Modeling and Simulation for multivariable Chemical System in Semadco Urea-Plant

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Abstract:

For target of stabilizing the operation of ammonia converter R-107 is Semadco (TALKHA II Fertilizer Company); that is by designing appropriate control system for the "HP BF Water heater E-127" High Pressure Boiler Feed Water heater which governs the system inlet temperature, it is very important to construct a mathematical model which simulates perfectly the practical system construction and operation.

Such a model is not clearly and accurately presented in references. So, this work deals with formulating and constructing suitable mathematical model for this E-127 heater. The modeling procedure is based on dividing the chemical system into subsystems coupled through boundary conditions.

The suggested mathematical model is tested numerically by computing the system open loop performances, which are then compared with the recorded experimental performances from the field.

The results obtained show good agreement between both of the suggested model and the physical system.
Introduction:

In the ammonia synthesis section of Sonaco urea plant shown in Fig.(1), the primary objective in the control of a high-pressure synthesis loop, and the entire ammonia plant is to produce the desired amount of product consistency (1200 metric tons per day); with low operating costs, minimum risk, long equipment life time and reduced down time. An optimization of the operation of the synthesis loop requires that careful attention be given to operating variables; the most important of which are: [1,8]

1. Converter temperature.
2. Loop pressure.
3. Inlet converter concentration.
4. $\frac{H_2}{N_2}$ ratio.
5. Gas circulation rate.

The main reaction in the ammonia converter R-107 is a highly exothermic one. Consequently, the hot reactor effluent is often used to preheat the reactor feeding from 30°C to 150°C through the ammonia converter feed effluent exchanger E-128. Such exchange may lead to serious stability problems in the reactor operation due to undesirable operating conditions.

As shown in Fig.(2-a), the relation between the reactor feeding temperature ($T_f$) and the reactor effluent temperature ($T_e$) follows a sigmoidal curve. In other way, a heat balance around the heat exchanger operating point is represented by a straight line linear relation.

Mostly, the unstable problems associated with the reactor operation are occurred due to the operating point "S" [3]. Thus, a secondary heater E-127 with BFW is added which can be designed with the aid of robust adaptive controller in purpose of modifying the sigmoidal curve to that suggested in Fig.(2-b).

This E-127 heater can give heat duty of $30.5 \times 10^6$ kcal/hr [8] during passing the hot effluent gases from ammonia converter R-107 at 327°C where the gas is cooled to 190°C.

Precisely constructed mathematical model for E-127 heater is helpful for designing appropriate controller. Such a model is not available, so, this work deals with building a suitable one; that is by considering the heater as a multivariable system, and depending on the practical knowledge and observations of the process feeds and parameters.
Model Building for the RP BFW heater E-127

Considering the E-127 subsystem under study, shown in Fig. (3) with associated chosen input and output variables which can be defined as:

- \( u_1 \): stroke of valve HVIII.
- \( u_2 \): stroke of valve FVB1.
- \( D \): input temperature to E-127 (TI0184).
- \( y_1 \): BFW flow (FT57) + interaction effect from (FT51).
- \( y_2 \): flow to E-127 (FT51) + interaction effect from (FT57).
- \( y_3 \): output temperature (TI0153).

and selecting the state variables as:

- \( X_1 \): BFW flow (FT57).
- \( X_2 \): flow to E-127 (FT51).
- \( X_3 \): output temperature (TI0153).
- \( X_4 \): gas circulation rate \( Q = \frac{54,64 \text{ A}}{T_i - T_f} \times \text{TRF} \) \[4,5\]

where A is the ammonia product in tons/day.

TRF is the temperature rise factor.

