Adaptive Kalman filter for on-line spectroscopic sensor corrections

Daniel Sbarbaro[1] and Tor Arne Johansen[2] and Jorge Yañez[3]

***Abstract*— Spectroscopic sensors provide online information about the composition and concentration of species in a sample by analyzing the interaction of light and matter. At the industrial scale, external variables such as temperature, pressure, and particle size distribution affect spectroscopic measurements. Thus, conventional quantitative analytical methods that do not consider these external factors provide poor estimates. Their effects have to be compensated through proper modeling and processing to improve the concentration estimation. This work presents an integrated discrete-time model considering the process dynamic and a physics-based sensor model. Then, we suggest a novel application of an adaptive Kalman filter to provide concentration estimates by correcting external factor effects. The convergence of the Kalman filter requires the fulfillment of uniform observability (persistent excitation) conditions for both inputs and external signals. Simulation results illustrate the modeling methodology and the main characteristics of the proposed Kalman filter approach for performing online correction of the spectroscopic sensor signals. The results show that the proposed adaptive Kalman filter can estimate concentrations with small error under temperature variations and measurement noise.**

I. Introduction

Spectroscopic sensors provide information about the composition of a sample by measuring and analyzing the radiation emitted, reflected, or transmitted by the sample. Sensors based on infrared and Raman spectral information are routinely used at the laboratory and industrial level for chemical analysis and process monitoring [1], [2]. Calibration methods usually perform quantitative analysis of the spectral information to estimate the concentration of a given component [3]. These methods are data-driven and they require a set of informative data for calibration. The calibration process is carried out offline.

In practice, physical interferences can affect the spectroscopic measurements. The effects produced by changes in temperature, viscosity, and optical path are, in general, nonlinear since they produce both additive and multiplicative deformations in the shape of the spectral response. For instance, [4] provides an overview of data-driven approaches to deal with the temperature influence on Near-infrared (NIR) spectra. Some of the representative algorithms are: Local and Global Partial Least-Squares calibration strategies [5], Extended Multiplicative Signal Correction, [6], Extended loading space standardization, and systematic error prediction [7]. On the other hand, several authors have proposed physics-based spectral methods to account for the physicochemical information of the elements [8][9]. These methods consider parametric models represented by a linear combination of peak functions having physicochemical significance. Under this approach, pure components can be modeled as parametrized peak models, accounting for nonlinear effects such as peak shifts and deformations. The sensor model combined with the process model leads to a nonlinear state space model. Kalman filters is the facto standard estimation method. Unfortunately, the model considered in this application does not have a standard structure, having a nonlinear output map with unknown parameters. However, following similar transformations as proposed for a continuous-time model in [10], the model can be transformed to a standard form with a time-variant linear output map. The design of Kalman filters for model structures similar to the one obtained in this application has been proposed by several authors. For instance, [11] offers an approach based on two interconnected Kalman-like filters and [12] one based on the combination of a Kalman filter and Recursive Least Square (RLS) algorithm. The main advantage of using a Kalman filter compared to an adaptive observer, such as the one presented in [13], is the convergence speed and the possibility of tuning the filter's dynamic. Hence, this work aims to combine parametric models based on a linear combination of peak functions and adaptive Kalman filter, as proposed by [12], to estimate the concentrations of components based on measurements affected by external factors. Thus, this contribution extends our previous work [10] to consider the discrete time implementation, more complex and realistic sensor models and the presence of disturbances. The paper's organization is as follows: Section 2 describes an integrated discrete-time model for the process dynamic and the spectroscopic information. Section 3 presents an adaptive Kalman filter for performing an online calibration. Section 4 provides a convergence analysis of the filter, considering the particular model structure to shade light over the conditions to be fulfilled. Section 5 illustrates the main characteristics of the proposed approach by addressing the problem of correcting the effect of an external variable over the mixture of two components. Conclusions and future works are summarized in section 6.

*This work was supported by Fondecyt project 1221225

[1]Daniel Sbarbaro is with Department of Electrical Engineering, Faculty of Engineering, Universidad de Concepcion, Concepcin, Chile dsbarbar@udec.cl

[2]Tor Arne Johansen with the Center for Autonomous Marine Operations and Systems (AMOS), Department of Engineering Cybernetics, Norwegian University of Science and Technology, Trondheim, Norway tor.arne.johansen@ntnu.no

[3]Jorge Yañez is with the Department of Analytical and Inorganic Chemistry, Faculty of Chemical Sciences, Universidad de Concepcion, Concepcin, Chile jyanez@udec.cl

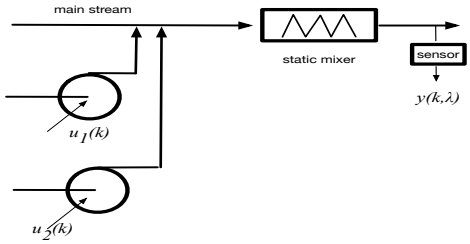

Fig. 1. Basic mixing process

II. Process and sensor modeling

Let us consider a mixing process where a constant main stream is mixed with several constituents as depicted in figure 1. The concentrations of each constituent are manipulated by the speed of peristaltic pumps and the resulting mixture is monitored by a spectroscopic sensor.

