Provision of facilities

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Abstract

For this year's EURECHA challenge we have made our report with two very different segments in mind. One is technical and is based on verifiable data, calculations and of course computer simulations, while the other segment is more illustrative, and serves only to give better representations. Of course bigger emphasis was put on the technical part.

The computer simulations done for technical part of this report cover electrical provision from the light ends of the crude oil, fertilizer production using ammonia, which is produced taking heavy oil as a raw material. Furthermore, water recycling at the refinery and of course provision of potable water for the growing city is also considered. The simulation results showed that using suitable technologies and process integration it is possible to obtain a sustainable development of the Sheikhdom.

The illustrative part is basically a city of 20,000 made in a computer game called "CITIES:Skylines". The game allows the user to import real life terrain data, that you can get from Google maps. In the game the city is divided into five regions where basic transport &logistics knowledge is applied for creating the Sheikhdom and connecting the regions.

1 Introduction

Discovering previously unknown underground or underwater oil reserves can mean a fast and dramatic change in the local society and of course the flora and fauna of that area. On the other hand it also represents the great opportunity for city development. The appropriate design of the chemical processes can on one hand contribute to the sustainable city development, and on the other hand the environmental impact can be negligible, or even positive.

Using oil, or some of its fraction, many chemicals can be produced. This study shows that almost all city needs, including electricity, water, fertilizer needed for crops, etc., can be covered using oil as a feedstock. Furthermore, the integration between processes is very important, and as it would be showed in the following chapters, the incorporation of mentioned process is possible and desirable.

The region of the Middle East is known as a desert region. That is why the efficient water management, including water recycling, is essential in order to ensure sustainable development of the Sheikhdom city and its region. That is why, the appropriate water treatment and management, was the main task of this study.

2 Sheikhdom overview

This chapter describes the basic principles that would govern the sustainable Sheikhdom, and also provide some illustrations. Hopefully the reader will get a better felling for what & how this report will try to solve all of the Sheikhs problems.

2.1 Sheikhdom

For the small sheikhdom and the non-technical aspects of this year's challenge, we decided to give "life, which we made in a game called "CITIES:Skyline". The purpose of this city is only to give a better illustration of the broad challenge. For the creation of our city, we decided to first try to locate a location that met our specification, and then create a terrain model in-game. So we set our eyes on the Middle East, where we used google maps, to locate the perfect spot. The location we had in mind had to be near an ocean.

The spot we found was in Kuwait, about 70 km south of Kuwait city. We used a terrain analysis tool, which gives 18km x 18km height map of the location, and the imported it into the game. We then added the finer details such as oil reserves, ocean flow direction, wind speed, local highway etc. manually.

Figure 1 - The in-game version of the location we took a s terain snapshot of. The first picture from the left shows the area which we took to be our Sheikhdom, the middle picture shows hot the terain looks like in the game and picture on the right shows where in this location did we place the newly found oil reserves.

The city with of about 20,000 residents was built near the coast, and was divided into five main sectors. The sectors are: industrial, old town, new town, agricultural area and student campus. The envisioned student campus location was chosen to be near the main residential area. Due to the page limitations of report and better representation of the Sheikhdom, a short video was made in order to describe the envisioned town: Tour of the Sheikhdom

As mentioned before the incorporation between refinery, electricity production, water management etc. is extremely important. Figure 2 represents the simplified overlook on integration of individual processes.

