COMPUTER SIMULATION OF AMMONIA COLD SHOT CONVERTER

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Abstract
A mathematical model is developed and tested with plant data for the ammonia cold shot converter of Razi Petrochemical Complex. The model is based on a material and energy balance in a differential element of beds and is subjected to the assumptions of uniform distribution of temperature and composition through a general cross section and negligible mass and heat transfer in axial direction. The governing differential equations are solved by Runge-Kutta of fourth order to obtain temperature and concentration profiles through the reactor. The agreement between calculated temperature and composition with plant data confirms the validity of the developed model.

Key Words
Computer Simulation, Mathematical Model, Ammonia Converter, Ammonia Cold Shot Converter, Razi Petro Chemical Complex

چکیده
یک مدل ریاضی برای واحد تولید آمونیاک پتروشیمی رازی ارائه شده است. این مدل بر اساس یک روش ساده برای مدلی برای محاسبه شرایط سطحی و غلظت در سطح محیطی رکتور استفاده می‌شود. در بدست آمده مدل ریاضی از فرآیند کشش بودن درجه و غلظت در سطح محیطی رکتور استفاده شده است و با استفاده از این اطلاعات، جرم و حرارت درجه جرم و حرارت درجه جرم درجه حرارت درجه حرارت و غلظت در سطح محیطی رکتور محاسبه می‌شود. ایجاد سخنرانی در مورد ویژگی‌های این رکتور با استفاده از نتایج باشندگی، دیده می‌شود که درجه حرارت و غلظت پیش‌بینی شده با مدل ریاضی با مقادیر موجود در واقع صفحه‌ای محاسبه می‌شود.

INTRODUCTION

Ammonia synthesis, one of the oldest commercial high-pressure processes, consists of reacting a hydrogen-nitrogen mixture over a catalyst at elevated temperatures and pressures. The reaction is exothermic and the high temperature in the reactor is sustained by the heat of reaction throughout the reactor length. The temperature is controlled between the catalyst basket beds by the cold feed gas. This process has been the subject of numerous studies and, with the aid of computers, mathematical models have proved to be adequate for prediction of plant data.

Several studies have considered the effects of various pertinent variables upon ammonia production and converter stability. Van Heerden calculated temperature and pressure profiles in a NEC-TVA (Nitrogen Eng. Corp.-Tennessee Valley Authority) converter by the concept of autothermal processes [1]. Badour, et. al. used a steady-state simulation of the T.V.A. reactor to determine the effects of design and operating parameters upon reactor stability, production rate, and the temperature profile of catalyst beds [2]. Dyson and Simon derived the rate expression of ammonia formation, with diffusion correction for an industrial catalyst, at pressures ranging from 150 to 300 atm. [3]. Porubsky, and his coworkers simulated the TVA-converter by a mathematical model in which they obtained the concentration profile in the reactor [4].

Gaines developed a steady-state model for a
quench-type ammonia converter [5]. Singh and Saraf considered diffusion effects within catalyst pores to describe the synthesis rate equation for catalysts of different types [6].

Reddy and Asghar Husain simulated the synthesis loop of a special ammonia synthesis converter called Casal [7]. Singh developed a generalized method for calculating an effectiveness factor. The ammonia synthesis reaction was utilized for testing the applicability of the procedure [8].

In the present work, a mathematical model has been developed for an ammonia cold shot converter. The ammonia plant chosen for this study is the Razi Petrochemical Complex, with 1000 TPD capacity with a design of Kellog, using a two stage reciprocating compressor. The plant is located in Imam Khomeiny Bandar which works under a low pressure (140 atm).

