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SIMULATION OF AMMONIA SYNTHESIS LOOP

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RESUME

Cet exposé présente les résultats d'un exercice de simulation effectué pour une boucle de synthèse d'une unité d'ammoniac de 1350 t/j. Le logiciel repose sur des principes physico-chimiques fondamentaux et il est commercialisé pour une unité donnée avec tout son équipement, tuyauterie, etc. Le programme peut répondre à la question "Quoi faire si ? c'est-à-dire que sera le comportement de l'unité si la température, la pression, le débit ou la composition en un point de la boucle est modifié. Le rendement, la consommation d'énergie pour le compresseur de gaz recyclé, la charge de réfrigération et la quantité et la qualité des purges sont calculés.

L'industrie indienne des engrais compte plus de 35 unités d'ammoniac, utilisant différentes matières premières, technologies et capacités de production, construites ces 30 dernières années. Dans chaque cas, la technologie choisie et la dimension de l'unité reposaient sur une technologie à jour et les facteurs économiques dominant au stade d'élaboration. Au fil des années, plusieurs modifications, améliorations dans les méthodes opératoires, réhabilitations ont entraîné des gains significatifs en terme d'accroissement de capacité, nombre de jours de fonctionnement, consommation d'énergie, etc.

Ayant atteint un coefficient élevé d'utilisation de la capacité et une consommation d'énergie proches de la valeur théorique, l'industrie de l'ammoniac en Inde vient de commencer à s'intéresser à l'emploi des techniques de simulation et d'optimisation pour rechercher de nouvelles améliorations dans le fonctionnement des unités. Plusieurs possibilités allant du simple traitement de données à une optimisation continue très avancée utilisant des concepts de contrôle sophistiqué ont été considérées et en sont actuellement à des stades divers de mise en oeuvre. Comme il y a un grand éventail de choix, les décisions concernant le type et le niveau d'application sont susceptibles de varier d'une unité à l'autre selon l'utilité perçue, la possibilité d'application et l'analyse coût-bénéfice. Les besoins en logiciel et matériel et les investissements varient aussi avec la nature de l'application de l'ordinateur.

Cet exposé examine le développement du logiciel pour une simulation discontinue en condition constante d'une boucle de synthèse d'ammoniac dans un atelier moderne de 1350 t/j marchant sur gaz. Avant de décrire l'ampleur du travail de simulation on donne un brève description de la boucle de synthèse.

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SYNTHESIS LOOP

The main components of the synthesis loop are the synthesis reactor, equipment for heat recovery from converter effluent gas, synthesis compressors, chillers and separator **(Figure 1)**. Ammonia synthesis is an exothermic reversible reaction. Nearly 30% of hydrogen is converted to ammonia in the reactor. Heat is recovered from the converter effluent gas in a steam boiler and boiler feed water preheater. The gas is further cooled in a gas-gas heat exchanger in which recycle gas to the reactor is heated. The converted effluent after gas-gas heat exchanger is at about 60°C and in gaseous state. This gas is cooled in water cooler where ammonia condensation starts. This gas-liquid stream is cooled in cold gas-gas heat exchanger where recycle gas from ammonia separator gets heated.

For further cooling of converter effluent gas, two chillers are used with ammonia as refrigerant. After the first ammonia chiller purge gas is removed and make up synthesis gas is added to the loop. After the second ammonia chiller the gas is separated and recycled, the liquid ammonia is sent for further separation.

The recycle gas after ammonia separator passes through the cold gas-gas heat exchanger, compressor and hot gas-gas heat exchanger in that order. In both the heat exchangers it gets heated by the converter effluent gas.

In the synthesis compressor, the make-up synthesis gas and recycle gas are compressed. The two-case compressor consists of a low pressure case and a high pressure case. In the low pressure case make-up synthesis gas is compressed in two stages from 26 to 52 to 104 atm. In the high pressure case the make up synthesis gas is compressed in the first stage from 104 to 196 atm and recycle gas in the second stage from 190 to 220 atm. All the stages are driven by a single shaft run by steam turbine.

SCOPE AND OBJECTIVE OF THE SIMULATION PACKAGE

Simulation packages can be developed to serve a variety of purposes and can vary in scope over a wide range. The present package was developed to be plant specific and to answer off-line "What if" question and serve as a guide and support to the plant personnel. In addition, it was desired that it should be usable on an inexpensive PC and complete the simulation in a short time.