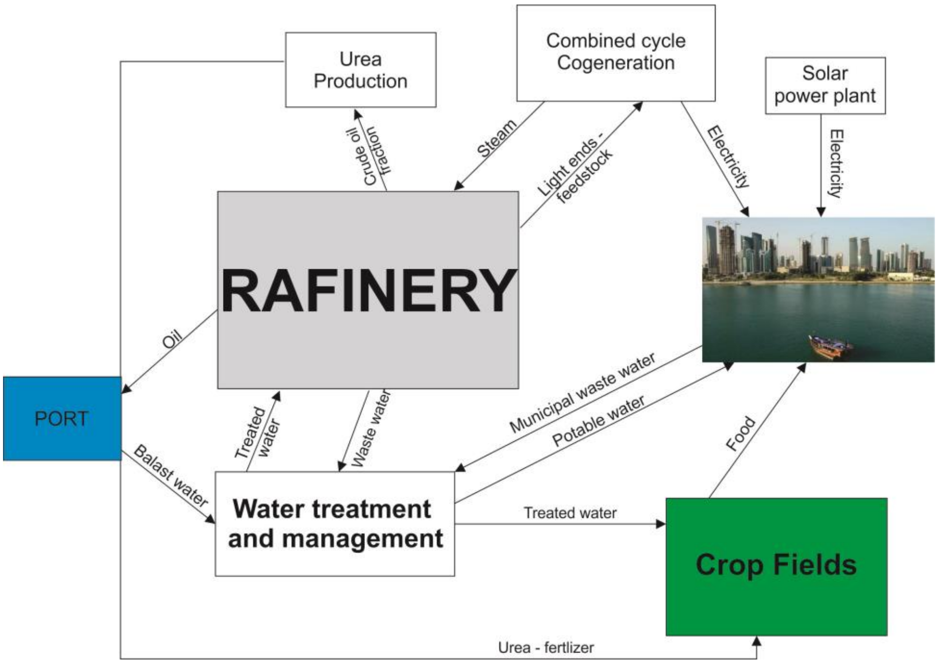

Figure 2 – Simplified overlook of the integration of process in the Sheikhdom.

As it can be seen in Figure. 2 it is possible to integrate separate processes. The refinery provides necessary feedstock for urea production and cogeneration. The assumed refinery capacity taken into account for this study is 150,000 bbl/day. This capacity falls into the average mid-range oil refinery[1]. On the other hand appropriate water treatment ensures minimal well water usage and wastewater discharge. Individual processes and possible connections between them are evaluated in the following chapters.

3 Provision of electrical energy

One of the main tasks for ensuring sustainable development of the Sheikhdom city is stable electricity production and supply. For that purposes, two types of energy sources can be used; renewable and non-renewable. Since the city is placed in the desert area, the only renewable source, which can be used for electricity production is the Sun. The region of Middle East is perfect for the implementation of solar power plant due to the large number of sunny hours per year [2]. The main advantage of solar power plant is the reduction of CO_2 emission, which is very important for the city due to the large industry present. The main issue of the mentioned electricity production is its weather dependence, meaning that the production capacity varies between full capacity during sunny hours, to the zero capacity during cloudy hours (in the modern solar plant, such variation can be partially be avoided using heat reservoirs). In order to ensure stable energy supply, it is essential to have also some other type of electricity production. Due to the limitation of the sources available, the only possibility is usage of oil, or some crude oil fraction, for power generation.

As mentioned before the projected city population is approximately 20,000 people. Taking this number into account, the provision of 65 MW electricity productions have to be ensured. This number is calculated considering the average electricity consumption of the Kuwait citizens, which is approximately 16000 kWh per year [3]. Also, some reserve should be taken into account.

The implementation of 23.8 MW solar power plants is taken into consideration for this study [4]. Taking the number of sunny hours into account, such power plant would cover approximately 1/3 of the Sheikhdom electricity consumption. As it can be expected the amount of electricity produced during summer period is greater compared to the winter period. Such power plant would cover the 50 ha large area, and it would contribute to the CO_2 emission saving of 35,000 tons. The investment cost, of such solar power plant is estimated to 50 M$.

Beside solar energy also some other energy source has to be considered in order to ensure sustainable electricity production. Due to the fact that the city is placed in desert area no other renewable source can be used. The existence of oil refinery leads to the reasonable choice of electricity production from some oil fraction. Cogeneration using combined cycle is taken into consideration for this study. There are several reasons why such production can be very suitable in this case.

As feedstock for cogeneration the lighter oil fraction can be used. It consists on light hydro-carbons including methane, ethane, butane and propane (also known as light-ends). Such combination is suitable for usage in the first part of combined cycle – gas turbine. The process scheme is represented on figure 3. The fuel is firstly combusted in the burning unit, using suitable amount of excess air. The fuel gases are than led to the gas turbine for electricity production.

