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INTRODUCTION

A PRTR is an environmental database or inventory of potentially harmful releases or transfer to air, water and soil as well as waste transported off site for treatment or disposal. In addition to collecting data for PRTR from stationary sources, PRTR are also designed to include estimates of releases from diffuse sources such as agriculture and transport activities.

PRTR data are useful in identifying some of the sources of pollutants and their possible risks to human health, these data represent a portion of all chemical releases and transfers in a given area from a range of industrial and non-industrial sources.

This document contains information about the role of process simulation in PRTR projects.

This document is divided in three parts:

- **the process simulator**, in which this category of software and related software is briefly described and their role in the PRTR project is evidenced;
- **the training program**, in which the description of training activities are reported, focusing on process simulation but also on other software as reported in the previous section;
- **the case studies**, in which a description of case studies of growing difficulties are presented; all the case studies have been developed within the PRTR project.

THE ROLE OF PROCESS SIMULATORS IN PRTR PROJECT

The Process simulator

A process simulator solves material and energy balances by means of a computer code. A description of a typical process simulation code is reported in figure 1 in which all the most important elements of a simulator and their connections are evidenced. Figure 1 shows clearly that a process simulator include cost estimation routines as well as economic evaluation. The importance of the database is shown in the figure as a necessary source of information for different objects in the structure.

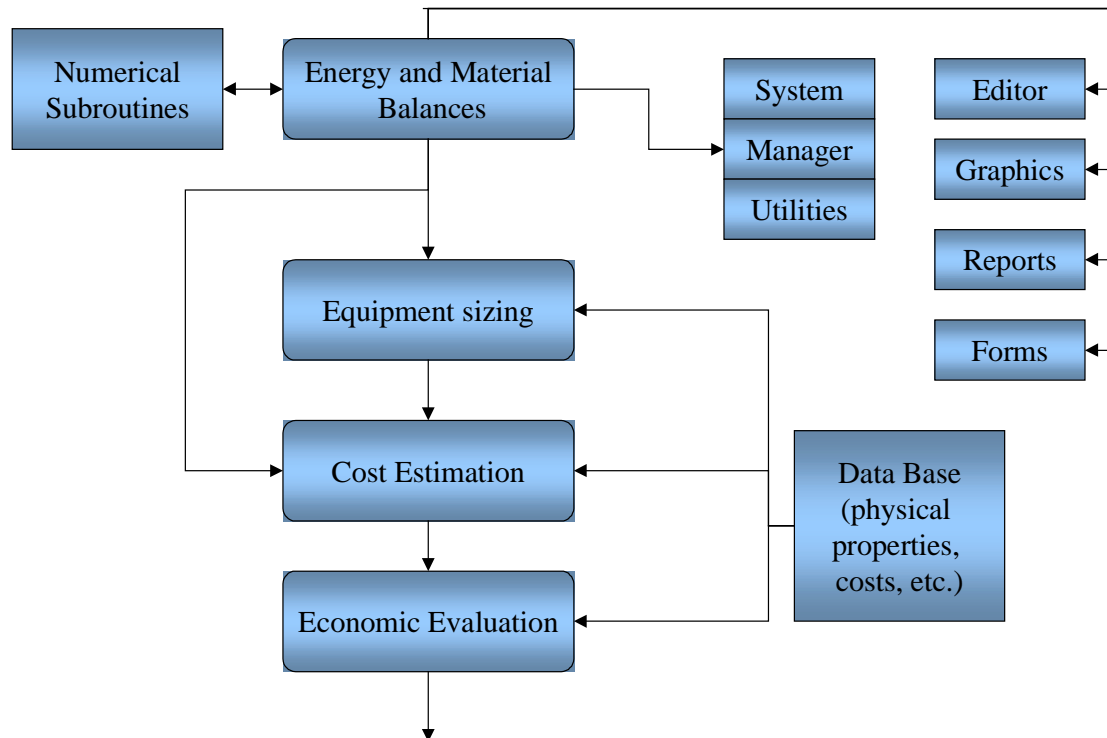


Figure 1: general scheme representing a steady state process simulator

Mathematically speaking a process simulator solves a set of n non linear material balances equations and 1 non linear energy balance equation. This gives as a result a set of differential - algebraic equations, if the dynamic simulation is considered, in presence of:

- Very many components;
- Complex thermo-physical models for phase equilibrium calculations
- A high number of subsystems (equipment)
- Rather complex equipment (distillation column,...)
- Recycle streams
- Control loops

The following different approaches are available in the process simulation:

- Steady state simulation which considers a snapshot in time of the process
- Dynamic simulation which considers the evolution in the time domain of the equations describing the process
- Integrated steady state - dynamic simulation, which combines the two previously, described approaches.

The approaches listed above may be used in three different philosophies when dealing with process simulation. One possibility is to perform a process analysis, in which an existing process is studied and alternative conditions as well as dynamic behavior is investigated for the appraisal of effectiveness of design. The second approach is the process synthesis, in which different process configurations are compared aiming to the identification of the optimal choice of units and the connections between them. The third possible use of process simulation is the process design and simulation, aiming at the establishment of the optimal operating conditions of a given process.

In all the possible philosophy of application process simulation impact on industry is pervasive rather than restricted to a single moment in the development of the process. Process simulation has affected strongly the way engineering knowledge is used in processes. The traditional way of using process simulation was mainly focused on flow sheet design and on equipment critical parameters definition, such as distillation column stages, column diameter, and so on.

Today engineers are oriented to a more comprehensive use of process simulation in the entire 'life' of the plant such as the control strategies design, the process parameters optimization, the time evolution of the process for understanding start up and shut down processes and performing risk analysis, the operator training and the definition of procedure to reduce the unsteady state operations.

The main benefits one can gain from such a comprehensive use of the process simulation are the partial or total replacement of Pilot Plant operations (reduction of the number of runs and runs planning), the reduction of time to market for the development of new processes, the fast screening of process alternatives to select the best solution in terms of economic aspects, environmental aspects, energy consumption aspects and flexibility of the proposed process.

The Role of Process simulators in the PRTR project

The development and implementation of a PRTR system adapted to national needs represents a mean for governments to track generation, release and the fate of various pollutants over time. A PRTR can therefore be an important tool in the total environment policy of a government and encouraging reporters to reduce pollution by implementation of cleaner technologies. PRTR can be complementary to industry programmes such as ISO14000.

PRTR have generally these defining characteristics:

- reporting on individual chemicals
- by individual industrial facilities
- on all releases and transfers
- to all environmental media (air, water, land)
- periodically
- with consistently structured data
- entered into a computer database
- actively disseminated to the public
- with limited data held as trade secrets
- with the aim to improve environmental quality and promote cleaner technology.

The main technical procedures for the implementation of PRTR are the quantification of releases by combining two approaches:

- Monitoring campaign for the emissions, effluents and industrial solid waste generated individually by the industrial partners
- Using the available software designed specially for the quantification and estimation of industrial releases.

An analysis to both approaches can be carried out, with the objectives of:

- Identifying the differences between the monitoring and estimation that are used for estimating releases of the same or similar sources.

- Identifying approaches for determining the accuracy and reliability of the estimation techniques and examines applicability, limitations and uncertainties of each technique.
- Preparing criteria for determining which techniques seem to work best in which situations and how techniques could be improved.

Process simulation software is the tool for providing description of process output, including releases and pollutants, by knowing process input and process parameters.

Process simulation is the mathematical representation of a group of operations that transfer input streams into product streams by means of chemical – physical transformations by using a computer, providing a reliable platform for solving material and energy balances using variations of the sequential modular or equation based approaches.

The role of process simulation in the PRTR project is depicted in figure 2, in which it is clear that the data base of the information on wastes and disposal is of prominent importance in the project. The data input to this data base can be provided in several ways by the industrial partners. Certainly the easiest way of providing data is the direct measure of the releases by means of a suitable measuring device. But not always these measurements are readily available or economically affordable: in such cases it is possible to calculate the emissions, both qualitatively and quantitatively by solving material and energy balances by means of computer codes.

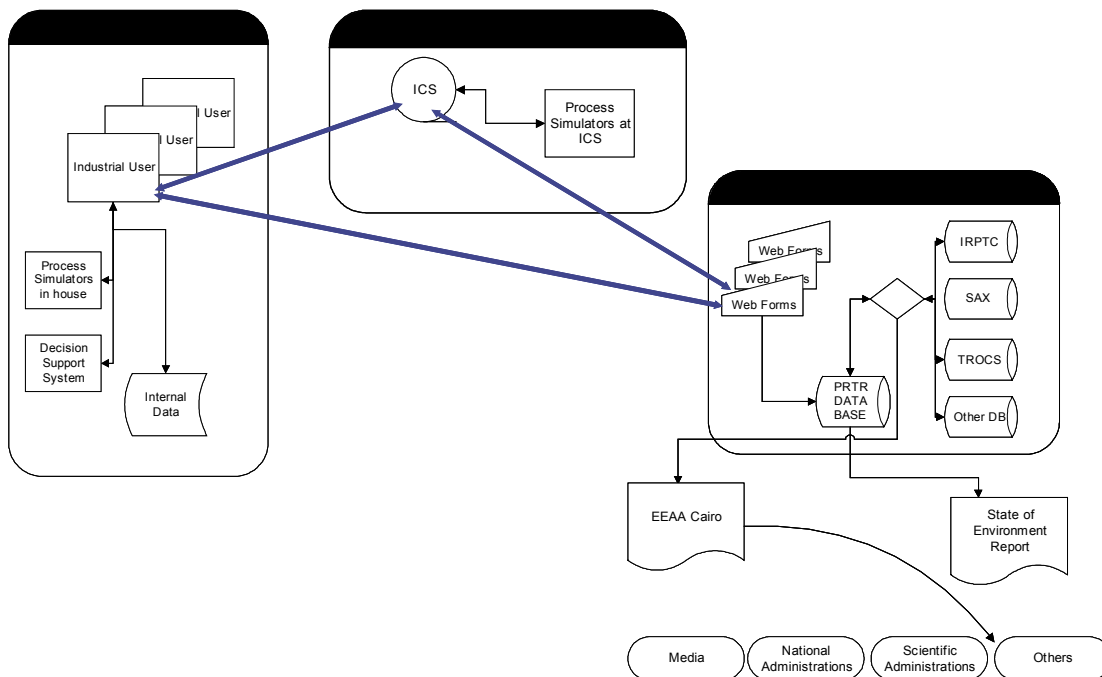


Figure 2: information flow and role of process simulators in PRTR project

Other Software

Process simulators can be integrated by other software which may be also useful in the PRTR project for determining the quality and quantity of emissions and releases when they cannot be directly measured.

