the complexity of those dynamic physiological processes, a model that fits the behavior of physiological variables in the time-domain is valuable.

The gas exchange dynamics has been largely studied related with chemical reactions and provide the easiest solution to investigate human physiology. Based on gas exchange (Wasserman et al., 1973) and (Beaver et al., 1986) described a method for identifying the use of aerobic or anaerobic metabolic pathways while exercising, which has been extensively accepted. Actually, the level of each pathway for energy production makes the difference in terms of the efficiency of human exerted power. In this sense, these physiological variables have been considered to solve bioenergetic optimization problems, for example in (Aftalion and Bonnans, 2014). Other works

about physiological-oriented control have been proposed in (Corno et al., 2015), where a Heart Rate control is addressed. See also (Fayazi et al., 2013), (Wan et al., 2014) and (Corno et al., 2016) where dynamical fatigue models are used for the electrical assistance control. However, validation of these fatigue models is difficult in practice since fatigue can not be measured. In the work (Rosero et al., 2017) it is proposed an energetic-chain based model for human-bike system analysis and control.

One of the main difficulties in the use of physiological models in optimization or control is that they are highly subject-dependent, therefore a common model structure that fits the main general dynamics is valuable, as it can account for model variability and uncertainty.

Here, a discrete-time linear parametric varying model is proposed. It could be used for simulation, estimation or prediction of gas exchange dynamics while cycling. The model is mostly intended for designing model-based control systems. It can be parametrized by using three measurable variables: the mechanical power at the pedal level as system input, and volumes per unit time of oxygen $\dot{V}O_2$ and carbon dioxide $\dot{V}CO_2$ as system outputs.

The model is also able to predict the excess of CO_2 while high intensity workout is performed. This has been possible by using a time-varying parameter which is scheduled according to the difference between the masses per unit time of O_2 and CO_2 . An illustration of the proposed methodology for identification and validation of the model is also presented in this paper. The model parameters, for a given individual, were obtained by using measured data of cycle-ergometer tests from two different cycling scenarios.

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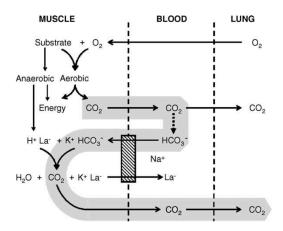


Fig. 1. The model for lactic acid buffering by bicarbonate and the control of hyperventilation above ventilatory threshold: from (Wasserman et al., 2005) redrawn by (Péronnet and Aguilaniu, 2006).

2. CO_2 PRODUCTION AND O_2 CONSUMPTION DURING CYCLING

While performing an exercise and for any human activity, the energy required comes from food transformation. In fact, through chemical reactions it is possible to obtain the energy currency in the body, which is the Adenosine Triphosphate (ATP).

There are mainly three ways to synthesize ATP: i) aerobic, ii) alactic anaerobic and iii) lactic anaerobic. The first is the most efficient way. However, as it requires an adequate supply of oxygen to the muscles, this pathway activates slowly. During the transient required to adapt the respiratory system, energy is produced through the alactic anaerobic pathway. This pathway use molecules of Phospocreatine (PCr) and Adenosine Diphosphate (ADP) to synthesize ATP. For example, during moderate and prolonged exercise, energy comes mainly through the aerobic pathway, using firstly glycogen stored in active muscles and liver glycogen, which provide almost the half part of the energy requirement, with the remainder from fat breakdown with minimal amounts from blood glucose. Examples of aerobic ATP synthesis from glucose and fat can be represented by the reactions (1) and (2), respectively (McArdle et al., 2006).

$$C_6H_{12}O_6 + Pi + ADP + O_2 \longrightarrow CO_2 + H_2O + ATP \tag{1}$$

$$CH_3(CH_2)_{14}COOH + Pi + ADP + O_2 \longrightarrow CO_2 + H_2O + ATP$$
 (2)

When an exhaustive exercise is performed lactic anaerobic pathway is used and the lactate clearance mechanisms acts to maintain proper acid base balance. Then CO_2 production increases more than oxygen consumption, the sodium bicarbonate $NaHCO_3$ in the blood buffers or neutralizes the lactate generated during anaerobic metabolism in the following reaction:

$$HLa + NaHCO_3 \longrightarrow NaLa + H_2CO_3 \longrightarrow CO_2 + H_2O$$
(3)

In the pulmonary capillaries, carbonic acid breaks down to its components carbon dioxide and water to allow carbon dioxide to readily exit through the lungs. Therefore, that buffering adds extra CO_2 to expired air above the quantity normally released during cellular energy metabolism. Relatively low CO_2 production occur after exhaustive exercise when carbon dioxide remains in body fluids to replenish bicarbonate that buffered the accumulating lactate.

