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A New Spinach Respiratory Prediction Method Using Particle Filtering Approach

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ABSTRACT Nowadays, agricultural and food technology require the integration of advanced computer technology and sophisticated computational approach for enhancing the characterization and quality of produces and their products. Huge amount of data was gathered and it needs to be processed and analyzed with confidence that the useful information is being extracted accurately. Therefore, sophisticated computing methods are the most important parts of the overall system. Particle filtering has been recognized as an efficient tool to deliver the accurate state model prediction especially in highly nonlinear and non-Gaussian dynamical systems. In this work, a particle filter (PF) was designed for parameter estimation of respiratory of spinach storage under modified atmosphere. The Michaelis-Menten model was examined in this work for spinach respiratory mechanism under different atmospheric storage conditions to illustrate the performance of the method. The estimating results from the PF were compared to the conventional estimation techniques widely used in literature. From the experimental and computational results, we found that the particle filtering method delivers higher accuracy, outperforming the existing conventional regression method and the extended Kalman filter.

INDEX TERMS Particle filter, Bayesian filtering, spinach, respiration, Michaelis-Menten model.

I. INTRODUCTION

Spinach (*Spinacia oleracea L.*), one of leafy vegetables, is ranked as a high nutrients food [1]. Its demand and production has been increasing recently. It is classified as a high respiration rate vegetable and susceptible to deterioration during transportation and storage. Respiration is an important metabolism causing the deterioration of fruits and vegetables after harvest. This process consumes O_2 in a series of enzymatic reactions to produce CO_2 and water, with release of energy. Therefore, this process must be reduced or controlled in order to diminish fresh produces deterioration. Modified atmosphere package (MAP) is a method used to reduce respiration rate and prolong shelf-life of fruits and vegetables. This technique relies on the modification of the atmosphere inside the package, typically into low level of O_2 and high level of CO_2 , resulting from respiration and gases exchange through packaging material [2]–[4]. However, the drawback of low O_2 packages is that a shift from aerobic respiration to fermentation when the O_2 concentration becomes lower

than lower O_2 limit and this leads to undesirable reactions [5], [6]. Therefore, modified atmosphere package should be carefully designed. In designing the MAP, respiration rate modelling is crucial depending on several factors, such as the produce characteristics, its mass, atmosphere composition, temperature and also permeability of the packaging materials; these factors should be taken into consideration [2], [7]. In this work, we consider a Michaelis-Menten model, an enzyme kinetics based model, that is generally used to describe the respiration of fresh fruits and vegetables. In this model, the reaction rate is controlled by one limiting enzyme reaction where O_2 is considered as a limiting substrate and CO_2 is a product of the reaction [2], [6], [8]. In MAP, this model is used to predict the dynamic change of gas composition in the package during storage and distribution chain. Therefore, Michaelis-Menten model can be used as a model of high respiration rate sample for capturing the respiration rate of spinach in this study [9], [10].

Particle filtering (PF) can be often referred to as data assimilation technique to seek for estimating the posterior probability density of the parameters where the observation or measurement data related to the estimating parameters

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is available. It has been received a great attention by researchers from various disciplines including the agriculture and food industry. Its popularity for parameter estimation and tracking problems can be found from many applications ranging from ocean acoustics, hydrology, speech processing, finance, and agricultures [11]–[16]. Efficient parameter estimation is important for tackling the challenges of model-based smart agriculture which is the crucial part of agricultural systems in the era of big data analytic over the intelligent system.

In literature, respiration rate models can be either theoretical-based or empirical best fitted models. Theoretical-based model method is frequently considered in respiration problems [17], [18]. To obtain the parameters involving the respiration of the produces, this approach is conventionally employed via regression analysis [7], [8], [17], [19]. To the best of our knowledge, a PF approach for spinach respiratory prediction has not been seen in literature. Therefore, the novelty of this work is the analysis and implementation of a PF for the prediction of spinach respiratory parameters in order to achieve better prediction results, respiration rate and O_2 concentration, in particular.

The rest of this paper is organized as follows. Section II describes a general concept of sequential Bayesian filtering and particle filtering, followed by a particle filtering. In section III, a particle filtering implementation for respiration rate and O_2 concentration estimation will be explained. Simulation results are discussed in Section IV. Conclusions can be found in Section V.