One software is the **Integrated Pollution Control (IPC)** software, which is used to assess rapidly the pollution situation in a specific geographic location, such as metropolitan area or water basin, and to analyze alternative pollution control strategies and policies.

IPC generates estimated pollution loads in a study area by applying standard emission factors to data on the scale of economic activities by industry/sector. These load estimates can be further processed to compute annual average concentrations in an area and/or water body and the impacts of selected pollution controls. The IPC extends this approach to calculating the costs of controls and outlining a cost-effective abatement strategy.

Computation modules can estimate:

- Air, water and solid waste emissions.
- Ambient concentrations of air and water pollutants.
- Total costs of control options.
- Long-run marginal cost schedules to achieve a certain level of emission reduction (or decline in ambient concentration) for a chosen pollutant.

Another software of interest for the project is the **Transport of Chemical Substances (TROCS)** which is a maritime transport-oriented database, used to assist the first responder in the decision-making process during marine oil or chemical spill situations.

The database presents a wide list of oil and chemical products (containing oil properties data, physical chemical data, transportation data), a list of the main oil shoreline countermeasures, and also some other items or tools (UN labels, marks and signs signification, unit Conversion programme, TNT equivalent calculation programme).

In addition to TROCS software, the chemical data bank (IRPTC) can also be used as information sources for PRTR project. The data bank on chemicals, operated by **The International Register of Potentially Toxic Chemical (IRPTC)**, has a series of files on all aspects of a chemical that are deemed important to hazard assessment, including a Waste Management File and a Legal file.

The information on these chemicals is presented in the form of data profiles which aim at providing comprehensive description of information needed to assess the hazard presented by a given chemical. IRPTC collects monitoring data concerning humans and the environment. In addition it provides chemical, physical and toxicological characteristics relevant for hazard assessment, information on production and consumption, main uses, and waste management, as well as recommendations and legal mechanisms for the control of risks posed by chemicals. IRPTC has the following goals:

- Enhance obtaining information on production, distribution, release, disposal and adverse effects of chemicals;
- Help to identify potential hazards from chemicals and wastes and to improve awareness of the dangers;
- Provide information about national, regional and global policies, controls and recommendations on potentially toxic chemicals;
- Promote the development and application of methodologies relevant for assessing health and environmental hazards and risks;
- Promote the development and application of methodologies and tools for the implementation of effective chemical management systems, ensuring safer and cleaner production, handling, use and disposal of chemical.

TRAINING ACTIVITY

The training is an important task for the PRTR pilot project implementation since skill in the use of simulation programs and related software is not common in process and environmental engineers in developing countries. Training activity on process simulation and related software has the following goals:

- Training on process simulation, process control and thermodynamic software as an estimation technique for quantification of releases in order to set up process simulation for industrial case studies in PRTR project.
- Training on analysis of the process of the industrial partners, implementation of the simulation schema, performing sensitivity analysis as an environmental application of process simulation.
- Training on the use of software IPC, for estimating releases of items on PRTR database based on production data and emission factor. This software is useful for application of PRTR if the authority needs to estimate releases from small and medium enterprises by economic sector. It can also be used to estimate releases from transportation and releases from agriculture sector.
- Using other software (TROCS and IRPTC) to support PRTR project with a wide range of information necessary for assessing and managing chemical risks and oil spill emergency plan.
-

Structure of the Training

The training activity for reaching all the goals listed in the previous section lasts approximately 3 months, including the development of some case studies. In this period, the first two months are devoted to training on advanced tools in process simulation with attention to model selection, thermodynamics and kinetics according to the following program:

- Introduction to process simulation: fundamentals and use, different approaches for process simulation,
- Numerical strategies and procedures of process simulation.
- The concept of base case, introductory examples to process simulation.
- The user interface of PRO II and Aspen+
- General concepts of material and energy balances.
- Data banks in process simulation software.
- Thermodynamic modeling and fundamental of phase equilibrium.
- Unit operations based on phase equilibrium: flash, distillation,...
- Interactive chemical process principles software for learning about unit operation principles.
- Chemical reaction: fundamentals and ideal reactors.
- Analysis tools: sensitivity, optimization, with examples.
- Elementary examples and environmental application of process simulation.

The third month is devoted to work with the other software, starting first with IPC software with an example of a given study area to obtain the following outputs:

- Air, water waste emissions.
- Ambient concentrations of air and water pollutants.
- Total costs of control options by using standardized engineering-type cost functions.

- Long-run marginal cost schedules to achieve a certain level of emission reduction (or decline in ambient concentration) for a chosen pollutant

The training program ends with the study and training on the last two software: TROCS and IRPTC. These software are used to obtain information on physical chemical properties, shore guide, sea guide information linked to the selected chemical.

Results of the Training

The result of the training can be summarized in the following:

- Gaining experience on using process simulation as an estimation technique for quantification of releases generated from industrial process.
- Applying simulation as process integration for sustainable industrial development by performing sensitivity analysis, optimization techniques.
- Using of other software (IPC) designed for quantification of industrial releases, pollution load, and releases from transport and agriculture.
- Using of other chemical database (TROCS and IRPTC) required for assessing and managing chemical risks, oil spill emergency plan.

After the training activity on the selected software the participant is able to perform the following actions within the PRTR project:

- Contact the industrial partners in order to obtain data required for simulation of the unit operations of the industrial partners, including:
 - Be able to develop a simplified process schema of the industrial units that will be simulated, the schema should indicate the units, streams including material and energy.
 - Get information concerning description of the general operating conditions of the process in terms of temperature, pressure, concentration, components, composition, and flow rate.
 - Detailed description of all input streams of the process, all material entering the process as liquid, gas and solid with conditions as temperature, pressure, total flow rate, reaction and other input information related to simulation of the process.
- Designing the flow sheeting of the process required to be simulated.
- Co-operate with ICS-UNIDO for better simulating the process in order to obtain the estimated releases generated from the processes of the industrial partners.
- Obtain input data required for operating IPC software from the industrial partners or from the PRTR database reported.
- Integrate the output information obtained from (TROCS) software concerning chemical and physical properties of chemicals together with IRPTC data bank and the estimated releases obtained from process simulation and IPC with PRTR database.

CASE STUDIES

This section includes some case studies developed during the training. More details is available upon request from ICS-UNIDO.

The case studies reported here as examples are the following:

- Methylene Chloride Recovery
- Ammonia Production
- Carbon Black Process

- Vinyl chloride Monomer Production
- Example of application of IPC software

1. Methylene Chloride Recovery

Application of steam stripping technology to the treatment of methylene chloride-contaminated process wastewaters has been shown to effectively recover solvent for recycling. Steam stripping of aliphatic halogenated solvent from contaminated wastewater allows recovery of solvent for recycle. Recovery permits reduced costs for raw solvent purchase, providing economic savings. In addition, reduction of solvent concentrations in process wastewater promotes facility compliance with environmental standards.

Description

The solvent recovery system from a chemical plant was used to recover methylene chloride from wastewater before it was discharged to the sewer.

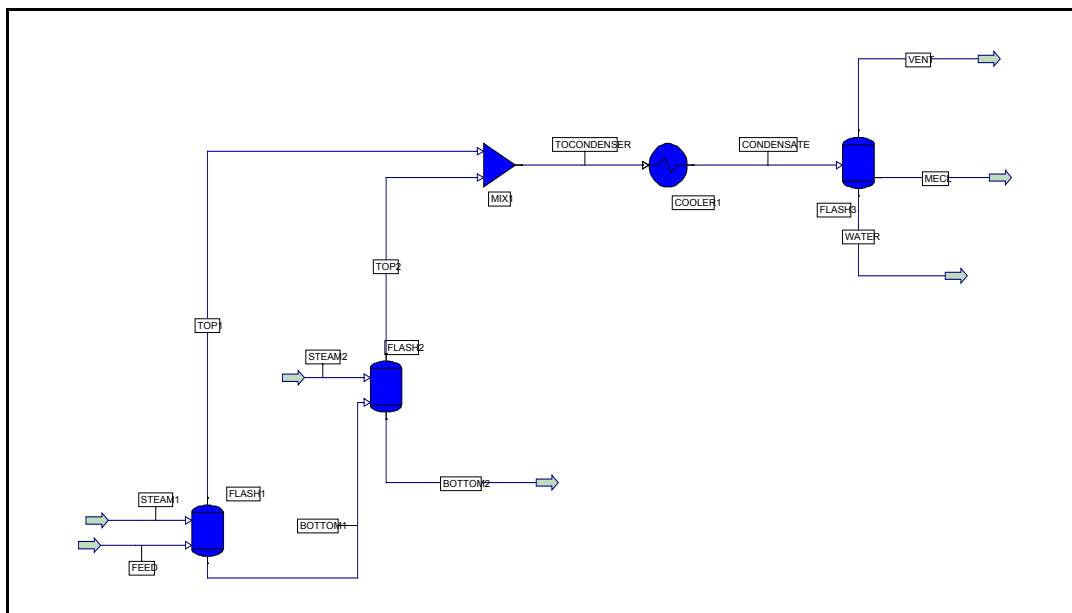


Figure 1.1. Flow sheet for Methylene Chloride recovery from waste.