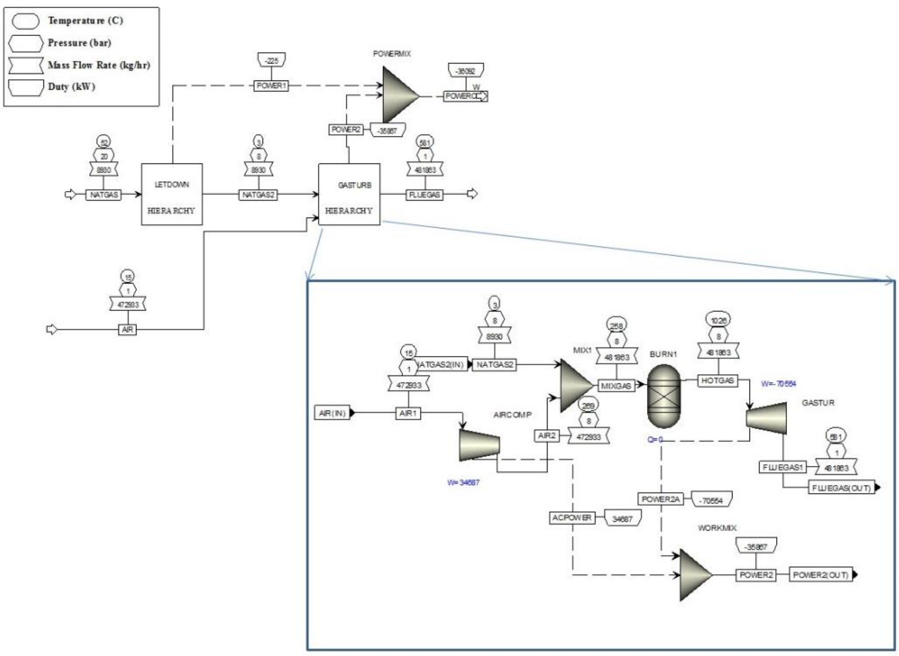

Figure 3: Combined cycle cogeneration

Some basic results of the mentioned process simulation are represented in the Table 1. The process is simulated for the natural gas as the main feedstock for the simplicity. The simulation can be seen as appendix B1 to this report. The process where before mentioned oil fraction would be used, is very similar to the one simulated, since the heating values are similar [5]. All thermal results and mass balances would be very similar, including the amount of the feedstock, electricity output, etc.

Table 1: Results of the cogeneration simulation

Amount of the feedstock	8930 kg/h
Electricity output of the gas turbine	36,1 MW
Isentropic efficiency of the gas turbine	0,9
Fuel gases temperature after the gas turbine	581 °C
Fuel gases pressure after the gas turbine	1,1 bar
Amount of the fuel gas	481,8 t/h

The amount of the feedstock is calculated taking the necessary electricity output into consideration. The mentioned amount represents approximately 50 % (48 % to be more accurate) of the total light ends produced in the refinery with the stated capacity. This value is calculating considering the amount of the crude oil feedstock, and the fraction of it representing light ends (approximately 2,5 %, depending on the type of the crude oil)[6]. The fuel gasses after the gas turbine can be used for both, heat and electricity generation. If carefully designed, the second part of the process can be flexible, and operate at different conditions regarding the weather conditions. During the summer days, when more electricity is produced using solar panels, the ratio of heat generation, in the second cycle of the combined cycle, would be higher. Heat can be used for steam generation for use in the refinery. On the other hand, during winter days, more electricity would be produced, due to the lower solar panel production. At these days, more steam would be generated by some other source. At the base case, approximately 35 % of the electricity produced in the gas turbine, can be produced in the second part of the cycle [6].

Finally, the combination of electricity production using solar panels and cogeneration would cover all city needs, and would provide stable electricity supply. Nonetheless, the integration of mentioned production with oil refinery can be established, since the heat generated in the cogeneration process can be used for covering the part of steam refinery needs.

