Development of Bilinear Models for Some Chemical Processes

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ABSTRACT Bilinear models of some chemical processes were developed. The
response to step input changes were obtained with and without implementa-
tion of a recursive parameter estimation algorithm. Bilinear models are
shown to be more accurate than the linear models. An approximation of a high order bilinear
model by a first order bilinear model is also presented, and shown to be satisfactory.

1. Introduction
Nonlinear systems are described by complex nonlinear differential equations whose
solution is difficult. Usually, linear approximation of a nonlinear system is possible
only when the behavior of the system is confined in the region around some normal
operating level.

The class of bilinear models has been introduced as a tool for examining many non-
linear phenomena[1]. As an approximation to general nonlinear plant, the bilinear model
may provide a more accurate representation than the linear one[2][3]. Many successful
applications results can be found in the literature[4][5] which illustrate the effectiveness
of the use of bilinear models as approximations for nonlinear systems. It has been
reported[6] that for a general plant in which the control appears linearly, a dynamically
equivalent bilinear model can be found.

In this paper, approximations of some nonlinear and bilinear chemical processes by
first order bilinear models are introduced. Comparison between linear and bilinear
approximations with and without parameter estimation is also presented.

2. Continuous Stirred Tank Reactor (CSTR)
The simulated continuous stirred-tank reactor (CSTR) process consists of an irre-
versible, exothermic reaction A → B, in a constant reactor cooled by a single coolant
stream which can be modeled by the following equations:

\[ C_A(t) = a_1 (C_{in} - C_A(t)) + k_0 C_A(t) \exp(a_0/T_0) \]  
\[ T(t) = a_2 \{ T_0 - T(t) \} + a_1 C_A(t) \exp(a_0/T_0) + a_2 C_A(t) \exp(a_0/T_0) \]  
\[ \] where,

\[ a_1 = \frac{\Delta H}{\rho C_p V} \]
\[ a_2 = \frac{(\rho C_p \Delta H)}{\rho C_p V} \]

The nominal CSTR parameters used in the simulation are as follows:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_A )</td>
<td>Measured product concentration = 0.1 mol/l</td>
</tr>
<tr>
<td>( T )</td>
<td>Reactor temperature = 441 K</td>
</tr>
<tr>
<td>( q_c )</td>
<td>Coolant flow rate = 100 l/m</td>
</tr>
<tr>
<td>( C_{AO} )</td>
<td>Feed concentration = 1 mol/l</td>
</tr>
<tr>
<td>( T_0 )</td>
<td>Feed temperature = 350 K</td>
</tr>
<tr>
<td>( T_{inj} )</td>
<td>Inlet coolant temperature = 350 K</td>
</tr>
<tr>
<td>( V )</td>
<td>CSTR volume = 100 l</td>
</tr>
<tr>
<td>( \Delta A )</td>
<td>Heat transfer term = ( 7 \times 10^5 ) cal min(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( k_0 )</td>
<td>Reaction rate constant = ( 7.2 \times 10^{10}) min(^{-1})</td>
</tr>
<tr>
<td>( E/R )</td>
<td>Activation energy term = ( 1 \times 10^8)</td>
</tr>
<tr>
<td>( \Delta H )</td>
<td>Heat of reaction = ( -2 \times 10^4) cal/mol</td>
</tr>
<tr>
<td>( \rho, \rho_c )</td>
<td>Liquid densities = ( 1 \times 10^2) g/l</td>
</tr>
<tr>
<td>( C_{AO1}, C_{AO2} )</td>
<td>Specific heats = ( 1 ) cal g(^{-1}) K(^{-1})</td>
</tr>
</tbody>
</table>