II. MATERIALS AND METHODS

A. SEQUENTIAL BAYESIAN FILTERING

The first step in sequential Bayesian framework is to represent the parameters of interest and the measurement data by the state-space transition and observation equations as

$$\mathbf{x}_n = f_n(\mathbf{x}_{n-1}) + \mathbf{v}_{n-1}, \quad (1)$$

and

$$\mathbf{y}_n = g_n(\mathbf{x}_n) + \mathbf{w}_n, \quad (2)$$

where n is time. The functions f_n and g_n are called the state transition or system function, and observation or measurement function, respectively. It should be noted that both functions are typically available. In practice, they are mostly nonlinear functions. Quantities \mathbf{v}_n and \mathbf{w}_n are process and measurement noise vectors. Both noise characteristics are known. Vectors \mathbf{x}_n and \mathbf{y}_n represent state and measurement vectors, respectively. Equation (1) describes how the state vector is updated from the previous time step, while Eq. (2) projects the relationship of the state vector and the measured data. In agriculture and especially for the produce properties, the state vector contains the parameters of the investigating model that we wish to estimate. The goal is to estimate the state vector \mathbf{x}_n using the measurement data \mathbf{y}_n obtained from the fields, farm, laboratory, or sensors at the working place.

In this work, the data was gathered from the experiments in the laboratory.

Let $p(\cdot|\cdot)$ stands for a generic conditional probability distribution, and symbol \sim for 'distributed as'. In the Bayesian approach, the transition equation is the evolution of the state and we can consider it as

$$\mathbf{x}_n \sim p(\mathbf{x}_n|\mathbf{x}_{n-1}). \quad (3)$$

Moreover, the measurement equation that constructs the likelihood function is given by

$$\mathbf{y}_n \sim p(\mathbf{y}_n|\mathbf{x}_n). \quad (4)$$

Equation (3) is referred to the transition density, the propagation of the state vector \mathbf{x}_n is propagated according to this density. PF takes this density as the importance density which can be considered as the prior for importance sampling. Let $\mathbf{Y}_n = [\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n]$ contains the measurement data up to time n . Equations (3) and (4) allow us to compute the probability density function of the state \mathbf{x}_n , i.e., $p(\mathbf{x}_n|\mathbf{Y}_n)$ by using Chapman-Kolmogorov equation and Bayes' rule as

$$\begin{aligned} p(\mathbf{x}_n|\mathbf{Y}_{n-1}) &= \int p(\mathbf{x}_n|\mathbf{x}_{n-1}, \mathbf{Y}_{n-1})p(\mathbf{x}_{n-1}|\mathbf{Y}_{n-1})d\mathbf{x}_{n-1} \\ &= \int p(\mathbf{x}_n|\mathbf{x}_{n-1})p(\mathbf{x}_{n-1}|\mathbf{Y}_{n-1})d\mathbf{x}_{n-1}, \end{aligned} \quad (5)$$

then,

$$p(\mathbf{x}_n|\mathbf{Y}_n) = \frac{p(\mathbf{y}_n|\mathbf{x}_n)p(\mathbf{x}_n|\mathbf{Y}_{n-1})}{p(\mathbf{y}_n|\mathbf{Y}_{n-1})}, \quad (6)$$

where $p(\mathbf{y}_n|\mathbf{x}_n)$ is the likelihood at time step n , $p(\mathbf{x}_n|\mathbf{Y}_{n-1})$ is the prior distribution, and $p(\mathbf{y}_n|\mathbf{Y}_{n-1})$ is the normalization factor and it can be computed as

$$p(\mathbf{y}_n|\mathbf{Y}_{n-1}) = \int p(\mathbf{y}_n|\mathbf{x}_n)p(\mathbf{x}_n|\mathbf{Y}_{n-1})d\mathbf{x}_n \quad (7)$$

The posterior probability density function (PDF) of the state variable is available from the sequential update given above, the interferences on the state can then be employed from this distribution. The expected value of the function and the covariance matrix $\mathbf{C}_n^{\mathbf{xx}}$ of the state can be computed by

$$\begin{aligned} \widehat{F(\mathbf{x}_n)} &= \mathbf{E}_{p(\mathbf{x}_n|\mathbf{Y}_n)}[F(\mathbf{x}_n)|\mathbf{Y}_n] \\ &= \int F(\mathbf{x}_n)p(\mathbf{x}_n|\mathbf{Y}_n)d\mathbf{x}_n, \end{aligned} \quad (8)$$

and

$$\mathbf{C}_n^{\mathbf{xx}} = \int (\mathbf{x}_n - \widehat{\mathbf{x}}_n)(\mathbf{x}_n - \widehat{\mathbf{x}}_n)^T p(\mathbf{x}_n|\mathbf{Y}_n)d\mathbf{x}_n, \quad (9)$$

respectively. The feasibility in computing the multi-dimensional integration to obtain the closed form of Eq. (6) is very limited for only the cases of linear systems and Gaussian noise assumption.

The Kalman filter (KF), a filter that is known as the very first filter designed for sequential Bayesian filtering under the linear and Gaussian assumption fails to deliver a successful parameter estimation [20], [21]. It is not a case that the problem that is investigating falls in the linear and

Gaussian category. Although KF variants were implemented [22]–[25] to handle these difficulties, KF family cannot provide satisfactory results for most cases. For practical treatment of utilizing the sequential Bayesian framework, a set of samples within the range of estimation is used to approximate the posterior distribution. Alternatively, the technique that represents a probability distribution using a set of random numbers with their associated weights, known as particle filtering method, was proposed to overcome these limitations. We will discuss this approach in the next subsection.