Accordingly, the main operating parameters which can be set or changed by the operators of this plant namely reactor inlet pressure and temperature, fraction of vapour part removed as purge, make up synthesis gas flow rate in addition to some temperatures are to be specified by the user of the package. Physico-chemical parameters are an inbuilt part of the package. The simulation package then computes the ammonia production, temperature, pressure, flow rate and composition of each of the 23 streams, compressor rpm and power, heat recovered by boiler feed water and in H.P. steam, chiller load and refrigeration power. In addition, incremental cost of additional ammonia produced and increase in profit/day using costs relevant to the current Indian conditions are computed.

REACTOR MODEL

Mathematical model based on fundamental physico-chemical principles was developed for the adiabatic two bed radial flow reactor with heat exchange (between the inlet gas and the outlet from the first bed and cold shot to adjust the temperature of the gas entering the first bed). Giving the feed gas flow rate, its composition, temperature and pressure, and knowing the heat exchanger configuration and the dimensions of the two catalyst beds, the performance of the reactor is calculated using the kinetic, thermodynamic and transport properties. The somewhat divergent literature information on the thermodynamic, transport and kinetic parameters required a careful choice of the values. Use of forward rate constant and cold shot fraction as adjustable parameters sufficed to tune the model to match the simulation results for the design case. The well-known feature of very low conversion obtained in such an auto-thermal reactor in case of high inerts level was predicted by the model as should be expected of a phenomenon based model.

VALIDATION OF SYN LOOP MODEL

The development of the model for the complete loop was initiated with the operating conditions of the design case which corresponds to 1350 MTPD ammonia production. The same plant has been operated at appreciably higher capacities for which the data were available. The model capability to predict the higher production levels was tested without adjusting any of the parameters, for a range of actual operating conditions with production varying from 1420 to 1550 MTPD ammonia. The plant performance and the model predictions are compared in **Table 1.**

Table 1: Model Validation

	Case I		Case II		Case III		Case IV	
	Design	Simulation	Plant	Simulation	Plant	Simulation	Plant	Simulation
Production, MTPD	1350	1350	1423	1421	1493	1492	1550	1547
Recycle Flow, 1000 Nm^3/hr	591	609	652	624	624	650	706	689
% Methane in Recycle	6.1	5.6	6.6	7.4	6.5	6.4	6.7	7.5
Reactor Exit, Temp °C	458	455	445	444	447	448	447	445
Compressor, rpm	-	10220	10150	10240	10350	10540	10200	10290

The above results substantiate the suitability of the simulation package to compute the plant performance over a wide range of operating conditions.

REACTOR PERFORMANCE

As part of the simulation results, temperature, concentration profile and local reaction rate are computed as a function of the reactor length for both the beds. Typical conversion versus bed length for two of the cases are shown in **Tables 2 and 3** from which it can be seen that only a part of the catalyst bed is utilised in attaining the conversion obtained e.g. for the first bed the final conversion obtained in less than 50% of the bed for 1350 MTPD and in not much more than 50% for 1550 MTPD. Similarly for the second bed less than 70% of the bed is required for 1350 MTPD and less than 90% for 1550 MTPD. The estimated catalyst requirement for production of 1350 and 1550 MTPD, other conditions remaining the same as those used for plant operation were 66 and 91 m^3 as against catalyst charge of 108 m^3. Of course, the amount of catalyst required would change with pressure, temperature, hydrogen-nitrogen ratio, the effect of all these can be calculated with the simulation package. The results thus show that there is sufficient catalyst in the reactor bed to produce more ammonia under a variety of combinations of operating conditions with regard to temperature, pressure, feed composition and feed flow rate.