The system can be represented by the suggested block diagram shown in Fig. (4); for which system transfer functions can be performed in the following matrix equation form \[(2,6)\]

\[
\begin{bmatrix}
  y_1 \\
  y_2 \\
  y_3 \\
\end{bmatrix}
= \begin{bmatrix}
  Gv_1 & (Gv_2 + Gp_{12}) \\
  (Gv_1 + Gp_{21}) & (Gv_2 + Gp_{22}) \\
  (Gv_1 + Gp_{31}) & (Gv_2 + Gp_{32}) \\
\end{bmatrix}
\begin{bmatrix}
  u_1 \\
  u_2 \\
  0 \\
\end{bmatrix}
+ \begin{bmatrix}
  0 \\
  0 \\
  Gp_{33} \\
\end{bmatrix}
\begin{bmatrix}
  D \\
\end{bmatrix}
\]

with the system output equations:

\[
\begin{align*}
  y_1 &= 1 \times x_1 \\
  y_2 &= c_k_1 x_1 + 0 \times x_2 + 0 \times x_3 \\
  y_3 &= 0 \times x_1 + 1 \times x_2 + 0 \times x_3 \\
\end{align*}
\]

where: \[(6,7)\]

\[
\begin{align*}
  Gv_1 &= \frac{TK_1}{TV_1 S + 1} \\
  Gv_2 &= \frac{TK_2}{TV_2 S + 1} \\
  Gp_{12} &= c_k_1 \\
  Gp_{21} &= c_k_2 \\
  Gp_{22} &= \frac{c_k_3}{TT_1 S + 1} \\
  Gp_{31} &= \frac{c_k_4}{TT_2 S + 1} \\
  Gp_{32} &= \frac{c_k_5}{TT_3 S + 1} \\
\end{align*}
\]
Thus, system state model can be deduced from (1) & (2) giving

\[
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\dot{x}_3 \\
\dot{x}_4
\end{bmatrix} =
\begin{bmatrix}
a_{11} & 0 & 0 & 0 \\
0 & a_{22} & a_{23} & 0 \\
a_{31} & a_{32} & a_{33} & a_{34} \\
a_{41} & a_{42} & a_{43} & a_{44}
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix} +
\begin{bmatrix}
b_{11} & 0 & 0 \\
0 & b_{22} & 0 \\
b_{31} & b_{32} & 0
\end{bmatrix}
\begin{bmatrix}
\nu_1 \\
\nu_2 \\
\nu_3
\end{bmatrix}
\]

\[\begin{bmatrix}
u_4
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
\gamma
\end{bmatrix} \begin{bmatrix}
D
\end{bmatrix}
\]  \( (3) \)

where all of \( a , b \) and \( \gamma \) parameters depend on the previous defined system constants by complicated relations which are omitted here for saving area. These parameters will be identified in the next section by the aid of experimental investigations.

Parameters Calculations and Results:

Experimental approach is used to investigate how the behavior of HP 3FW heater E-127 changes with time under the influence of changing external disturbances and manipulated variables. Table (1) summarizes the recorded changes in the E-127 outputs under deliberately 1% step change in the FV31 valve stroke \( (\nu_3) \).

From these data, system specification parameters can be calculated giving final values as shown in Table (2).

Consequently, the different transfer function components will be:

\[
G_{\nu_1} = \frac{1.8}{0.05\, S + 1}
\]

\[
G_{\nu_2} = \frac{0.925}{0.08\, S + 1}
\]

\[
G_{\nu_3} = C_{\nu_1} = 0.0
\]

\[
G_{p_{\nu_3}} = C_{\nu_2} = 0.3
\]

\[
P_{\nu_3} = -0.155
\]

\[
P_{\nu_4} = \frac{-0.23}{10\, S + 1}
\]

\[
P_{\nu_3} = \frac{0.155}{10\, S + 1}
\]

\[
P_{\nu_2} = \frac{0.925}{10\, S + 1}
\]

and the final state model with the corresponding output equations will be:
\[
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\dot{x}_3 \\
\dot{x}_4
\end{bmatrix} = 
\begin{bmatrix}
-4.7 & 0 & 0 & 0 \\
0 & -16.7 & 0 & 0 \\
0 & 0 & -0.1 & -1 \\
-0.355 & -0.257 & -0.801 & -0.2
\end{bmatrix} + 
\begin{bmatrix}
0.0 \\
0.0 \\
0.0 \\
0.0
\end{bmatrix}
\] (4)

\[
[10]
\begin{bmatrix}
2.0 & 0 \\
0 & 12.75 \\
0 & 0 \\
0.09 & 0.213
\end{bmatrix}
[\begin{bmatrix}
u_1 \\
u_2
\end{bmatrix}] + 
[\begin{bmatrix}
0.0 \\
0.0 \\
0.0 \\
0.0
\end{bmatrix}]
\] (5)

According to this deduced mathematical model, and considering nominal values of \( w = 0.35; u_2 = 0.8 \) and \( D = 0.874 \), transient response calculations are carried out on IBM Personal Computer using Runge-Kutta technique. Calculated state variables are plotted together with that recorded in Fig.(5).