**AMMONIA SYNTHESIS CONVERTER**

In the above mentioned plant, the converter feed gas is split into five fractions. The bulk of the gas enters the bottom of the converter and flows upward around the outside of the catalyst section to the exchanger at the top of the converter as shown in Figure 1. The gas is heated in the exchanger and passes to the first quench zone where it is mixed with cold feed gas before entering the first bed. Ammonia is formed according to Equation 1 as the gas flows through the bed.

\[
\frac{3}{2} H_2 + \frac{1}{2} N_2 = NH_3
\]  

(1)

The reaction is exothermic and the heat released increases the energy of the reaction mixture. The first bed is followed by three quench zones and beds, each receiving portion of the feed. The hot gas out of the forth bed after passing through the riser is cooled on the tube side of the exchanger before leaving the converter. This transfer of heat is necessary to bring the cold feed gas to reaction temperature.

**RATE EXPRESSIONS**

The intrinsic rate of reaction used in this study is a modified form of the Temkin-Pyzhev equation [9].

\[
R_{NH_3} = K_2 \left[ K_3^2 a_1^{\frac{1}{3}} (a_2^{\frac{3}{2}} - a_3^{\frac{3}{2}})^{1-\alpha} \right]
\]  

(2)

where \( R_{NH_3} \) = reaction rate (Kg - Mole of \( NH_3 \)/Hr, \( M' \) Catalyst), \( K_2 \) = velocity constant for the \( NH_3 \) decomposition, \( \alpha \) is a parameter which should have a value between 0.0 and 1.0, and \( a_1, a_2, \) and \( a_3 \) are the activities of nitrogen, hydrogen, and ammonia respectively. \( K_2 \), equilibrium constant, is calculated from the equation of Gillespie and Beattie [10].
\[ \log_k K_w = -2.691122 \log_10 T + 5.519265 \cdot 10^{-5} T + 1.848863E-7 T^2 + 2001.6/T + 2.6899 \]  

(3)

where \( T \) is in K.

The activity of various components are obtained by the application of the Lewis and Randall rule [11]. The activity coefficients of the gases involved in the synthesis of ammonia can be easily found in the literature. This information for hydrogen, nitrogen and ammonia is provided by Cooper [12], Shaw et al. [13], and Newton [14] respectively.

The fugacity of a component may also be calculated from an equation of state [5]. But in this research the equations given by Cooper, Shaw et al., and Newton, for fugacity of hydrogen, nitrogen and ammonia are used.

Two types of catalyst (Iron Oxide) have been used in the converter of this study, both manufactured by Catalysts and Chemical Inc. (C-73-1-01 and C-73-2-07). They are similar in composition except for the concentration of promoters which give different ranges of temperature application. Therefore, the C-73-2-01 catalyst is being used mainly at the top of the reactor, occupying around 15% of the total volume, while the rest is being filled in by the C-73-1-01. From the experimental data given by Guacci, et al. [15] for many catalysts, the corresponding values for \( \alpha, E_z, \log K_{w0} \) were estimated for the C-73-1-01 and C-73-2-01 types. Here the velocity constant, \( K_w \) is estimated by an Arrhenius relation of the form \( K_w = K_{w0} \exp \left( E_z / RT \right) \). The respective values for the C-73-1-01 catalyst were \( \alpha = 0.55, E_z = 44303 \text{Kj/Kg-mole}, \log (K_{w0}) = 16.2380 \) and for the C-73-2-01 were \( \alpha = 0.55, E_z = 39057 \text{Kj/Kg-mole} \) and \( \log (K_{w0}) = 14.7102 \). Where \( K_w \) has the unit of Kg.Mole / Hr. / M³ and T is in K.

Since the catalyst particles are 6-12 mm in size, evidently there exists internal pore diffusion that reduces the reaction rate. This effect is taken care of by an effectiveness factor \( \zeta \) and its calculation is done following the procedure recently reported by Singh and Saraf [6] using an expression of the type

\[ \zeta = \left[ \frac{n_0 Y_{NH_3}}{dY_{NH_3} / dt} \right] = 1 / \left[ R_p \left( 1 + Y_{NH_3} \right) R_{NH_3} / C D_{NH_3} \left( 1 - \varepsilon \right) \right] \]  

(4)

where \( Y_{NH_3} \) is the ammonia mole fraction at any point in the pellet, \( \zeta \) is a dimensional radius given by \( R_p = R_p' \varepsilon, R_p' \) is the radius of a spherical particle, \( Y_{NH_3} \) is the ammonia mole fraction in the gas bulk phase, \( C \) is the total concentration of the reacting gas mixture (Kg mole / M³), \( D_{NH_3} \) is the effective diffusion coefficient for ammonia in the particle, \( \varepsilon \) is the void fraction of packed bed, and \( R_{NH_3} \) is the rate of reaction given by Equation 2.