The process dynamic can be represented by a discrete-time linear model

$$\begin{aligned} x_j(k+1) &= \sum_{l=1}^{n} a_{jl}x_l(k) + \sum_{l=1}^{n_u} b_{jl}u_l(k) + \omega_j(k), \\ & \qquad j = 1,..,n \qquad (1) \\ w_i(k) &= \sum_{j=1}^{n} c_{ij}x_j(k), \qquad i = 1,...,m \end{aligned}$$

where n is the number of state variables, $x_j(k)$ are state variables, $u_l(k)$ input variables, $\omega_j(k)$ are input disturbances, and $w_i(k)$ concentrations. The constants a_{ij}, b_{ij}, and c_{ij} represent the parameters of the dynamical system. We also assume that the concentration of each constituent is manipulated by an independent input; i.e. the number of outputs is equal to the number of inputs, $m = n_u$. This model has demonstrated to represent adequately this process [14].

Thus, according to the Beer's law the relationship between the sensor output $y(k,\lambda) \in R$ and the constituent concentrations can be written as follows:

$$y(k,\lambda) = \sum_{i=1}^{m} w_i(k)\phi_i(\lambda, v(k)) \quad + d(\lambda) + \nu(k,\lambda), \qquad (2)$$

$$\lambda \in \Lambda, k \geqslant 0 \qquad (3)$$

where the variable $\lambda \in \Lambda$ represents the spectral coordinate as a wavelength value, Λ is the wavelength interval, $\phi_i(\lambda, v(k))$ is the absorbance of the $i-th$ element, $w_i(k)$ is the corresponding concentration, and $d(\lambda)$ a baseline offset. The output noise is noted as $\nu(k,\lambda)$. Notice that the absorbance of the different components is affected by an exogenous variable, $v(k)$. This baseline is sensor specific, and in practice the offset compensation can be performed off-line and therefore it will not be considered in this work.

Following physics-based methods [8], the absorbance model of the constituent considers a linear combination of N_i peaks functions

$$\phi_i(\lambda, v(k)) = \sum_{j=1}^{N_i} \alpha_{ij}(v(k))\psi_{ij}(\lambda) \qquad (4)$$

where $\psi_{ij}(\lambda)$ are peak functions required to model the i^{th} element, $\alpha_i(v(k))$ models the effect of the exogenous variable, $v(k)$, over constituent spectra.

Each linear coefficient can be modeled as a linear combination of known functions

$$\alpha_{ij}(v(k))) = \sum_{l=1}^{N_{\alpha_{ij}}} \beta_{ijl}\varphi_{ijl}(v(k)) \qquad (5)$$

where β_{ijl} are the calibrating factors and $\varphi_{ijl}(v(k))$ are a set of $N_{\alpha_{ij}}$ known functions.

Using equations (4) and (5), the sensor model (2) can be written as a linear parametrization in terms of the calibrating factors collected in a single vector $\boldsymbol{\theta} = [\beta_{111} \cdots \beta_{m\, N_m\, N_{\alpha_m\, N_n}}]^T$ as follows

$$y(k,\lambda) = \sum_{q=1}^{N_p} \theta_q \Psi_q(\lambda, v(k))\mathbf{w}(k) + \nu(k,\lambda) \qquad (6)$$

where $\Psi_q(\lambda, v(k))$ is a row vector having the cross products between $\varphi_{ijl}(v(k))$ and $\psi_{ij}(\lambda)$. The vector $\mathbf{w}(k) = [w_1(k),..,w_m(k)]^T$ is the concentration vector. The length of $\boldsymbol{\theta}$ is $N_p = \sum_{i=1}^{m}\sum_{j=1}^{N_i} N_{\alpha_{ij}}$.

Remark 1: The parametrization given by (6) can also accommodate models derived from data-driven methods. For instance, as suggested in [2], the effect of temperature over the absorbance of each element can be modeled as a second order polynomial; i.e. $\phi_i(\lambda, T(k))$

$$\phi_i(\lambda, T(k)) = \phi_{i0}(\lambda) + \phi_{i1}(\lambda)T(k) + \phi_{i2}(\lambda)T^2(k) \qquad (7)$$

where all the coefficients are wavelength dependent. These coefficients can be calculated by means of Standard Loading Space Standardization. However, this model can be casted as (6), if each wavelength dependent function $\phi_{ij}(\lambda)$ is modeled by a parametric model as follows:

$$\phi_{ij}(\lambda) = \sum_{l=1}^{l_j} c_{jl}\psi_{jl}(\lambda) \quad j = 0, 1, 2. \qquad (8)$$

where l_j is the number of basis functions $\psi_{jk}(\lambda)$ and c_{jk} are parameters to be estimated. The basis functions can be predefined using mathematical considerations or the available knowledge about the absorbance spectrum of each constituent; see for instance [15], [16]. □