A stream with 10.000 lb/hr of Water and Methylene Chloride is fed to a first tower and combined with a stream of saturate vapour at 200 psi.

Two streams are obtained in this operation, the bottom stream is fed to a second flash, where the top product is separated and mixed with the top stream of the first flash. The mixed vapours are conducted to a condenser and next to a decanter, where is recuperated methylene chloride. The figure 1.1 shows the simulation flow sheet.

The situation requires disposing water with the lower organic content to less than 150 ppm of Methylene Chloride. The simulation conditions are given in the tables 1.1 and 1.2.

TEMPERATURE (F)		100
PRESSURE (atm)		24.7
TOTAL FLOWRATE (lb/h)		100.000
Mass Composition	Methylene Chloride	0.014
	Water	0.986

Table 1.1 Stream feed conditions, in the methylene chloride recovery study.

Stream	Steam1 (first tower)	Steam2 (Second Tower)
Pressure (psi)	200	200
Flow rate (lb/h)	5.000	10.000

Table 1.2. Stream vapour conditions, in the methylene chloride recovery study.

Objectives

- Recovery methylene chloride from the waste
- Sensitivity analysis of the flow rate of steam on the primary tower with fixed secondary tower steam flow rate in 5.000 lb/h
- Sensitivity analysis of the flow rate of steam on the secondary tower with fixed primary tower steam flow rate in 10.000 lb/h

Results

A simulation model was developed to calculate steam consumption, which could constitute the biggest operating cost. In this process the NRTL thermodynamic model was used. It is very important to define a liquid-liquid–vapour equilibrium with the purpose of obtaining results similar to the experimental information.

Recovery methylene chloride from the waste

The table 1.3 resumes the information obtained in this simulation.

With these conditions, the content of methylene chloride is 934.9 ppm (0.0002 mole fraction en BOTTOM2 stream), which does not enough to dispose the wastewater. It is necessary to change the steam flow rates to reach the objective. The total recuperated of Methylene Chloride is 90.86%.

Stream	FEED	BOTTOM1	BOTTOM2	TOP2	TOP1	MECL	WATER	VENT
Phase	Liquid	Liquid	Liquid	Vapor	Vapor	Liquid	Liquid	Mixed
Temperature F	77.00	181.14	218.001	218.001	181.143	75.000	75.000	0.000
Pressure PSIA	14.70	19.70	18.700	18.700	19.700	14.700	14.700	0.000
Molecular Weight	18.22	18.11	18.028	25.689	58.590	84.270	18.311	
Total Lb-mol/h	5489.71	6031.37	6247.020	61.897	13.434	15.127	60.204	0.000
Component Mole Fract.								
CL2M	0.003	0.001	0.0002	0.1147	0.6063	0.9901	0.0044	0.000
H2O	0.997	0.9986	0.9998	0.8853	0.3937	0.0099	0.9956	0.000

Table 1.3. Results obtained in the initial methylene chloride simulation.

Sensitivity analysis of the flow rate of steam on the primary tower with fixed secondary tower steam flow rate in 5.000 lb/h.

The results of this analysis can be observed in the figure 1.2. The goal is reached with a flow rate of 13.247 lb/h of vapor in STEAM1. The total consumption of steam was 18.247 lb/h.

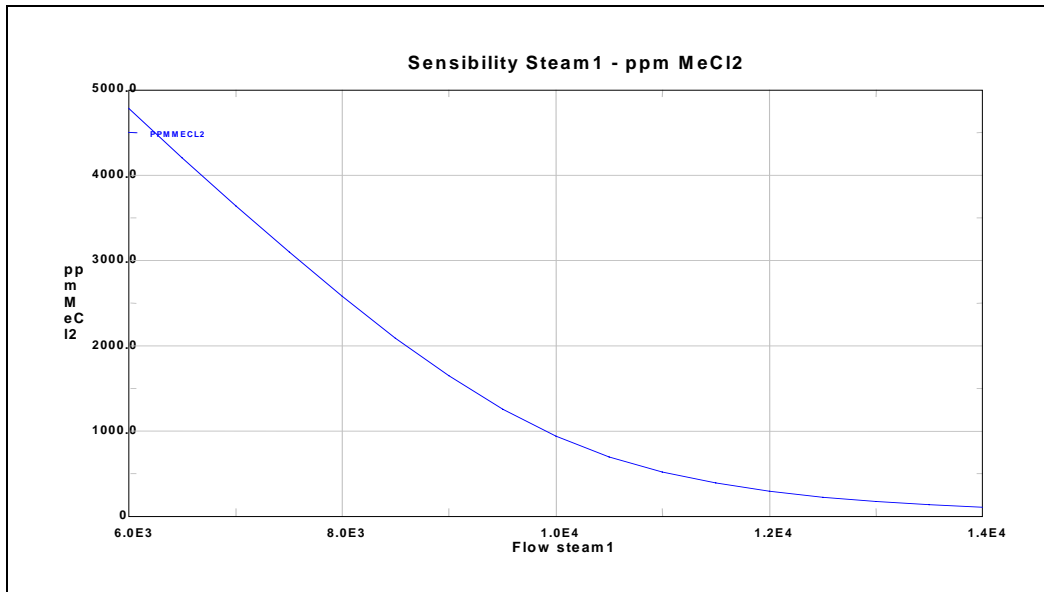


Figure 1.2. Sensibility Analysis for STEAM1 Stream flow rate (lb/h) versus composition of Methylene Chloride (ppm) in BOTTOM2 stream.

Sensitivity analysis of the flow rate of steam on the secondary tower with fixed primary tower steam flow rate in 10.000 lb/h.

The results of this analysis can be observed in the figure 1.3. The goal is reached with a flow rate of 12.036 lb/h of vapor in STEAM2. The total consumption of steam is 22.036 lb/h.

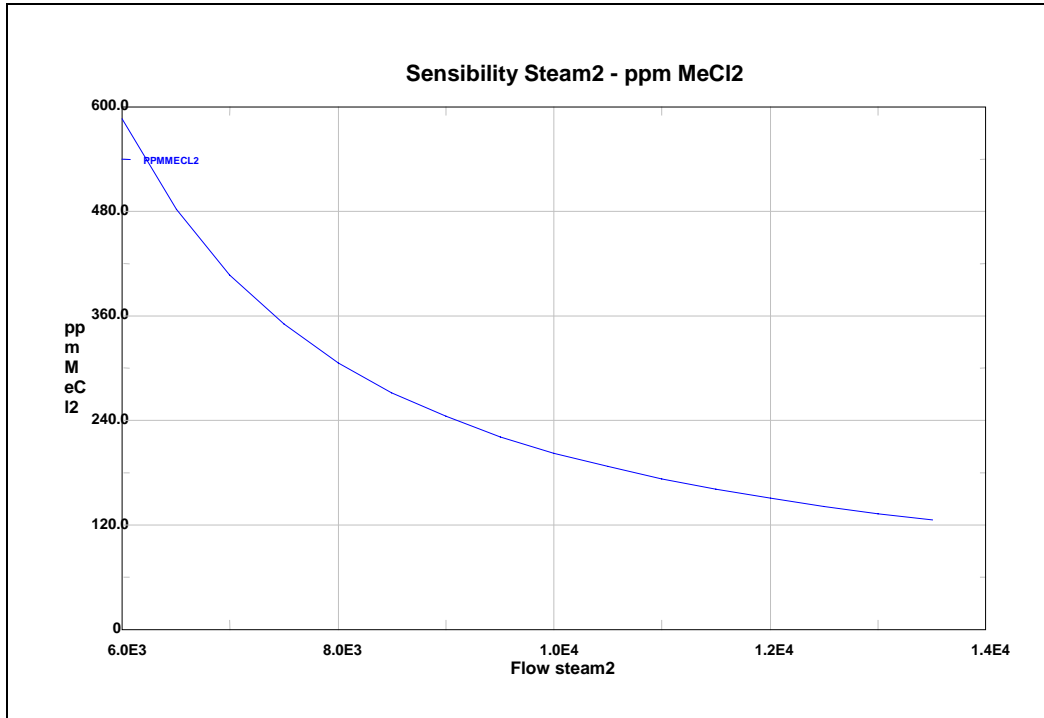


Figure 1.3. Sensibility Analysis for STEAM2 Stream flow rate (lb/h) versus composition of Methylene Chloride (ppm) in BOTTOM2 stream.

2. Ammonia Production

Ammonia is one of the most highly produced chemicals in the world. In the U.S alone more than 17 million tons of ammonia are produced every year. Ammonia is not only used as a direct fertilizer but is also to produce a number of other fertilizers. It is used as a coolant in refrigeration and cooling processes. It is also used to produce a wide variety of other chemicals such as pharmaceuticals, specialty chemicals, polymers and plastics, and even explosives.

The main raw materials for ammonia production are nitrogen (from air) and a hydrogen source (which can be water or hydrocarbons such as natural gas, fuel oils, and coal). The most widely used and environmentally safe method is the production of ammonia by natural gas. According to the International Fertilizer Industry (IFA) nearly 77% of the world ammonia production is based upon natural gas. Steam reforming of natural gas is the most commonly used ammonia production process. The work was focused in the simulation of the reaction stage.

Description

The catalytic reaction for producing ammonia through the Haber process was simulated. The figure 2.1 shows the diagram for the process. The conversion per pass is 65% of N₂. The reaction products are refrigerated to separate 75% of NH₃ product per pass (no pressure drop in mixer). The remaining product is recycled back after purge (10%)

The reaction carried out is shown in the equation (1)



Other conditions for the reaction are given in the table 2.1.

TEMPERATURE (F)		930
PRESSURE (psi)		7350
TOTAL FLOW RATE (lbmol/h)		100
FLOWRATE (lbmol/h)	Hydrogen	74.0
	Nitrogen	24.5
	Methane	1.2
	Argon	0.3

Table 2.1. Reaction conditions in the ammonia production.

