CPD NR 3301
Conceptual Process Design

Process Systems Engineering
DelftChemTech - Faculty of Applied Sciences
Delft University of Technology

Subject

Removal of N_2O and Isoflurane from the exhaust stream of the operation rooms in hospitals.

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Preface

This is an assignment of the second year Masters students in Delft University of Technology. This is a course where it is expected that all the students will learn to design a chemical plant on a conceptual level. The assignment is about treatment of waste anesthetic gases from the operation rooms. The waste gases considered are mainly Isoflurane and N_2O.

It was a nice and learning experience with three nationalities and six team members, three members from China (Sarah, Max, Yiling), two from India (Vani, Nikhil), one from Suriname (Dinesh).

According to the team we have a successful solution for the assignment. The assignment deals with the treatment of waste anesthetic gases from the operation theatres. We all were excited to solve this assignment creatively, as this was the main task of the course. Of course, different culture, different thinking, qualities and weaknesses of each and every team member were studied and maximum focus had been given to the optimum result.

We all believe that this solution could be used in reality, as we all are quite confident about our design. We have proposed two designs for the N_2O removal in the solutions i.e. Catalytic Decomposition and Thermal Decomposition The purpose behind pursuing two options was not to increase the workload, but to come up with the options and above all future aspects are also taken into serious considerations. Thermal decomposition can be used for the countries like Netherlands where the weather is cold in winter and every hospital has a centralized heating system, which can be used as a N_2O decomposer. The catalytic approach is more for developing countries or the countries where there is relatively hot climate.

We think the design discussed in this assignment could be used as a guideline and the proposed design is capable to apply in reality after detailed and exact data considerations, as we had to use some assumptions. Choosing right approach and creative design was the main consideration of this assignment. After going through several processes and possible options we have narrowed down to two different processes of same functions. Recycle of Isoflurane and decomposition of N_2O by thermal and catalytic means are the two options.

Recycle of Isoflurane has two units and the process is semi continuous. Putting an adsorber in the main venting system of all the operation rooms and the zeolite will selectively remove one of the components from the mixture. A new one will replace the used adsorber and the used adsorber will be desorbed to get back the selectively adsorbed component. The vapor of the desorbed component is condensed by means of the low condensation temperature and the liquefied component can be recycled and used again.

Adsorption is a continuous process, while desorption and condensation are batch processes.

During an adsorption operation the components that are not adsorbed will move further and sent to the decomposition section, where they can be treated by thermal or catalytic means. Creativity and logical reasoning is used for the thermal and catalytic section. Natural gas fired centralized heating system and monolithic reactor, are the choices for the N_2O decomposition. The high temperature in the heating system is used for the thermal decomposition of N_2O and the monolithic reactor can be operated at low temperatures as compared to the thermal system.

During the completion of the Conceptual Process Design course I hope all the team members must be having lots of good and trace of bitter memories, but nevertheless the output and the learning that counts finally.

26th Nov 2003

Nikhil D Shindgikar

Acknowledgements

To show our sincere gratitude we would like to thank all the people who helped us during this assignment. We are the last group of the first quarter of 2003, who are doing CPD (Conceptual Process Design 3301, *NSYMVD*). The group has three Chinese and two Indians and one Surinam member. All the team members worked hard and tried to make a good and creative process design.

We would like to thank Dr. Guido Mul, our principal, who gave us this interesting assignment. Dr. Albert Goossens, our creativity coach, we were the third team for him. He always encouraged us to think in different and better routes to solve this assignment. The discussions with Albert were very helpful to solve group problems and he personally tried to maintain the healthy atmosphere in the group. He was more of a team member rather than a creativity coach.

We would like to thank Ir. Pieter Swinkles, who is the coordinator of this course and whose remarks and criticism helped us to make a better reporting and detailed design.

We visited some of the hospitals in the Netherlands for detailed information for our assignment. The information and cooperation received by the following experts was very satisfactory, and we would like to thank all of these experts for their information, help and immense hospitality.

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- Dr. A.G. L Burm (HOD, Anesthesiologist, LUMC, Leiden)

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- Ir. Peng.Du (Doctor, Catalysis group, TU Delft)

We would like to thank some people who have nothing to do directly with the assignment; they are our friends and fellow students with whom we discussed not only the technical concepts but also various other things and spent nice time. If somehow we forgot to mention some names here, then please forgive us.

22nd Nov 2003
Nikhil D Shindgikar

Contents

1 Introduction

Anesthetic gas, contains N_2O, O_2 and Isoflurane, is widely used for some operations in hospitals all over the world. Since N_2O and Isoflurane are all green house gases, the emission of this gas without any treatment is very harmful to environment especially to ozone layer. Nowadays, scientists are working on solving this problem. Some of them suggest using so called "reflecting" system to save Isoflurane during the operation. However, Isoflurane is still released to environment directly, even it is reused during one operation. It calls for a clean, efficient and simple process for anesthetic gas treatment. The consideration is given to the fact that the design is going to be installed in the hospital.

There are no processes available so far commercially in the hospitals to treat the waste gases, but there are some primary methods i.e. carbon filters being used for the removal of one of the anesthetic gases. The attention is given to the treatment of the waste anesthetic gases, because of their green house effect.

1.1Brief Background

N_2O and Isoflurane are major anesthetic gases used in hospitals to provide anesthesia for patients and the exhaled gases are emitted through a separate venting system in the hospital or re-circulated. The two main systems applied in Dutch hospitals are the non re-breathing and the re-breathing system. Re-breathing and non re-breathing system differentiate according to the recycle of the exhaust gases. In non re-breathing system the exhaust gases from the patient are not recycled back, but in re-breathing system they do. [1]

The non re-breathing system is the classical process. This system is now mainly used for small children. The gas flow rate in the non re-breathing system is approximately 3-10L/min. The patient is provided with a fresh anesthetic gas mixture and the exhaled gas from the patient, that contains not only anesthetic gas mixture but also carbon dioxide, water vapor, which is released in the operating room.

The price of Isoflurane is high and Isoflurane may destroy the ozone layer, the non re-breathing system has unfavorable effects on environmental and economical aspects. Things become even much worse for that N_2O is a very important green house gas, which has effects on atmosphere equals to 300 times than CO_2 does. One thing has to be taken into account that for re-breathing or for non re-breathing system the vol% of anesthetic gas i.e. Isoflurane is always higher (5-8%) in the beginning to saturate the body, especially lungs with the anesthetic gas.

1.2 Problem definition

The treatment of green house gases with possibly cheaper means is expected from the hospitals.

- 5-8 lit/min of waste gas (Anesthetic gas) emission from the hospital operation theatre.
- The waste anesthetic gas contains 55-65% vol N_2O and 2% vol Isoflurane and 33-48% vol Oxygen.

The proposed design should meet the following conditions from the given data:

- More than 99% of N_2O conversion to N_2 and O_2 by decomposition either by Thermal or Catalytic means.
- Maximum possible recycle of Isoflurane with a purity of 99.99 %, as Isoflurane is costly.
- The proposed design should be simple and economical.
- 10 operation rooms work 6hrs/day, so total 60 hrs/day of emission.
- Sensitivity analysis is important as the feed composition and flow rate may not be constant, but the average flow rate of 5.5 lit/min and 2% Isoflurane, 40% Oxygen and 58% Nitrous oxide is assumed.

The solution is expected to satisfy the following qualities:

- Creativity.
- Innovation.
- Technical feasibility and safety.
- Economical feasibility.

The solution will not consider the following points:

- For Thermal Decomposition process option, improvements in heating system
- Consideration of natural gas as a utility in a Thermal Decomposition process option.
- Blower design for Catalytic Decomposition process option to create a 0.2 bar_a in the vent system.
- Electrical usage for preheating the exhaust feed to the reactor inlet in the Catalytic Decomposition system.
- Improvements in the flue gas heat recovery for the Catalytic Decomposition process.

Consider the hospital is not a commercial organization and Isoflurane is an expensive chemical, we designed Volatile organic coumpound separation and recycle to recover high purity Isoflurane. The similar separation method is tested for desflorane [2]. Since it has high green house effect, complete decomposition of N_2O is considered here in this proposed design to treat the waste gases. Our concept of using the high temperature to get

the decomposition done is quite an innovative. N_2O can be decomposed to N_2 and O_2 at high temperature around 700°C- 800°C and the conversion could be 70%-80%.
Chapter2 has a selection of chosen process options. One option for separation and two for N_2O decomposition defeat others. Catalysts and reactors for catalytic decomposition are also chosen.