Linearization around the steady state values of reactor temperature (\( T_{SS} \)) and coolant flow rate (\( q_c \)) is carried out for the exponential terms; \( \exp(a_1/T(t)) \) and \( q_c(t) \) \( \exp(a_0/T_{SS}) \). Using Taylor series expansion yields:

\[ \exp(a_1/T_{SS}) \approx 1 + a_1/T_{SS} \]  
\[ \exp(a_0/T_{SS}) \approx 1 + a_0/T_{SS} \]  
\[ \exp(a_0/T(t)) \approx 1 + a_0/T(t) \]  
\[ \exp(a_1/T(t)) \approx 1 + a_1/T(t) \]  
\[ \exp(a_0/q_c(t)) \approx 1 + a_0/q_c(t) \]  
\[ \] where

\[ a_0 = \frac{-\Delta H}{\rho C_p V} \]

Substitution of equations (3) and (4) into equations (1) and (2) and rearranging will yield the following bilinear model for CSTR:

\[ T(t) = b_1 T(t) + b_2 C_A(t) + b_3 C_A(t)^2 + b_4 q_c(t) + b_5 \]  
\[ C_A(t) = b_6 C_A(t) + b_7 C_A(t)^2 + b_8 \]
where

\[ b_1 = -a_1 + \alpha_1 q_c \exp (a_2 / q_c) - \alpha_2 q_c \exp (a_3 / q_c) \]
\[ b_2 = \alpha_1 \exp (a_2 / q_c) + \alpha_2 q_c \exp (a_3 / q_c) \]
\[ b_3 = \alpha_1 \exp (a_2 / q_c) - \alpha_2 q_c \exp (a_3 / q_c) \]
\[ b_4 = \alpha_1 \exp (a_2 / q_c) - \alpha_2 q_c \exp (a_3 / q_c) \]
\[ b_5 = \alpha_1 T_0 - \alpha_2 T_0 \exp (a_2 / q_c) - \alpha_2 q_c T_0 \exp (a_3 / q_c) \]
\[ b_6 = -a_1 - b_4 \exp (a_2 / q_c) - (a_2 T_0 / q_c) \exp (a_3 / q_c) \]
\[ b_7 = (a_2 T_0 / q_c) \exp (a_3 / q_c) \]
\[ b_9 = \alpha_1 \exp (a_2 / q_c) - \alpha_2 q_c \exp (a_3 / q_c) \]

The parameters of Equations (5) and (6) are estimated at each sampling period using a recursive least square method (RLS) with a variable forgetting factor[6]. The coolant flow rate was changed from an initial value of 1001 min\(^{-1}\) to 110, to 100, to 90, and back to 100, at 7 min intervals.

Figures 1 to 4 show the concentration and temperature responses to step changes in the coolant flow rate (\( q_c \)) with and without recursive parameters estimation. The figures show the results for the simulated CSTR, the bilinear models, and the linear models. It can be seen from the figures that bilinear models describe the dynamics of the CSTR more accurately than linear models which are included for the sake of comparison. Considerable improvement in the predictions of bilinear and linear models is observed when parameters estimation algorithm is implemented.

![Fig. 1. Concentration response of CSTR without parameter estimation.](image-url)
Fig. 2. Concentration response of CSTR with parameter estimation.

Fig. 3. Temperature response of CSTR without parameter estimation.
3. Plate Heat Exchanger (PHE)

In modeling PHE, the following assumptions were made[7]:
1. Heat losses to the surroundings are negligible.
2. Heat transfer within the fluid in any channel is by convection only.
3. The fluid will split equally between the parallel channels for each stream.
4. Thermal capacity of the plate wall is negligible.
5. The temperature distributions in all channels belonging to the same streams are identical.
6. The heat-transfer film coefficient depends mainly on the hot fluid velocity.
7. The physical properties of the fluid are constant over the range of temperature employed.
8. The rate of change of the cold-stream outlet temperature is identical to that of the hot stream.