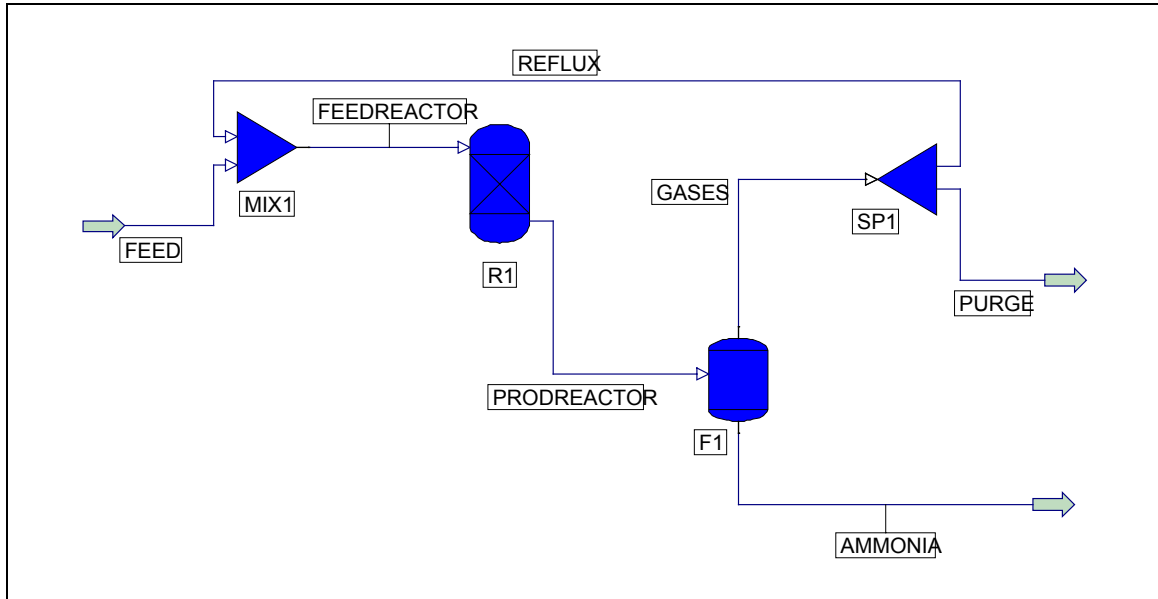


Figure 2.1. Flow Sheet for Ammonia production

Objectives

Simulate the problem with the initial conditions.

- Adjust the purge rate so that the combined feed to the reactor contains 18% CH₄ (mass fraction).
- Calculate all the streams for two additional values of input methane flow rates (2 and 3 lbmole/hr).
- Optimization: maximize the product value. Ten times the difference between the flow rate in of NH₃ in *AMMONIA* and *PURGE* streams, with the constrain that the *FEEDREACTOR* stream cannot exceed 500 lbmole/h. (see figure 2.1).

Results

A simulation model was developed to resolve the problem. In this process the PENG ROBINSON thermodynamic model was used due to the system is working at high pressure.

Simulate the problem with initial conditions

The table 2.2 resumes the information obtained in this simulation.

STREAM		FEED	FEED REACTOR	PROD REACTOR	AMMONIA	GASES	REFLUX	PURGE
Temperature	F	300.000	184.468	930.000	42.212	42.212	42.212	42.212
Pressure	PSIA	500.000	500.000	7350.000	500.000	500.000	500.000	500.000
Molecular Weight		8.667	9.910	13.542	17.038	11.604	11.604	11.604
Component Molar Rates	LB-MOL/HR							
H2		74.000	111.053	41.355	0.093	41.262	37.136	4.126
N2		24.500	35.743	12.510	0.018	12.492	11.243	1.249
METHANE		1.200	10.700	10.700	0.069	10.630	9.567	1.063
AR		0.300	2.260	2.260	0.068	2.191	1.972	0.219
AMMONIA			13.490	59.955	44.967	14.989	13.490	1.499
Total	LB-MOL/HR	100.000	173.245	126.779	45.215	81.564	73.408	8.156

STREAM	FEED	FEED REACTOR	PROD REACTOR	AMMONIA	GASES	REFLUX	PURGE
Component Mole Fractions							
H2	0.7400	0.6410	0.3262	0.0021	0.5059	0.5059	0.5059
N2	0.2450	0.2063	0.0987	0.0004	0.1532	0.1532	0.1532
METHANE	0.0120	0.0618	0.0844	0.0015	0.1303	0.1303	0.1303
AR	0.0030	0.0130	0.0178	0.0015	0.0269	0.0269	0.0269
AMMONIA	0.0000	0.0779	0.4729	0.9945	0.1838	0.1838	0.1838

Table 2.2. Results obtained in the initial simulation for ammonia production.

In this situation, a notable quantity of Ammonia is eliminated in the stream PURGE, in order to 2.5%. It is necessary to increase the recycled relation with the purpose of recovery more Ammonia in the Stream AMMONIA.

Adjust the purge rate so that the combined feed to the reactor contains 18% CH₄ (mass fraction).

With this objective, it was necessary to make a plot of the reflux relation (product fraction recycled) versus the CH₄ composition in the reactor feed (FEEDREACTOR Stream). The information obtained is shown in the figure 2.2. For an 18% of Methane, the Fraction Recycled obtained by interpolation is 0.9624. With this recycle condition; the table 2.3 gives the simulation results. In this case, we can observe a decrease in the ammonia loss and the product flow is increased due to the reactor works with more high flows. The limit to minimize the purge is given for the kinetics and design of the reactor.

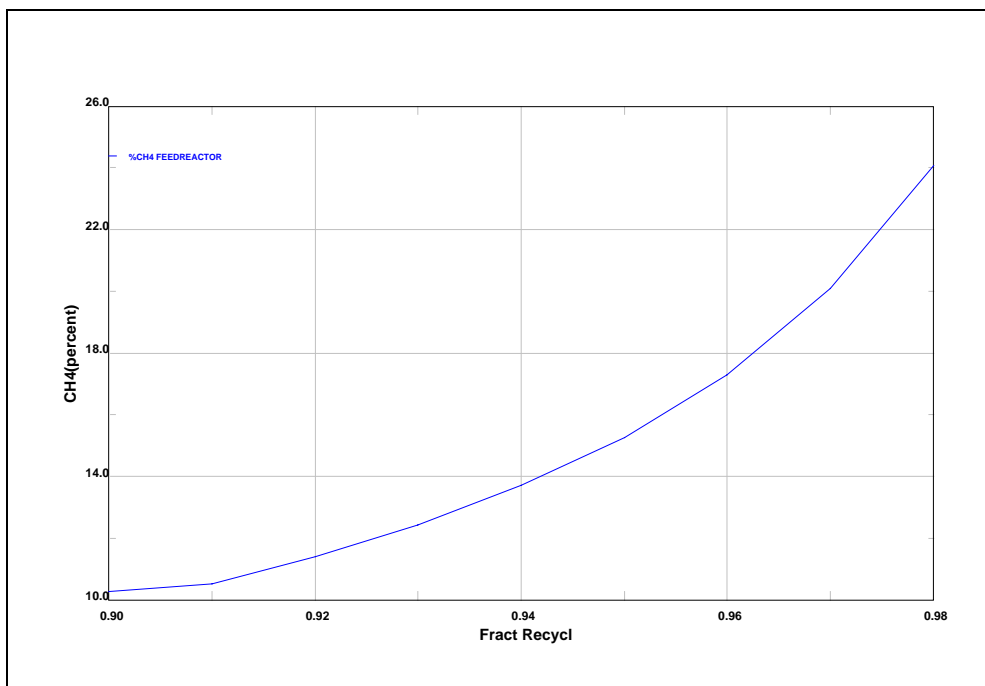


Figure 2.2. Sensibility analysis for the percent of Methane in the FEEDREACTOR Stream, in function of Products Fraction Recycled.

<i>Stream</i>		FEED	FEED REACTOR	PROD REACTOR	AMMONIA	GASES	REFLUX	PURGE
Temperature	F	300.000	157.914	930.000	31.605	31.605	31.605	31.605
Pressure	PSIA	500.000	500.000	7350.000	500.000	500.000	500.000	500.000
Molecular Weight		8.667	10.404	13.684	17.059	12.144	12.144	12.144
Comp.Molar Rates	LB-MOL/HR							
H2		74.000	120.516	48.514	0.081	48.434	46.612	1.821
N2		24.500	36.924	12.923	0.014	12.910	12.424	0.485
METHANE		1.200	23.280	23.280	0.115	23.165	22.294	0.871
AR		0.300	4.357	4.357	0.110	4.247	4.088	0.160
AMMONIA			15.207	63.208	47.406	15.802	15.208	0.594
Total	LB-MOL/HR	100.000	200.283	152.282	47.725	104.557	100.626	3.931
Component Mole Fractions								
H2		0.7400	0.6017	0.3186	0.0017	0.4632	0.4632	0.4632
N2		0.2450	0.1844	0.0849	0.0003	0.1235	0.1235	0.1235
METHANE		0.0120	0.1162	0.1529	0.0024	0.2216	0.2216	0.2216
AR		0.0030	0.0218	0.0286	0.0023	0.0406	0.0406	0.0406
AMMONIA			0.0759	0.4151	0.9933	0.1511	0.1511	0.1511

Table 2.3. Results obtained when is fed methane to reactor with an 18% concentration.

Calculate all the streams for two additional values of input methane flow rates (2 and 3 lbmole/hr).

The estimation for these two flows was realized. The information generated is given in the table 2.4.