3. PROBLEM STATEMENT

From the above reactions for ATP synthesis, it is possible to consider the bioenergetic process as an unknown system consuming O_2 and substrates and producing CO_2 as a consequence of producing mechanical power. Considering chemical reactions as these stated by equations (1) and (2), it is possible to simplify the ATP synthesis in a general reaction of the form: 1) for aerobic reactions:

$$Substrate + O_2 \longrightarrow CO_2 + ATP + others \tag{4}$$

and 2) for anaerobic reactions:

$$Substrate \longrightarrow CO_2 + ATP + others \tag{5}$$

The latter does not require O_2 for synthesizing ATP. In addition, this equation collects all the sequence of multiple reactions producing CO_2 as a consequence of producing ATP (power) and other sub-products, as it is illustrated in equation (3). Thus, the term "others" in (4) and (5) involves the amount of produced water, used enzymes and other substances different from substrates that participate into the chemical reactions. These "others" substances will not be taken into account in this work. For simplicity, the above presented chemical reactions only mention the kind of molecules involved into the chemical reaction without indication of the quantity of molecules. However, in this work we will be more concerned with the equivalent mass balance equations.

During the modeling process we keep in mind the following statement: "The mass that enters a system must, by conservation of mass, either leave the system or accumulate within the system".

In the model proposed by Wasserman et al. (2005), see Fig. 1, the relationships between produced power, oxygen consumption and carbon dioxide production have been widely accepted into the research community. However, this model can not be used for control-design purposes. The model proposed in this paper does not pretend to reproduce all these chemical reactions, instead of that it keeps only the dynamical relations between variables. Since the model is intended to be used for control-design of electrical assistance for bicycles, it has not been derived from laws of physics or chemical sciences, but from dynamical systems relationships observing system inputs and outputs.

It concerns a mathematical dynamical model relating three variables: O_2 , CO_2 and excess of CO_2 denoted here as εCO_2 , that are function of the produced power. However those variables, can be also dependent of themselves if we consider that such dynamical systems are formed by storage elements of O_2 and CO_2 . From the aerobic reactions, for instance the reactions in the form (4), we suppose

there exists a mechanism that controls the available O_2 for performing such reactions, then the variations of O_2 will depend of both produced power and CO_2 .

In this work, we assume that εCO_2 dynamics can be modeled as a function of itself, the produced power and the CO_2 . Therefore, all functions describing the time evolution of the system variables can be expressed in terms of the following differential equations:

$$\dot{O}_2 = \mathbf{f}_1(O_2, CO_2, power) \tag{6}$$

$$\dot{CO}_2 = \mathbf{f}_2(CO_2, power)$$
 (7)

$$\varepsilon \dot{C}O_2 = \mathbf{f}_3(\varepsilon CO_2, CO_2, power) \tag{8}$$

where the functions \mathbf{f}_1 , \mathbf{f}_2 and \mathbf{f}_3 will be considered as linear and time-invariant functions. Remark that these relationships describe the system state evolution $(O_2, CO_2, \varepsilon CO_2)$ with respect to the system input, i.e. the *power*. For simplicity, the time-varying part of the model is associated to a particular output which will concatenate the aerobic and the anaerobic contributions of CO_2 . That is,

$$y_1(t) = O_2(t) \tag{9}$$

$$y_2(t) = CO_2 + \rho(t)\varepsilon CO_2 \tag{10}$$

where $0 \le \rho(t) \le 1$ will be a state-dependent time-varying parameter.

4. PROPOSED MODEL OF GAS EXCHANGE DYNAMICS

Consider the following discrete-time system:

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}u_k + \mathbf{B}w \tag{11}$$

$$\mathbf{y}_k = \mathbf{C}(\rho_k)\mathbf{x}_k \tag{12}$$

where the state vector $\mathbf{x}_k = [x_1, x_2, x_3]^T$ with x_1 stands for the consumed oxygen mass per unit time (in g/min), x_2 stands for the aerobic-produced carbon dioxide mass per unit time (in g/min) and x_3 stands for the anaerobic-produced carbon dioxide mass per unit time (in g/min). The input u_k stands for the mechanical power (in Watts) at pedal level at the instant k. The symbol w models an additional unknown power consumption (for instance, power required for other physiological tasks that also perform oxygen consumption and carbon dioxide production). Remark that, at rest (e.g. $u_k = 0$), the input w is the only responsible of O_2 consumption and CO_2 production. The matrix \mathbf{B} multiplying this input, allows obtaining w in the same units than u_k , i.e. in Watts.