Summarizing, equations (1) and (6) can be written as

$$\begin{aligned} \mathbf{x}(k+1) &= \mathbf{A}\mathbf{x}(k) + \mathbf{B}\mathbf{u}(k) + \boldsymbol{\omega}(k) \qquad (9) \\ \mathbf{w}(k) &= \mathbf{C}\mathbf{x}(k) \\ y(k,\lambda) &= \sum_{i=1}^{N_p} \theta_i \Psi_i(\lambda, v(k))\mathbf{w}(k) + \nu(k,\lambda) \end{aligned}$$

where $\mathbf{u}(k) = [u_1(k),..,u_{n_u}(k)]^T$, $\mathbf{x} = [x_1(k),..,x_n(k)]^T$, $\mathbf{w}(k) = [w_1(k),..,w_m(k)]^T$, $\boldsymbol{\omega}(k) = [\omega_1(k),..,\omega_m(k)]^T$ and $\Psi(\lambda, v(k)) = [\Psi_1(\lambda, v(k))....\Psi_{N_p}(\lambda, v(k))]$. Matrices $\mathbf{A} \in R^{n\times n}$, $\mathbf{B} \in R^{n\times m}$, and $\mathbf{C} \in R^{m\times n}$ define the state space model. Since the dynamic equations represent transportation and mixing dynamics, we also assume that $\mathbf{A}$

is Hurwitz. Equation (9) represents a linear dynamic model with a nonlinear output map given by the product of the concentrations, $\mathbf{w}(k)$, with the unknown parameters θ_i.

III. On-line correction

The on-line correction methods estimate the concentrations based on the spectral measurements, even though they are affected by exogenous variables. Thus the on-line calibration problem can be defined as follows:

Given the process and sensor models, equations (1) and (2) respectively, the measurements of $\mathbf{u}(k)$, $y(k,\lambda)$ and $v(k)$ estimate the concentrations $\mathbf{w}(k)$ and the calibration factors θ_i.

We consider the unknown parameters to satisfy the following equation

$$\theta_i(k+1) = \theta_i(k), \quad i = 1, \dots N_p \tag{10}$$

To obtain time-variant linear model, we define a new variable $\mathbf{q}_i(k) = \theta_i(k)\mathbf{x}(k)$, as in [17] for continuous-time, then by equation (10) it follows $\mathbf{q}_i(k+1) = \theta_i(k)\mathbf{x}(k+1)$. Thus, multiplying the recursive equation of (9) by $\theta_i(k)$ we obtain:

$$\begin{aligned} \mathbf{q}_i(k+1) &= \mathbf{A}\mathbf{q}_i(k) + \theta_i(k)\mathbf{B}\mathbf{u}(k) + \theta_i(k)\boldsymbol{\omega}(k) \\ y(k,\lambda) &= \textstyle\sum_{i=1}^{N_p} \Psi_i(\lambda, v(k))\mathbf{C}\mathbf{q}_i(k) + \nu(k,\lambda) \end{aligned} \tag{11}$$

Summarizing the dynamical equations and the output map:

$$\begin{aligned} \mathbf{x}(k+1) &= \mathbf{A}\mathbf{x}(k) + \mathbf{B}\mathbf{u}(k) + \boldsymbol{\omega}(k) \\ \theta_i(k+1) &= \theta_i(k), \quad i = 1, 2, ..N_p \\ \mathbf{q}_i(k+1) &= \mathbf{A}\mathbf{q}_i(k) + \theta_i(k)\mathbf{B}\mathbf{u}(k) + \theta_i(k)\boldsymbol{\omega}(k), \\ &\qquad i = 1, 2, ..N_p \\ y(k,\lambda) &= \sum_{i=1}^{N_p} \Psi_i(\lambda, v(k))\mathbf{C}\mathbf{q}_i(k) + \nu(k,\lambda) \end{aligned} \tag{12}$$

Remark 2: Model (12) is an overparametrized time-variant linear model representation of the non-linear model (9). The downside of the overparametrized model is that it neglects some of the relationships between redundant variables and also the nice state and output noise properties of the original model become quite complex and correlated. □

By defining $\mathbf{p} = [\mathbf{x} \;\; \mathbf{q}_1 \cdots \mathbf{q}_{N_p}]^T$ and $\boldsymbol{\theta} = [\theta_1 \;\; \cdots \theta_{N_p}]^T$ the system equations (12) can be written as

$$\begin{aligned} \mathbf{p}(k+1) &= \mathbf{A}_p\mathbf{p}(k) + \mathbf{B}_p\mathbf{u}(k) + \mathbf{B}_\theta(k)\boldsymbol{\theta}(k) \\ y(k,\lambda) &= \mathbf{C}_p(k,\lambda)\mathbf{p}(k) \end{aligned} \tag{13}$$

where

$$\mathbf{A}_p = \begin{bmatrix} \mathbf{A} & 0 & 0 & 0 \\ 0 & \mathbf{A} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \mathbf{A} \end{bmatrix} \quad \mathbf{B}_p = \begin{bmatrix} \mathbf{B} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{14}$$