B. PARTICLE FILTERING

For particle filtering, the recursive propagation of the posterior density can be done using a discrete random measurements to approximate the continuous distribution. Let $\Gamma = \{\mathbf{x}_n^i, w_n^i\}_{i=1}^N$ be a set of random vector and scalar, where N is number of particles; \mathbf{x}_n^i is the i th particle and w_n^i is its corresponding weight. The weight of each particle corresponds to its probability. From Eq. (5), we have

$$\begin{aligned} p(\mathbf{x}_n | \mathbf{Y}_{n-1}) &= \int p(\mathbf{x}_n | \mathbf{x}_{n-1}, \mathbf{y}_{n-1}) p(\mathbf{x}_{n-1} | \mathbf{y}_{n-1}) d\mathbf{x}_{n-1} \\ &= \int p(\mathbf{x}_n | \mathbf{x}_{n-1}) p(\mathbf{x}_{n-1} | \mathbf{y}_{n-1}) d\mathbf{x}_{n-1} \\ &= \int p(\mathbf{x}_n | \mathbf{x}_{n-1}) \sum_{i=1}^N w_{n-1}^i \delta(\mathbf{x}_{n-1} - \mathbf{x}_{n-1}^i) d\mathbf{x}_{n-1} \\ &= \sum_{i=1}^N w_{n-1}^i \int p(\mathbf{x}_n | \mathbf{x}_{n-1}) \delta(\mathbf{x}_{n-1} - \mathbf{x}_{n-1}^i) d\mathbf{x}_{n-1} \\ &= \sum_{i=1}^N w_{n-1}^i p(\mathbf{x}_n | \mathbf{x}_{n-1}^i). \end{aligned} \quad (10)$$

Using this setting, the posterior PDF can be approximated by [26], [27]

$$p(\mathbf{x}_n | \mathbf{y}_n) \approx \sum_{i=1}^N w_n^i \delta(\mathbf{x}_n - \mathbf{x}_n^i), \quad (11)$$

where $\delta(\cdot)$ denotes the Dirac delta function. It can be seen obviously that the expectation of the state vector is obtained as

$$\hat{\mathbf{x}}_n = \sum_{i=1}^N w_n^i \mathbf{x}_n^i. \quad (12)$$

According to Eq. (3), we take a sample \mathbf{x}_n^i from $p(\mathbf{x}_n^i | \mathbf{x}_{n-1}^i)$ which is equivalent to propagating the state vector at time $n-1$, \mathbf{x}_{n-1}^i , to the new value at time n . Taking samples from the posterior is not feasible, an alternative way is to use a sequential proposal density to produce a set of particles in such a way that the ratio between the posterior density and the proposal density is defined as w_n^i . Therefore, to approximate $p(\mathbf{x}_n | \mathbf{y}_n)$ using $\{\mathbf{x}_n^i\}_{i=1}^N$, we draw samples from an importance density $q(\mathbf{x}_n | \mathbf{y}_n)$ and their weights can be defined as

$$w_n^i \propto \frac{p(\mathbf{x}_n^i | \mathbf{y}_n)}{q(\mathbf{x}_n^i | \mathbf{y}_n)}. \quad (13)$$

If we use the results from the previous step, and select the following importance density

$$q(\mathbf{x}_n | \mathbf{y}_n) = q(\mathbf{x}_n | \mathbf{x}_{n-1}, \mathbf{y}_n) q(\mathbf{x}_{n-1}, \mathbf{y}_{n-1}), \quad (14)$$

we can then obtain the posterior PDF as:

$$p(\mathbf{x}_n | \mathbf{y}_n) = \frac{p(\mathbf{y}_n | \mathbf{x}_n) p(\mathbf{x}_n | \mathbf{x}_{n-1})}{p(\mathbf{y}_n | \mathbf{y}_{n-1})} p(\mathbf{x}_{n-1}, \mathbf{y}_{n-1}). \quad (15)$$

By substituting Eqs. (14)–(15) into Eq. (13), the weight of the i th particle at time step n can be given as [27]:

$$w_n^i \propto \frac{p(\mathbf{x}_{n-1}^i | \mathbf{y}_{n-1}) p(\mathbf{y}_n | \mathbf{x}_n^i) p(\mathbf{x}_n | \mathbf{x}_{n-1}^i)}{q(\mathbf{x}_{n-1}^i | \mathbf{y}_{n-1}) q(\mathbf{x}_n^i | \mathbf{x}_{n-1}^i, \mathbf{y}_n)}, \quad (16)$$

or

$$w_n^i \propto w_{n-1}^i \frac{p(\mathbf{y}_n | \mathbf{x}_n^i) p(\mathbf{x}_n^i | \mathbf{x}_{n-1}^i)}{q(\mathbf{x}_n^i | \mathbf{x}_{n-1}^i, \mathbf{y}_n)}. \quad (17)$$