From Equation 4 an effective rate of formation of \( NH_3 \) per unit volume is defined as

\[ R_{NH_3} = \zeta R_{NH_3} \]  

(5)

For the deactivation of catalyst after prolonged use, a mean activity coefficient, \( v \), is incorporated into Equation 5. Therefore, Equation 5 can be written as follows

\[ R_{NH_3} = v R_{NH_3} \]  

(6)

The catalyst activity, \( v \), deteriorates at high temperatures because of changes in catalyst structure. Here the activity is defined as the ratio of the rate at which the pellet is forming \( NH_3 \) to the rate of reaction with a fresh pellet. A concentration - independent deactivation was assumed and the value of \( v \) [2,16,17,18,19] is adjusted in each bed for the steady-state simulation of the reactor at the actual operating conditions.

**MATHEMATICAL MODEL**

The converter contains three concentric tubes. The catalyst basket is kept in the middle tube. The other
tubes, outer and inner tubes are called annulus and riser respectively. The catalyst basket is coated with insulation to minimize heat transfer from the hot catalyst to the cold feed gas. An uninsulated riser tube transports gas from the last bed to the heat exchanger section. Minimal heat transfer to the riser gas is due to a small heat transfer area and due to the fact that the riser gas has been heated to near reaction temperature. The catalyst section is nearly adiabatic and an assumption of uniform radial temperature is made. A uniform velocity profile in the bed may also be assumed since the bed diameter is much larger than the catalyst diameter. The assumptions of uniform radial temperature and velocity reduce the equations to an easily usable from while retaining the desired accuracy of the model.

**MATERIAL BALANCE**

The ammonia produced in a differential element of a catalyst bed is given by

$$ F_i \delta x = R_{NH_3} A \delta z = R_{NH_3} \delta V $$

where $A$ is the cross-sectional area of the bed in $\text{m}^2$ and $\delta x$ is the change in the conversion of ammonia within the increment. $F_i$ is the flow rate of $\text{NH}_3$ into the bed, in kg.mole/ht. Figure 2 is a simplified diagram of the synthesis converters which shows flows and temperatures used in the following equations.

The flow of other components at any point in the bed may be computed from the inlet flow rate by:

$$ F_i = F_{i-1} - 0.5 F_{j-1} \delta x $$
$$ F_i = F_{i-1} - 1.5 F_{j} \delta x $$

$$ F_i = F_{i-j} (1 + \delta x) $$
$$ F_i = F_{i-1} $$
$$ F_i = F_{i-1} $$

(8)

where $F_1, F_2, F_3, F_4$ and $F_5$ are molar flow rates of nitrogen, hydrogen, ammonia, methane and argon respectively. The pressure is assumed to vary linearly through the beds with the fraction of catalyst which is traversed. It could be said that:

$$ P_i = P_n - W V_i $$

$i = 1, \ldots, N$

(9)

where, $W = (P_n - P_o) / V_n = \delta P / V_{bed}$

(10)

In which the units of pressure and $W$ are in atmosphere and atm. / $\text{m}^3$ respectively.