Chapter 3 is the basis of the design. Background information is introduced and key data, like battery limit, process definition, Basic assumptions, are demonstrated.

Chapter 4, study is done to present reliable data on thermodynamic properties and reaction kinetics. Definition of vapor pressure, Specific heat, condensation temperature, and reaction kinetics are valid for the ranges of the process operating conditions.

Chapter 5 gives the knowledge of the process structure and description. It also emphasizes the simulation part of the separation of Isoflurane and thermal Decomposition.

Chapter 6 gives the information of process controls of each unit in the process, and the working of each unit is explained in detail.

Chapter 7 focuses on the mass and heat balance calculations, equations and assumptions of the separation and decomposition processes.

Chapter 8 includes design criteria, layout, and conceptual approach for each unit in the separation and decomposition process.

Chapter 9 gives information about the waste in the designs. It is supposed that the design will produce less amount of waste, as the process design is for treatment of waste gases.

Chapter 10 has safety issues related to the designed units. HAZOP analysis and Explosion limits are studied to cross check the conceptual design approach as a safety point of view.

Chapter 11 is giving detailed information of economics of both the processes of separation and Thermal Decomposition and separation and Catalytic Decomposition.

Chapter 12 gives information about the creativity tool, which is used to solve the assignment

Chapter 13 gives the conclusion and recommendation of the two design options.

1.3 Market of the Product

There is no direct formation of any product in this process. The income is only the money that can be saved from the maximum possible recycle of the Isoflurane. Isoflurane is very costly anesthetic and there are not many companies who produce this anesthetic. The price of the 99.999% pure Isoflurane is approximately 1 Euro for 1 ml. The purity required for the medical purpose is very high about 99.999% and as the purity increases the cost increases as well. Isoflurane is a volatile organic compound and normally it comes in a bottle of 250 gm in liquid form.

1.4 Uncertainties

There are some uncertainties during the design considerations which have overcame during the design are:

- Adsorption and desorption capacity of zeolite for Isoflurane is not given accurately in any literature source, but as the molecular structure is similar Disflurane capacities are used in the Separation process.
- For Thermal Decomposition process the Dutch laws are not known for putting some external means for burning to the heating system.
- It is estimated that the temperature in the heating system will be sufficient for the Thermal Decomposition even in the summer time, as the flame temperature is very high and at least some hot water supply is needed for other purposes than room heating.
- For the Catalytic Decomposition, there are various possible reaction kinetics that depends on the reaction model and on the catalyst type. In this design, simple square channel monolith for first order N_2O decomposition reaction kinetics is used.

2 Process Options and Selection

2.1 Volatile Organic Compound Separation and Recycle

In the coming chapters, this process is also called "Separation" for convenience.

2.1.1 Introduction

The exhaust gas mixture from the operation rooms contains organic and inorganic components. Isoflurane is an expensive chemical and the single volatile organic compounds. The idea is to separate high purity Isoflurane from mixing gas and recycle as much Isoflurane as possible. Another true story we have to weigh on our mind is the hospital is not a commercial organization but a public service section. Hence, the investing cost become an important criteria on options chosen.

2.1.2 Options

Option 1 - Condensation

Generally, Condensation is preferred for gas separation of light components*. When the partial pressure of the constituent in the gas phase reaches or exceeds the vapor pressure of the pure component in liquid form under the same conditions [3], this compound will liquefied from the gas phase into the liquid phase. Consequently, the efficiency of separating volatile organic compounds depend on, the pressure and temperature applied in the condenser, the concentration of the compound, and vapor pressure of the pure compound.

It is obviously that the components being considered in our process have big difference in thermodynamic properties. i.e. Compared to Isoflurane, oxygen and nitrous oxide have much lower boiling points. The temperature difference is even larger than 120 ℃. We can observe that the components can be separated by phase change easily. And highly pure component could be gained at the end.

Option 2 – Adsorption

Adsorption is commonly used to remove relatively low concentrations of pollutants from a gas stream by trapping them on a solid with a large surface area. TSA (Temperature-Swing Adsorption) and PSA (Pressure-Swing Adsorption) are two most widely used methods.

Pressure Swing Adsorption (PSA) is a very effective and clean method of removing one, or several, target gases from another carrier gas. PSA requires an elevated pressure for adsorption and a low pressure for desorption [4]. PSA is normally used for the separation of residual carbon dioxide from methane after a scrubbing unit. On a larger industrial scale PSA is also used to separate oxygen from nitrogen. [5] For a continuous process, at least two units must be used in parallel; one is adsorbing while the other is being regenerated. The adsorbent is expected to have a service life equal to that of the plant.

*Components that have boiling point lower than that of propylene (-48°C) are called "light component" and are normally considered cannot be condensed at high pressure with cooling water.

Temperature (Thermal) Swing Adsorption (TSA) is especially suited for organic compounds that have molecular weight range of 40 to130 and boiling point between 21°C and 150°C. With this properties, the organic molecular is easy to be adsorbed at normal condition and easily removed from adsorbents at higher temperature. Adsorption may be regarded similar to distillation process, because the heavier components are retrained better than lower boiling components.

Adsorbent
We have two choices on adsorbent: active carbon and high-silica zeolite.
Considering the goal of separation, we list the criteria for adsorbent choosing:

- high selectivity on Isoflurane;
- high adsorption capacity and easy recovery;
- tolerant to high temperature.

Because of the bad selectivity and the lack of desorption information about active carbon and very good properties of zeolite, we choose zeolite as adsorbent rather than active carbon.

Option 3 - Membrane

Membrane, such as molecular sieve, is also a good separation method for gases. The molecular sieve, as its name suggests, is based upon a naturally occurring mineral, zeolite, which can filter gases at a molecular level. It is only where the molecular dimensions of the carrier gas and the target gas are very close that this separation principle will not operate effectively.

Molecular sieves are synthetic zeolites or metal alumino silicates and strictly defined by pore diameter. Molecular size of Isoflurane is about 5-7Å and N_2O 1.6Å and O_2 1.2 Å. [6] Molecular sieves give selective adsorption.

By using molecular sieves, the membrane technology is similar to adsorption. Unfortunately, not enough information on applying molecular sieves as membrane is found; hence, we regard membrane as an alternative technology for adsorption.

2.2 N_2O Removal

2.2.1 Introduction

The environmental impacts of N_2O are severe and it is almost 300 times more hazardous than CO_2. It has high density, so it will remain in the atmosphere for a long time. The N_2O decomposition produces N_2 and O_2. From several options two options are chosen to remove N_2O from the system. Thermal decomposition and catalytic decomposition are the two options for N_2O removal.

2.2.2 Options

- Thermal decomposition

- Catalytic decomposition
- Biological process
- Purification and sell

Option 1- N_2O Thermal Decomposition:

At high temperatures N_2O can be decomposed to N_2 and O_2. The temperature range can be 700°C-800°C for approximately 70% N_2O conversion. The dissociation of N_2O starts at 300°C-320°C [9]. At higher temperatures it is expected to have more conversion, as the reaction is temperature dependent. Maintaining the temperature required for the decomposition needs high amount of energy.

Option 2 – N_2O Catalytic Decomposition:

N_2O decomposition is possible at low temperature by using a catalyst. There are various catalysts for the decomposition of N_2O. Either a fixed bed or monolith can be used as a reactor. The advantage of using catalyst is low operating temperature i.e. approximately 320°C-400°C, and the conversion could be more than 90%.

Catalyst options:

- *Rh/Al_2O_3*

Among Rh/Al_2O_3, Pd/Al_2O_3, and Pt/Al_2O_3, Rhodium gives the highest activity and conversion at the temperature 573 K. Over 823 K, the decomposition reaches nearly 100%. [7]

- *$Ex\text{-}feZSM_5$*

This catalyst is reported very active (almost 100% conversion of N_2O, ppm level, 500 – 800 K). [8] It is stable at high temperature and has high contact area. But it is not available for commercial use.

- Other catalysts:

Ex-framework FeMFI catalysts, e.g. ex –[Fe,X]MFI where X= Al,Ga,-, also show significant N_2O conversion at > ~700 K. They were tested in a condition of 1.5 mbar N_2O in He. This catalyst is not commercial available and is only available at lab-scale.