Conclusion:

It is clear from these simulation that \( x_1, x_3, x_4 \) agree well with recorded values. However, \( x_3 \) in spite of tuning parameter values for this variable, the result is not satisfactory. For the time being, the result is stated as it, however, more work on this point is undergoing.

Partially satisfactory results are obtained which indicate enough and acceptable similarity between each of experimentally recorded, and the theoretically calculated state changes for the HP-BFW heater (E-127) in the ammonia plant of Semadco.

Thus the suggested mathematical model can be considered suitable for simulating the real system after some further adjustment, and consequently helpful when used in future for designing appropriate controllers for governing and modifying operation.
<table>
<thead>
<tr>
<th>Time (hr)</th>
<th>FT57(y1) m³/hr</th>
<th>FT51(y2) m³/hr</th>
<th>T10152(y3) °C</th>
<th>T10164(D) °C</th>
<th>T10151(Tc) °C</th>
<th>Q(X4) m³/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>182</td>
<td>92</td>
<td>195</td>
<td>341</td>
<td>173</td>
<td>5603.00</td>
</tr>
<tr>
<td>1</td>
<td>175</td>
<td>110</td>
<td>205</td>
<td>351</td>
<td>165</td>
<td>5964.00</td>
</tr>
<tr>
<td>2</td>
<td>170</td>
<td>110</td>
<td>195</td>
<td>350</td>
<td>162</td>
<td>5900.62</td>
</tr>
<tr>
<td>3</td>
<td>168</td>
<td>110</td>
<td>192</td>
<td>345</td>
<td>163</td>
<td>5995.14</td>
</tr>
<tr>
<td>4</td>
<td>168</td>
<td>110</td>
<td>192</td>
<td>345</td>
<td>163</td>
<td>6095.14</td>
</tr>
<tr>
<td>5</td>
<td>168</td>
<td>110</td>
<td>191</td>
<td>345</td>
<td>163</td>
<td>6095.14</td>
</tr>
<tr>
<td>6</td>
<td>168</td>
<td>110</td>
<td>189</td>
<td>345</td>
<td>162</td>
<td>6061.84</td>
</tr>
<tr>
<td>7</td>
<td>168</td>
<td>110</td>
<td>189</td>
<td>345</td>
<td>160</td>
<td>5996.30</td>
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<td>168</td>
<td>110</td>
<td>189</td>
<td>345</td>
<td>161</td>
<td>6061.84</td>
</tr>
</tbody>
</table>

*Calculated values according to corresponding mentioned equation*

Table (1)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>TK1</td>
<td>1.0 Kg/min</td>
<td>CK5</td>
<td>8.5</td>
</tr>
<tr>
<td>TK2</td>
<td>0.825 Kg/min</td>
<td>TV1</td>
<td>0.06 min</td>
</tr>
<tr>
<td>CK1</td>
<td>0.0</td>
<td>TV2</td>
<td>0.06 min</td>
</tr>
<tr>
<td>CK2</td>
<td>0.3</td>
<td>TT1</td>
<td>10.0 min</td>
</tr>
<tr>
<td>CK3</td>
<td>-0.23</td>
<td>TT2</td>
<td>10.0 min</td>
</tr>
<tr>
<td>CK4</td>
<td>-0.155</td>
<td>TT3</td>
<td>10.0 min</td>
</tr>
</tbody>
</table>

Table (2)

References:

4. ICI report, 1983 "Semadoor ammonia loop problem".
5. ICI report, 1989 "Ammonia converter specifications".
Simplified AMM SYNTHESIS SECTION

(a) Reactor heat balance:
(a) Without secondary balance heater.
(b) With secondary balance heater.
SECONDARY BALANCE HEATER

FIG. (3)

FIG. (4)
Fig. (6): Transient response of system state variables.