In the sequential importance sampling (SIS) PF, the importance density $q(\mathbf{x}_n | \mathbf{x}_{n-1}, \mathbf{y}_n) = p(\mathbf{x}_n | \mathbf{x}_{n-1})$ is chosen to minimize the importance sampling error [28]. A simple variant of the SIS can be obtained by choosing the transition density as:

$$q(\mathbf{x}_n | \mathbf{x}_{n-1}, \mathbf{y}_n) = p(\mathbf{x}_n | \mathbf{x}_{n-1}), \quad (18)$$

which is independent of the current observation \mathbf{y}_n [29]. From this choice, the weight of Eq. (17) is finally expressed as

$$w_n^i \propto p(\mathbf{y}_n | \mathbf{x}_n^i) w_{n-1}^i, \quad (19)$$

with the condition $\sum_{i=1}^N w_n^i = 1$. The process just described above is referred to sequential importance sampling (SIS) algorithm.

A common problem with the SIS particle filter is that, after a few iterations, the weights of most particles are negligible and few particles with large weights are survived. The variance of the importance weights always increase over time, causing the problem of degeneracy [30]. This loss of sample diversity may result in poor filtering performance. To remedy this problem, a second sampling stage called resampling is used. It creates more significant weight particles from the original set of particles to obtain a better quality set of particles, this process is called sequential importance resampling (SIR) [31]–[33], and this stage is widely used in most PF applications. A block diagram of the SIR particle filter is shown in Fig. 1.

III. PARTICLE FILTER FOR RESPIRATION RATE MODEL

A. THE MICHAELIS-MENTEN MODEL

Based on the performance in describing the spinach respiration as reported in [6], the Michaelis-Menten Model without Inhibition is considered for interpreting the respiratory metabolism and employed for the validation of the particle filtering method. The model is given by

$$r_{O_2} = \frac{r_{max} [O_2]}{K + [O_2]}, \quad (20)$$

where r_{O_2} is oxygen consumption rate in mmols/kg-hour, $[O_2]$ is oxygen concentration in mmols/l, r_{max} represents

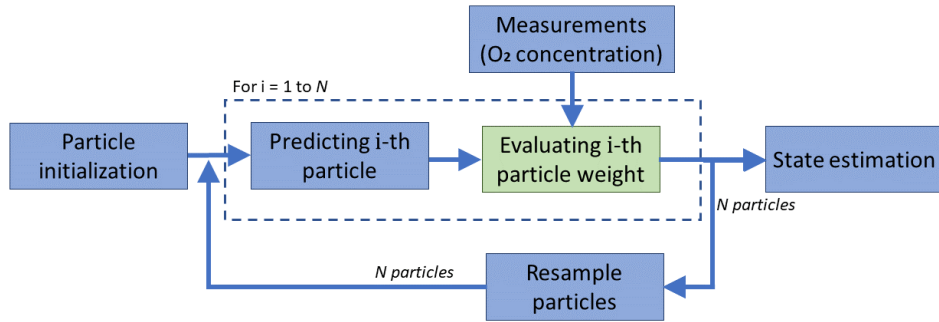


FIGURE 1. SIR particle filtering structure (N particles): Particle initialization, particle prediction (state transition), particle weight calculation (likelihood), and resampling.

maximum O_2 consumption rate in mmols/kg-hour, K is Michaelis-Menten constant in mmols/l. The parameters r_{max} and K are what we desire to estimate using the PF. These parameters are typically considered as constant quantities in conventional model fitting. For particle filtering, in contrast, we estimate them recursively and the PF is capable of capturing the uncertainty of these parameters, resulting in obtaining the better estimates of these parameters than the convention regression model fitting, under the noisy dynamical system. Consequently, the prediction of oxygen concentration can be more accurate than a conventional method and this results in better description and characterization of spinach respiration. Therefore environmental and packaging design for spinach can be employed more effectively.

The respiration rate can be computed by the rate of oxygen consumption that was determined by gas concentration per unit time and sample mass W between two measurements. The oxygen consumption rate in Eq. (20) can be calculated as:

$$r_{O_2} = \frac{[O_2](n) - [O_2](n - 1) V}{\tau W}, \quad (21)$$

where $[O_2](n)$ and $[O_2](n - 1)$ are oxygen concentrations at time steps n and $n - 1$, respectively. The quantity τ is time between the two samples. V stands for the void volume of the storage chamber in liters, and W represents spinach sample mass in kilograms.

