



Simulation of fed-batch fermentation process using single-term HAAR wavelet series

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ABSTRACT

In recent years it has been acknowledged that to significantly improve biological system performance and productivity, control, including optimal control, should be implemented online. The dynamics of biological processes are highly non-linear and key variables are difficult to measure. As an aid to contributing solutions to the twin difficulties of complex dynamics and measurement difficulty a relatively simple mathematical model has been developed for the purpose of evaluating optimal controllers. In this paper a simulation of fed-batch fermentation is developed which includes the non-linear dynamics of the process using single-term Haar wavelet series (STHW) method.

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Introduction

The control of a biological process is based on the measurement of physical, chemical or biochemical properties and environmental parameters of the process. Often many important variables and parameters have to be calculated or estimated because of their unmeasurability, such as cell mass and substrate concentrations in a fermentation process. Most of estimation technique is to run the simulation models of the process in real-time and in parallel with the real process giving both the same inputs. Instead of the dynamics of the systems, the simulation technique can be applied to the systems for optimal control because lots of non-linear systems are generally very complex and not completely known, like a fermentation process from [1-8 and 19].

This paper describes in detail the dynamic models of two non-linear systems fed-batch and batch fermentation processes in detail and discusses results of the analysis. In order to solve the state equations for the non-linear systems a STHW for the integration of the nonlinear differential equations were developed. The state models have been expanded to include the various nonlinearities.

Structure of a Non-Linear System

Description of Dynamics

A fermentation process is a classical complicated, non-linear, time varying system. Its dynamics are not non measurable, such as biomass and substrate concentrations. The dynamics of the system are described by a series expanded models. In fact, a fed-batch, batch, continuous culture of baker's yeast or also many other organisms, can be described in fully aerobic conditions by the following (non-linear) models:[7]

(i) Biomass:

$$\frac{dX(t)}{dt} = [\mu - D(t)]X(t) \quad (1)$$

(ii) Substrate:

$$\frac{dS(t)}{dt} = -K_1 \cdot \mu \cdot X(t) + D(t) \cdot [S_{fi} - S(t)] \quad (2)$$

(iii) Fermentor volume of the growth culture:

$$\begin{aligned} \frac{dV}{dt} &= F_{in} - F_{out} \\ F_{in} &= DV \\ F_{out} &= 0 \end{aligned} \quad (3)$$

(iv) Oxygen concentration

$$\begin{aligned} \frac{dO}{dt} &= OTR + OUR \\ OUR &= -\frac{dX(t)}{dt} \left(\frac{1}{Y_{x0}} \right) \\ OTR &= K_{la} (X_{O2} O_1 - O) \end{aligned} \quad (4)$$

(v) Carbon dioxide concentration

$$\begin{aligned} \frac{dC}{dt} &= CEP + CTR \\ CEP &= K_{c2} \cdot \mu \cdot X(t) \\ CTR &= K_d \cdot K_2 \cdot (X_{CO2} \cdot C_1 - C) \end{aligned} \quad (5)$$

(vi) Ethanol concentration

$$\begin{aligned} \frac{dE}{dt} &= EPR - ECR \\ EPR &= \left(\frac{\xi_{max}}{\left(1 + \frac{E}{K_{et}} \right)} \right) \cdot \left(\frac{S}{(K_s + S)} \right) \\ ECR &= \left(\frac{K_{PO} \cdot O}{(O + K_{O2})} \right) \cdot \left(\frac{E}{(K_e + E)} \right) \end{aligned} \quad (6)$$

Where X, S, O, C and E are the concentration of biomass, substrate, oxygen, carbon-dioxide and ethanol respectively, X and S are nonmeasurable; O, C and E can be measured; OUR is the oxygen uptake rate. OTR is the oxygen transfer rate. CEP is the CO_2 transfer rate. ECR is the ethanol concentration rate. D is the dilution rate. S_{fi} is the substrate in the influent. μ is the specific growth rate with maximum value μ_{max} . K_1 is the yield coefficient. O_1 is dissolved oxygen and C_1 is CO_2 concentrations. $K_s, K_a, K_{c1}, K_{c2}, K_{et}, K_{la}, K_c, K_{po}$ and ξ_{max} are known.