**ENERGY BALANCE**

The converter may be divided into three major sections: catalyst beds, quench zones, and heat exchanger. The energy balance for the converter may be obtained from the energy balance equations for the three sections by combining them in the proper order. The energy balance equations for each major section are developed. The energy balance for a horizontal differential element of catalyst bed involves four heat terms.

$$ dQ_{\text{reaction}} + dQ_{\text{gas}} + dQ_{\text{flow}} + dQ_{\text{exchanger}} = 0 $$

(11)

of which the last two are small as already indicated but are included in the model. The finalized equation is as
follows:

\[
\frac{dT}{dV} = \left[ \frac{-\delta H_{\text{Net}}}{M_i C_{\text{pmax}}} \right] + \left( \frac{U_A}{M_i C_{\text{pmax}}} \right) \times \left( \frac{dA_a}{dV} \right) \left( T_A - T \right) + \left( \frac{U_g}{M_i C_{\text{pmax}}} \right) \times \left( \frac{dA_d}{dV} \right) \left( T_D - T \right)
\]
(12)

where:

\[
dA_a/dV = 4D_a / (D_b^2 - D_a^2) \quad \text{and} \quad dA_d/dV = 4D_d / (D_b^2 - D_a^2)
\]
(13)

The heat transfer from the bed to either the gas flowing in the annulus on the outside of the catalyst basket or the gas in the riser is computed as follows:

\[
dQ_{\text{annulus}} = U_A dA_a (T_A - T) = f_i \frac{M_i C_{\text{pmax}} (T_A, P_i)}{4D_a / (D_b^2 - D_a^2)}
\]
(14)

where

\[
U_A = \frac{1}{\delta / K'} = \frac{K'}{\delta}
\]
(15)

Therefore, we have:

\[
\frac{dT_A}{dV} = \left( \frac{(K' (T_A - T))}{\delta f_i M_i C_{\text{pmax}} (T_A, P_i)} \right) \times \left( \frac{dA_a}{dV} \right) = \left( \frac{(K' (T_A - T))}{\delta f_i M_i C_{\text{pmax}} (T_A, P_i)} \right) \times \left( \frac{dA_d}{dV} \right)
\]
(16)

Since the primary resistance to heat transfer is the catalyst basket insulation, neglecting all other heat transfer resistance reduces computational effort without substantially affecting the accuracy of the simulation. For converters without insulation, heat transfer to the feed gas would be considerable and an overall heat transfer coefficient would be necessary. Since the riser is uninsulated, an overall heat transfer coefficient \(U_R\) is considered in calculating this heat term.

\[
dQ_{\text{rISR}} = U_R dA_a (T_A - T) = M_i C_{\text{pmax}} (T_A, P_i) dT_R
\]
(17)

Therefore we have:

\[
\frac{dT_R}{dV} = \left( \frac{U_R}{M_i C_{\text{pmax}} (T_A, P_i)} \right) (T_R - T) \times \left( \frac{4D_R}{(D_b^2 - D_a^2)} \right)
\]
(18)

The overall heat transfer coefficient is given by:

\[
\frac{1}{U_R} = \frac{1}{h_b} + \frac{1}{h_a} + \left( \frac{r_b}{r_a} \ln \left( \frac{r_b}{r_a} \right) / K_w \right) + R_f
\]
(19)

\(h_b\) is calculated for heat transfer inside packed tubes as described by Leva [20].

\[
h_b = \tau \cap \Omega^{0.7}
\]
(20)

where \(\Omega\) is the mass flow in Lb / HR. The geometric factor \(\tau\) is calculated from

\[
\tau = 3.5 \exp \left( -4.6 \frac{D_p}{D_b} \right) \left( \frac{D_p}{A} \right)^{0.7} / D_b
\]
(21)

where \(D_p\) is the catalyst diameter in feet and \(D_b\) is the bed diameter.

The bed heat transfer factor \(\cap\) is a function of reaction gas thermal conductivity \(K\) and gas viscosity and is given by

\[
\cap = K / \mu^{0.7}
\]
(22)

The colburn [21] equation is used to calculate the heat transfer coefficient inside the riser.

\[
h_b = 0.23 G C_{\text{pmax}} (T_R, P_i) N_{\text{Pr}}^{-0.25} N_{\text{Re}}^{-0.2} \left( \frac{r_b}{r_a} \right)
\]
(23)

\(G\) is the mass velocity Lb- mole / Hr. Ft² and the Prandtl number is computed as:

\[
N_{\text{Pr}} = C_{\text{pmax}} (T_R, P_i) \mu / K
\]
(24)

The thermal conductivity of the riser material is \(K_w\), and \(R_f\), the fouling factor, was assumed to have a value of .001.