3.1 Energy Balances

3.1.1 Cold Stream Side

\[ V_c \frac{dT_{c1}}{dt} = F_c T_{c0} - F_c T_{c1} + \left( U_A h c_p \right) \Delta T_{in} \]  

(7)

where,

\[ \Delta T_{in} = \left( T_{i1} - T_{c0} \right) + \left( T_{i0} - T_{c1} \right) \log \left( \frac{T_{i0} - T_{c0}}{T_{i1} - T_{c1}} \right) \]  

(8)

3.1.2 Hot Stream Side

\[ V_h \frac{dT_{h1}}{dt} = F_h T_{h0} - F_h T_{h1} - \left( U_A h c_p \right) \Delta T_{in} \]  

(9)
The nominal operating conditions used in this paper can be summarized as follows:

- \( C_p \): specific heat = 1 cal g\(^{-1}\) °C\(^{-1}\)
- \( F_v \): volumetric flow rate of cold stream = 3.5 \( \text{L min}^{-1}\)
- \( F_s \): volumetric flow rate of hot stream = 2 \( \text{L min}^{-1}\)
- \( T_i \): inlet temperature of cold stream = 31°C
- \( T_{r,0} \): outlet temperature of cold stream = 40°C
- \( T_{r,0} \): inlet temperature of hot stream = 60.5°C
- \( T_{h,0} \): outlet temperature of hot stream = 40.5°C
- \( V_c \): volume of cold side channels = 1.0 l
- \( V_s \): volume of hot side channels = 1.0 l
- \( A \): heat transfer area = 1.062 \( \text{m}^2\)
- \( \rho \): liquid density = 1000 g/l

The overall heat-transfer coefficient \((U)\) is a function of the hot stream mass flow rate \((\rho F_s)\) as follows:\(^{(10)}\):

\[
\frac{1}{U} = \frac{1.2 \times 10^{-2}}{(T_{r,0})^{0.85}} + 7.06 \times 10^{-3} \rho F_s \]

Experimental data reported by Al-Azehran\(^{(11)}\) indicates that \(T_{h,0}\) is very close to \(T_{r,0}\). Therefore, they can be substituted for each other without appreciable error. The following first-order discrete bilinear model can be obtained by incorporating the above assumptions into Equations (7) and (9):

\[
\frac{\dot{T}_r}{T_r} = \left(1 - \frac{1}{2 V_c} \frac{F_r}{T_r} \right) (k-1) + (\frac{1}{2 V_s} F_s)(k-1) + \frac{F_r}{2 V_r} T_p(k-1) + \frac{F_s}{2 V_s} T_p(k-1)
\]

which can be rewritten as follows:

\[
\frac{\dot{T}_r}{T_r} = \left(1 - \frac{1}{2 V_c} \frac{F_r}{T_r} \right) (k-1) + \frac{F_r}{2 V_r} T_p(k-1) + \frac{F_s}{2 V_s} T_p(k-1)
\]

where \( \dot{T}_r \): \(T_r \) process output; \( T_r \): model output; \( \dot{T}_r \), \( T_r \), \( \dot{F}_r \), \( \dot{F}_s \) are model parameters; \( F_r \) : manipulated variable; \( T_p \) : sampling time.

Similarly, second and higher order bilinear models can be constructed depending on the degree of approximation of the derivative terms in Equations (7) and (9).

Figure 5 shows the responses of the outlet temperature of the cold stream to step changes in the flow of the hot stream, which was changed from an initial value of 2 \( \text{L min}^{-1}\) to 5, 2, to 1, and back to 2, at 5 min intervals. The figure shows the results of the simulated PHE, the bilinear model and the linear model when a parameter estimation algorithm is implemented. As can be seen from Fig. 5, the bilinear model approximates the simulated PHE dynamics more accurately than the linear one. The response of the linear model shows a large deviation from the simulated model for the negative step in the flow rate of the hot stream; \( (1 \text{ L min}^{-1}) \). For positive steps, small deviations are observed.
4 Bilinear Processes

Bilinear models arise naturally in many chemical processes, where mass and energy balances contain products of flows and temperatures or concentrations. The order of those bilinear models may be high, which makes controller design complex. As an example of such processes, assume that a process can be described completely by a third order discrete, bilinear model of the form:

\[ Y(k) = 0.6Y(k-1) - 0.35Y(k-2) + 0.25U(k-2) + 0.3Y(k-1) + 0.5U(k)\]
\[ + 0.4U(k-2) + 0.3U(k-3) + d(k) \]  

where \( Y \) is the process output, \( U \) is the process input, and \( d \) is a step disturbance.