Table 2: Conversion Profile in First Bed

Production (MTPD)	1350	1550
Bed Volume%	Hydrogen	Conversion
10	0.0379	0.0265
30	0.1414	0.0950
50	0.1618	0.1718
70	0.1619	0.1820
90	0.1619	0.1822
100	0.1619	0.1822

Table 3: Conversion Profile in Second Bed

Production (MTPD)	1350	1550
Bed Volume%	Hydrogen	Conversion
0	0.1619	0.1822
50	0.2798	-
70	0.2830	0.3053
90	-	0.3089
100	0.2830	0.3091

COMPRESSOR

Another major equipment in the synthesis loop is the compressor. The simulation results showed that the compressor rpm for plant load of 1550 MTPD is 10290 **(Table 5)** as against the upper recommended rpm of 10840 showing a considerable margin to compress larger quantities of gas.

OFF-LINE SIMULATION AND OPTIMISATION

In light of a valid model, excess catalyst and sufficient margin in compressor rpm the package was used for exploring its use for off-line simulation to answer "What If" questions with regard to each of the variables which the operator can change and to which the package responds. The findings for two of these variables namely fraction of vapour part removed as purge and make-up syn gas flow rate are discussed below:

Fraction of Vapour Part Removed for Purge

With sufficient catalyst in the reactor and margin in the compressor it should be possible to increase ammonia production by reducing the purge quantity. This would of course increase the inerts in purge and in recycle, increase the recycle flow rate and the chilling load simultaneously reducing the heat available to the reformer as reduced purge of lower calorific value. Since the software takes all these into account the simulation package was used to explore the effect of this variable at several levels of production achieved in the plant from 1350 to 1550 MTPD. Typical results are shown in Tables **4** and **5.**

Table 4: Production Increase by purge Reduction
(Base Case - 1350 MTPD Operation)

Make-up syn gas flow, 1000 Nm^3/hr	161	161	161	161
Production, MTPD	1350	1381	1401	1419
% Inerts in purge	10.4	13.6	16.4	20.9
Compressor power, 1000 KW	21.5	21.8	22.2	22.4
Refrigeration load, million Kcal/hr	8.5	8.8	9.9	9.4
Heat recovered, 10^6 Kcal/hr	36.1	36.7	36.9	37.2
Heating value of purge	2320	1620	920	800
Equivalent NG, Nm^3/hr, compressor, rpm	10230	10240	10250	10290
Increase in production, MTPD	-	31	51	69
Incremental cost of production, Rs/MT	-	1760	1750	1890
Additional profit Rs/day	-	99600	163600	213900

Increase in inerts in the reactor beyond a limit may stop the reaction. The increase in compressor rpm and refrigeration load and reduction in heating value of purge gas may be noted. Since no change in front end is required, the incremental cost of additional ammonia can be easily worked out. Using the costs relevant to the current Indian scenario the software also computes the additional profit per day which is reported in the **Table 4**.

Table 5 reports the results of simulation at base production level of 1547 MTPD. The numbers change but the trends are similar to those for the case of 1350 MTPD in that the purge quantity can be decreased to production obtain additional ammonia resulting in good addition to profit and production. It may be observed that the maximum permissible % inerts in purge goes only up to 18.2% .

Table 5: Production Increase by Purge Reduction
Base Case - 1547 MTPD

M.U. syn gas, 1000 Nm^3/hr	182	182	182	182
Production, MTPD	1547	1563	1579	1583
% Inerts in purge	13.2	15.1	17.7	18.2
Compressor power, 1000 KW	24.1	24.4	24.8	25.0
Refrigeration load, million Kcal/hr	6.6	6.8	7.1	7.2
Heat recovered, million Kcal/hr	40.7	40.9	41.1	41.1
Heating value of purge Eq. NG, Nm^3/hr	1960	1600	1240	1150
Compressor, rpm	10290	10320	10360	10370
Increase in production, MTPD	-	16	32	36
Incremental cost of production, Rs/MT	-	2070	2210	2220
Additional profit, Rs/day	-	46900	89250	100800

Influence of make up syn gas flow rate

The results discussed above were obtained under the constraint of make up syn gas flow rate which had been already achieved in the plant (182,000 Nm^3/hr) as against the design case of 161,000 Nm^3/hr. Since the synthesis reactor, compressor and chilling unit were not fully utilised even at a production level of 1583 TPD the feasibility of increased production by increased syn gas make up flow rate was explored by using the simulation package. The results are shown in **Table 6**.