The energy balances for the quench zones are developed assuming each zone to be adiabatic and
perfectly mixed. The corresponding equation for the Lth quench zone is

\[ M_{2L-1} H(T_{2L-1}, P) + f_{L-1} M_{L} H(T_{L}, P) = M_{2L} H(T_{2L}, P) \]  

(25)

\[ M \] is the molar flow from the previous bed and \( H \) is the enthalpy, Kcal/Kg-mole. The enthalpy of the quench is obtained by multiplying the fraction of feed used for quenched in the Lth zone by the total enthalpy of feed. Flow rate of a component out of the zone is equal to the sum of the flows in since no reaction occurs.

The energy balance for the heat exchanger located at the top of the converter may be obtained from the heat transfer equations. The cold gas flowing from the annulus passes downward through the exchanger shell side into the beds and reacted gas flows counter current and is cooled on the side. The energy balance for the gas in the heat exchanger shell side is

\[ M_{2} \int_{z} C_{p,m} (T_{2}, P_{2}) dT_{z} = -U_{h} A' (T_{2} - T_{2}) \]  

(26)

where \( A' \) is the heat transfer area in \( m^{2} / M \) of heat exchanger height and \( T_{2} \) and \( T_{2} \) are shell side and tube side temperature, respectively. \( U_{h} \), the overall heat transfer coefficient for the heat exchanger. The energy balance for the reacted gas in the exchanger tubes yields

\[ M_{2} C_{p,m} (T_{2}, P_{2}) dT_{2} = -U_{h} A' (T_{2} - T_{2}) \]  

(27)

Equations 26 and 27 may be solved analytically as suggested by Shah [22] if \( C_{P} (T_{2}, P_{2}) \) and \( C_{p} (T_{2}, P_{2}) \) are assumed to be constant and calculated at average temperature of shell and tube sides. The solution may be obtained by letting

\[ \beta = f_{L} M_{L} C_{p,m} (T_{L}, P_{L}) \]  

(28)

and

\[ \emptyset = M_{2} C_{p,m} (T_{2}, P_{2}) \]  

(29)

yields after integrating the following equation.

\[ T_{p} = \left( (c \beta / \emptyset) (T_{2} - T_{A}) \right) + T_{RT} \]  

(30)

**PHYSICAL DATA EVALUATION**

The heat capacities are taken to be a function of temperature and pressure. The temperature and pressure dependencies are expressed by Hougen and Watson [23] as polynomials. For \( N_{2}, H_{2}, CH_{4} \) and Ar the pressure dependence of the heat capacity is negligible. Mixture enthalpies are computed using the BWR equation of state. Mixture constants are computed according to Ried and Sherwood [24]. Mixture viscosity and thermal conductivity are calculated by methods suggested by Reid and Sherwood [24]. Pure component viscosities for \( N_{2}, NH_{3}, CH_{4}, Ar \) are obtained by using the theoretical treatment of Stiel and Thodos, but for \( H_{2} \) are obtained by using the theoretical treatment of Chapman and Enskog. Low pressure mixture gas viscosities are then computed by the method of Dean and Stiel, and corrected for high pressure by the equation proposed by Dean and Stiel. Pure component thermal conductivity is computed as suggested by Bromley and mixture thermal conductivities are computed according to the method of Lindsay and Bromley; the mixture value is then corrected for high pressure by the equations of Stiel and Thodos.

The basic Equations 7,8, 11, 16 and 18 have been solved by method of Rung-Kutta of fourth order. The activities used in the solution of above mentioned equations are .46, .53, .6, .61 for beds number 1,2,3,4 respectively [25].

**RESULTS AND DISCUSSION**

The calculation results for an ammonia cold shot
Table 1. Comparison between results from the simulation model and plant data of Razi Petrochemical Complex.