A first order bilinear model approximation of the process represented by Equation (13) gives:

\[ y_n^M = a_0 y_{n-1} + b_0 u_{n-1} + c_0 d_{n-1} \]  

where \( y_n^M \) is the model output.

The parameters of Equation (14) are estimated at each sampling instant using RLS with forgetting factor.

Figure 6 shows the responses of the process (Eq. 13) and the bilinear model (Eq. 14) to step changes in \( U \) which was changed from 0 to 1, to 0, to -1, and back to 1, at 5 min intervals. The figure shows that the response of the first bilinear model is very close to that of high order bilinear process (Eq. 13). The simulation was also conducted using a
second order bilinear model as an approximation for Equation (17), but no improve-
ment in the approximation was observed over that of the first order one. Simulations
were also conducted for higher order bilinear processes using bilinear model approxi-
mations with different orders whose parameters are estimated via RLS. The first order
bilinear model approximation was found to be satisfactory.

![Graph](image)

**Fig. 6.** Response of bilinear process with parameter estimation.

5. Conclusion

Approximations of CSTR and PHE by bilinear models have been described. The
predictions of the bilinear models and the linear one for various input changes are
obtained. The results are obtained with and without implementation of a parameter esti-
mation algorithm (RLS). Simulations show that bilinear model approximates the
process more accurately than the linear one. A considerable improvement in the
responses is observed when a parameter estimation algorithm (RLS) is implemented.
An approximation of a high order bilinear process with a first order bilinear model is
also presented. The approximation was found to be satisfactory for various input
changes.

References


902 (1975).
\[\begin{align*}
A & \text{ heat transfer area \text{[m}^2\text{]} } \\
C_a & \text{ measured product concentration \text{[mol/l]} } \\
C_{sa} & \text{ heat concentration \text{[mol/l]} } \\
C & \text{ heat capacity \text{[J g}^{-1}\text{C}^{-1}\text{]} } \\
E/R & \text{ activation energy term \text{[K]} } \\
F & \text{ volumetric flow rate of cold stream \text{[l min}^{-1}\text{]} } \\
F_B & \text{ volumetric flow rate of hot stream \text{[l min}^{-1}\text{]} } \\
\Delta h & \text{ heat transfer coefficient \text{[J m}^{-2}\text{K}^{-1}\text{min}^{-1}\text{]} } \\
\alpha & \text{ reaction rate constant \text{[min}^{-1}\text{]} } \\
\psi & \text{ coolant flow rate \text{[l min}^{-1}\text{]} } \\
T & \text{ inlet temperature \text{[K]} } \\
T_{in} & \text{ outlet temperature \text{[K]} } \\
T_0 & \text{ inlet temperature of cold stream \text{[C]} } \\
T_r & \text{ outlet temperature of cold stream \text{[C]} } \\
T_v & \text{ inlet temperature of hot stream \text{[C]} } \\
\Phi & \text{ outlet temperature of hot stream \text{[C]} } \\
V & \text{ volume of cold side channels \text{[l]} } \\
V_v & \text{ volume of hot side channels \text{[l]} } \\
\rho & \text{ liquid density \text{[g/l]} } 
\end{align*}\]
تطوير فن إنتاج شبه خطية لبعض العمليات الكيميائية

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المستخلص: تم تطوير فن إنتاج شبه خطية لبعض العمليات الكيميائية. كما
تمت دراسة استخدام النماذج لاعتماد تأثيرات خارجية باستخدام مبادلات للنماذج
كاملاً أو جزئياً. وقد نتجت النتائج أن النماذج الدقيقة تضرورة
لتقييم العمليات الكيميائية بدقة أكثر من النماذج الخاطئة. كما تم دراسة
إمكانية توصيف العمليات الكيميائية باستخدام مجموعة من أدوات الدرجة العليا للنماذج
الدقيقة من الدرجة الأولى، وكانت النتائج مرضية.