For sequential filtering framework, the first order Markov chain is applied to the state space model, so do the state equations in this work. This stems from the fact that the parameters to be estimated evolve with time and the measured data in this work is actually the time-series of the oxygen concentration. To formulate the state equations from the respiratory models, assuming that the measurement noise in the experiment is additive, a set of state equations for particle filtering according to the respiratory models is now ready to be created.

The state transition equation and measurement equation for this model are given by:

$$\begin{bmatrix} r_{max}(n) \\ K(n) \end{bmatrix} = \begin{bmatrix} r_{max}(n - 1) \\ K(n - 1) \end{bmatrix} + \begin{bmatrix} v_r(n - 1) \\ v_K(n - 1) \end{bmatrix} \quad (22)$$

and

$$[O_2](n) = \frac{r_{O_2}(n)K(n)}{r_{max}(n) - r_{O_2}(n)} + w(n). \quad (23)$$

Quantities $v_r(n)$ and $v_K(n)$ represent the state perturbations, they dictate the momentum of the state movement. In this work we assume these quantities to be additive white Gaussian perturbations. Next, $w(n)$ is the additive white Gaussian noise in the measurement equation and this quantity leads us to formulate likelihood function and the update of particle weight. In addition, most practical consideration of the noise characteristics is found to be a Gaussian type, this is a reasonable assumption for this problem as well. Therefore, the likelihood for r_{max} and K is expressed as:

$$l(O_2(n)|r_{max}(n), K(n)) \propto \exp\left(-\frac{1}{2\sigma_w^2} \left\{ [O_2](n) - \frac{r_{O_2}(n)K(n)}{r_{max}(n) - r_{O_2}(n)} \right\}^2\right), \quad (24)$$

where σ_w^2 is the noise variance of $w(n)$.

B. FILTER IMPLEMENTATION

In this part, we outline the steps for parameter estimation according to the analysis provided above. Given the observation $[O_2](n)$, a set of noisy oxygen concentration along with the underlying state-space models of Eqs. (22) and (23), we implement the PF to determine maximum O_2 consumption rate r_{max} and Michaelis-Menten constant K . Since the model of measurement equation is highly non-linear structure, the KFs are not suitable. To implement a PF, the following steps are needed.

- **Initialization** At the beginning, $n = 0$, the PDFs of parameters are unknown. To form the joint PDF of all unknown parameters, the prior densities of the estimating parameters must be initiated at the beginning of the filtering process. The initial particles are sampled from these prior PDFs. Using Bayes theorem, the likelihood of Eq. (24) must be multiplied by the priors of all unknown parameters. In this work, prior densities for r_{max} , and K are chosen as uniform distributions.
- **Prediction** The prediction step begins with a set of uniform weight particles obtained from the previous time. The particles from the precedent step are propagated

via Eq. (22), two Gaussian densities act as small perturbations in the transition density, i.e. $v_r \sim \mathcal{N}(0, \sigma_{v_r}^2)$ and $v_K \sim \mathcal{N}(0, \sigma_{v_K}^2)$. It should be noted that this stage corresponds to the implementation of Eq. (5).

- **Updating** Updating process begins with a set of equal weight particles, $w_{n-1}^i = 1/N$. From the measurement equation and the noise in the data acquisition process, the weight of each particle is evaluated using the data just arrived and then normalized by

$$w_n^i = \frac{p(\mathbf{y}_n | \mathbf{x}_{n|n-1}^i)}{\sum_{i=1}^N p(\mathbf{y}_n | \mathbf{x}_{n|n-1}^i)} \quad (25)$$

where $p(\mathbf{y}_n | \mathbf{x}_{n|n-1}^i)$ is the likelihood function computed using Eq. (24). Therefore, we can calculate the weight of i th particle as

$$w_n^i = \frac{l(O_2(n) | r_{max}^i(n), K^i(n))}{\sum_{i=1}^N l(O_2(n) | r_{max}^i(n), K^i(n))}. \quad (26)$$

- **Resample** This is a crucial step, introduced to remedy the sampling degeneracy. A new set of particles $\{\mathbf{x}_n^j, w_n^j = 1/N\}_{j=1}^N$ are sampled from an approximated density $p(\mathbf{x}_n | \mathbf{Y}_n)$ computed at the updating stage. Resampling creates new particles according to the weights of their parent particles w_n^i by generating more particles where the parents have high weights and removing low weight particles. After resampling, all particles occupy the same weight and will be used for the next time step.