The system matrices are considered to be described as follows:

$$\mathbf{A} = \begin{bmatrix} \theta_1 & \theta_2 & 0 \\ 0 & \theta_3 & 0 \\ 0 & \theta_5 & \theta_6 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} \theta_4 \\ \theta_4 \\ \theta_7 \end{bmatrix}$$
 (13)

The matrix $\mathbf{C}(\rho_k)$ depends on a time-varying parameter ρ_k as follows

$$\mathbf{C}(\rho_k) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \rho_k \end{bmatrix} \tag{14}$$

This varying parameter changes according to the intensity of the exercise. If the exercise is classified as aerobic, then $\rho_k = 0$, otherwise it will be varying between 0 and 1 for mixed aerobic/anaerobic exercises

The parameter $\rho_k := \rho(z_k)$ can be modeled as a function of a certain physiological index z_k which will be responsible of

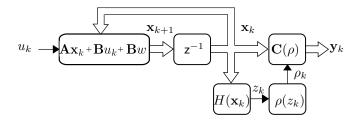


Fig. 2. Equivalent block diagram of the proposed model.

the aerobic or mixed aerobic/anaerobic use of substrates. Because the parameter ρ_k verifies $0 \le \rho_k \le 1$, it can be modeled using a fixed structure in terms of z_k as follows:

$$\rho(z_k) = 0.5 + 0.5 \tanh\left(\frac{\mathbf{z}_t - z_k}{h}\right) \tag{15}$$

In this work we assume that the physiological index z_k can be written in terms of the system states and/or system inputs, that is:

$$z_k = H(\mathbf{x}_k, u_k) \tag{16}$$

For instance, this index can be a function of the mechanical power, or the produced CO_2 , or a linear combination of states and inputs. In this paper we explore a novel index which considers the real-time difference between O_2 and CO_2 mass per unit time, i.e.

$$z_k = y_1(k) - y_2(k) (17)$$

The main motivation for using this index concerns the fact that the mass of oxygen minus the mass of carbon dioxide has to be equal to the mass associated to the produced ATP, water and other substances minus the amount of used substrates (i.e. considering equation (3) written in a mass balance equation form). Thus, this index can be interpreted as an image of the substrates over-consumption during aerobic and/or anaerobic reactions for producing ATP. The more negative this index is, the more substrate is used for producing a similar amount of ATP. Remark that this index is quite similar to that proposed and analyzed in Issekutz and Rodahl (1961) for estimation of excess CO_2 production. Here the varying parameter $\rho(z_k)$ could be interpreted as the percentage of anaerobic contribution in the total energy expenditure.

Remark that the index z_k can be written in terms of VCO_2 and VO_2 , as follows:

$$z_k = \delta_{O_2} \dot{V}O_2(k) - \delta_{CO_2} \dot{V}CO_2(k)$$
 (18)

where the constants δ_{O_2} and δ_{CO_2} correspond to the volumetric mass density in g/l (or equivalently kg/m^3) of O_2 and CO_2 , respectively.

Figure 4 depicts the proposed model structure. The mechanical power is considered to be the input of the system, denoted u_k , and the vector \mathbf{y}_k , formed of mass per unit time of O_2 and CO_2 , are the system outputs that can be calculated from $\dot{V}O_2$ and $\dot{V}CO_2$ measured in practice. The model provides the evolution of states at every time instant, denoted \mathbf{x}_k formed of the mass per unit time of O_2 , aerobic CO_2 and excess εCO_2 . The function $H(\mathbf{x}_k, u_k)$, that here will be only state dependent, permits the calculation of the index z_k , which determines the value of the varying parameter ρ_k into the matrix $\mathbf{C}(\rho_k)$.

5. IDENTIFICATION AND VALIDATION

5.1 Parameter identification by optimization

In this work we consider the availability of several sequences of N uniform-sampled measured data for system input (pedal power) and outputs of mass per time units of O_2 and CO_2 . Even if the measures have not the same time sampling, interpolation methods can be applied for obtaining vectors with data each second. The outputs are calculated from measurements of oxygen consumption $\dot{V}O_2$ and CO_2 production $\dot{V}CO_2$. In the sequel, we use the proposed model structure to find a vector of parameters \mathbf{p} that minimizes the prediction output error. The identification problem will be:

Find the vector of parameters $\mathbf{p}=[\theta,w,\mathbf{z}_t,h]$ which minimizes

$$J := \sum_{k=1}^{N} \|(\mathbf{y}_k - \mathbf{y}_k^{measured})\|_2$$
 (19)

subject to

$$\mathbf{x}_{k+1} = \mathbf{A}(\theta)\mathbf{x}_k + \mathbf{B}(\theta)u_k + \mathbf{B}(\theta)w \tag{20}$$

$$\mathbf{y}_k = \mathbf{C}(\rho_k)\mathbf{x}_k \tag{21}$$

$$z_k = H(\mathbf{x}_k) \tag{22}$$

$$\rho_k = \rho(z_k) \tag{23}$$

for $k = \{1, \dots, N\}$, with:

$$\rho(z_k) = \begin{cases} 0 & \text{for case } 1 : \text{mostly aerobic} \\ 1 & \text{for case } 2 : \text{mostly anaerobic} \\ 0.5 + 0.5 \tanh\left(\frac{\mathbf{z}_t - z_k}{h}\right) & \text{for case } 3 : \text{mixed} \end{cases}$$

Due to the nature of the problem and the available data, this optimization problem can not be solved in one shoot. In practice, it is necessary to solve the problem in three different steps, as it will be described in the following subsection.

5.2 The proposed methodology

Parameter identification is performed using 3 steps:

- (1) Identify the model parameters associated to the aerobic reactions consuming O_2 and producing CO_2 by using data obtained during moderate intensity workout. That is, the used measured data is considered to be obtained during a dominant aerobic situation, i.e. $\rho \approx 0$. Therefore, find the parameter vector $[\theta, w]$ concerning the first and the second state equations for x_1 and x_2 .
- (2) Fixing the parameters obtained in step 1, identify the model parameters associated to the anaerobic contribution of CO_2 (i.e. the state equation for x_3) by using data obtained during high intensity workout. That is, the used measured data is considered to be obtained during a anaerobic situation, i.e. $\rho \approx 1$.
- (3) Identify parameters of the function $\rho(z_k)$ characterizing the varying parameter ρ_k , i.e. $[\mathbf{z}_t, h]$ with respect to a given physiological index z_k . Here, the used measured data has to include aerobic and anaerobic situations, i.e. $0 \le \rho \le 1$.

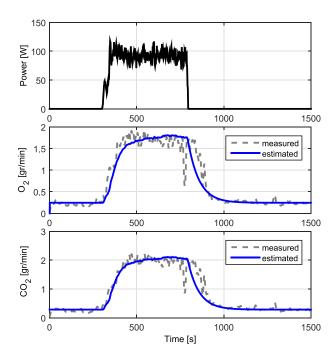


Fig. 3. Sequence used for parameter identification of the aerobic dynamics, $\rho_k = 0$.

Validation can be based on the evaluation of the model fit using other sequences of data and comparing the outputs (measured and simulated) using the same input. Data for validation has to be obtained during aerobic and mixed scenarios. Here we will use data obtained from two tests for model validation.

6. ILLUSTRATION OF THE METHODOLOGY USING REAL DATA

For identification and validation of the model two tests are done with the same subject. The test 1, consists in power bursts, with different torque and cadence characteristics, but with the same energy reached in each step.

The test 2 consists in a Incremental Cycling Test scenario (ICT) with resistance protocol, which is performed at 80 rpm while the resistance power is incremented stepwise every 30 seconds. The test runs till exhaustion. The available measures are: pedal torque and angular speed or, cadence and power provided by a cycle-ergometer, and gas exchange measures using a SensorMedic Vmax device. Here, the Heart Rate is also available but is not used.

6.1 Identification

Moderate workout: A scenario of moderate intensity is chosen to identify parameters of aerobic pathway contribution. The subject performs an exercise with power around 100 W during 500 s. The initial state and post-exercise recovery (rest time with power = 0) are taken into account. All data were treated to have an uniform sampling of $t_s = 1$ s.

At this step, the parameters $[\theta_5, \theta_6, \theta_7]^T$ and ρ are fixed at zero, while we are finding $[\theta_1, \theta_2, \theta_3, \theta_4]^T$. The Fig. 3 shows the input (power at pedal level) and the outputs: mass per unit time of O_2 and CO_2 .

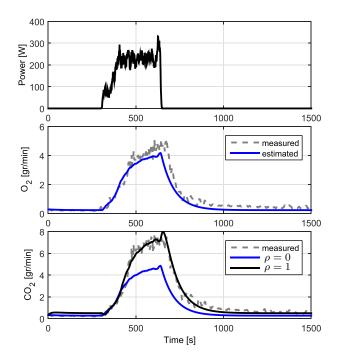


Fig. 4. Scenario used for parameter identification of the anaerobic dynamics $\rho_k = 1$ and, a comparison with respect to the aerobics dynamics $\rho_k = 0$.