Option 3 – N_2O Biological Decompostition:

N_2O decomposition by special kind of cultured microbes is possible. Those microbes are anaerobic and don't required O_2. Handling the microbes and maintaining cleanliness is very important and special care has to be taken for this purpose.

Option 4 – N_2O Purification and sell:

Only N_2O decomposition is not a possible option, but purification and ell could be one of the options, even if not sounds convincing. N_2O can be used as a fuel enhancer in automotive industry, so N_2O can be sold to those companies at cheap price.

2.3 Options Chosen

2.3.1 Volatile Organic Compound Separation and Recycle

The goal of volatile organic compound separation and recycle is to save the most expensive chemical compound Isoflurane and offer good conditions for N_2O removal.
The original stream has every small amount of Isoflurane. Neither condensation nor adsorption alone can get large amount of pure Isoflurane easily. The idea comes that we'd better combine adsorption and condensation to reach our goal.
Two main options we shall consider:

1. The sequence of adsorption and condensation;
2. Adsorption method chosen between PSA and TSA.

- *Sequencing:*

First of all, a continuous operation would be better than a batch. Second, to get high purity Isoflurane by condensation, high molar concentration of Isoflurane in gas phase is necessary. The molar concentration of Isoflurane in the original stream is too low (2%) for condensation. The last but not the least, condensation is normally the most expensive step in most separation process, because it requires big amount of energy and sometime expensive utilities. That suggests us concentrate the gas mixture before sending it into condensation.

We choose using adsorption followed by condensation.

- *PSA or TSA:*

PSA: In our project, the process pressure is only 0.2 atm and the gas flow rate is 5.5 L/min. If we apply PSA to our project, a gas compressor will be necessary for getting an elevate pressure, which indicate PSA may cost lot of energy and increase investing cost.
Besides, the stream containing N_2O and O_2 gets an elevate pressure after passing the PSA adsorber. But we have to notice that the downstream treatment to this stream is N_2O decomposition proceeding at high temperature, which is willing to accept low-pressure stream (< 1Atm). In another word, the elevate pressure does not bring benefits but maybe safety troubles. As the Isoflurane can only be released from adsorbents under low pressure, it is also no help for condensation section.

Table. 2-1 Advantages and Disadvantages of PSA.

Advantages	Disadvantages
o High efficiency o Clean o High selectivity on molecular size o Continuous operation, o No temperature change	o Safety problems for N_2O decompositions o Long life time adsorbent needed o Compressor needed.

TSA: Isoflurane is the sole organic component and its molecular weight is 84 with boiling point 49 °C. It is possible to separate Isoflurane from the gas mixture by TSA. For a hospital, increasing temperature is much easier than increasing pressure.

Table. 2-2 Advantages and Disadvantages of TSA

Advantages	Disadvantages
o Suit for organic compounds o Easy operation o Work well with a wide range of adsorbate concentration o Continuous operation o Wide choice on adsorbents o No pressure change	o Slower compare to PSA. o Needs special equipments for desorption o Temperature change (not good for condensation)

TSA dominates PSA mainly for safety considering.

Conclusion: As explained above, the option we chose for volatile organic compound separation and recycle is TSA followed by condensation.

2.3.2 N_2O Removal

Two ideas for N_2O removal are N_2O decomposition and Purification of N_2O from the gas mixture of N_2O and O_2. As the molecular size of N_2O and O_2 are similar (N_2O 1.6Å and O_2 1.2 Å [6], purification is very difficult. Besides, the selling price of N_2O is not high. Purification becomes unnecessary. The main idea narrowed down to decomposition.

We are not allowed to put any flow control for the vent gases, as time of the operations and number of operations are unknown and we want to treat the gases whenever they are coming through the venting system.

Criteria for chosen options;

1. Safety of the treatment
2. Efficiency of the technology
3. Controllability
4. Investing and operating cost

There are other criterions as well other than those four mentioned above. Other important criterions could be Sustainability, Return On Investment, Innovative design, etc. but more importance is given to the four criterions, which could be important to this assignment consideration.

The options for decomposition are:

1. Thermal;
2. Catalytic;

3. Biological.

Thermal:

Safety: Decomposition of N_2O is an exothermic process. N_2O is not flammable and it has no explosion limits, so it can be transferred to the heating system directly. Moreover N_2O is a fuel enhancer and it will give oxygen for combustion process.

Efficiency: The temperature in a heating system is around 1500°C-1800°C, where the conversion could reach around 90% -95% or more [9].

Controllability: Temperature and pressure controllers are required. Natural gas flow rate can be controlled and that is dependent on the temperature inside the heating system.

Investing and operating cost: N_2O decomposition is an exothermic reaction, so use of N_2O can reduce the natural gas requirement to some extent. Temperature and pressure controllers are common controllers to any heating system. No additional investment for fuel to decompose N_2O.

Catalytic:

Safety: The maximum flow rate of 82 gram per second is not high, and the plant is not operating 24 hours. So the heat releasing is not harmful to catalysts and reactor. For a heat in integrating system the heat of the reaction can be used to preheat the feed stream.

Efficiency: The catalytic decomposition of N2O can reach 100% at a certain temperature (~250°C for the feed temperature).

Controllability: Operating a monolithic reactor is easy and safe. Negligable pressure drops on the length of the reactor. Temperature and pressure controllers can be used for operating reasons.

Investing and Operating cost: The cost of the total decomposition of nitrous oxide depends on the price of the catalyst. The price of a monolith reactor is about 1-2 Euro per m^3. If we use Fe/Al_2O_3, or Pb/Al_2O_3 then the price is almost negligible because Fe and Pb is almost free, but if we use Rh/Al_2O_3, the price of Rhodium is high. No information is found about the price of Rhodium. If a fixed bed is used as a reactor, the price of Rh/Al_2O_3 of the palletized particle is known, 25 gram of 0.5% Rh/Al_2O_3 cost 96.50 Euro [10]. The operating pressure is almost 1 bar. For the heat transfer a heat exchanger has to be installed.

Biological:

Safety: Handling of microbes needs special attention, especially in the hospitals. The operating temperature and pressure conditions are safe, as they are standard room temperature and atmospheric pressure.

*Efficiency: A*round 60% - 70%

Controllability: Cultured microbes need anaerobic environment for their growth. Absence of oxygen is not possible in this case, as O_2 is in the gaseous mixture and difficult to be separated from N_2O.

Investing and Operating cost: Buying cultured microbes and their maintenance are the major issues for the cost. The operating temperature and pressure conditions are normal, so no additional investment has to be done.

Conclusion: From the criterions it is quite obvious to focus on two processes for N_2O removal i.e. Thermal Decomposition and Catalytic Decomposition.

2.4 Basic Process Block Scheme

After options are selected, the process block scheme can be formed to indicate the main design of the process. The block flow scheme is an overview of all the flows in the process and the units considered in the system. Here we combine Volatile organic compound separation with either Thermal decomposition or Catalytic decomposition. The temperature and pressure conditions for each unit and the flow rates of inlet and outlet streams are mentioned.

The block schemes can be found in Appendix 2.1.

3 Basis of Design

N_2O and Isoflurane are major anesthetic gases used in hospitals to provide anesthesia for patients. The most normal anesthetic systems are re-breathing system (fig3. 1) and non re-breathing system (fig. 3.2). The former one is applied to adults while the later to small patients, like children. The exhaled gases are emitted through a separate venting system in the hospital.