Models of the Specific Growth Rate (μ)

The specific growth rate μ is a key time-varying parameter for description of biomass growth, substrate consumption and products formation. For a fermentation process, the most commonly used models for μ are presented as follows: [6] [7]

(i) Monod's model:

A functional relationship between the specific growth μ and an essential compound's concentration was proposed by Monod.

$$\mu(s) = \mu_{max} \cdot \frac{S(t)}{[K_s + S(t)]} \quad (7)$$

(ii) Ollson's model:

Aerobic fermentation are processes where the microorganism need oxygen to develop properly. In such case, dissolved oxygen (O) in the culture medium can be considered an additional substrate. This law which has Monod similarities is often referred to as the Ollson model for specific growth rate μ .

$$\mu(S, O) = \mu_{max} \cdot \left(\frac{S}{K_s + S} \right) \cdot \left(\frac{O}{K_{O_2} + O} \right) \quad (8)$$

This model considers the influence of substrate concentration S and biomass concentration X. [7].

(iii) Contois model:

The biomass growth is often presumed to slow down at high biomass concentrations. A possible model in this case is the following form:

$$\mu(S, X) = \mu_{max} \cdot \left(\frac{S}{K_C \cdot X + S} \right) \quad (9)$$

This model considers the influence of substrate concentration S and biomass concentration X. [7].

Computer Simulation

In order to assess the system dynamics and to optimize controller design, the system models were simulated in computer software. The principle of all numerical integration methods is to estimate the system states at time $(t + \Delta t)$ given the state at time " t " where " Δt " is the sampling period [2]. For a general equation of the form

$$\dot{\theta} = f(\theta, u, t) \quad (10)$$

At each step computation are done by some formula normally based upon the Taylor series,

$$\theta(t + h) = \theta(t) + \Delta t \cdot \dot{\theta}(t) + \frac{(\Delta t)^2}{2!} \cdot \ddot{\theta}(t) + \dots \quad (11)$$

If Δt is chosen to be sufficiently small and if sufficient higher order derivatives of " θ " and powers of " θ " are taken, then the value $\theta(t + \Delta t)$ can be accurately found.

A classical first order Euler method and STHW have been applied to the models for integration and are compared to the experimental data. These techniques are widely used in engineering for a non-linear system.

Euler Method

The Euler method is the simplest. For equation (11), only a first power of Δt is considered assuming the terms in $\Delta t^n (n > 1)$ are very small compared to Δt . This is valid only if $\Delta t \ll 1$. The Euler method has the form,

$$\theta(t + \Delta t) = \theta(t) + \Delta t \cdot f(\theta, u, t) \quad (12)$$

Sthw

The orthogonal set of Haar wavelets $h_i(t)$ is a group of square waves with magnitude of ± 1 in some intervals and zeros elsewhere Sekar et al. [9-17]. In general,

$$h_n(t) = h_1(2^j t - k), \quad \text{where } n = 2^j + k, \quad j \geq 0, 0 \leq k < 2^j, n, j, k \in Z$$

$$h_1(t) = \begin{cases} 1, & 0 \leq t < \frac{1}{2} \\ -1, & \frac{1}{2} \leq t < 1 \end{cases}$$

Namely, each Haar wavelet contains one and just one square wave, and is zero elsewhere. Just these zeros make Haar wavelets to be local and very useful in solving stiff systems.

Any function $y(t)$, which is square integrable in the interval $[0, 1]$. Can be expanded in a Haar series with an infinite number of terms

$$y(t) = \sum_{i=0}^{\infty} c_i h_i(t), i = 2^j + k, \quad (13)$$

where $i = 2^j + k, j \geq 0, 0 \leq k < 2^j, n, j, t \in [0, 1]$ where the Haar coefficients

$$c_i = 2^j \int_0^1 y(t) h_i(t) dt$$

are determined such that the following integral square error \mathcal{E} is minimized:

$$\mathcal{E} = \int_0^1 \left[y(t) - \sum_{i=0}^{m-1} c_i h_i(t) \right]^2 dt, \quad \text{where } m = 2^j, j \in \{0\} \cup N$$

Usually, the series expansion Eq. (13) contains an infinite number of terms for a smooth $y(t)$. If $y(t)$ is a piecewise constant or may be approximated as a piecewise constant, then the sum in Eq. (13) will be terminated after m terms, that is

$$y(t) \approx \sum_{i=0}^{m-1} c_i h_i(t) = c_{(m)}^T h_{(m)}(t), t \in [0,1]$$

$$c_{(m)}(t) = [c_0 c_1 \dots c_{m-1}]^T, \quad (14)$$

$$h_{(m)}(t) = [h_0(t) h_1(t) \dots h_{m-1}(t)]^T,$$

where “T” indicates transposition, the subscript m in the parantheses denotes their dimensions. The integration of Haar wavelets can be expandable into Haar series with Haar coefficient matrix $P[3]$.