,

$$\mathbf{B}_\theta(k) = \begin{bmatrix} 0 & 0 & 0 \\ \mathbf{B}\mathbf{u}(k) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \mathbf{B}\mathbf{u}(k) \end{bmatrix} \tag{15}$$

$$\begin{aligned} \mathbf{C}_p(k,\lambda) = [0 \;\; &\Psi_1(\lambda, v(k))\mathbf{C} \;\; \Psi_2(\lambda, v(k))\mathbf{C} \;\; \cdots \\ &\cdots \;\; \Psi_{N_p}(\lambda, v(k))\mathbf{C}] \end{aligned}$$

Augmenting the system with the dynamic of the parameters it follows:

$$\begin{bmatrix} \mathbf{p}(k+1) \\ \boldsymbol{\theta}(k+1) \end{bmatrix} = \begin{bmatrix} \mathbf{A}_p & \mathbf{B}_\theta(k) \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{p}(k) \\ \boldsymbol{\theta}(k) \end{bmatrix} + \begin{bmatrix} \mathbf{B}_p \\ \mathbf{0} \end{bmatrix} \mathbf{u}(k) \tag{16}$$

For this structure, Zhang [12] proposed an adaptive Kalman filter with different error dynamics for the state and parameters. The recursive equations for the estimates are:

$$\begin{aligned} \hat{\mathbf{p}}(k) = &\mathbf{A}_p\hat{\mathbf{p}}(k-1) + \mathbf{B}_p\mathbf{u}(k-1) + \mathbf{B}_\theta(k)\hat{\boldsymbol{\theta}}(k-1) + \\ &\mathbf{K}(k)e(k) + \Upsilon(k)[\hat{\boldsymbol{\theta}}(k) - \hat{\boldsymbol{\theta}}(k-1)] \\ \hat{\boldsymbol{\theta}}(k) = &\hat{\boldsymbol{\theta}}(k-1) + \Gamma(k)e(k) \end{aligned}$$

where the estimation error is

$$\begin{aligned} e(k) = &y(k,\lambda) - \mathbf{C}_p(k,\lambda)[\mathbf{A}_p\hat{\mathbf{p}}(k-1) + \mathbf{B}_p\mathbf{u}(k) \\ &+ \mathbf{B}_\theta(k)\hat{\boldsymbol{\theta}}(k-1)] \end{aligned}$$

The gain matrix $\mathbf{K}(k)$ associated to the state is updated as follows:

$$\begin{aligned} \mathbf{P}(k|k-1) &= \mathbf{A}\mathbf{P}(k-1|k-1)\mathbf{A}^T + \mathbf{Q} \\ \Sigma(k) &= \mathbf{C}_p(k,\lambda)\mathbf{P}(k|k-1)\mathbf{C}_p(k,\lambda)^T + \mathbf{R} \\ \mathbf{K}(k) &= \mathbf{P}(k|k-1)\mathbf{C}_p(k,\lambda)^T\Sigma(k)^{-1} \\ \mathbf{P}(k|k) &= [\mathbf{I} - \mathbf{K}(k)\mathbf{C}_p(k,\lambda)]\mathbf{P}(k|k-1) \end{aligned}$$

where $\mathbf{Q}$ and $\mathbf{R}$ in a deterministic setting can be considered as tuning parameters.

The gain matrix $\Gamma(k)$ associated to the parameters update is given by the following recursive equations:

$$\begin{aligned} \Upsilon(k) &= [\mathbf{I} - \mathbf{K}(k)\mathbf{C}_p(k,\lambda)]\mathbf{A}\Upsilon(k-1) \\ &\quad + [\mathbf{I} - \mathbf{K}(k)\mathbf{C}_p(k,\lambda)]\mathbf{B}_\theta(k) \\ \Omega(k) &= \mathbf{C}_p(k,\lambda)\mathbf{A}\Upsilon(k-1) + \mathbf{C}_p(k,\lambda)\mathbf{B}_\theta(k) \\ \Lambda(k) &= [\gamma\Sigma(k) + \Omega(k)\mathbf{S}(k-1)\Omega(k)^T]^{-1} \\ \Gamma(k) &= \mathbf{S}(k-1)\Omega(k)^T\Lambda(k) \\ \mathbf{S}(k) &= \frac{1}{\gamma}\mathbf{S}(k-1) - \frac{1}{\gamma}\mathbf{S}(k-1)\Omega(k)^T\Lambda(k)\Omega(k)\mathbf{S}(k-1) \end{aligned}$$

where $\Upsilon(k)$ is an auxiliary variable and $\gamma \in (0,1)$ is a forgetting factor.