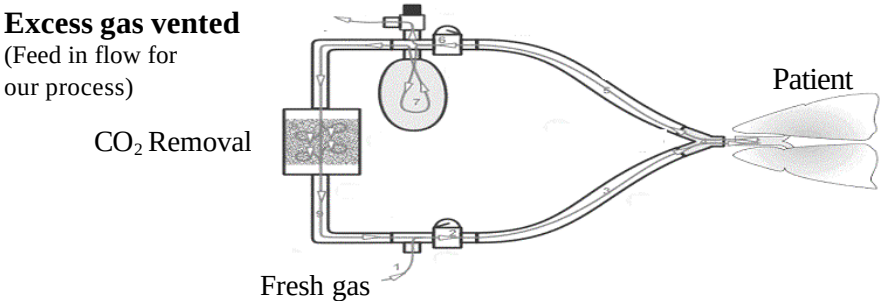


Fig 3.1 Re-breathing system:

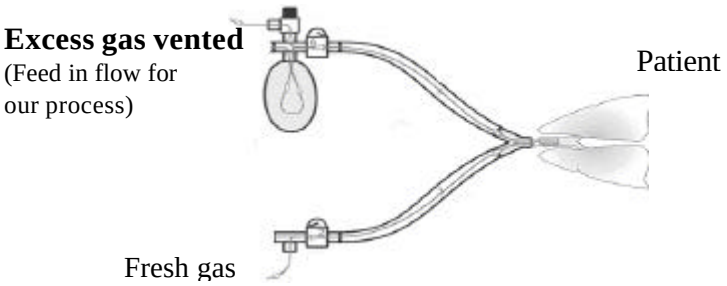


Fig 3.2 Non re-breathing system:

3.1 Description of the design

The exhaust gas stream has a flow rate range of 1L/min approximately (in the re-breathing system) to 3-10L/min (in the non re-breathing system). Generally composition of the exhaust gas stream from the operation rooms is Isoflurane 2% vol, nitrous oxide 50%-65% vol, oxygen 33%-48% vol, little amount of water vapor (ppm) and carbon dioxide (ppm).

N_2O is a green house gas, which effects environment 300 times more than CO_2 does. Isoflurane is an expensive chemical and is likely to contribute to the green house effect and destroy ozone layer. Until now, no special treatment is observed for the N_2O or Isoflurane recycle from exhaust streams in the hospitals in Netherlands.

3.1.1 Design objective

The goal of this design is to carry out a conceptual process that removes both the Isoflurane and N_2O from the exhaust streams of major hospitals. Refer to previous background; the project undertaken is intended to overcome the loss of expensive anesthetic medicine and to reduce the impacts to environment. As the hospital is taken into account, the processes we need to design must be easy to be controlled and economically favorable.

The solution will include:

- Process design and control
- Safety analysis
- Economy estimation

Those will not be considered in this assignment are:

- The anesthesia system inside the operation room
- The composition change in the exhaust gas from the operation room
- The water and electricity supply in the hospital

3.2 Process Definition

3.2.1 Continuous/Batch

The feed rate for this process is only 11.522 ton/yr, which is much less than 5000 tons/yr. Theoretically; it is not necessary to use continuous process. For a hospital, the operation rooms have no regular working hours. And once there is an operation, which uses Isoflurane and N_2O as anesthetic gases, this process is necessary. Hence, the main process is designed to be continuous while desorption and condensation of Isoflurane are semi-continuous.

3.3 Basic Assumptions

3.3.1 Plant Capacity

The plant capacity assumption of 5.5 L/min is based on average value of 3-8L/min (given in the project description) for one operation room. For ten operation rooms in a day is 55 L/min of feed stream that contains 2 % Isoflurane, 58 % N_2O, and 40% O_2. The average time the use of anesthetic gas is assumed 6 hours a day in one operation room. This gives a flow rate of whole hospital is 7227000L/yr, which equals 11.522 ton/yr.

3.3.2 Feedstock's

In hospitals, N_2O is used as an anesthetic gas in combination with Isoflurane (a chlorine and fluorine containing ether). The feedstock is essentially a waste gas mixture of these gases from the operation room send to the atmosphere without any treatment.

Base chemical, feedstock, product, byproduct and waste:

In this process to treat the exhaust gas from the operation room of hospitals, there is no base chemical. The feedstock of the process is a gas mixture, which combines re-breathing gas and non re-breathing gas. There is no valuable product; since almost 99.98 % of the Isoflurane in exhaust gas is separated and 70% of separated Isoflurane is being recycled back to the process, other 29.98% Isoflurane can't be condensed will be sent back to adsorption section. The nitrous oxide is converted (80-90%) to nitrogen and oxygen, which is emitted to the air. There is no waste formation.

3.3.3 Economic plant life

This design is based on the fact that there will always be operations in hospitals where anesthetic gases will be used. If in some years there will be another new alternative of the anesthetic gases like air combine with Isoflurane, the volatile organic compound separation section of the plant can also be used for a long period of time. Because there is no selling of product the only income is the money that is saved from the Isoflurane recycle. That means the Isoflurane do not have to be bought frequently anymore, once the process recycles it. That recycled amount can be re-used for the next operation. The assumed economic plant life has been taken to 15 years, because the operating machines are also designed for 15 years.

3.3.4 Location

The location shall be outside of the operation room in a large Dutch hospital (e.g Erasmus Rotterdam in south west Holland)

3.3.5 Battery Limit

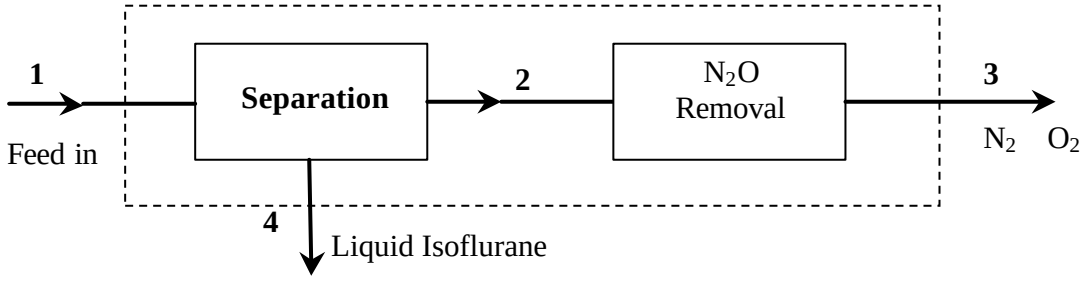


Fig 3.3 block scheme of battery limit

Block scheme of battery limit:

The battery limit is previously described in the block diagram in figure 3.1 the total process can be divided into two sub processes, which are the separation part and the conversion part. In the separation part an absorber and condenser is used and in the conversion part a monolithic reactor is used. The condition is mentioned in the Table 3.1.

Definition of the units inside the battery limit:

There are options in the separation processes: condenser, adsorption and two in the conversion part: *Thermal decomposition* and *Catalyst decomposition.*

Facilities:
Table 3.1 facilities of inside and outside battery limit

Inside Battery Limit	**Outside Battery limit**
For separation: Temperature Swing Adsorber • For adsorption (0.2 atm 25 °C) • For desorption (0.01 atm 130 °C) • Condenser (1 atm 4°C) **For removal:** • Catalyst decomposition: Reactor (1 atm 300°C - 500°C) Heat exchanger • Thermal decomposition: Heating system (inside the heating chamber) (9.6 atm 2000 °C)	• Safety equipment (fire extinguisher etc.) • Storage tank (Storage of Isoflurane that is being recycled (1 atm 4°C))

4 Thermodynamic Properties and Reaction Kinetics

4.1 Introduction

In separation section, thermodynamic properties are very important for energy balance calculations and consequently guide equipment designs.
In our case, the thermodynamic properties we focus on are heat capacity, vapor pressure, gas density, reaction kinetics, and reaction enthalpy.

4.2 Vapor pressures

Vapor pressure is the pressure exerted by a vapor in equilibrium with the solid or liquid phase of the same substance. Vapor pressures of each component are calculated from Antoine Equation:

$$\log_{10}(P/mmHg) = A - B/(t/°c + C)$$

The Antoine constants for each component are listed [11] :

Compound	A	B	C
Isoflurane	8.056	1664.581	273.152
Nitrous Oxide	7.003	654.260	247.163
Oxygen	6.691	319.013	266.697

Calculated by Antoine Equation, vapor pressures (P/atm) at different temperatures for these three compounds are listed.

Table 4.1 Vapor pressures of Isolurane, N2O and O2 at –5 °C to 30°C

T(°C)	K	P/atm Isoflu	P/atm N_2O	P/atm O_2
30	303.15	0.483327	57.75645	543.2148
25	298.15	0.390983	52.26764	520.6445
20	293.15	0.314002	47.12398	498.2739
15	288.15	0.250267	42.31895	476.1215
10	283.15	0.197877	37.84527	454.207
5	278.15	0.155138	33.69488	432.5502
0	273.15	0.120551	29.85912	411.1722
-5	268.15	0.092799	26.32807	390.0944

The values for oxygen are useless, since the temperatures are much higher than the critical temperature of oxygen (158K). More vapor pressures for other temperatures are listed in App. 4.1.