<i>STREAM</i>		FEEDREACTOR		PRODREACTOR		AMMONIA		PURGE	
<i>FLOW METHANE (lbmole/h)</i>		2	3	2	3	2	3	2	3
Temperature	F	140.412	167.186	930.000	930.000	22.767	32.070	22.767	32.070
Pressure	PSIA	500.000	500.000	7350.000	7350.000	500.000	500.000	500.000	500.000
Molecular Weight		10.899	10.441	13.950	13.831	17.060	17.038	12.749	12.349
Comp. Molar Rates	LB-MOL/HR								
H2		121.358	111.107	49.248	41.397	0.063	0.070	1.721	4.133
N2		36.980	35.749	12.943	12.512	0.010	0.013	0.453	1.250
METHANE		41.416	26.955	41.416	26.955	0.161	0.135	1.444	2.682
AR		4.764	2.303	4.764	2.303	0.103	0.059	0.163	0.224
AMMONIA		15.285	13.492	63.359	59.965	47.519	44.974	0.554	1.499
Total	LB-MOL/HR	219.803	189.606	171.730	143.132	47.857	45.251	4.336	9.788
Component Mole Fractions									
H2		0.5521	0.5860	0.2868	0.2892	0.0013	0.0016	0.3971	0.4222
N2		0.1682	0.1885	0.0754	0.0874	0.0002	0.0003	0.1044	0.1277
METHANE		0.1884	0.1422	0.2412	0.1883	0.0034	0.0030	0.3330	0.2740
AR		0.0217	0.0121	0.0277	0.0161	0.0022	0.0013	0.0376	0.0229
AMMONIA		0.0695	0.0712	0.3689	0.4190	0.9929	0.9939	0.1279	0.1532

Table 2.4. Comparative information between different flows of Methane in the feed.

Optimization: maximize the product value.

The tables 2.5 and 2.6 resume the information obtained in this simulation.

RESULT	FINAL VALUE
BEST OBJECTIVE FUCTION	487.8
CONSTRAINT	336.2
VARIABLE	0.997

Table 2.5. Optimization results.

In this simulation, the variable employed is the reflux relation, where it takes the unitary value at total recirculation of the products from the reactor. This optimization gives a minimization in the ammonia losses. These losses were calculated in 0.046 lbmole/h (0.071% of the PRODREACTOR stream); table 2.6.

Stream		FEED	FEED REACTOR	PROD REACTOR	AMMONIA	GASES REFLUX	PURGE
Temperature	F	300.000	75.305	930.000	-6.520	-6.520	-6.520
Pressure	PSIA	500.000	500.000	7350.000	500.000	500.000	500.000
Molecular Weight		8.667	11.792	13.794	17.099	13.113	13.113
Comp. Molar Rates	LB-MOL/HR						
H2		74.000	160.623	87.339	0.042	87.296	87.052
N2		24.500	37.582	13.154	0.004	13.150	13.113
METHANE		1.200	107.401	107.401	0.176	107.225	106.925
AR		0.300	14.902	14.902	0.180	14.722	14.680
AMMONIA			16.157	65.014	48.760	16.254	16.208
Total	LB-MOL/HR	100.000	336.666	287.809	49.162	238.647	237.979
Component Mole Fractions							
H2		0.7400	0.4771	0.3035	0.0009	0.3658	0.3658
N2		0.2450	0.1116	0.0457	0.0001	0.0551	0.0551
METHANE		0.0120	0.3190	0.3732	0.0036	0.4493	0.4493
AR		0.0030	0.0443	0.0518	0.0037	0.0617	0.0617
AMMONIA			0.0480	0.2259	0.9918	0.0681	0.0681

Table 2.6. Final information generated in the optimization of the ammonia production.

3. Carbon Black Process

Introduction

Carbon black is produced by the reaction of a hydrocarbon fuel such as oil or gas with a limited supply of combustion air.

Due to its excellent pigmentation properties, especially its light stability and universal insolubility, carbon black has been used as a black pigment since early times. The principal uses of carbon black are as a reinforcing agent in rubber compounds (especially tires) and as a black pigment in printing inks, surface coatings, paper, and plastics.

The process for the production of carbon black also is important due the reactions are used in the hydrogen generation.

Approximately 90% of all carbon black sales are to rubber industry. However, while the major portion of carbon black is sold to the tire industry, carbon black is also used by printing industry (for pigments blacks in printing inks) and by the plastic industry.

Process Description

The increasing demand for carbon black led to new production process. The most important process today is the *Furnace Black process*. Developed in the United States in the 1930s and substantially improved after World War II, it is continuous process, which allows the production of a variety of carbon black grades under carefully controlled conditions. Nevertheless, other processes, such as Gas black, Lamp Black, Thermal Black and Acetylene Black processes, are still used for the production of specialties.

The principal raw materials are mixtures of gaseous or liquid hydrocarbons, which can be vaporized. Since aliphatic hydrocarbons give lower yields than aromatic hydrocarbons, the latter are primarily used. Unsubstituted polynuclear compounds with 3-4 rings give the best yield. The material rich in these compounds are certain fractions of coal tar oils and petrochemical oils from petroleum refining or the production of ethylene from naphtha (aromatic concentrates and pyrolysis oils). These aromatic oils, which are mixtures of variety of substances, are most important feedstock today. The aromatic portion of typical petrochemical oil consists of 10-15% monocyclic, 50-60% bicyclic, 25-35% tricyclic, and 5-10% tetracyclic aromatics.

In particular, the catalytic activity of carbons produced from different hydrocarbons can be arranged in the following order:

Naphthalene > benzene > ethylene > propane > methane

It is also clear that in the presence of ethylene and polyaromatics increase the aliphatics decomposition rate.

Furnace black process

The furnace black process was developed in the United States in the 1920s and since then, it has been refined (see figure 3.1).

The process use two feed stocks, the primary usually is converted to carbon black (high content in aromatics), while the secondary is used to generate energy (natural gas).

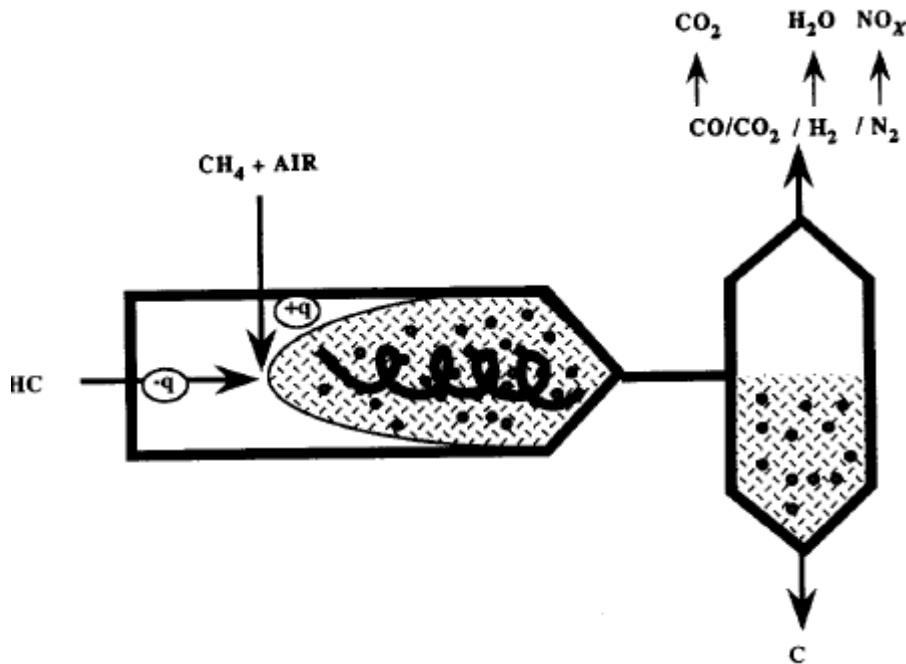
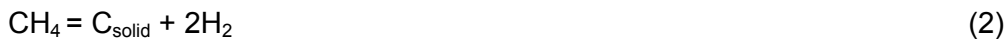


Figure 3.1. Reactor diagram used in the production of carbon black

Carbon black is produced by the reaction of a hydrocarbon fuel such as oil or gas with a limited supply of combustion air at temperatures of 1200 to 1900°C. The temperature is achieved by burning the secondary feedstock with air. The oxygen, which is in excess with respect to the secondary feedstock, is not sufficient for complete combustion of primary feedstock. The majority of which is therefore pyrolysed to form carbon black. The reaction mixture is then quenched with water and further cooled in heat exchanger, and the carbon black is collected from the tail gas by a filter system. The unburned carbon is collected as an extremely fine black fluffy particle, 10 to 500 nanometers (nm) in diameter.

Primary quench water-cools the gases to 500°C to stop the cracking. The exhaust gases entraining the carbon particles are further cooled to about 230°C by passage through heat exchangers and direct water sprays. The black is then separated from the gas stream, usually by a fabric filter. A cyclone for primary collection and particle agglomeration may precede the filter.

Methane decomposition reaction is moderately endothermic process. The energy requirement per mole of hydrogen produced (37.8 kJ/mol H₂) is considerably less than that for the steam reforming process (63.3 kJ/mol H₂). Due to this relatively low endothermicity of the process, less than 10% of the heat of methane combustion is needed to drive the process.



However if the target product is hydrogen, steam catalytic reforming is preferred:



The carbon monoxide obtained in this process is transformed to hydrogen by the shift-reaction:



The synthesis gas replaces natural gas fuel for the carbon black reactor and its upgraded heating value allows for overall reduction of natural gas consumption or an increase in carbon black production.

The recovered carbon black is finished to a marketable product by pulverizing and wet palletizing to increase bulk density. Water from the wet pelletizer is driven off in a gas-fired rotary dryer. From 35 to 70 percent of the dryer combustion gas is charged directly to the interior of the dryer, and the remainder acts as an indirect heat source for the dryer. The dried pellets are then conveyed to bulk storage.

The properties of carbon black depend on the ratios of primary feedstock, secondary feedstock and air, which therefore must be controlled carefully. The particle size of carbon black generally decreases with increasing amounts of excess air relative to the amount needed for the complete combustion of the secondary feedstock. Since the excess air reacts with the primary feedstock, a greater amount of air leads to higher oil combustion rates, resulting in rising temperatures in the reaction zone. As a consequence, the nucleation velocity and the number of particles formed increase, but the mass of each particle and the total yield decrease.