4 Provision water

In Kuwait there is practically no permanent renewable surface water, so they must rely on other sources. Total well water withdrawal by source in 2002 was 46% from desalinated water, 45% from Groundwater and 9% from reused treated wastewater. In general groundwater quality and quantity are deteriorating due to continuous pumping of water. Because of this wells with high-quality water are seen as a long term strategic assets and are used almost entirely as potable water [7].

4.1 Provision of process water

Refineries are quite known to be huge water consumers, so inadvertently they produce a lot of wastewater. Recent trends however, are pointing towards a concept called “Zero liquid discharge” (ZLD), which means that no liquid waste is discharged into the environment. Existing infrastructure, coupled with new technologies can bring facilities close to the zero discharge goal. Improved water management results in reductions in wastewater flow or contaminant load or both. Lower flow and contaminant load may result in lower wastewater treatment operating and maintenance costs and ultimately the environmental impact of a refinery's discharge.

4.1.1 Refinery wastewater

Wastewater from the refinery is typically categorized into low total dissolved solids (LTDS) stream or non-oily wastewater, and a high total dissolved solids (HTDS) or oily wastewater stream. LTDS stream is more versatile and need less treatment before being reused or discharged, while the same cannot be said for the HTDS stream. Some of the more problematic contaminants usually seen in discharges of various process units include Cyanides, phenols, hydrocarbons, ammonia, etc.

4.1.2 Oil tanker ballast wastewater

Nowadays, most ships are constructed with dual hull design, so they have segregated ballast water meaning that the ballast water doesn't come into direct contact with the leftover oil in the tanker. But this poses a new problem in its own. Since tanker pump the ballast water at one port and discharge it at another, the introduction of alien species to a local flora and fauna can be recognized. The transferred species may survive to establish a reproductive population in the host environment, becoming invasive, out-competing native species and multiplying into pest proportions. Furthermore, this can have a very negative influence on fishing, which represents one of the main food source. The process of pumping ballast water into and out of a tanker usually happens via on-board pumps. The typical ballast water cycle can be seen on figure 4.

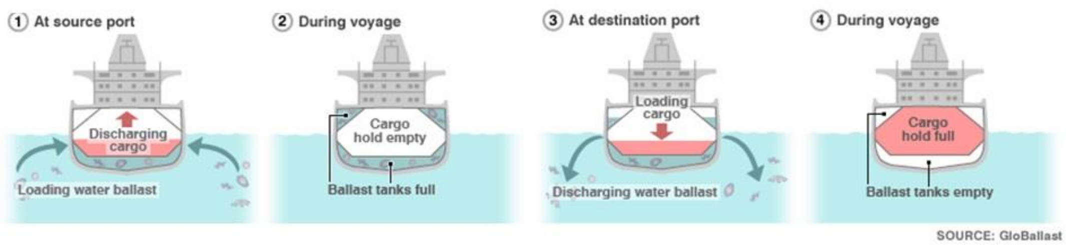

Figure 4 Typicall ballast water cycle of a modern oil tanker.

The international maritime organization adopted resolution A.868(20). This resolution requires all ships to implement a ballast water management (BWM) plan, meaning that ships have to carry out BWM procedures to a certain standard. As of October 2014 there are 51 management systems which received type approval certification by Maritime Environment protection committee (MEPC), many of which incorporate some kind of advanced particle filtration in combination with other techniques (UV, active components, etc.) [8]. Because of this we can assume that ballast water in general gets cleaned of its suspended solids to some degree.

Our proposal here is that instead of discharging the partially treated water (which has some value) back into the ocean, the water would be pumped into a storage facility near the harbor and then further treated to create a usable water source (either potable or process water for refinery). A quick check at the oil tanker freight rates going shows, that about ten tankers carrying an average of 250,000 tones enter and leave the Gulf each day [9]. The proposed refinery of 150,000 bbl/day would represent about 0,7% of the Gulf refining capacity, so we can assume that out of all the tankers entering the gulf this refinery would also account for 0.7% of that tanker traffic. This means that on average about 42 tankers would come to our refinery each year. Given that oil tankers of this size carry a lot of ballast water (as much as 40% of their carrying capacity)[10], we are looking at about 500 tons of ballast water on averate each hour for the whole year.