4.3 Condensation Temperature [calculation of this part see Appendix 4.2]

Condensation is the technology that removes one or more components from a gas mixture by phase changing. When the partial pressure of the component reach or excess the vapor pressure of the pure component at the same condition, we may get this component in liquid phase:

$$P_{i,T}^{*} = P_{total,T} \cdot n_i$$

Where, $P^{*}_{i,T}$ is the saturated vapor pressure of component i at temperature T. $P_{total,T}$ is the total pressure of the gas mixture at that temperature and n_i is the molar concentration of i. In the temperature range of 30°C to -10°C, oxygen is impossible to be liquified because of its pretty high vapor pressure. Nitrous oxide has vapor pressures 300 times more than those of Isoflurane at corresponding temperatures.

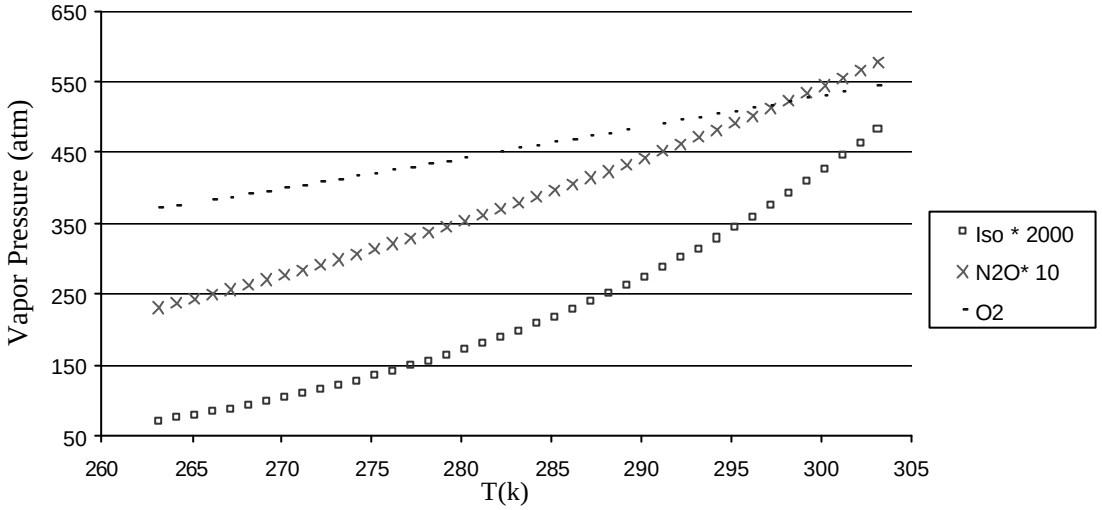


Fig.4.1Vapor pressures at different temperatures

Under the help of "SuperPro Designer", we found the purity of Isoflurane liquid excess 99.9% throughout the temperature range. Based on this fact, the criteria for choosing a condensation temperature are:

1. large amount of Isoflurane could be gained at that temperature in liquid phase;
2. Small energy consuming;
3. Low total investment cost;
4. Cheap coolant available.

Table4.2. Recovery of Isoflurane at different condensation temperatures (without 'feedback stream"):

Temperature °C	15	10	8	5	3	0	-10
Isoflurane (liq) kg/hr	0.05237	0.06482	0.06877	0.07383	0.07672	0.08047	0.08915
Recovery %	52.37	64.82	68.877	73.83	76.72	80.47	89.15

We choose 4°C as condensation temperature. Latent heat of vaporization would be the amount of energy (heat) needed to evaporate a unit mass (e.g. one gram) of the liquid into vapor.
Isoflurane = 41 cal/gm = 31.84 kJ/mol

4.4 Specific heat

Specific heat is a product of mass and specific heat capacity. Substances with high specific heat have strong bonds, as they require high amount of energy to break into small molecules. It is a highly temperature dependent quantity.

To determine specific heat, several parameters are given. They are A, B, C, D and even E, F. Parameters from different reference match different equation to obtain correct specific heat. Equation 4.1.1 is one of those equations and the most popular one.

$$C^{ig}{}_p = A + BT + CT^2 + DT^{-2} \quad \text{----------(4.1.1)}$$

Parameters of nitrous oxide, methane, nitrogen and oxygen are easily found in lecture books. As Isoflurane is a new compound that appears after 1980, its heat capacity coefficients are not found directly from books but calculated by a so-called Jacback group method [App.4. 3, 12]. This group method is clearly explained in Appendix.4.3
Parameters for Isoflurane are then obtained as below, which match the equation 4.1.2.

$$C_p = A + B\cdot T + C\cdot T^2 + D\cdot T^3 \quad \text{----------(4.1.2)}$$

A= 41.17; B=4.29E-1; C= -3.09E-4; D= 6.96E-7

Table 4.3 Specific heat capacities of the gases at STP (298 K, 1atm) and 1273K, 1atm

Cp kJ/mol/k	CH_4	CO_2	H_2O	CO	O_2	N_2O	N_2
298K, 1 atm	0.0350515	0.0371265	0.033575	0.02915784	0.0293831	0.038617	0.0291136
1273K, 1atm	8.11E-02	5.58E-02	4.43E-02	3.39E-02	3.55E-02	5.67E-02	3.36E-02

4.5 Reaction constants and kinetics

Reactions in the decomposition section are

1) $2N_2O \rightarrow 2N_2 + O_2$

2) $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ (Only for Thermal Decomposition)

4.5.1 Thermal Decomposition

Reaction constants

For components

Enthalpy:

$$\triangle H^{ig} = \int_{T_0}^{T} C_P{}^{ig}\, dT + \triangle H^0{}_{form} \quad \text{----------(4.2)}$$

A thermodynamic function of enthalpy change is given as $H = U + PV$. The enthalpy change is the heat energy exchange with the surrounding at constant pressure. It is

independent of pressure. e.g. In case of enthalpy of formation, for the components which releases heat during their formation have a negative sign.

Entropy:

$$\Delta S^{ig} = \int_{T_0}^{T} C_P{}^{ig} \frac{dT}{T} - \ln \frac{P}{P_0} \text{ ----------(4.3)}$$

It is the amount of energy in a physical system, which is unable to do work. The entropy of the chemical reaction always tends increase. It is a function of temperature and pressure.

Gibb's free energy:

$$\Delta G = -R * T * \ln \frac{P_0}{P} \text{ ----------(4.4)}$$

This is the amount of free energy, which is available for useful work. If the system changes, the free energy tends to decrease. It is a function of temperature and pressure.

Table4.4 Entahlpy, Entropy, Free energy of the gases at STP (298 k, 1atm)

Component	CH_4	CO_2	H_2O	CO	O_2	N_2O	N_2
?$Hf_{(298)}$ kJ/kmol	-74.52	-393.509	-235.129	-110.525	0	82.1	0
? $Gf_{(298)}$ kJ/kmol	-0.03682	-0.044868	-8.8098	-33.011	-0.0312	104.22	0
? $Sf_{(298)}$ kJ/kmol	-0.08053	0.00302	-0.04427	0.08955	0	-0.01738	0

Table 4.5 Entahlpy, Entropy, Free energy of the gases at 1273 K, 1 atm

Component	? $Hf_{(1273)}$ kj/kmol	? $Gf_{(1273)}$ kj/kmol	? $Sf_{(1273)}$ kj/kmol
CH_4	4.5578298	-2.08	0.01
CO_2	-339.069	-2.12	-0.26
H_2O	-191.9774	-1.97	-0.15
CO	-77.426389	-1.91	-0.06
O_2	34.60621	-1.92	0.03
N_2O	137.35279	-1.70	0.11
N_2	32.727424	-1.90	0.03

For reaction

Enthalpy: (kJ/mol)

$$\Delta H_{reaction} = \sum \Delta H_{products} - \sum \Delta H_{reactants} \text{ ----------(4.5)}$$

Entropy: (kJ/mol)

$$\Delta S_{reaction} = \sum \Delta S_{products} - \sum \Delta S_{reactants} \text{ ----------(4.6)}$$

Gibb's free energy: (kJ/mol)

$$\Delta G_{reaction} = \sum \Delta G_{products} - \sum \Delta G_{reactants} \text{ ----------(4.7)}$$

Table 4.6 Entahlpy, Entropy, Free energy of the reactions at 1273 K, 1 atm

Rxn	?Hf$_{(1273)}$ kJ/kmol	?Gf$_{(1273)}$ kJ/kmol	?Sf$_{(1273)}$ kJ/kmol
1	-174.64	-2.31	-0.14
2	-796.79	-0.13	-0.63

Equilibrium constant

$$\ln K = \frac{\Delta G}{-R*T} \text{ ----------(4.8)}$$

Table 4.7 Reaction rate constant: The reaction is approximately second order reaction [App. 4.4]

Rxn	K sec^{-1}.(gmol/lit)
1	1.2441482
2	1.0119531

Reaction Kinetics

The method that we use here to determine the reaction kinetics is half-life method. The half-life of a reaction, $t_{1/2}$ is defined as the time it takes for the concentration of the reactant to fall to half of its initial value. By determining the half-life of a reaction as a function of the initial concentration, the reaction order and specific reaction rate can be determined.