<table>
<thead>
<tr>
<th>Variables</th>
<th>Simulated Value</th>
<th>Plant Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inlet</td>
<td>Outlet</td>
</tr>
<tr>
<td>Pressure, atm.</td>
<td>140</td>
<td>135.3</td>
</tr>
<tr>
<td>H₂ / N₂ ratio</td>
<td>3.02</td>
<td>3.02</td>
</tr>
<tr>
<td>Temperature to the converter, °C</td>
<td>135</td>
<td>-</td>
</tr>
<tr>
<td>Total molar flow rate, Kg. Mole / Hr.</td>
<td>22616.6</td>
<td>20589</td>
</tr>
<tr>
<td>% of gross feed to 1st bed.</td>
<td>.6149</td>
<td>-</td>
</tr>
<tr>
<td>% of gross feed as quench to 1st bed.</td>
<td>0.0</td>
<td>-</td>
</tr>
<tr>
<td>% of gross feed as quench to 2nd bed.</td>
<td>.1379</td>
<td>-</td>
</tr>
<tr>
<td>% of gross feed as quench to 3rd bed.</td>
<td>.1477</td>
<td>-</td>
</tr>
<tr>
<td>% of gross feed as quench to 4th bed.</td>
<td>.0995</td>
<td>-</td>
</tr>
<tr>
<td>Catalyst volume of 1st bed, M³</td>
<td>10.1</td>
<td>-</td>
</tr>
<tr>
<td>Molar composition of 1st bed.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas %</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nitrogen.</td>
<td>21.00</td>
<td>19.661</td>
</tr>
<tr>
<td>Hydrogen.</td>
<td>63.350</td>
<td>59.348</td>
</tr>
<tr>
<td>Ammonia.</td>
<td>2.050</td>
<td>6.763</td>
</tr>
<tr>
<td>Argon.</td>
<td>3.350</td>
<td>3.505</td>
</tr>
<tr>
<td>Methane.</td>
<td>10.250</td>
<td>10.723</td>
</tr>
<tr>
<td>Temperature, °C</td>
<td>420</td>
<td>490.9</td>
</tr>
<tr>
<td>Catalyst volume of 2nd bed, M³</td>
<td>13.2</td>
<td>-</td>
</tr>
<tr>
<td>Molar composition of 2nd bed.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas %</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydrogen.</td>
<td>60.109</td>
<td>57.514</td>
</tr>
<tr>
<td>Ammonia.</td>
<td>5.867</td>
<td>8.923</td>
</tr>
<tr>
<td>Argon.</td>
<td>3.475</td>
<td>3.576</td>
</tr>
<tr>
<td>Methane.</td>
<td>10.633</td>
<td>10.940</td>
</tr>
<tr>
<td>Temperature, °C</td>
<td>429.06</td>
<td>473.75</td>
</tr>
<tr>
<td>Catalyst volume of 3rd bed, M³</td>
<td>19.7</td>
<td>-</td>
</tr>
<tr>
<td>Molar composition of 3rd bed.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas %</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydrogen.</td>
<td>58.524</td>
<td>56.189</td>
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<tr>
<td>Ammonia.</td>
<td>7.733</td>
<td>10.484</td>
</tr>
<tr>
<td>Argon.</td>
<td>3.536</td>
<td>3.627</td>
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<tr>
<td>Methane.</td>
<td>10.821</td>
<td>11.097</td>
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<tr>
<td>Temperature, °C</td>
<td>414.6</td>
<td>453.8</td>
</tr>
<tr>
<td>Catalyst volume of 4th bed, M³</td>
<td>27.8</td>
<td>-</td>
</tr>
<tr>
<td>Molar composition of 4th bed.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas %</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nitrogen.</td>
<td>18.859</td>
<td>18.144</td>
</tr>
<tr>
<td>Hydrogen.</td>
<td>56.954</td>
<td>54.817</td>
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<tr>
<td>Ammonia.</td>
<td>9.583</td>
<td>12.099</td>
</tr>
<tr>
<td>Argon.</td>
<td>3.597</td>
<td>3.680</td>
</tr>
<tr>
<td>Methane.</td>
<td>11.007</td>
<td>11.259</td>
</tr>
<tr>
<td>Temperature, °C</td>
<td>416.74</td>
<td>452.1</td>
</tr>
<tr>
<td>Produced ammonia, (T.E.NH₃ / DAY)</td>
<td>-</td>
<td>1016.4</td>
</tr>
<tr>
<td>Product temperature, °C</td>
<td>-</td>
<td>444.73</td>
</tr>
</tbody>
</table>