4.1.3 Wastewater recycle and reuse optimization

For the creation of a wastewater recycle and optimization model, we first had find out what are the typical water cycles inside refineries. Literature has shown, that typically there is a pretreatment unit for creating water of specified quality, and a treatment unit for the wastewater generated in the refinery process. The pretreatment unit can be fed from different water sources (sea water, well water, municipal wastewater etc.), but here special emphasis is given on using the wastewater generated within the refinery [11,12].

The water cycle superstructure was modeled for a 150,000 bbl/day refinery. The model is made of four process units (PU1=crude oil desalted, PU2=atmospheric & vacuum distillation unit, PU3=catalytic cracking unit, and a PU4=cooling tower), five water treatment units, four water sources, and the water itself could carry five contaminants (A- total suspended solids, B- total dissolved solids, C-hydrocarbons, D- Phenols, E-various Sulphur compounds). The contaminants were set up so that water sources (well water, ballast tank water, sea water and municipal wastewater) are mostly contaminated with contaminants A and B, while contaminants C, D and E are picked up in the refinery section.

A typical refinery nowadays needs about 400L of water for every tone of crude oil. So for our refinery of 150,000 bbl/day this would mean about 350 m^3/h[12]. Our simulation brings this number down to about 30, due to the extensive recycle and reuse optimization. About 80% of the water entering is used to cover evaporation loses at the cooling tower, and the rest is sent to other parts of the refinery. All of this was incorporated into the GAMS model [11,12]. The superstructure of the model can be seen in Figure 5.

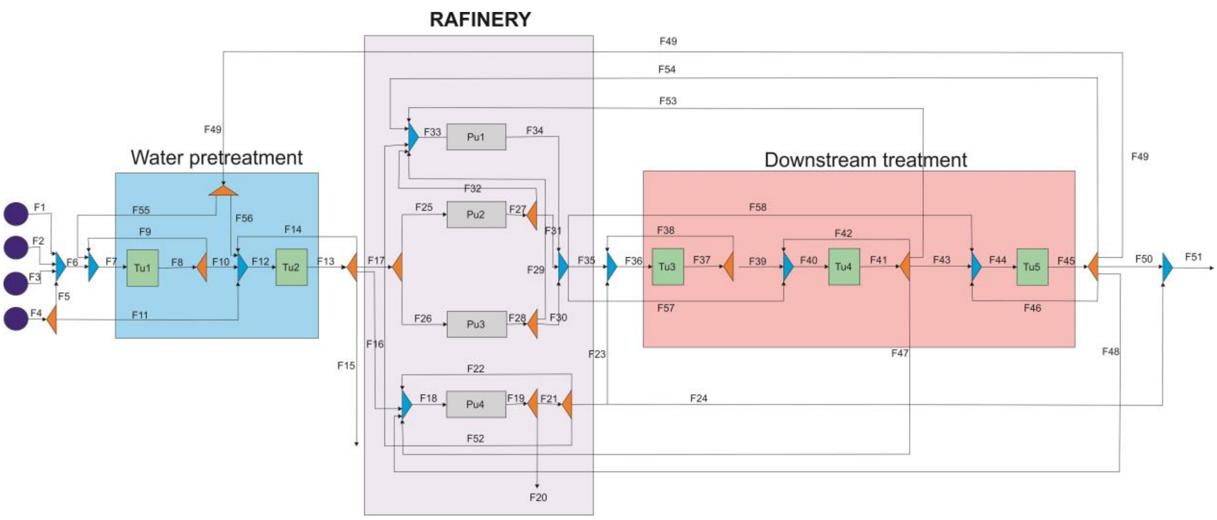

Figure 5 – The wastewater superstructure comprised of four process units (PU1,PU2,PU3,PU4) in the purple section, two pretreatment units (TU1, TU2) in the light blue section, and three treatment units for cleaning used process water in the red section.

The concentrations leaving each process unit, entering water specifications for each unit and of course the state of each water source were checked with literature so that the concentrations given into GAMS were as close to the real ones as possible[11,12].

Based on the concentrations and water flows through each unit, the mass loads for all the contaminants for each process unit were then calculated. The mathematical model of the superstructure was then written in GAMS software, with freshwater use minimization being the objective function.