C. RESPIRATION RATE MEASUREMENT AND PARAMETER ESTIMATION

The data in this work is based on the experiment detailed in [6]. An experiment was operated to compute the baseline parameters, Spinach sample was stored in a closed storage chamber with initial condition of 21% Oxygen, 299 mmol O_2 / kg spinach, controlling at 25°C for 77 h. To generate a uniform storage atmosphere in a storage chamber, the need of a circular fan is necessary. During the storage, the change of O_2 concentration inside the chamber was measured using optical sensor (21G Foxy-R sensor, Ocean optics, Inc., USA) and respiration rate was calculated by O_2 concentration change per unit time and sample weight every 4 h time interval. The O_2 consumption rate and O_2 concentration were then used to estimate the model parameters (K and r_{max}) using nonlinear regression. This experiment acts as the baseline results for this work since the nonlinear regression method is a conventional technique widely used in many model fitting problems including foods and agricultures [34], [35]. Results from this experiment will be presented in Section IV.

IV. RESULTS AND DISCUSSION

This section provides results from nonlinear regression analysis, estimating results obtained from the PF using the experimental data, and performance comparison between nonlinear regression, extended Kalman filter, and PF.

TABLE 1. Estimated parameters from nonlinear regression analysis.

Parameters		
K	1.21	mmols/l
r_{max}	5.79	mmols/kg-hour

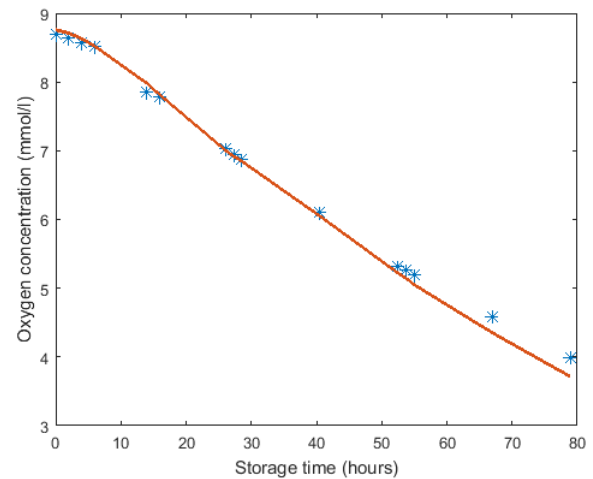


FIGURE 2. Measured and simulated O_2 concentration during storage for 77 hours at 25°C.

A. BASELINE PARAMETER: RESULTS FROM CONVENTIONAL NON-LINEAR REGRESSION

An experimental condition containing initial condition of 21% Oxygen, 299 mmol O_2 / kg spinach at 25°C was used to conduct gas concentration measurement. This initial condition can be converted into 8.69 mmol/l of O_2 / concentration in storage chamber head space [6]. This setting was employed to acquire the data for nonlinear regression obtaining the seeking parameters K and r_{max} of the model. The fitted parameters are present in Table 1. The R^2 of this fitting is 0.96.

Figure 2 shows the measured and simulated O_2 concentration during storage for 77 hours at 25°C. Fourteen data points were used in the regression analysis as displayed using the dots, and a solid line displays the estimated O_2 concentrations obtained from the nonlinear regression.

B. RESULTS FROM PARTICLE FILTER

A particle filtering method was implemented based on the data from the experimental setting described in section III-B. The parameter initialization is based on the values obtained from nonlinear regression analysis. As mentioned, the uniform distribution was applied in this work. i.e.,

$$K(n=0) = \mathcal{U}[K_{reg} - 0.5, K_{reg} + 0.5] \quad (27)$$

and

$$r_{max}(n=0) = \mathcal{U}[r_{max,reg} - 0.5, r_{max,reg} + 0.5] \quad (28)$$

where $\mathcal{U}[a, b]$ is a uniform density with parameters a and b . The quantities K_{reg} and $r_{max,reg}$ are obtained from the nonlinear regression found in Table 1, therefore,

$$K(n=0) = \mathcal{U}[0.71, 1.71], \quad (29)$$

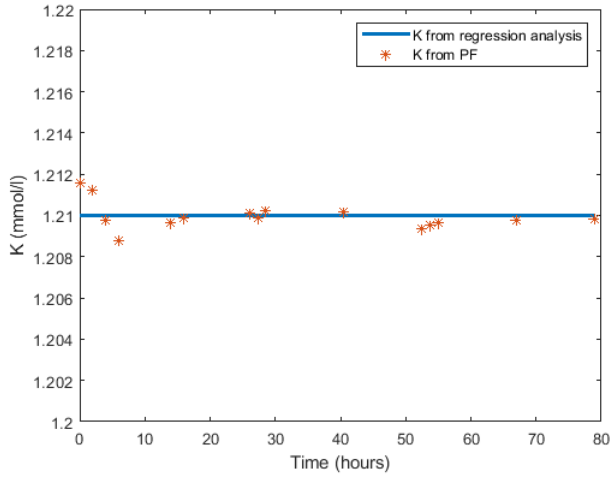


FIGURE 3. Michaelis-Menten constant; calculated from nonlinear regression is plotted by a solid line, and obtained by MAP estimator from the PF are plotted by markers.

and

$$r_{max}(n = 0) = \mathcal{U}[5.29, 6.29]. \quad (30)$$

These distributions are reasonable and dictate the initial set of particles used in the PF. It should be noted that the parameters of the uniform distributions can be different from these values, but this selection can save time consumption of the PF. In addition, number of particles used for computation can be tremendously reduced by choosing the initialized parameters that are closed to the true values.