Table 6: Production Increase with Make up Syn Gas Flow

Syn gas flow, 1000 Nm^3/hr	175	190	200	203	205	220
Production, MTPD	1446	1626	1712	1738	1755	1883
Recycle flow, 1000 Nm^3/hr	685	740	779	790	798	857
% Inerts in Purge	12.6	16.4	16.4	16.4	16.4	16.4
Compressor, power, 1000 KW	23.7	26.5	28.4	28.9	29.4	32.3
Refrigeration load, million Kcal/hr	9.00	10.20	10.75	10.90	11.00	11.80
Heat recovered, million Kcal/hr	38.9	42.5	44.5	45.1	45.4	48.3
Compressor, rpm	10390	10620	10790	10820	10870	11120

The simulation results demonstrate that compressor rpm constraint will become operative at a production level of about 1720 MTPD although the reactor would suffice to go to still higher production. At a production level of 1720 MTPD make up syn gas flow rate required would be about 202,000 Nm^3/hr. The front end of the plant has already been used to produce 182,000 Nm^3/hr. It may be noted that the results of fine tuning of inlet pressure, temperature and purge quantity are not included in the about result.

The software discussed in the present paper can be implemented on a PC 386. A single run is implemented in less than 2 minutes.

CONCLUSION

To sum up, a simulation package for off-line simulation based on physico-chemical modeling of key equipment has been developed. The package which can be used on an inexpensive PC is capable of quickly answering several "What If" questions with which the plant operator is concerned. The answer can be used to guide the operator to implement changes in operating conditions that become desirable for efficient plant operation in light of changing scenario.

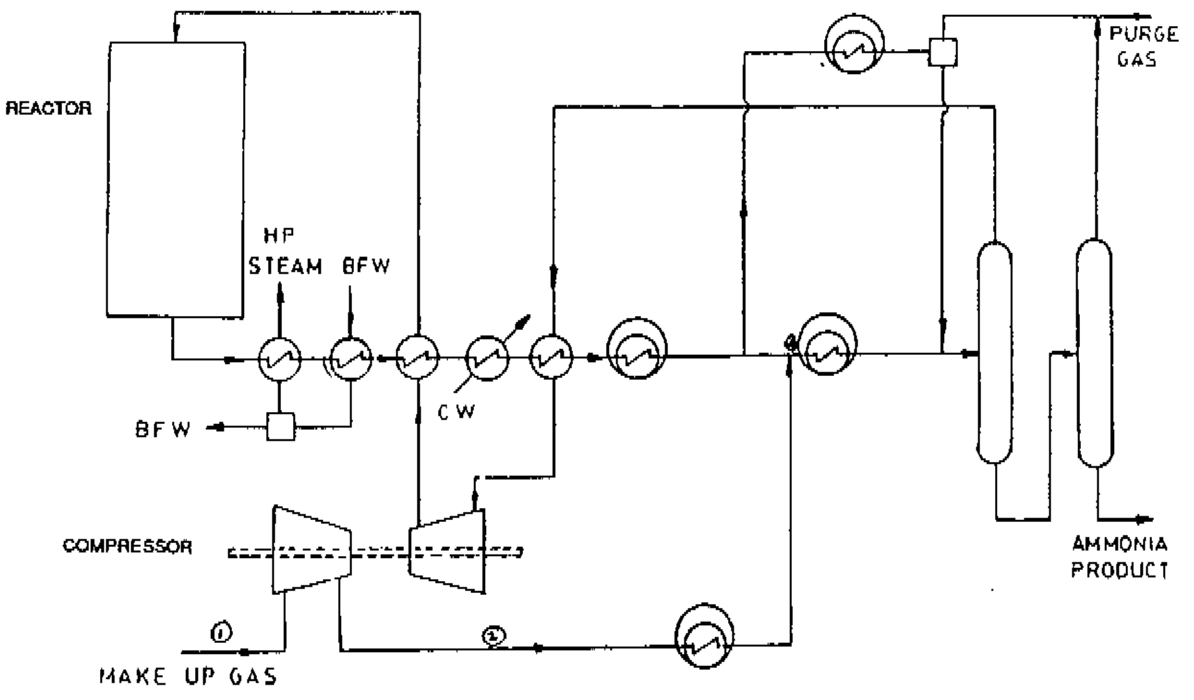

FIGURE 1 AMMONIA SYNTHESIS LOOP