$$\int h_{(m)}(\tau) d\tau \approx P_{(m \times m)} h_{(m)}(t), t \in [0,1]$$

where the m -square matrix P is called the operational matrix of

integration and single-term $P_{(1 \times 1)} = \frac{1}{2}$. Let us define [12]

$$h_{(m)}(t) h_{(m)}^T(t) \approx M_{(m \times m)}(t), \quad (15)$$

and $M_{(1 \times 1)}(t) = h_0(t)$. Eq.(15) satisfies

$$M_{(m \times m)}(t) c_{(m)} = C_{(m \times m)} h_{(m)}(t),$$

where $c_{(m)}$ is defined in Eq.(14) and $C_{(1 \times 1)} = c_0$.

Applying a simple Euler approximation and STHW to the system models, the equations (1), (2), (3), (4), (5), (6), (7), (8), (9) have the following values given in tables and graphs.

Fig 1: Solution curve for Monod's Model

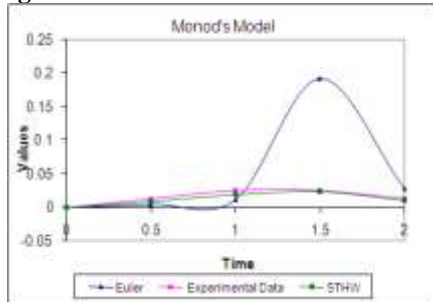


Fig 2: Solution curve for Ollson's Model

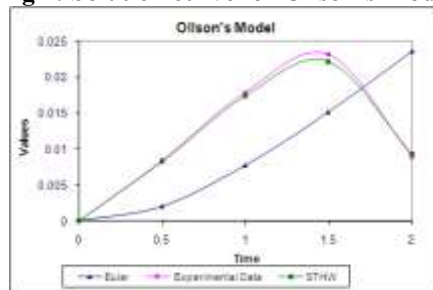
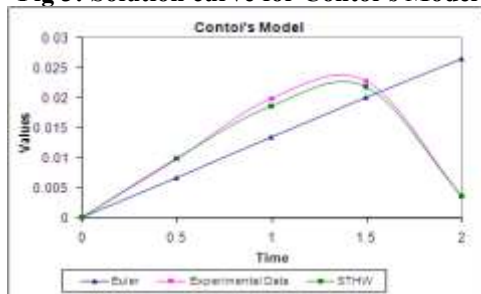


Fig 3: Solution curve for Contoi's Model



Conclusions

The obtained discrete solutions using the STHW give more accurate values when compared to the Euler's method. From the tables 1 – 9, we observe that the solutions obtained by the STHW match well with the experimental data of the fed-batch fermentation process, but the Euler's method yields a error. It is to be noted that from figures 1, 2 and 3. From the error graph presented in figures 1, 2 and 3, we can observe that the STHW yields very less error (almost no error) when compared to Euler's method in Mond's Model, Ollson's Model and Contoi's Model.

Hence, the STHW is more suitable for studying the simulation of the fed-batch fermentation process.

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Table-1 : Values for Experimental Data – Mond's Model

S.No	Experimental Data – Mond's Model							
	Time	Biomass	Substrate	Volume of fermentor	Oxygen	Carbon-dioxide	Ethanol	Mond's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.6179	0.6395	1.6567	0.0496	0.0249	0.0154	0.0132
3	1.0	2.6504	0.9814	2.7446	0.0536	0.0970	0.0374	0.0255
4	1.5	4.3963	1.4563	4.5470	-0.0929	0.2672	0.0517	0.0257
5	2.0	7.3839	2.0895	7.5329	-0.6511	0.6312	0.0141	0.0140

Table-2 : Values for Euler Method – Mond's Model

S.No	Euler Method – Mond's Model							
	Time	Biomass	Substrate	Fermentor Volume	Oxygen	Carbon-dioxide	Ethanol	Mond's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.4750	0.5980	1.5050	0.0533	0.0000	0.0013	0.0050
3	1.0	2.1941	0.8703	2.2650	0.0927	0.02122	0.0042	0.01141
4	1.5	3.2911	1.2413	3.4089	0.0841	0.0945	0.0106	0.1923
5	2.0	4.9778	1.7412	5.1303	-0.0545	0.2818	0.0234	0.0284