The reaction volume is constant,. Because the volume of the furnace is not been changed any more. The equation that used is:

$$-\frac{dC_A}{dt} = -r_A = kC^a{}_{N_2O} \text{ ----------(4.9)}$$

This equation is described in more detail in Equation 4.5.1 to 4.5.8, Appendix 4.5, the half-life is defined as the time required for the concentration to drop to half of its initial value:

$$t_{1/2} = \frac{2^{a-1}-1}{k(a-1)}\left(\frac{1}{C_{A0}{}^{a-1}}\right) \text{ ----------(4.10)}$$

Draw the plot of ln $t_{1/2}$ as a function of ln C_{A0} is equal to 1 minus the reaction order

$$a = 1 - Slope \text{ ----------(4.11)}$$

The corresponding rate law is;

$$-r_A = kC^2{}_{N_2O} \text{ ----------(4.12)}$$

Finally, in this process the Rate of reaction:

$$-r_A = 0.708C^{1.728}_{N_2O}$$

More details about the calculations and values are described in Appendix 4.5.
All the data and equations are referred from Van Hess-Smith, thermodynamic book. [18]

4.5.2 Catalytic decomposition

Reaction kinetics

Generally catalysts selection depends upon its activity, selectivity, stability, cost, deactivation time on a certain condition etc, of the catalysts. Some catalysts that are used for N_2O decomposition are based on some supported metal with the presence of other metal as promoter. (e.g., Cu, Rh, Co, Fe, etc.). The effect of promoters is to increase the reaction rate and reduce catalyst deactivation. A rhodium based catalysts (Rh/Al_2O_3) is selected for the application of the monolith reactor because of its high activity, high stability (~900 K).

The chemistry of the reaction is the direct decomposition of nitrous oxide.
$2N_2O \rightarrow 2N_2 + O_2$

The kinetic expression.

1st order	$r = k_{obs} \cdot p_{N2O}$	}	The power law expression
Strong O_2 inhibition:	$r = k_{obs} \cdot \frac{p_{N2O}}{(p_{O2})^{0.5}}$	}	
Moderate O_2 inhibition:	$r = \frac{k_{obs} \cdot p_{N2O}}{1+(p_{O2}/K_3)^{0.5}}$	→	The LHHW expression.

As the gas mixture contains 38% O_2, and O_2 is fair inhibiter to N_2O decomposition. We choose LHHW expression for simulation calculation.

For high temperature, we can assume that the rate of mass transfer in the catalyst surface is very high, so only the reaction at the surface of the catalyst is rate-determining.

The activation energy is137 J/kmol [13]
The calculated kinetic expression, k_obs = 1.05 e3 S^{-1} (first order reaction)

4.6 Properties of compounds

Other chemical and physical properties of compounds are listed in a big table as Appendix 4.6.

4.7 Data Accuracy

Data are reliable for the design only with sufficient accuracy. The sensitivities are then analyzed. Mass and energy sensitivities of the process are then tested and results are satisfied. (App. 4. 7 Sensitivity Analysis)

5 Process Structure and Description

5.1 Process Structure

The structure of the process we designed is: *Volatile organic compound separation* followed by *N_2O removal.*

3 steps in Separation part are: Adsorption; Desorption; Condensation. 2 options for N_2O removal are: Thermal Decomposition; Catalytic Decomposition.

Inlet of the process is a gas mixture comes from operation rooms at room temperature (~25 ºC) 0.2 Atm. Gas flow rate is 3-8 lit/ min with the following compositions:

- Isoflurane = 2 %,
- N_2O = 50 -65%,
- oxygen = 33 -48%,
- small amount (ppm) of water vapor and carbon dioxide.

There are no commercial products produced in the process, but the separation and recycle of Isoflurane saves considerable amount of money. Besides that, N_2O decomposition generates energy.

5.1.1 Catalysts and reactor selection (for Catalytic Decomposition)

Catalyst selection:
In section 2.2, we list the options for catalysts. Here we chose the most suitable catalyst for our process. The candidates are Rh/Al_2O_3 Ex-$feZSM_5$ and other catalysts.

Table5.1: catalyst weighing (+ is good; ++ is very good; - = bad; -- = very bad)

Criteria	**Rh/Al_2O_3**(1)	**Ex-$feZSM_5$** (zeolite)(1) and others
Activity	++	++
Stability at high temperature (900 K)	++	++
Price (2)	++	- -
Availability	++	--
Influence of oxygen (Inhibition effect)	-	++
Effect of impurities (deactivation)	-	-
Total	8+ 2-	6+ 5-

(1) tested on ppm level of N_2O.
(2) see table 5.1 (app. 5.1) for the price of pellet catalyst.

Based on the analysis of the Table 5.1, ***Rh/Al_2O_3*** is the best choice.

Reactor selection:
This strategy is based on the three strategies level of Krishna and Sie [14].
The details of this method is given in Appendix 5.2

Depending upon the criteria, a weighing factor is given to these two options:

Table 5.2 Reactor weighing (+ is good; ++ is very good; - = bad; – = very bad)

Criteria	**Fixed bed**		**Monolith**	
Pressure drop	High	-	Low	++
Operability	Easy	+	Easy	+
Heat exchange	Easy	++	Not easy	--
Equipment cost	Low	+	Low	++
High effectives factor	Low	-	High	++
Catalyst refreshing	Possible	+	Not possible	-
Space velocity (relative)	low	+	low	+
Total	6 + 2 -		8+ 3-	

The main advantages of the monolithic reactor are:

- High surface to volume ratio (high contact area)
- Low or negligible pressure drop
- A negligible axial dispersion
- Very good mass transfer properties
- Short diffusion distances

The disadvantages of the monolith reactor with respect to mass and heat transfer characteristics are the application in situations only if: the flow through the channels is laminar, no interconnectivity between the channels, poor heat transport or conductivity [15].

The process flow scheme is shown in Appendix 5.3

5.2 Volatile organic compound separation

The separation process starts from an adsorber, which is replaceable and contains high-silica zeolite as absorbent. The adsorption is continuous process.

Desorption happens at higher temperature (130ºC) in a vacuum oven. The effluent of desorption containing high concentrated Isoflurane and is sent to condensation. Condensation works continuously at 8ºC with pressure at least 1 atm. We simulate the separation process under the help of “SuperPro Design”.

5.2.1 Adsorption

The aim of adsorption is to remove Isoflurane from gas mixture.
Isoflurane adsorption:

Almost all (>98%) Isoflurane existing in exhausted gas stream (inlet stream) is adsorbed by zeolite. After adsorbing a certain amount of Isoflurane (here we refer to the reference, 90 g desflurane/620 g zeolite, for Isoflurane and desflurane have similar structure and molecular weight), exhausted zeolite bed is replaced by fresh zeolite bed and is sent to desorption section. The components remaining in gas phase from adsorption section are mainly N_2O and O_2, along with ppm of Isoflurane. The gas mixture is then sent to N_2O removal section.

N_2O and O_2 adsorption:

N_2O can be adsorbed when concentrations of Isoflurane and oxygen are low. Maximum amount of N_2O that can be adsorbed by 620gram zeolite is 9 gram. [16] As in our process, the concentration of oxygen is 40% vol and that of Isoflurane is 2% vol, N_2O and O_2 are more likely to be partially adsorbed.

5.2.2 Desorption

Concentrated Isoflurane vapor is got in this section and zeolite is recycled.

A microwave oven is applied in desorption and temperature rise to 130 °C lasting for 2 hrs. All adsorbed components, i.e. Isoflurane, O_2 and N_2O, are released to gas phase. This Isoflurane-rich gas mixture is sent to condensation unit continuously during this 2 hrs. After desorption, zeolite can be recovered and reused.