The yields, which depend on the carbon black type and the type of primary feedstock, range between 40 and 65% for some types of carbon black. High surface area pigment blacks with markedly smaller particle size than rubber blacks give lower yields (10-30%). Other parameters influencing carbon black quality are the manner in which the oil is injected, atomized, and mixed with the combustion gases, the type and amount of additives, the preheating temperature of the air and the quench position.

During the reaction time, several reactions on the carbon surface occur, so that the chemical nature of the carbon black surface is modified with increasing residence time. Varying the pelletising and drying conditions can also further modify carbon black surface properties.

Thermal process

The thermal process is a cyclic operation in which natural gas is thermally decomposed (cracked) into carbon particles, hydrogen, and a mixture of other organics. Two furnaces are used in normal operation. The first cracks natural gas and makes carbon black and hydrogen.

When methane is heated to high temperature, the methane decomposes or cracks to carbon and hydrogen:



Or Propane decomposes to produce carbon and Hydrogen



Temperatures above 700 C are required and, although lower pressures allow higher feedstock conversions since the reaction is equilibrium limited, higher pressures favor higher rates of reaction. The endothermic energy required to perform this reaction is only 18 Kcal/mole to produce 2 moles of hydrogen. The carbon produced is usually in particulate form and must be separated from the hydrogen gas stream. The main gaseous product is hydrogen. The system is a semi-continuous process.

The effluent gas, from the first reactor, is cooled by water sprays to about 125°C, and the black is collected in a fabric filter. The filtered gas (90 percent hydrogen, 6 percent methane,

and 4 percent higher hydrocarbons) is used as a fuel to heat a second reactor. When the first reactor becomes too cool to crack the natural gas feed, the positions of the reactors are reversed, and the second reactor is used to crack the gas while the first is heated. Normally, more than enough hydrogen is produced to make the thermal black process self-sustaining, and the surplus hydrogen is used to fire boilers that supply process steam and electric power.

The thermodynamics of the thermal decomposition of methane can be determined from the decomposition reaction $\text{CH}_4 = \text{C} + 2\text{H}_2$. The figure 3.2 represents an equilibrium diagram of the mole fraction left in the gas phase as a function of temperature and pressure. Hydrogen and methane are in equilibrium with carbon in the solid phase. The figure 3.2 indicates that above temperatures of 800 C at one atmosphere total pressure, very little methane remains and the gas phase hydrogen content is over 95%. At higher pressure the equilibrium shifts to higher methane concentrations and thus higher temperatures are required to decompose most of the methane. It has also been shown that the rate of decomposition can be increased by presence of catalysts, the most practical of which is carbon itself.

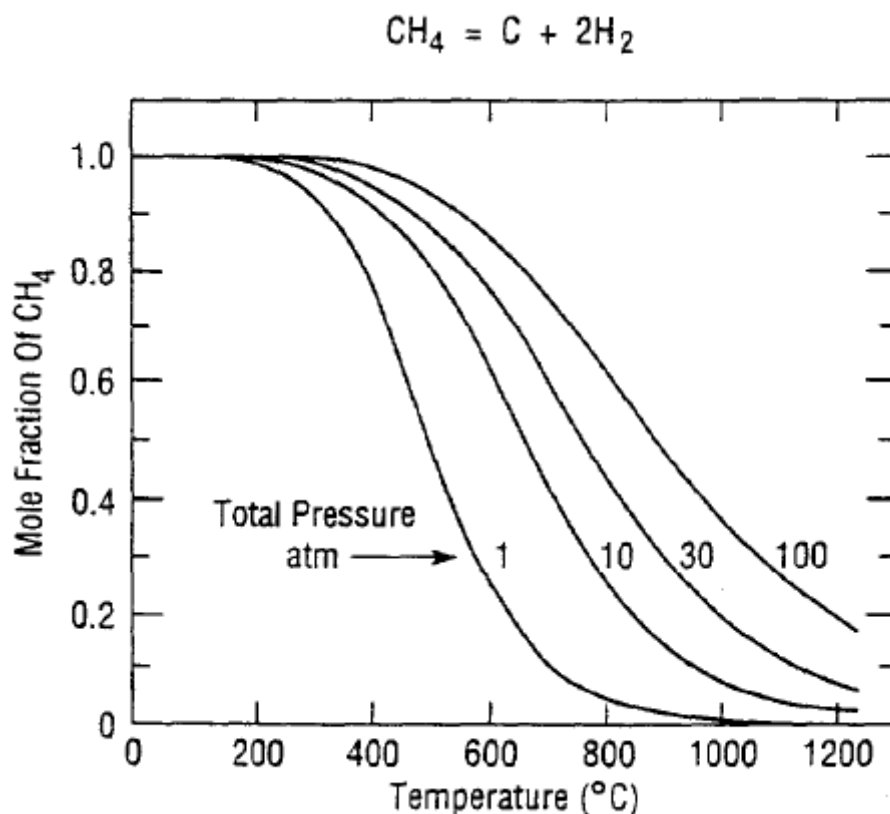


Figure 3.2. Equilibrium Diagram for methane decomposition in the carbon black production.

Carbon catalysts offer the following advantages over metal catalysts: No catalyst regeneration is required, no sulfur poisoning, high fuel flexibility, and significant reduction in CO₂ emissions.

The Simulation

As a first exercise in the carbon black process was developed a simulation about the Furnace Black Process.

The Methane was the principal raw material in the simulation and stoichiometric quantities were used with the exception of air, which was employed in a 20% in excess. It was

considered a methane flow of 1 Kmol/h preheated at 700 C and airflow of 4.14 Kmol/h (20% in excess) at the same temperature. The pressure was assumed in 1 atmosphere.

The following diagram (figure 3.3) resumes the process simulated.

The process diagram has two reactors, where the first (R1) is carried out with the following reaction:



The second reactor (R2) is used to generate heat and synthesis gas. The latter will be used as the combustible in R2.

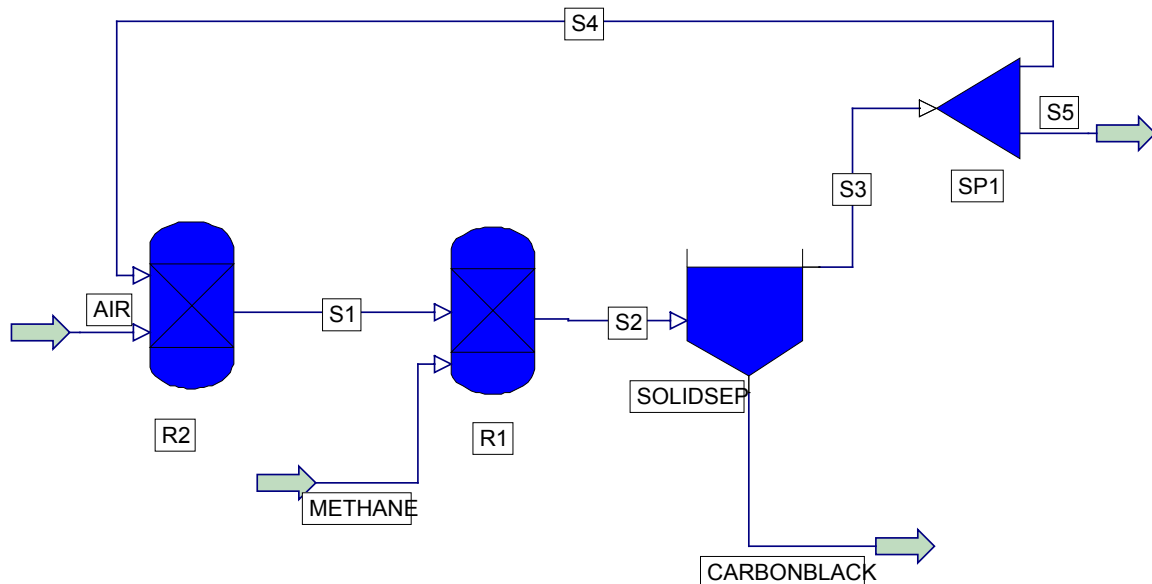
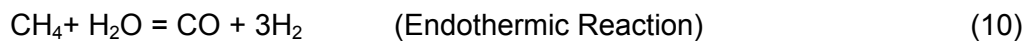
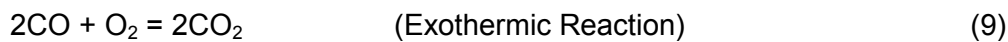


Figure 3.3. General diagram used in the simulation. Carbon Black Production.

For this simulation, a 95% of conversion was supposed for all reactions and the separation efficiency of carbon was of 100%.

Stream		AIR	METHANE	S1	S2	S3	S4	S5	CARBON BLACK
Rate	Kg-mol/h	4.140	1.000	5.890	8.791	7.840	1.960	5.880	0.951
	Kg/h	120.757	16.043	162.554	178.597	167.179	41.795	125.384	11.418
Temp.	C	700.00	700.00	1297.40	866.01	866.01	866.01	866.01	866.01
Pressure	Atm	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Enthalpy	M*Kcal/h	0.020	0.010	0.066	3.224	0.057	0.014	0.043	3.167
Molar Flowrates		Kg-mol/h							
METHANE		0	1.00000	0.00063	0.05000	0.05000	0.01250	0.03750	0
H2O		0	0	0.60530	0.60530	0.60530	0.15130	0.45390	0
H2		0	0	0.06020	1.96140	1.96140	0.49030	1.47100	0

Stream	AIR	METHANE	S1	S2	S3	S4	S5	CARBON BLACK
CO2	0	0	0.00381	0.00381	0.00381	0.00095	0.00286	0
CARBON	0	0	0	0.95060	0	0	0	0.95060
O2	1.20000	0	1.28750	1.28750	1.28750	0.32190	0.96570	0
N2	2.94000	0	3.92000	3.92000	3.92000	0.98000	2.94000	0
CO	0	0	0.01200	0.01200	0.01200	0.00301	0.00902	0

Table 3.1 Mass balance and conditions in the carbon black process.