The results in Table 1 show that in general the calculated values are in good agreement with the

Journal of Engineering, Islamic Republic of Iran
Vol. 8, No. 2, May 1995 - 67
plant data. Maximum difference in plant data and calculated ammonia concentration exists at the exit from the second bed; nevertheless, this error is under one percent and is well within expected range of error. The difference in temperature is maximum in outlet of the forth bed with a measured value of 11°C higher than the calculated one which leads to 1.6 percent error.

Once the validity of the proposed model is confirmed by the plant data, the concentration and temperature profiles along the beds and the temperature profile along the annulus and riser are obtained. Figures 3 and 4 show the temperature and ammonia concentration profiles along the beds. Figure 5 shows the temperature profiles along the annulus and riser.

* Financial support of the Shiraz University Office of Research is appreciated.

**NOMENCLATURE**

A = cross sectional area of bed (m²).
A' = heat transfer area per meter of exchanger (m²/M).
A_r = circumference of riser (m²).
A_ś = circumference of catalyst section (m²).
a_i = activity of component i (dimensionless).
C = total concentration of reacting gas mixture (Kg - Mole /M³).
C_p = specific heat of reacting gas mixture (Kcal/Kg - Mole /K).
D_a = annulus diameter (m).
D_n = catalyst basket diameter (m).
\[ D_{NH_3} = \text{effective diffusion coefficient of ammonia (M}^2/\text{S}). \]

\[ D_s = \text{catalyst particle diameter (Ft)}. \]

\[ D_r = \text{riser diameter (M)}. \]

\[ F_i = \text{inlet molar flow rate of component i to each compartment (Kg - Mole / Hr)}. \]

\[ F_j = \text{outlet molar flow rate of component i from each compartment (Kg - Mole / Hr)}. \]

\[ f_i = \text{fraction inlet flow (dimensionless)}. \]

\[ G = \text{mass velocity (Lb - Mole / Hr / Ft}^2). \]

\[ (H) = \text{molar enthalpy of mixture (Kcal / Kg - Mole)}. \]

\[ \delta H = \text{heat of reaction (Kcal / Kg - Mole)}. \]

\[ h_o = \text{outside heat transfer coefficient (Btu / Hr.Ft.Ft}^2). \]

\[ h_t = \text{tube side heat transfer coefficient (Btu / Hr.Ft.Ft}^2). \]

\[ i = 1 \text{ refers to } N_{es}, 2 \text{ refers to } H_{es}, 3 \text{ refers to } NH_{es}, 4 \text{ refers to } CH_4, 5 \text{ refers to } A. \]

\[ K = \text{thermal conductivity of gas mixture (Btu / Hr. (sq. ft)). (Ft / Ft)}. \]

\[ K_s = \text{equilibrium constant in terms of activities (dimensionless)}. \]

\[ K'_s = \text{thermal conductivity of catalyst basket insulation (Kcal / Hr. M}^2. C/M). \]

\[ K_w = \text{thermal conductivity of riser tube (Btu / Hr. (sq. ft). Ft/Ft)}. \]

\[ K_z = \text{rate constant for decomposition of ammonia (Kg - Mole / Hr / M}^2). \]

\[ L = \text{subscript refers to converter zone (dimensionless)}. \]

\[ M_f = \text{molar flow rate of feed (Kg - Mole / Hr)}. \]