Remark 3: Tuning matrices $\mathbf{Q}$ and $\mathbf{R}$ can be challenging since they can no longer be associated with the noise covariances due to the model's overparametrization. Hence, it is worth exploring approaches without overparametrized models, such as the Double Kalman Filter (DKF) approach [18]. As future work, we will explore the DKF discrete versions [19] and [20] to improve performance and ease filter tuning. □

IV. Convergence properties

The Kalman filter will converge if a set of key assumptions associated to the model structure and persistency of excitation are satisfied [12]. These conditions depend on the structure of the system and the input signals; i.e. $\mathbf{u}(k)$ and $v(k)$.

Assumption 1: The pairs $[\mathbf{A},\ \mathbf{C}_p(k,\lambda)]$ and $[\mathbf{A},\ \mathbf{Q}]$ are uniformly completely observable and controllable, respectively.

The conditions for uniform observability and controllability are defined in terms of the the controllability and observability Grammians, which are defined as follows

$$W_c(k,k_0) = \sum_{i=k_0}^{k} \Phi(k,i+i)\mathbf{Q}\mathbf{Q}^T\Phi^T(k,i+i) \tag{17}$$

$$W_o(k,k_0) = \sum_{i=k_0+1}^{k} \Phi^T(i,k_0)\mathbf{C}_p(k,\lambda)^T\mathbf{C}_p(k,\lambda)\Phi(i,k_0) \tag{18}$$

where $k \geq k_0 \geq 0$ and $\Phi(k,k_0) = \mathbf{A}^{k-k_0}$.

The pair $[\mathbf{A},\ \mathbf{Q}]$ is uniformly completely controlable if there exits constants $c_c \in \mathbb{R}$ and $N_c \in \mathbb{N}$ such that

$$W_c(k+N,k) \geq c_c\mathbf{I}\ \ \forall k \geq 0 \tag{19}$$

Given that $\mathbf{A}$ is Hurwitz, it is always possible to chose a positive definite matrix $\mathbf{Q}$ so that the pair $[\mathbf{A},\ \mathbf{Q}]$ satisfies (19).

On other hand, the pair $[\mathbf{A},\ \ \mathbf{C}_p(k,\lambda)]$ is uniformly completely observable if there exits constants $c_o \in \mathbb{R}$ and $N_o \in \mathbb{N}$ such that

$$W_o(k+N_o,k) \geq c_o\Phi^T(k+N_o,k)\Phi(k+N_o,k)\ \ \forall k \geq 0 \tag{20}$$

This condition imposes a constraint over $\mathbf{C}_p(k,\lambda)$ so that (20) is satisfied. Since $\mathbf{C}_p(k,\lambda)$ depends on $v(k)$, it means that the exogenous signal must satisfy a kind of persistently excitation condition.

Finally, the last assumption deals with the evolution of the regressor term in (13) and imposes conditions over the input signal, $\mathbf{u}(k)$.

Assumption 2: The input signal $\mathbf{u}(k)$ is persistently exciting in the sense that exists an integer $h > 1$ and a constant $\alpha \in R$ such that $\sum_{l=0}^{h-1} \Omega^T(k+l)\Sigma(k+l)^{-1}\Omega(k+l) \geq \alpha\mathbf{I}_p\ \ \forall k \geq 0$

Remark 4: The assumptions 1 and 2 require the input and external variable satisfy persistent excitation condition; which in practice is not always satisfied. Recent works have addressed this problem [21] [22], and the analysis of these approaches in the context of this application is subject of future work. □

V. Simulation results

To illustrate the main ideas, we consider a simulated mixing example of two components. These components are mixed in a static mixer. A spectrometer measures the spectra at the output of the mixing stage, as depicted in figure 1,

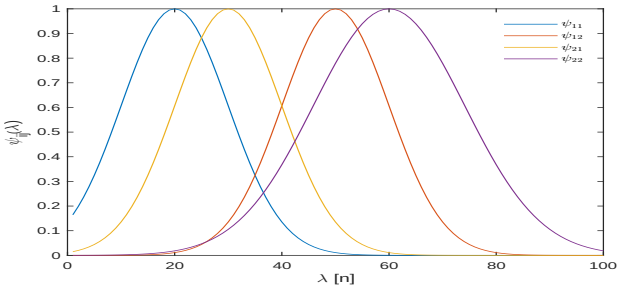

Fig. 2. Basis spectral response of each component

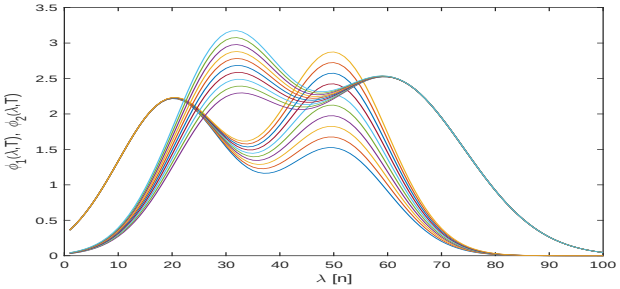

Fig. 3. Spectral response of each component for different temperature.

where $F(t)$ is the main stream, $u_1(t)$ and $u_2(t)$ are the flow rates of each component, $v(t)$ is the mixture temperature and $y(t,\lambda)$ is the measured spectra.