Table-3 : Values for STHW – Mond's Model

S.No	STHW – Mond's Model							
	Time	Biomass	Substrate	Volume of fermentor	Oxygen	Carbon-dioxide	Ethanol	Mond's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.6181	0.6395	1.6570	0.0496	0.0179	0.0086	0.0093
3	1.0	2.6512	0.9813	2.7456	0.0536	0.0862	0.0228	0.0190
4	1.5	4.3984	1.4561	4.5494	-0.0934	0.2756	0.0391	0.0239
5	2.0	7.3891	2.0887	7.5383	-0.6530	0.7302	0.0413	0.0108

Table-4 : Values for Experimental Data – Ollson's Model

S.No	Experimental Data – Ollson's Model							
	Time	Biomass	Substrate	Volume of fermentor	Oxygen	Carbon-dioxide	Ethanol	Ollson's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.6179	0.6395	1.6567	0.0495	0.0249	0.0156	0.0084
3	1.0	2.6504	0.9814	2.7446	0.0536	0.0970	0.0374	0.0179
4	1.5	4.3963	1.4563	4.5470	-0.0929	0.2673	0.0517	0.0232
5	2.0	7.3839	2.0895	7.5329	-0.6511	0.6312	0.0141	0.0089

Table-5 : Values for Euler Method – Ollson's Model

S.No	Euler Method – Ollson's Model							
	Time	Biomass	Substrate	Fermentor Volume	Oxygen	Carbon-dioxide	Ethanol	Ollson's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.4750	0.5980	1.5050	0.0533	0.0000	0.0013	0.0020
3	1.0	2.1941	0.8703	2.2650	0.0927	0.0212	0.0042	0.0078
4	1.5	3.2911	1.2413	3.4089	0.0841	0.0945	0.0106	0.0151
5	2.0	4.9778	1.7412	5.1303	-0.0545	0.2817	0.0234	0.0236

Table-6 : Values for STHW – Ollson's Model

S.No	STHW – Ollson's Model							
	Time	Biomass	Substrate	Volume of fermentor	Oxygen	Carbon-dioxide	Ethanol	Ollson's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.6181	0.6395	1.6570	0.0496	0.0179	0.0086	0.0083
3	1.0	2.6512	0.9813	2.7456	0.0536	0.0862	0.0228	0.0174
4	1.5	4.3984	1.4561	4.5494	-0.0934	0.2746	0.0392	0.0222
5	2.0	7.3891	2.0887	7.5383	-0.6530	0.7302	0.0413	0.0093

Table-7 : Values for Experimental Data – Contoi's Model

S.No	Experimental Data – Contoi's Model							
	Time	Biomass	Substrate	Volume of fermentor	Oxygen	Carbon-dioxide	Ethanol	Contoi's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.6178	0.6395	1.6567	0.0496	0.0249	0.0156	0.0098
3	1.0	2.6503	0.9813	2.7446	0.0536	0.0970	0.0374	0.0199
4	1.5	4.3963	1.4563	4.5470	-0.0929	0.2672	0.0517	0.0228
5	2.0	7.3839	2.0895	7.5328	-0.6511	0.6312	0.0141	0.0036

Table-8 : Values for Euler Method – Contoi's Model

S.No	Euler Method – Contoi's Model							
	Time	Biomass	Substrate	Fermentor Volume	Oxygen	Carbon-dioxide	Ethanol	Contoi's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.4750	0.5980	1.5050	0.0533	0.0000	0.0013	0.0067
3	1.0	2.1940	0.8703	2.2650	0.0927	0.0212	0.0042	0.0134
4	1.5	3.2911	1.2413	3.4089	0.0841	0.0945	0.0106	0.0200
5	2.0	4.9778	1.7412	5.1303	-0.0545	0.2818	0.0234	0.0265

Table-9 : Values for STHW – Contoi's Model

S.No	STHW – Contoi's Model							
	Time	Biomass	Substrate	Volume of fermentor	Oxygen	Carbon-dioxide	Ethanol	Contoi's Model
1	0.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.5	1.6181	0.6395	1.6570	0.0496	0.0179	0.0086	0.0099
3	1.0	2.6512	0.9813	2.7456	0.0536	0.0862	0.0228	0.0187
4	1.5	4.3984	1.4561	4.5494	-0.0934	0.2746	0.0392	0.0209
5	2.0	7.3891	2.0887	7.5383	-0.6530	0.7302	0.0413	0.0036