In practice, the parameters K and r_{max} vary with time. By view of conventional non-linear regression analysis, each of these parameters is considered as a constant and valid for any experimental condition. The PF, on the other hand, relaxes this assumption. The nature of Bayesian framework allows the parameters to evolve with time, the justification of the parameter validity is done via the likelihood function. The PF can capture the uncertainty of these parameters, therefore we do not need them to be fixed and this aim is the essential in using the PF approach to obtain more accurate parameters.

We show in Figs. 3 and 4 the parameters K and r_{max} obtained by the PF, respectively. Each quantity for a specific time was obtained from the maximum a posteriori (MAP) estimator by using the posterior PDF generated by PF. We see in the figures that the filter took a few time steps to acquire enough information in order to achieve the values that are almost closed to the parameters provided by non-linear regression analysis. As mentioned earlier, the fluctuations occur because of capturing process behavior of the filter to follow the variations of the parameters which is the result of measurement uncertainty and noise process during the experiment. By view of PF, these fluctuations trace the valid values K and r_{max} by means of minimizing the prediction error. The number of particles used in this computation was 5,000.

In addition to the parameter estimates displayed in Figs. 3 and 4. The main feature of the sequential Bayesian filtering

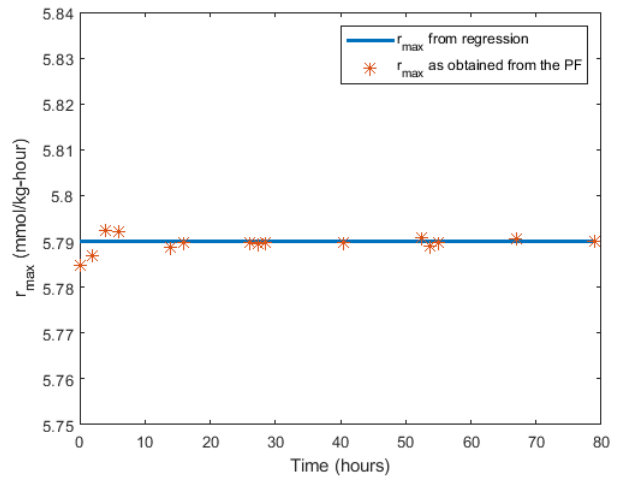


FIGURE 4. Maximum O_2 consumption rate; calculated from nonlinear regression is plotted by a solid line, and obtained by MAP estimator from the PF are plotted by markers.

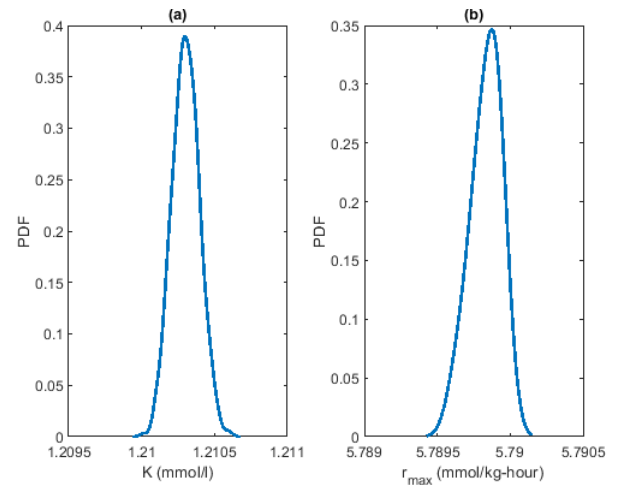


FIGURE 5. The PDFs of the estimated parameters (a) Michaelis-Menten constant and (b) maximum O_2 consumption rate. Number of particles used to obtain the PDFs was 5,000.

framework is the ability to provide the PDF of the estimating parameter. The approximated PDFs for the two parameters at time 40.5 h are given in Fig. 5. As observed in the figure that the PDF of each parameter has normal-like distribution but not exactly. This stems from the fact that the true PDFs of both parameters are not exactly Gaussian distributions, and the variation in errors of the measurement data, therefore the PF reveals the approximated PDFs via this results. The MAP estimates of the PDFs at this time step are 1.2103 mmol/l and 5.7899 mmol/kg-hour, respectively.