The absorbance of each component is modeled as a linear combination of two gaussian peaks, depicted in figure 2. The effects of the external variable $v(k)$ on the absorbance of each component are depicted in figure 3. These are described by the following equations:

$$\begin{aligned}\phi_1(\lambda,v(k)) &= \theta_1\psi_{11}(\lambda) + (\theta_2+\theta_3 v(k))\psi_{12}(\lambda) \\ \phi_2(\lambda,v(k)) &= (\theta_4+\theta_5 v(k))\psi_{21}(\lambda) + \theta_6\psi_{22}(\lambda)\end{aligned} \tag{21}$$

and illustrated in . Functions $\psi_{ij}(\lambda)$ represents gaussian peaks associated to the model of each component i. The parameters nominal values are $\theta = [2.2\ \ -1.5\ \ 0.15\ \ -0.02\ \ 0.1\ \ 2.5]^T$ and the vectors $\Psi_i(\lambda,v(k))$ are:

$$\Psi_1 = \begin{bmatrix}\psi_{11}(\lambda)\\ 0\end{bmatrix},\ \Psi_2 = \begin{bmatrix}\psi_{12}(\lambda)\\ 0\end{bmatrix},\ \Psi_3 = \begin{bmatrix}\psi_{12}(\lambda)v(k)\\ 0\end{bmatrix} \tag{22}$$

$$\Psi_4 = \begin{bmatrix}0\\ \psi_{21}(\lambda)\end{bmatrix},\ \Psi_5 = \begin{bmatrix}0\\ \psi_{21}(\lambda)v(k)\end{bmatrix},\ \Psi_6 = \begin{bmatrix}0\\ \psi_{22}(\lambda)\end{bmatrix}$$

The sensor model combines the absorbance spectra of each components and the temperature effects; i.e.

$$y(\lambda,v(k)) = w_1(k)\phi_1(\lambda,v(k)) + w_2(k)\phi_2(\lambda,v(k)) \tag{23}$$

Using (21) and (22), the sensor model can be written as a linear in the parameter model as (6).

The dynamics representing the transport and mixing of the two componentes is modeled by a discrete space state model obtained for a sampling time of one second and having the

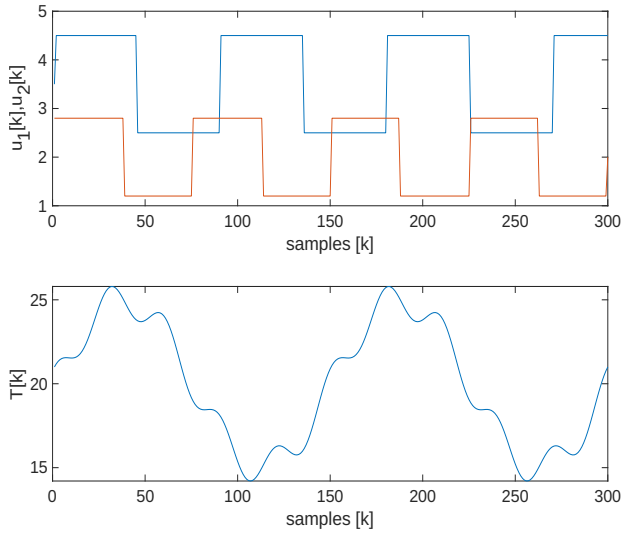

Fig. 4. Input variables and external variable.

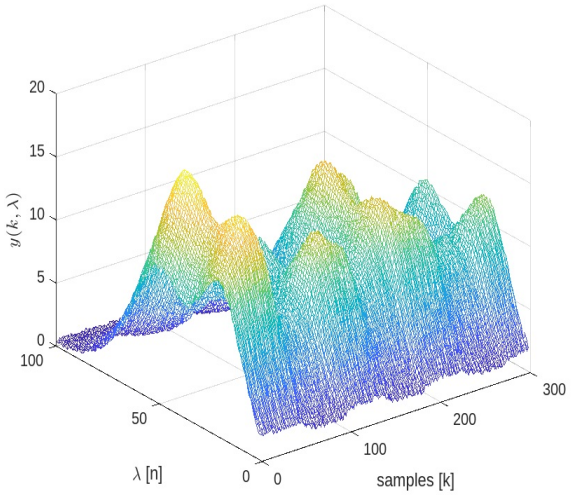

Fig. 5. Spectral response

following parameters

$$\mathbf{A} = \begin{bmatrix} 1.6 & -0.8 & 0 & 0 \\ 0.8 & 0 & 0 & 0 \\ 0 & 0 & 1.7 & -0.85 \\ 0 & 0 & 0.85 & 0 \end{bmatrix} \mathbf{B} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad (24)$$

$$\mathbf{C} = \begin{bmatrix} 0 & 0.05 & 0 & 0 \\ 0 & 0 & 0 & 0.0265 \end{bmatrix} \quad (25)$$

In addition, zero mean gaussian disturbances are considered in both the sensor measurements and the state equations, with variances $\sigma_\nu = 0.5$ and $\sigma_\omega = 0.1$ respectively.