The process shown in fig. 5 can be explained in the following way. Firstly water from different sources enters, and gets treated to the desired specification in treatment units 1 and 2. These two units are meanly there perform filtration and desalination (destination, reverse osmosis) processes. Cleaned water then goes towards process units 2, 3 and 4 and the wastewater generated here goes either to the cleaning sections or is directed towards process unit one, which has the highest allowable entering concentrations for all five contaminants. Stream F15 is meant to be clean water supply for various other areas in the refinery, which are not covered here (but they represent a small overall water consumption). Stream F20 represents evaporation loses from cooling towers, since this type (evaporative cooling water system) is the most popular way to lower the temperatures in hot streams of the refineries [11].

From here water goes towards the downstream cleaning section, (which is represented with red color in figure. 5), where it can again be sent to numerous destinations once it gets cleaned, or discharged if necessary. TU1 was set to have a maximal water flow of 300 m^3/h, while the other four had a maximal flow of 150 m^3/h.

4.1.4 GAMS simulation in the results

Scenario 1

When no constrains on which water source to use, GAMS calculated that a flow of 31,95 m^3/h from the well water source, and 2,91 m^3/h from the tanker ballast water was the optimal solution. There was no flow in pipes F2, F3, F6, F22, F23, F24, F29, F31, F50, F51, F56, F57, F58. It is interesting to note that the results give us a zero liquid discharge system, since the wastewater stream F51, is also zero. This is because our simulated refinery is a net consumer of water, since there are quite a lot of evaporation loses (F20). Detailed model, results and superstructure can be seen in the appendix A1 to this report.

Scenario 2

Because there is a large emphasis on recycling, oil tanker ballast water would be a prime candidate for a water source. We decided to put a constraint on well water (F3=0) because it could be in low supply or better used elsewhere, and also municipal waste water (F1=0), since it has great potential for plant irrigation [13].

The new results that we got were, 31,95 m^3/h from oil tanker ballast source (F4).This shows us that the system prefers ballast water since it has been already partially cleaned by the ship BWT systems. Detailed model, results and superstructure can be seen in the appendix A2 to this report.

4.2 Potable water provision

The average water consumption per capita in Kuwait is about 0,45 m^3/day [7], this mean that for our city of about 20,000 we would have to supply about 375 m^3/h of potable water. One possible solution for potable water provision could be to raise flowrates for Stream F15 shown in Figure 5, which provides high purity water for other processes in the refinery, and at the same time put higher restrictions on allowable concentrations of contaminants C, D and E. This would mean that absolutely no water from the downstream end of the refinery could be pumped around for pretreatment (TU1,TU2), because of the said contaminants. So for this part we borrowed the simulation from chapter 4.

4.2.1 Gams simulation and the results

Scenario 3

Like we said before, the following constraints on treating refinery wastewater at TU1 and TU2 were placed streams (F55=0 and F56=0). At the same time we would have to increase the flowrate from F2 and F4, and for them to be properly treated the maximum flowrate capacity at Treatment unit 1 had to be increased from 300 to 1750 m^3/h, and at treatment unit 2 from 150 to 800m^3/h.

The optimal solution was such that all of the feed water was chosen from the tanker ballast water supply (F=404), and again we got the ZLD system (F51=0). Detailed model, results and superstructure can be seen in appendix A3 to this report.

5 Fertilizer production

One of the most commonly used fertilizers is the UREA. It is produced using ammonia and CO_2 as feedstock, in the molar ratio 2:1. The reason why urea is chosen for this study is possibility of obtaining all necessary feedstock using some oil fraction. Ammonia can be produced via several synthesis routes, depending on the resources available. Furthermore, one of the main reasons why urea is chosen is the fact that usage of urea is suggested for warm climate areas.

The main feedstock needed for urea production is ammonia. The following table contains the possible ways of ammonia synthesis. Due to the time limitation the process of ammonia synthesis is not simulated.