C. O_2 CONCENTRATION PREDICTION

To show how the method is applicable in practice, we illustrate the prediction performance of the PF as compared to the nonlinear regression analysis in Fig. 6. As demonstrated in the figure, the PF prediction outperforms the fitted model obtained from the nonlinear regression analysis. The predicted O_2 concentrations from PF coincide with the

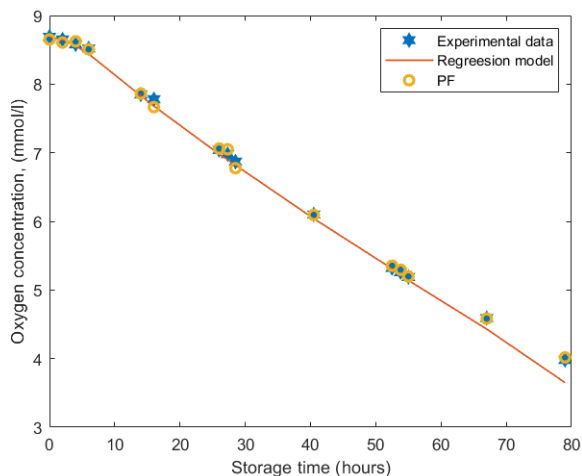


FIGURE 6. Measured and predicted O_2 concentrations during storage for 77 hours at 25°C. The predicted O_2 concentrations as obtained by a PF are plotted by orange circle, and red solid line is the fitted model from nonlinear regression analysis.

measured values from the experiment. It can be seen from the figure that the errors from nonlinear regression arise severely after 60 hours of experiment, but the PF can deliver excellent prediction in that period of time.

To validate the method, five different storage conditions were set and operated for gathering the data. To specific, each condition contains different initial oxygen concentrations. The O_2 concentration inside the chamber was measured according to the method already described in Section III-C. Nonlinear regression analysis was performed to obtain the Michaelis-Menten constant and the maximum consumption rate for each case. A PF was employed for each storage conditions and the estimates from the PF for O_2 concentration prediction at the different storage conditions were computed.

In addition to demonstrating the performance of the PF via O_2 concentration prediction, we also employed the PF for O_2 concentration prediction for various initial O_2 concentration and compared the predicted results to the conventional method. In this work, not only nonlinear regression analysis which is widely used in the analysis of respiratory of produces was considered, we also compared the performance of the PF with another sequential Bayesian filtering framework. In particular, the extended KF (EKF) was implemented to estimate the two parameters of the model, and prediction of O_2 concentration was also conducted for performance comparison. Predicted values of the O_2 concentration from these methods will then be evaluated by comparing to the measured data.

The predicted O_2 concentration was evaluated by the root mean squared error (RMSE) which is defined by

$$RMSE = \sqrt{\frac{1}{D} \sum_{k=1}^D \|C_{meas,k} - C_{est,k}\|^2}, \quad (31)$$

where $C_{meas,k}$ is the measured gas concentration, $C_{pre,k}$ is the predicted gas concentration, and D is number of data points.

TABLE 2. The RMSE for O_2 concentration at different storage conditions.

Condition	$[O_2]$ mmols/kg	$RMSE_{(reg)}$	$RMSE_{(EKF)}$	$RMSE_{(PF)}$
1	280	0.323	0.292	0.235
2	379	0.901	0.713	0.446
4	455	0.544	0.422	0.239
3	503	0.985	0.664	0.415
5	602	0.282	0.215	0.142

Shown in Table 2 are the RMSE for O_2 concentration predictions from nonlinear regression analysis, EKF, and PF. From the table, it is obviously seen that the performance of the PF is superior to that of the regression analysis and the EKF at all conditions. The results emphasize the reliability of the filter that it could achieve better predictions than the nonlinear regression analysis which is the conventional method in literature. Moreover, as mentioned previously that the EKF can only handle mildly nonlinear system, but the Michaelis-Menten model is not a linear model and leads to the highly nonlinear observation equation. Therefore, the KF prediction performance is lower than that of the PF.

V. CONCLUSION

In this paper, we presented a particle filtering approach for the prediction of spinach respiratory metabolism. The approach proposed in this work relies on the sequential Bayesian filtering method where the estimating parameters are considered to evolve with time. The main goal was to accurately estimate the Michaelis-Menten constant and maximum O_2 consumption rate in the Michaelis-Menten model without inhibition. The key feature of the approach is that the posterior PDFs of the estimating parameters can be obtained, resulting in a better interpretation of the estimates computed by the filter, and the uncertainty of the parameters can be revealed via these distributions. We showed a practical utilization of the proposed method for predicting the O_2 concentration, and the results illustrate the excellent prediction performance of the PF over the nonlinear regression analysis. Moreover, the estimates of the O_2 concentration for various initial conditions were obtained by the PF and the performance of the proposed method was validated by the RMSE. Results confirmed a superior performance of the proposed method to that of the conventional nonlinear regression analysis and the EKF, a benchmark filter in sequential Bayesian filtering framework.

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