The simulations consider a sampling time of one second and step changes in the flow-rates of each components and periodic variation in external variable, as shown in figure 4. The effect of these changes and the disturbances noises over the spectral response can be seen in figure 5.

The matrix $\mathbf{Q} = 10^{-4}\mathbf{I}$ was chosen to be a constant diagonal matrix, $\mathbf{P}(0) = 10^{3}\mathbf{I}$ and $\lambda = 0.9$. The observer initial conditions states are set to zero. The estimated concentrations converge fast to the real values. However, the convergence of some parameters are slower, as shown in figure 6. The variability of the input variables; i.e. flow rates and temperature, ensures the convergence of estimated concentrations and parameters, as seen in figure 6. The state error asymptotically converges to zero as depicted in figure 7.

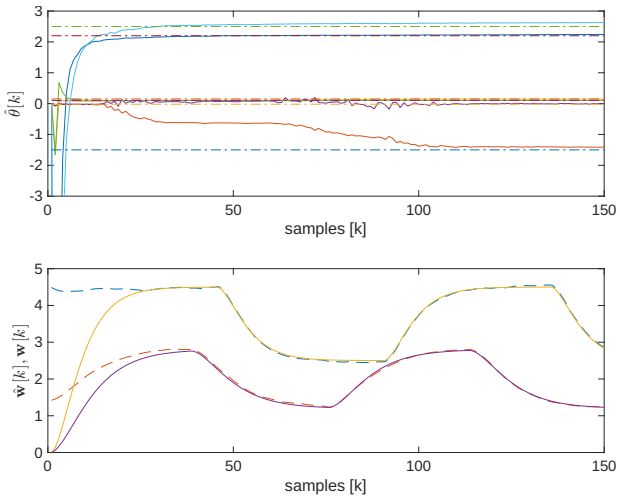

Fig. 6. Parameters and concentrations evolution. Solid line: estimated values

VI. Final Remarks

The problem of online correction of spectroscopic measurements subject to external perturbations is critical from a practical point of view. This work has proposed a novel discrete-time correction algorithm based on an adaptive Kalman filter for spectroscopic applications. The algorithm estimates the system states and the calibration factors associated with the sensor model considering the effects of external variables. The conditions for ensuring the asymptotic convergence of the Kalman filter imposes persistent excitation condition over the input and external variables. Since these conditions for online applications are not always satisfied, we will analyze relaxed convergence conditions to ensure the graceful degradation of the filter performance induced by the lack of excitation. In addition, we will also explore the use discrete DKF filters to improve performance and ease filter tuning.

A simple mixing simulation example has illustrated the sensor model's principal elements and shown the Kalman filter's performance under the presence of zero mean gaussian disturbances. The estimated concentrations converge fast with small error. These results are encouraging, and we will

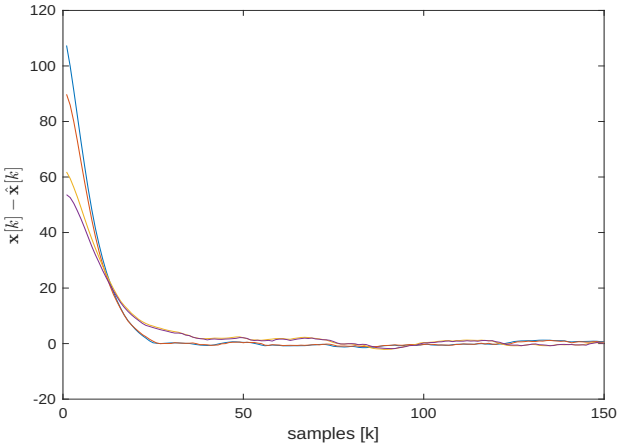

Fig. 7. State error.

further work on their real-time validation in a laboratory setup for NIR and Raman applications.

REFERENCES

[1] K. A. Bakeev., Ed., *Process analytical technology*. Oxford: Blackwell Publishing Ltd, 2005.

[2] Z. Chen, D. Lovett, and J. Morris, "Process analytical technologies and real time process control a review of some spectroscopic issues and challenges," *Journal of Process Control*, vol. 21, no. 10, pp. 1467–1482, 2011.

[3] H. Mark and J. Workman Jr., *Chemometrics in Spectroscopy*. Elsevier, 2007.