Table 2: Cost components of ammonia production for different raw materials

Raw material	Electricity consumption (kWh/t of NH_3)	Process water (m^3/t of NH_3)	Cooling water (m^3/t of NH_3)	Labor (work hours/t of NH_3)
Natural gas	/	1.1	210	0.3
Naphtha	/	1.1	280	0.3
Heavy oil	530	0.6	216	0.4
Coal	624	0.6	216	0.7

The majority of ammonia, for different application, is nowadays produced using natural gas. The main reasons are the lowest capital and operating costs. In this study the chosen raw material is heavy oil. There are two main reasons. First is the amount of process water needed. Since the city is placed in the desert area, it is reasonable to choose the process with lowest water consumption. Also, since the refinery is placed near the city, the raw material – heavy oil (one of the crude oil fraction) is available in the large quantities. Furthermore, the usage of heavy oil for ammonia is becoming more attractive due to the large decrease in the price of the crude oil. For production of one tone of ammonia 0.76 tone of heavy oil (HO) is typically needed. In addition, about 0.14 tone of HO or equivalent is required for generation of steam and electricity, or 530 kWh can be obtained using some other source [14].

The urea plant is designed to cover the fertilizer needs of the near crop fields. Duo to the data published by Food and Agriculture Organization (FAO) approximately 0.5 hectares of arable land per capita is necessary for obtaining a sustainable food security and diversified diet [15]. The average annual usage of fertilizer (in this case) per hectare in the region of Middle East is 800 kg/ha[16]. Taking these two vales, and the number of the citizens, into account approximately 7300 tons of urea have to be produced annually. The simplified process scheme of the urea production is represented on figure 6 [6].

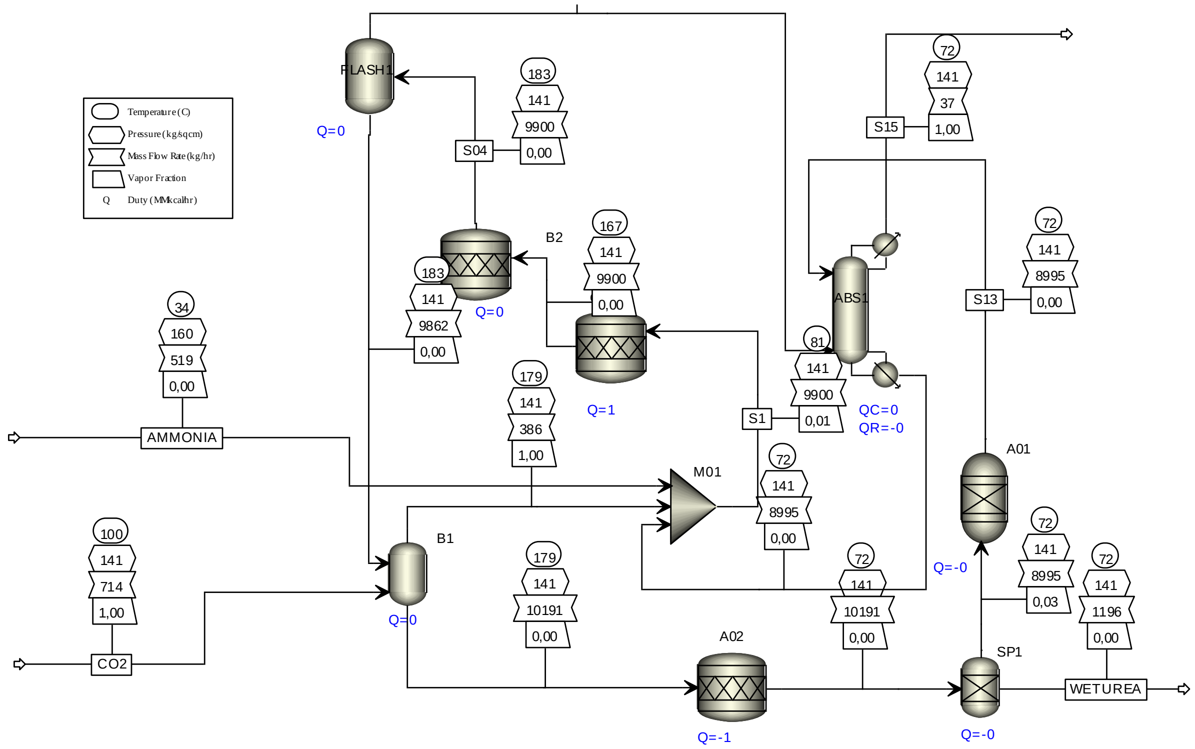

Figure 6 - Process scheme for urea production.