REACTION	REACTOR R1	REACTOR R2
Total Heat of reaction at 25C (M*Kcal/h)	0.0169	-0.0265
Inlet Temperature (C)	1135.65	753.86
Outlet Temperature (C)	865.99	1297.38

Table 3-2. Reactor conditions in the carbon black process.

It was necessary to achieve a sensibility analysis with the recycled fraction of tail gas (S3/S4 flow rate). The objective is to obtain the same temperature in the exit of the reactor R1 that the temperature given for the literature. The figure 3.2 gives the conditions, which is improved the conversion. The temperature must be 800 C and the conversion 95% of methane at one atmosphere of pressure.

The stream S3 is the tail gas, which usually is used to produce heat in a combustion process, but is not necessary to burn the whole of the gas. The recycled fraction adjusts the thermal conditions (temperature) in the reactor.

The initial fraction recycled of tail gas was fixed in 0.25. With all this information, the results of the simulation are given in the tables 3.1 and 3.2. The thermodynamic model used in the simulation was Peng Robinson.

The change of temperatures due to the chemical reaction is high. In the figure 6 is shown the effect of the fraction recycled in the exit temperature of the reactor R1. The temperature is very sensible to the changes in the fraction recycled, due to that this fraction is the combustible in R2.

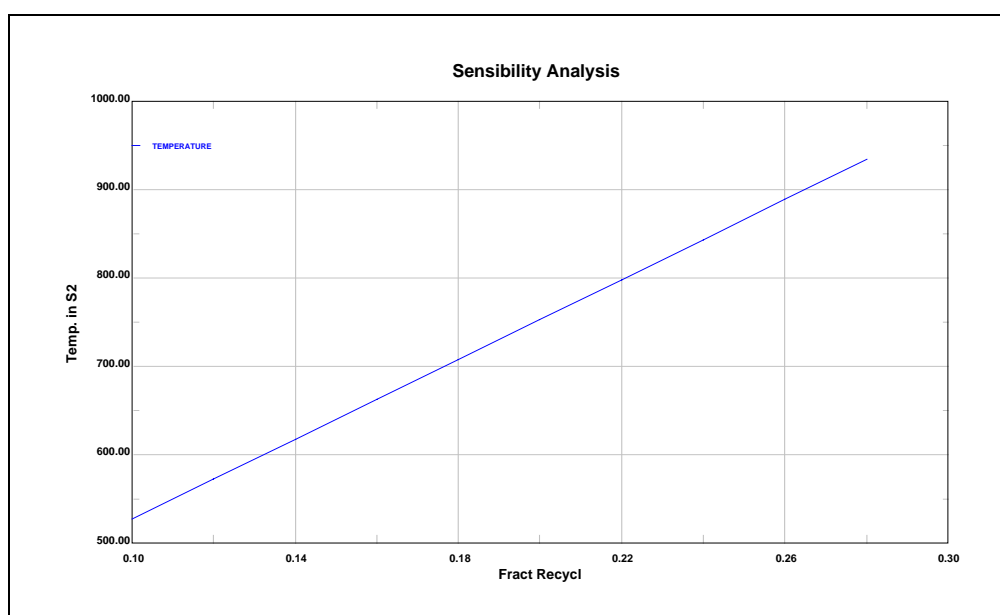


Figure 3.4. Sensibility analysis of tail gas recycled fraction.

The fraction recycled at 800 C (experimental condition) is near to 0.22. The optimization of the Stream flow in S4 is important because the principal goal in the process is the hydrogen production. The carbon Black is a byproduct. The table 3.3 shows the flow rates in the splitter. The stream S5 has the valuable product (hydrogen) in the process.

Stream	S4	S5
Temperature (C)	797.9	797.9
Component Molar Rates	Kg-mol/h	
METHANE	0.0110	0.0390
H2O	0.1122	0.3980
H2	0.4299	1.5240
CO2	0.0006	0.0022
CARBON	0	0
O2	0.2806	0.9947
N2	0.8292	2.9401
CO	0.0023	0.0082
Total (Kg-mol/h)	1.666	5.906

Table 3.3. Component flow rates in the splitter.

As a second point in this work, it was to compare the results obtained using ASPEN PLUS with the results generated by PRO/II. The process conditions used in the simulation are the same employed in the simulation with PRO/II. The following diagram (figure 3.5) resumes the process simulated using ASPEN PLUS.

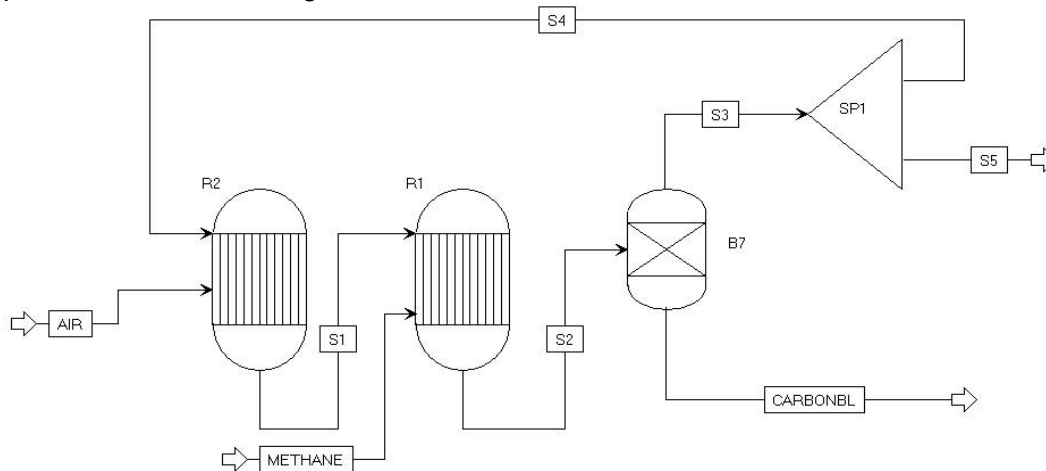


Figure 3.5. General diagram used in the simulation. Carbon Black Production in ASPEN PLUS.

The tables 3.4, 3.5 and 3.6 are given the comparative results in the simulation.

Stream		S1		S2	
SOFTWARE		ASPEN +	PRO/II	ASPEN +	PRO/II
Rate	Kg-mol/h	5.889	5.89	7.84	8.791
	Kg/h	162.553	162.554	167.178	178.597
Temp.	C	1281.55	1297.4	818.65	866.01
Pressure	Atm	1	1	1	1
Enthalpy	M*Kcal/h	0.092	0.066	0.041	3.224

Table 3.4. Comparative Results in the carbon black simulation.

Stream		S4		S5		CARBON BLACK	
SOFTWARE		ASPEN +	PRO//I	ASPEN +	PRO//I	ASPEN +	PRO//I
Rate	Kg-mol/h	1.96	1.96	5.88	5.88	0.951	0.951
	Kg/h	41.794	41.8	125.383	125.38	11.418	11.418
Temp.	C	818.67	866	818.67	866.01	818.67	866.01
Pressure	Atm	1	1	1	1	1	1
Enthalpy	M*Kcal/h	0.01	0.014	0.031	0.043	0.015	3.167

Table 3.5. Comparative Results in the carbon black simulation.

REACTION SOFTWARE	REACTOR R1		REACTOR R2	
	ASPEN +	PRO//I	ASPEN +	PRO//I
Total Heat of reaction at 25C (M*Kcal/h)	0.0169	0.0169	-0.013	-0.0265
Inlet Temperature (C)	N/A	1135.65	N/A	753.86
Outlet Temperature (C)	818.67	865.99	1281.59	1297.38

Table 3.6. Reactor conditions in the carbon black process.

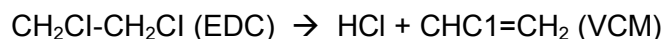
The simulations presented have similar results. There is a small difference in the total heat of reaction in R2 (Table 3.5). This difference induces an import variation in the temperature between both models (table 3.6). The discrepancy in the temperature does not affect the material balance because it was not used a kinetic model in the simulation.

4. Vinyl chloride Monomer Production

This simulation performed as a trial to simulate Vinyl Chloride Monomer (VCM) Production Process of an industrial partner in PRTR project. The VCM production process simulated by Aspen Plus. The source of input data for the simulation obtained by review of literature regarding VCM production process.

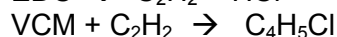
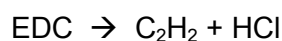
Process description

Vinyl chloride monomer (VCM) is produced through a high-pressure, noncatalytic process involving the pyrolysis of 1,2-dichloroethane (EDC), according to the following reactions:



The process flow diagram is shown in Figure 4.1.

The cracking of EDC occurs at 900°F and 300 psia in a direct-fired furnace. The pure EDC feed enters the furnace at 60°F and 390 psia, with a rate of 2000 lbmol/hr. Byproducts of pyrolysis consist principally of acetylene and chloroprene through the following reactions:



Overall EDC conversion is maintained at 55%, with a selectivity of 98% for VCM production and 2% for acetylene production. 75% of the acetylene produced is converted to chloroprene.

The hot gases from the furnace are quenched to 10 degrees below saturation, prior to fractionation. Two distillation columns are used for the purification of the VCM product. In the first column, anhydrous HCl is removed overhead and sent to the ox chlorination unit. In the second column, VCM product is delivered overhead, and the bottoms stream containing unreacted EDC is recycled back to the cracker.

Objectives

Base case simulation by ASPEN PLUS for VCM flow sheet, using the following specifications.

- The reactor effluent quenches by using the HEATER, Assuming 10 degrees sub cooling and a pressure drop of 5 psia across the quench.
- HCl recovery of 99.9% in the overhead, VCM recovery of 99.9% in the bottoms of the distillation column 1.
- VCM recovery of 99.9% in the overhead, EDC recovery of 99.9% in the bottoms of the distillation column 2.
- Assuming the flow rate of recycle EDC is 1600 lbmol/hr.