[4] J. Hageman, J. Westerhuis, and A. Smilde, "Temperature robust multivariate calibration: An overview of methods for dealing with temperature influences on near infrared spectra," *J. Near Infrared Spectrosc.*, vol. 13, no. 2, pp. 53–62, Apr 2005. [Online]. Available: https://opg.optica.org/jnirs/abstract.cfm?URI=jnirs-13-2-53

[5] F. Wülfert, W. Kok, and A. Smilde, "Influence of temperature on vibrational spectra and consequences for the predictive ability of multivariate models," *Analytical Chemistry*, vol. 70, no. 9, pp. 1761–1767, 1998.

[6] H. Martens and E. Stark, "Extended multiplicative signal correction and spectral interference subtraction: new preprocessing methods for near infrared spectroscopy," *Journal of Pharmaceutical and Biomedical Analysis*, vol. 9, no. 8, pp. 625–635, 1991.

[7] Z. Chen, J. Morris, and E. Martin, "Modelling temperature-induced spectral variations in chemical process monitoring," in *IFAC Proceedings Volumes*, vol. 37, no. 9, 2004, pp. 553–558.

[8] F. Alsmeyer, H.-J. Koß, and W. Marquardt, "Indirect spectral hard modeling for the analysis of reactive and interacting mixtures," *Applied Spectroscopy*, vol. 58, no. 8, pp. 975–985, 2004, pMID: 18070391. [Online]. Available: https://doi.org/10.1366/0003702041655368

[9] J. Wöhl, W. A. Kopp, I. Yevlakhovych, L. Bahr, H.-J. Koss, and K. Leonhard, "Completely computational model setup for spectroscopic techniques: The ab initio molecular dynamics indirect hard modeling approach," *The Journal of Physical Chemistry A*, vol. 126, no. 18, pp. 2845–2853, 2022, pMID: 35476427. [Online]. Available: https://doi.org/10.1021/acs.jpca.2c01061

[10] D. Sbarbaro and T.-A. Johansen, "On-line calibration of spectroscopic sensors based on state observers," *IFAC-PapersOnLine*, vol. 53, no. 2, pp. 11 681–11 685, 2020, 21st IFAC World Congress.

[11] A. Ticlea and G. Besancon, "Adaptive observer design for discrete time ltv systems," *International Journal of Control*, vol. 89, no. 12, pp. 2385–2395, 2016. [Online]. Available: https://doi.org/10.1080/00207179.2016.1157901

[12] Q. Zhang, "Adaptive Kalman filter for actuator fault diagnosis," *Automatica*, vol. 93, pp. 333–342, 2018.

[13] A. Guyader and Q. Zhang, "Adaptive observer for discrete time linear time varying systems," *IFAC Proceedings Volumes*, vol. 36, no. 16, pp. 1705–1710, 2003, 13th IFAC Symposium on System Identification (SYSID 2003), Rotterdam, The Netherlands, 27-29 August, 2003.

[14] T. A. Johansen and D. Sbarbaro, "Lyapunov-based optimizing control of nonlinear blending processes," *IEEE Transactions on Control Systems Technology*, vol. 13, no. 4, pp. 631–638, 2005.

[15] J. Dubrovkin, *Mathematical Processing of Spectral Data in Analytical Chemistry*. Cambridge Scholars Publishing, 2018.

[16] T. Kärnä, F. Corona, and A. Lendasse, "Gaussian basis functions for chemometrics," *Journal of Chemometrics*, vol. 22, no. 11-12, pp. 701–707, 2008.

[17] D. D. Martino, A. Germani, C. Manes, and P. Palumbo, "State observers for systems with linear state dynamics and polynomial output," in *43rd IEEE Conference on Decision and Control*, 2004, pp. 3886–3891.

[18] T. A. Johansen and T. I. Fossen, "Nonlinear filtering with exogenous kalman filter and double kalman filter," in *2016 European Control Conference (ECC)*, 2016, pp. 1722–1727.

[19] M. Abdollahpouri, M. Haring, T. A. Johansen, G. Takács, and B. Rohaľ-Ilkiv, "Nonlinear state and parameter estimation using discrete-time double kalman filter," *IFAC-PapersOnLine*, vol. 50, no. 1, pp. 11 632–11 638, 2017, 20th IFAC World Congress.

[20] M. Abdollahpouri, M. Haring, T. A. Johansen, G. Takács, and B. Rohal'-Ilkiv, "Double moving horizon estimation: Linearization by a nonlinear transformation," in *2018 European Control Conference (ECC)*, 2018, pp. 1148–1153.

[21] A. Pyrkin, T. M. Son, N. Q. Cuong, and M. Sinetova, "Adaptive observer design for time-varying systems with relaxed excitation conditions*," *IFAC-PapersOnLine*, vol. 55, no. 12, pp. 312–317, 2022, 14th IFAC Workshop on Adaptive and Learning Control Systems ALCOS 2022.

[22] V. Rodrigo Marco, J. C. Kalkkuhl, J. Raisch, and T. Seel, "Regularized adaptive Kalman filter for non-persistently excited systems," *Automatica*, vol. 138, p. 110147, 2022.