High intensity workout: The parameters estimated at the previous step were tested in a in a high intensity workout scenario. In this case, the subject applies a power around 190 W during 250 s. The results shown in Fig. 4 with $\rho=0$ exposes a good fitting for O_2 , however there is an over production of CO_2 that can not be modeled by just the aerobic dynamics. This result is expected. The over-production of CO_2 belongs to the contribution of the anaerobic pathway, therefore a new identification process is performed for obtaining the values of θ_5 , θ_6 and θ_7 , with fixed $\rho=1$.

Obtained model parameter values: The obtained system matrices, after performing the proposed optimization process for identification, are:

$$\mathbf{A} = \begin{bmatrix} 0.168 & 0.701 & 0 \\ 0 & 0.986 & 0 \\ 0 & 0.073 & 0.933 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 0.259 \\ 0.259 \\ -0.670 \end{bmatrix} \times 10^{-3} \quad (25)$$

and the parameters w = 14.0130, $\mathbf{z}_t = -1.17$ and h = 0.5054

The improvement of the fit in CO_2 by using $\rho = 1$ can be seen in Fig. 4. The results in the fit of O_2 suggests that is not necessary an additional adjustment for this variable.

6.2 Validation of the obtained model

Test 1. The parameter vector **p**, calculated in the procedure described in Section 6.1, are used during a longer data set. Here, three steps of different power and same energy are performed. The Fig. 5 shows the results of the obtained model fit in contrast with the measured data.

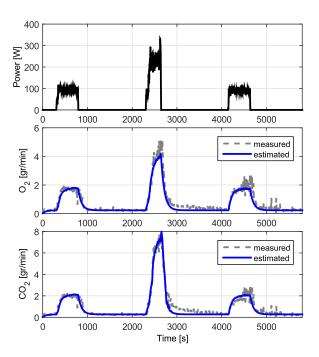


Fig. 5. Validation of the model using data of the test 1, by considering z_k as a function of the estimated model states.

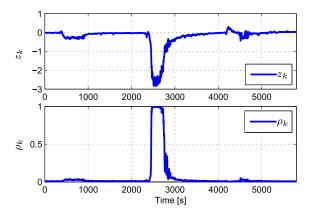


Fig. 6. Evolution of the index z_k and the varying parameter ρ_k for test 1.

The function (17) was implemented to update the value of z index at each instant k. Remark that the values of ρ are different to zero, even in the case of moderate intensity.

Test 2. The Fig. 7 shows the obtained model fit for an ICT scenario. It is observed an abrupt change in ρ around 250 s which corresponds nearly to the first ventilatory threshold, i.e. the model predicts the point where relation $\dot{V}CO_2/\dot{V}O_2>1$ and which is usually related with the onset of lactate production.

7. CONCLUSIONS AND PERSPECTIVES

In this paper a model for gas exchange dynamic during cycling has been proposed. An example of parameter identification and model validation were performed using real data from different scenarios with the same cyclist. The model includes a time-varying parameter which models the aerobic and anaerobic mode transitions for producing

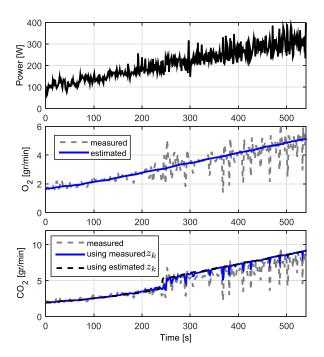


Fig. 7. Validation of the model using test 2, by considering z_k as a function of the estimated model states or z_k from measurements

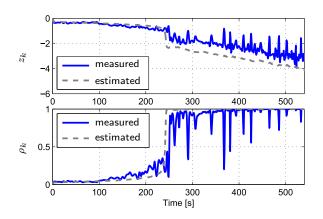


Fig. 8. Evolution of the index z_k and the varying parameter ρ_k during test 2. Comparison of the obtained index using real data or estimated one from the model.

mechanical power. This varying parameter also allows improve the model fit during mixed cases. Recovery dynamics after a high intensity workout is not power dependent (power is zero at this time), which turns difficult the fitting with the proposed model. Further work will treat this aspect.

The proposed model is relatively simple and can be used for both off-line and on-line bio-energetic dynamics simulation and/or filtration of available real-time data. It could be also useful for estimation and control of excess CO_2 .

This work can be considered as a first contribution in the modeling of gas exchange dynamics for future model-based control design. In addition, the model could be useful for non-invasive applications for monitoring physiological variables using few number of sensors. This aspect will be investigated in a future work.

ACKNOWLEDGEMENTS

This work was partially supported by the French CNRS PEPS 2017 in the context of the IMPROVED project.

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