\[ M_o = \text{molar flow rate out of converter (Kg - Mole / Hr)}. \]

\[ M_t = \text{molar flow rate through the reactor length (Kg - Mole / Hr)}. \]

\[ N_{fr} = \text{prandtl number (dimensionless)}. \]

\[ N_{Re} = \text{reynolds number (dimensionless)}. \]

\[ P = \text{pressure (atm)}. \]

\[ P_f = \text{pressure of feed (atm)}. \]

\[ P_j = \text{pressure at the inlet of bed (atm)}. \]

\[ P_k = \text{pressure at any point in the bed (atm)}. \]

\[ P_o = \text{pressure at the outlet of bed (atm)}. \]

\[ P_r = \text{pressure out of converter (atm)}. \]

\[ Q = \text{heat term (Kcal)}. \]

\[ R = \text{gas constant (Kcal / Kg - Mole / K)}. \]

\[ R_s = \text{fouling factor (dimensionless)}. \]

\[ R_{NH_3} = \text{reaction rate (Kg - Mole NH}_3/\text{Hr / M}^2\text{.Cal}). \]

\[ R_{eff} = \text{effective rate of NH}_3\text{ formation per unit of bed volume (Kg - Mole NH}_3/\text{Hr / M}^2). \]

\[ r_p = \text{radius of spherical particle (M)}. \]

\[ r_i = \text{inside tube diameter (M)}. \]

\[ r_o = \text{outside tube diameter (M)}. \]

\[ T = \text{temperature (K)}. \]

\[ T_a = \text{temperature in annulus f(K)}. \]

\[ T_c = \text{temperature in Lth zone (K)}. \]

\[ T_f = \text{temperature of feed (K)}. \]

\[ T_o = \text{temperature out of converter (K)}. \]

\[ T_r = \text{temperature in riser (K)}. \]

\[ T_AB = \text{temperature at bottom of annulus (K)}. \]

\[ T_AT_P = \text{temperature at top of annulus (K)}. \]

\[ T_BS = \text{temperature at bottom of riser (K)}. \]

\[ T_BT_R = \text{temperature at top of riser (K)}. \]

\[ T_S = \text{temperature on shell side of exchanger (K)}. \]

\[ T_T = \text{temperature on tube side of exchanger (K)}. \]

\[ U_{an} = \text{overall heat transfer coefficient of annulus (Kcal / K.Ft.Ft. Hr)}. \]

\[ U_{ex} = \text{overall heat transfer coefficient of exchanger (Kcal / K. Ft.Ft. Hr)}. \]

\[ U_{rs} = \text{Overall heat transfer coefficient of riser (Kcal / K. Ft.Ft. Hr)}. \]

\[ V = \text{volume of catalyst bed (M}^3). \]

\[ V_f = \text{the volume of catalyst up to any point of the bed (M}^3). \]

\[ V_b = \text{volume of bed (M}^3). \]

\[ V_{cat} = \text{catalyst activity (dimensionless)}. \]

\[ W = \text{constant in Equation 9 (atm. / M}^3). \]

\[ X_i = \text{mole fraction of component i (dimensionless)}. \]

\[ \delta X = \text{conversion of ammonia (dimensionless)}. \]

\[ Z = \text{distance from top of bed (M)}. \]

**GREEK SYMBOLS**

\[ \alpha = \text{Kinetic parameter (dimensionless)}. \]

\[ \beta = \text{defined by Equation 28 (Kcal / Hr / K)}. \]
\( \varepsilon \) = void fraction (dimensionless).
\( \mu \) = viscosity of gas mixture (Lb. / Ft. Hr).
\( \Omega \) = mass flow rate (Lb. / Hr).
\( \zeta \) = effectiveness factor (dimensionless).
\( \tau \) = geometric factor.
\( \gamma \) = bed heat transfer factor.
\( \phi \) = defined by Equation 29 (Kcal. / Hr / K).
\( \delta \) = thickness of insulation (M).

**REFERENCE**