A temperature sensor is added to test the temperature of the effluent gas stream and the temperature controller will adjust the electricity applied for the oven.

5.2.3 Condensation

Condenser is prepared vacuum before condensation by a vacuum cleaner. Temperature of condensation is 4°C and pressure is 1 atm. Under these conditions, N_2O and O_2 stay in gas phase and Isoflurane is liquefied. The gases remaining in condenser, which contains mainly N_2O and O_2 and little amount of Isoflurane, are pumped to adsorption section after being mixed with inlet gas stream. We call this gas recycle *feedback stream*'. The recovery of Isoflurane is 70% without 'feedback stream' and more than 90% with 'feedback stream'.

Condensation is operated along with desorption continuously for more than 2 hours.
After pumping remaining gas, the condenser will be vacuum and ready for the next cycle.

5.3 N_2O removal

5.3.1 Thermal Decomposition

The exhaust gas after the separation unit is transferred to the continuously operating decomposition section. No regulation is found for injecting N_2O in the heating system for decomposition section, but that would be very useful and important to know.

The exhaust gas will be mixed with the natural gas flow stream and passed to the heating system for decomposition purpose. The high temperature inside the radiation section of the heating system is enough for the decomposition of N_2O. Inline mixer is used to mix the two streams of exhaust gas and natural gas. The difference in flow rates and pressure will make the inline mixing possible [Fig 5.2].

The gas flow rate of exhaust gas is low and these gases can be directly put into the heating system without any flow control. We cannot put any flow control for the vent gases, as time of the operations and number of operations are unknown and we want to treat the gases whenever they are coming through the venting system.

N_2O is not flammable and it has no explosion limits, so it can be transferred to the heating system directly. Decomposition of N_2O is an exothermic process. The sensitivity analysis for the molar flow rate of N_2O and heat changes in the heating system has to be done to know the behavior of the system when the flow rate of N_2O changes. Moreover N_2O is a fuel enhancer and it will give oxygen for combustion process. The process option is discussed in detail in the following chapters.

5.3.2 Catalytic Decomposition

The gas flow from the separation part can be treated directly with the monolith reactor. Monolith reactor is proven to treat exhaust gas flow: e.g. Tree Way Catalytic reactor and in the nitric acid plant. Car exhaust is also a monolithic reactor to treat the outlet gas of the car motor. In this process we also have an exhaust stream of the operation room in a hospital.

The monolith reactor contains many small channels, which increases the contact area of the gas flow and the solid catalyst on the wall of the channel. This construction of the monolith has a very high activity due to the very high contact area. In figure 5.3 a visual description is given of the interaction of the flow and the catalyst. The flow is laminar and while he N_2O molecule is traveling along the channel it reacts on the wall. At the outlet of the reactor there is no N_2O left anymore. More details are given in reactor design in chapter 8

5.4 Process Modeling

Modeling gives a quick and clear overview of the whole process. After the description of the whole process, modeling will be easy to be understood. Modeling can prove whether the process is possible and suitable to be operated in real life. It also offers some valuable

theoretical data for the further work. Two soft wares are used for modeling. They are *Aspen* and *SuperPro* Designer (SPD for short).

Isoflurane is a new component, which is not defined in Aspen data bank Special efforts have been made to assign Isoflurane through user-defined mode in Aspen, but failed for the lack of some of the thermodynamic properties. *Adsorption Unit and Condensation Unit* is not possible to be modeled by Aspen. The information for Isoflurane is sufficient to assign it in SPD. Based on modeling by SPD, there is no Isoflurane present after adsorption unit. Then using Aspen to do the modeling becomes possible for the units, which are operated after adsorption unit.

5.4.1 Volatile organic compound Separation

As explained above, the software used for simulation is Super Pro Designer, which asks for relatively less properties of Isoflurane than Aspen does.

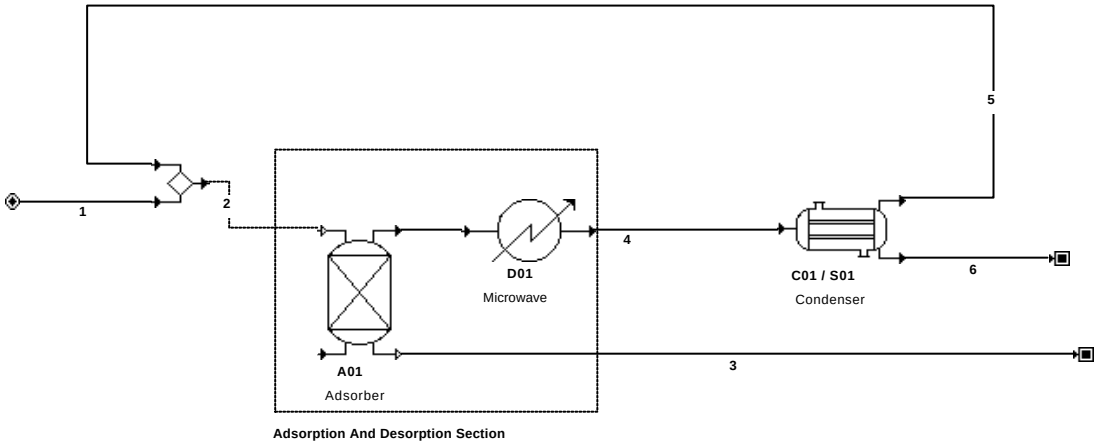


Fig.5.1 Simulation of Volatile organic compounds Separation and recycle by SPD.

The figure 5.1 shows what the model is like. Stream 1 is the original gas mixture we get from hospital. Stream 3 contains N_2O and O_2 and connects N_2O removal section. Stream 6 is the liquefied Isoflurane, which will be gained and reused.

Stream 5 is what we called “feedback stream” in 5.2.3, which connecting condenser to original feed in. By running this model, we found some Isoflurane (~30% of the total quantity) remaining in gas phase after condensation. Without stream 5, we are losing Isoflurane by venting the gas phase remained in condenser to atmosphere.

5.4.2 Aspen Model selection

Aspen thermodynamic model is used for Thermal as well as catalytic Decomposition.
Two major groups will decide the thermodynamic models:

- Activity coefficient
- Equation of state

The activity coefficient method is mostly applicable to describe liquid and vapor phase. It covers the liquid-vapor phase equilibria for hydrocarbon/ water solutions.

Equation of state related two properties to the third one e.g. P*v = R/M* T i.e. an ideal gas law. For inorganic gases there are some options in the Aspen simulation. The options are;

-RK Aspen
-RK Soave
-Soave Redlich Kwong (SRK)
-Peng-Robinson etc.

It was not easy to decide the option, but RK Soave model has been selected from the Aspen SYSOP wizard developed by the PSE group TU Delft.

5.4.3 Thermal Decomposition

Aspen is used to simulate the decomposition part of the process and results are used as a back up, as there are results from excel calculations as well [Appendix Table 5.4.1, 5.4.2]. The flow scheme of thermal decomposition includes five main units viz. Adsorption unit, Condensation unit, Mixer, Compressor, Heating system. Though the heating system is outside the battery limit, we won't consider that it is entirely outside the battery limit and necessary actions are required to maintain the steady state operation of the heating system when exhaust gas is fed to the heating system. All the controls are explained in the process control section [Ref. Chapter 6]

In the heating system there is radiation section and convection section. In Aspen we have solved the system by putting a cooler after a reactor. The cooler will be used to satisfy the real process conditions. The vent temperature is 110°C and the pressure is 1.03 bar_a. The temperature loss will be because of the convection section in the heating system and the pressure loss will be also because of the convection section.