The part of downstream processes, including drying and granulation, is missing. The simulation is done using the Aspen template, and it is modified in order to meet process specifications. It can be seen as appendix C1 to this report.

As it can be seen from the figure 6, there are several recycles taking place. Because of that, the Aspen software had some problems regarding convergence. Based on previous experience the process is firstly simulated using Wegstein convergence method. Secondly, using obtained results the process is run once again using Newton method. Final results are obtained using final run, where Wegstein method is used once more.

As stated before two main raw materials are ammonia and CO_2. The following equations are simultaneously occurring in the urea synthesis reactor [17]:

formation of ammonium carbamate (AmmC) - $2NH_3 + CO_2 \Leftrightarrow NH_2COONH_4$

urea formation $NH_2COONH_4 \Leftrightarrow H_2O + NH_2CONH_2(urea)$

As it can be seen, both reaction are equilibrium ones, which is why the control of reaction conditions is very important. The reaction mixture after the reactor is led to the flash separator. The gaseous phase, mainly consisting on non-reacted reactants is led to the absorber. The liquid phase, containing wet urea, AmmC, and other components is firstly stripped using fresh CO_2 feed, and then cooled down. During the cooling process, the remaining amount of AmmC is converted to urea, due to the equilibrium conditions. Finally, urea containing some amount of water and other impurities is separated using flash separator (liquid product – WET UREA). Final results are collected in table 3.

Table 3 - Final results of the urea process simulation

Amount of CO_2 needed (kg/h)	**714**
Amount of NH_3 needed (kg/h)	519
Amount of urea produced (kg/h)	915
The reactor temperature (°C)	183
Amount of purge stream (kg/h)	37

5.1 Insecticide production

The production of maleic anhydride from n-butenes is a catalyzed reaction occurring at approximately 400–440°C and 2–4 atmospheres. A special catalyst, constituted of an oxide mixture of molybdenum, vanadium, and phosphorous, may be used. Approximately 45% yield of maleic anhydride could be obtained from this route [18]:

Figure 7 – Reaction for production of Maleic anhydride.

As an intermediate, maleic anhydride is used to produce malathion, an important insecticide, and maleic hydrazide, a plant growth regulator. So for covering the Sheikhdom with insecticides this compound could be the answer.

6 Conclusion

The short overview this report provides on the problem of »Sheikhdom«, shows that sustainable development can be achieved. Electrical energy provision from the cogeneration in the refinery and also from the solar power plant would more than cover its current and future needs. Like elsewhere in the world, the government could encourage the local population with subsidies on household solar panels or efficient heat pumps, to further increase the energy self-sustainability.

A somewhat complex water and water treatment network would be needed if one would wish to minimize the already low groundwater. In fact this should minimize as much as possible in the eyes of the authors. From cited literature and calculations done here we see that ocean and oil tanker water can be used from provision high quality water, while moderately treated municipal wastewater with its useful components is ideal for irrigation. How these components affect on lowering the fertilizer use was not studied, but would be an interesting further investigation.

The fertilizer chosen for this report was urea, and it was produced using ammonia as the main feedstock. The output of this production facility was based on calculations made on the needs for the local agricultural industry. Other smaller aspects of this year's problem were also looked at and mentioned but were not studied in such detail.

7 References

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Appendices

Appendix A – water provision

A1 – A GAMS file of the model, table of main results, and the resulting optimal water superstrucutre.

A2 – A GAMS file of the model, table of main results, and the resulting optimal water superstrucutre.

A3 – A GAMS file of the model, table of main results, and the resulting optimal water superstrucutre.

Appendix B – electricity provision

B1 – Aspen plus simulation file of the electricy production via cogeneration.

Appendix C – Urea production

C1 – Aspen plus simulation file of the urea production