Thermodynamic Method

Redlich-Kwong-Soave equation of state used to represent the physical properties of the system.

Results

**VINYL MONOMER CHLORIDE PROCESS
STREAM SECTION**

1 2 3 4 5

STREAM ID	1	2	3	4	5
FROM :		CRACK	QUENCH	COL1	COL1
TO :	CRACK	QUENCH	COL1		COL2

SUBSTREAM: MIXED

PHASE:	Liquid	Vapor	Liquid	Liquid	Liquid
COMPONENTS: LBMOL/HR					
HCL	0	1980	1980	1978.02	1.98
VCM	0	1980	1980	1.98	1978.02
EDC	2000	1620	1620	0	1620
C2H2	0	0	0	0	0

TOTAL FLOW:

LBMOL/HR	2000	5580	5580	1980	3600
LB/HR	1.9792+05	3.5625+05	3.5625+05	7.2244+04	2.8401+05
CUFT/HR	2514.053	2.6834+05	2461.589	1248.991	5375.653

STATE VARIABLES:

TEMP F	60	900	90.2308	29.2493	296.5944
PRES PSI	390	300	295	367	372
VFRAC	0	1	0	0	0
LFRAC 0	1	0	1	1	1
SFRAC	0	0	0	0	0

**VINYL MONOMER CHLORIDE PROCESS
STREAM SECTION**

6 7 8

STREAM ID	6	7	8
FROM :	COL2	COL2	
TO :			CRACK

SUBSTREAM: MIXED

PHASE:	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR			
HCL	1.98	1.4290-07	0
VCM	1976.042	1.978	0
EDC	1.62	1618.38	1600
C2H2	0	0	0

TOTAL FLOW:

LBMOL/HR	1979.642	1620.358	1600
LB/HR	1.2373+05	1.6028+05	1.5833+05
CUFT/HR	2298.057	548.6044	2011.243

STATE VARIABLES:

TEMP F	123.525	333.8221	60
PRES PSI	115	118	390
VFRAC	0	0	0
LFRAC	1	1	1
SFRAC	0	0	0

Figure 4.1: flows sheet of the VCM production process

5. Example of application of IPC software

Overview of the system

The DSS/IPC system has been developed by the World Bank, in collaboration with WHO/PAHO, to assess rapidly the pollution situation in a specific geographic location, such as metropolitan area or water basin, and to analyze alternative pollution control strategies and policies.

This approach generates estimated pollution loads in a study area by applying standard emission factors to data on the scale of economic activities by industry/sector. These load estimates can be further processed to compute annual average concentrations in an area and/or water body and the impacts of selected pollution controls. The DSS/IPC extends this approach to calculating the costs of controls and outlining a cost-effective abatement strategy.

The DSS/IPC system is a personal computer software package that comprises a set of extensive databases and a number of computation modules. Computation modules enable a user to estimate:

- Air, water and solid waste emissions based on inventory of economic activities for a given location;
- Ambient concentrations of air and water pollutants by using simple (screening) dispersion models with minimum meteorological and hydrological data;
- Total costs of control options by using standardized engineering-type cost functions; and
- Long-run marginal cost schedules to achieve a certain level of emission reduction (or decline in ambient concentration) for a chosen pollutant.

In support of the calculation and analysis, the DSS/IPC software contains the following data bases, compiled by media of discharge:

- Pollution-intensive technological processes across all sectors of economic activity, including mining, manufacturing industries, energy, transport and municipal sector, that are grouped according to the UN International Standard Industrial Classification (ISIC) at 4-digit level;
- Principal control options available for each process, including “good housekeeping” and waste prevention programs;
- Emission factors, associated with these processes and “process-control option” combinations;
- Normalized cost units and parameters for control technologies; and
- Health guidelines for air and water pollutants where applicable.

Case study: Emerald City Pollution Analysis

General information on the study area

The Emerald City of 900,000 people covers the area of 100 km². It is situated along Winkie River. Within and near the city, the river has a width of 500 m, average depth of 5 m and an average flow of 250m³/sec. Upstream of the city, water in the river is considered clean. Near the city, there is also Skeezer Lake whose area is 125,000 m² and average depth is 10 m. Total annual inflow to the lake (precipitation, catchment drainage, direct discharges) is on average 80,000,000 m³; annual evaporation - near 10,000,000 m³. Up to recently, water in the lake was almost pristine. Annual mean of water temperature for both river and lake is 10 degrees Celsius. Atmospheric conditions in terms of frequencies of atmospheric stability / wind speed combinations, that greatly affect dispersion patterns of air emissions, illustrated in the following table:

Atmospheric stability	Wind speed (m/s)	Frequency Factor (0 -1)
Unstable	Very low (2 m/s)	0
	Low (2-5 m/s)	0
	Moderate (5-7.5 m/s)	0.1
	High (>7.5 m/s)	0.2
Neutral	Very low (2 m/s)	0.1
	Low (2-5 m/s)	0.2
	Moderate (5-7.5 m/s)	0.2
	High (>7.5 m/s)	0.1
Stable	Very low (2 m/s)	0.1
	Low (2-5 m/s)	0
	Moderate (5-7.5 m/s)	0

Industries, transport and services

Major industries include a steel mill that produces 800,000 ton of metal per year at its two facilities, one large cement plant with five emission stacks processing annually 10 million ton of clink. Three textile factories that process 330,000 ton of cotton, 120,000 of wool and 150,000 of synthetics per year, respectively; and two meat processing plants with the overall capacity of 100,000 ton LWK (life weight of animals killed). One of the meat plants started operations two years ago, and is currently the only industrial facility that discharges its wastewater into the lake (its discharges make 50 percent of total discharges from the meat industry). All other industries, as well as two main municipal sewers, serving the entire population of the city, discharge into the river. Also, 30 large industrial and district heat boilers burn 1.5 million ton of coal per year; and 200,000 ton of coal is used in small boilers and stoves by a hundred of other industrial and commercial establishments. Road transport in the Emerald City consists of 100,000 gasoline-powered cars (average annual mileage per car - 10,000 km), and 60,000 diesel-powered buses and trucks (average annual mileage per vehicle - 20,000 km). Average wage is US\$ 5/hour; energy and material prices are at the world market level. Commercial interest rate is 10 percent.

Pollution control.

Currently, pollution controls are few and include only primitive cyclones (removal efficiency - 75 %) at the cement plant and primary wastewater treatment at the cotton-processing factory. Recently, however, the government made commitments to pay much greater attention to the quality of the environment and set some ambient quality targets (in terms of annual mean concentrations of key pollutants), including the following:

Air quality: 1st step - reduce the ambient level of particulates to or below 70 $\mu\text{g}/\text{m}^3$; 2nd step - reduce the ambient level of particulates below 50 $\mu\text{g}/\text{m}^3$;

Water quality: the ambient level of BOD5 should not exceed 4 mg/l for both river and lake.

Case study: Emerald City Results

The program estimated the following outputs:

- Air, water waste emissions.
- Ambient concentrations of air and water pollutants.
- Total costs of control options.
- Long-run marginal cost schedules to achieve a certain level of emission reduction (or decline in ambient concentration) for a chosen pollutant.

From Tables and Graphs obtained from DSS/IPC we can conclude that:

1. Air Pollution

- Pollutants whose levels exceed the health guidelines are TSP (120 $\mu\text{g}/\text{m}^3$), SO₂ (58 $\mu\text{g}/\text{m}^3$) and NO_x (184 $\mu\text{g}/\text{m}^3$).
- Major contributors to the ambient levels:
 - For TSP - cement industry, large coal boilers; and diesel transport; then, small coal boilers and stoves, and steel industry;
 - For SO₂ - small coal boilers and stoves; diesel transport; and large coal boilers;
 - For NO_x - road transport.
- The least-cost strategy to achieve the level of less than 70 $\mu\text{g}/\text{m}^3$ TSP includes the following measures: (i) - high PM controls (~90 %), supported by WPP/GH, at the

cement plant; (ii) WPP/GH at the steel mill; and (iii) moderate PM controls (~75%) at large coal boilers.

- To achieve the level of less than 50 ug/m³ TSP, the following measures should be implemented: (i) high controls (~90%) at large coal boilers; (ii) very high control (~98 %) at the steel mill; and (iii) very high controls (~98 %) at the cement plant. The transport sector measures are not included in the analysis.
- The annualized cost is US\$ 1.3 million for the first set of measures, and increases to near US\$ 11 million for the second set of measures. In order to achieve the targeted level of pollution abatement, the emission charge on TSP should be set at the level of:
 - US\$ 13/ton - for the program (A);
 - US\$ 363/ton - for the program (B).
- The second set of measures largely exhausts the potential for controlling large sources. Further improvement in the pollution situation, i.e. reducing the ambient levels of particulates below 40 ug/m³, requires to control transport and small source emissions.

2. Water Pollution

- The annual average BOD5 level is slightly higher in the river (12.5 mg/l) than in the lake (11.6 mg/l), but in both cases exceeds the target level.
- There is only one pollution source for the lake - a new meat processing plant. The major sources of BOD5 in the river are textile manufactures (especially, cotton and wool) and municipal sewerage. The contribution by the other meat plant is small.
- The least-cost set of measures to reduce the average ambient level of BOD5 in the river below 4 ug/m³ includes: adoption of WPP/GH at the wool processing textile factory and the meat plant; biological and chemical treatment of municipal sewerage; upgrading wastewater treatment at the cotton processing factory from primary to secondary and tertiary treatment, complemented by WPP/GH, and secondary treatment (with WPP/GH) at the textile factory manufacturing synthetics materials. The annualized costs of this program are US \$20.3 million.
- To reduce the level of BOD5 below 4 ug/m³ in the lake, it is necessary to implement primary (with chemicals) treatment at the meat plant, in addition to WPP/GH. The costs are US \$ 48,000 per annum.