Thermal Decomposition Process Scheme

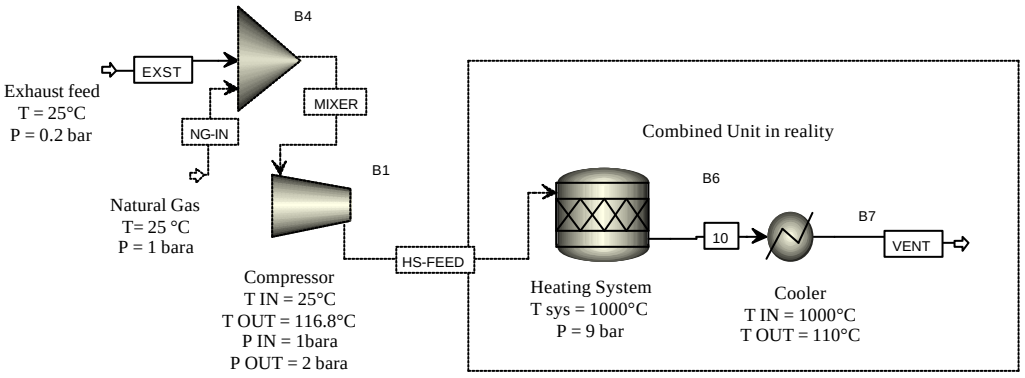


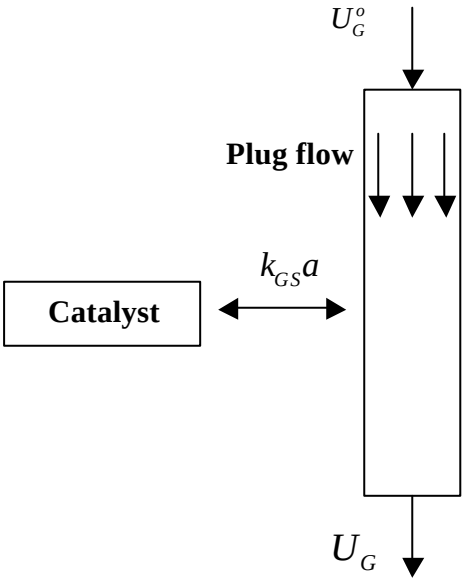
Fig. 5.2 Thermal decomposition process flow scheme

Table 5.2.1 Utilities: [17] [Appendix 5.6]

Utility	Units		Energy per quantity	Units costs, Nfl/unit			
				Quant		Energy	
	Quant	Energy	LHV	Min	Max	Min	Max
Natural gas	M^3	MJ	31.65	0.26	0.43	0.00821	0.01358
	kg	MJ	37.68	0.31	0.51	0.00821	0.01358
	ton	MJ	37678.57	309.52	511.90	0.00821	0.01358
Cooling water	M^3			0.05	0.10		
BFW/Process water	M^3			0.10	2.50		

5.4.4 Catalytic decomposition

The process is simulated in Aspen separately. The feed of the reactor is just the outlet feed of the separation part. Simulation is done with the average value of the flow rate (N_2O: 14.35 gm/min, and O_2 7.16 gm/min). The pressure is 0.2 bars and the stream temperature is preheated from 25 to 253 ^oC. The control of this part is explained in the control part section. Simulation results are given in chapter of reactor design. No utility is needed, besides the preheating of the feed stream electrically during the startup of the process.



A plug flow model

The molar flow rate of the gas phase will change due to the reaction. From the chemical reaction it is clear that for two moles of nitrous oxide gives three moles of components. The superficial velocity will increase but this will not effect the total concentration. So we neglect further the volume change by reaction. The results of the Aspen simulation can be seen in Appendix 5.4.2

Fig 5.3 Hydrodynamic Model

Stream summary of the two processes i.e. Separation and Thermal Decomposition and Separation and Catalytic Decomposition are given in Appendix 5.5

6 Process controls

This chapter explains in detail all the controls in the system. Placing appropriate controls in the system is always an important thing, as the safety totally depends on the controls of the system. All the units from the process scheme are discussed in this chapter. The streams contains anesthetic gases are all "wild" streams, means no controller shall be added to them. The reason is these streams are connected directly or indirectly to operating rooms and the quantity of them shall be only determined by operations.

6.1 A01/A02-- Adsorber:

Adsorption is a continuous process that has almost no temperature and pressure changes (only small pressure drop of 0.836 Pa [App 8]). The parameter we need to consider in this section is only the amount of Isoflurane be adsorbed by zeolite and the change of gas flow to adsorber bed. The weight of adsorber bed is measured and when it exceeds the specified value is the sensor sends the signal to the switch to change the gas flow to the secondary adsorber.

6.2 F02-- Microwave oven for desorption:

The temperature of the zeolite bed and outlet gas is to be considered. With the increase in temperature the desorption efficiency of zeolite bed increases and also zeolite can withstand up to 400 ^{o}C. So the temperature effect on zeolite bed can be ignored. The sensor TC1 measures the temperature of the outlet gas and it provides the feedback signal to control the power supplied to the oven.

6.3 C01& V01-- Condenser:

Condensation is the last and the most important section for Isoflurane recycle. To get large amount of highly pure Isoflurane, accurate temperature and pressure are supposed to be provided. The sensor TC2 measures the temperature of gas phase and sends the signal to manage cooling utility supplying. PC1 will open only when the pressure inside the condenser exceeds a certain pressure that may lead to poor purity of Isoflurane because of N_2O or O_2 liquefying.

6.4 M01-- Mixer (Inline Mixer)

The mixer is inline mixer and operates on the pressure and viscosity difference of fluids. Exhaust stream (stream no. 1) of 0.2 bar_a [Appendix 5.3] is mixed with the natural gas and air mixture (stream no. 8) [Appendix 5.3] of 1 bar_a. The mixer will mix both the gases, which will depend on the viscosity and pressure. Outlet Pressure of both the streams will be same, so no difficulty is expected. If the temperature inside the heating system is more than the set point, then the temperature controller will act on the feed stream of the natural gas to decrease the flow rate of the fuel. Exhaust gas neither be

decreased nor be regulated, so there is no flow indicator or control valve on stream no.1 [Appendix 5.3]

6.5 K01: Compressor

Stream no. 9 of 1 bar_a is the inlet for compressor. High flow rates and the existing use of compressor in reality makes the choice of using compressor easy, otherwise to compress 1 bar_a to 2 bar_a blower can also be used and it could be cheaper. It is highly possible that the flow rate of incoming stream changes, but this is not expected to change a lot, as the stream no.1 has maximum value of 4.8 m^3/hr compared to 200m^3/hr of natural gas stream no. 8

6.6 F01: Heating system

Temperature inside the heating system can be controlled by the fuel inlet i.e. stream no. 8 There are two methods to reduce the temperature in the heating system.

1. Reduce or close fuel inlet
2. Reduce or close air inlet

A temperature controller is mounted on the heated water outlet. If the outlet water temperature is higher than the set point, then the temperature controller will increase the flow rate of water that has to be heated and vice-versa. This temperature controller also helps to maintain the liquid phase of the heated water.

The pressure in the radiation section is approximately 9 atm. If this pressure is increased there is a pressure controller that is connected to a blower. The blower helps to remove the combustion gases. If the pressure inside the heating system is high, then the blower will rotate fast to remove the combustion gases from the system, so that the pressure is reduced. Emergency pressure relief valve is also mounted on the system for opens automatically if the blower cannot reduce the pressure fast enough or in a certain period.

6.7 R01: Monolithic Reactor

The most important variable we interested is the temperature of the reactor feed. This temperature should be controlled and fixed at ~250 ^oC, depending on the activation energy. Monoliths are highly selective and can withstand high temperatures. A feed stream 3 at 0.2 bar and 25 °C is transferred to the reactor. During the startup of the process the feed steam temperature must be raised till the set point (~250) temperature is reached. The outlet reactor stream is used to preheat the feed stream. Therefore a heat exchanger is designed. A temperature controller is installed between the heat changer and the reactor.

6.8 Electric heater

The temperature we are interested for catalytic decomposition is the temperature of stream 7. A temperature sensor is settled between heat exchanger (**E01**) and electric

heater to monitor the temperature of reactor feed in stream. At the time of start up and the continuous process, electric heater supplies heat to stream 7 to provide temperature at least 250℃. The power of electric heater is controlled by temperature sensor **TC3**.

7 Mass and Heat balance

The feed for our process is from the exhaust air stream of the operating rooms. The average inlet flows assumed for the heat and mass balance is 55 L/min. The process is a combination of continuous and batch process, as the adsorption of Isoflurane on zeolite bed and decomposition of N_2O don't have influence of the inlet flow rate, but after separation i.e. the desorption and condensation of Isoflurane simply depends upon the amount of zeolite in each adsorber bed, bed exhaustion time and number of beds used.

Heat and mass balance

Our mass and heat balances are considered for each day, as it's difficult to calculate for each hour. So the units of our streams, either for mass or for heat, are all based on day. The streams summery for mass and heat balance for two processes are provided in the Appendix 5.2.

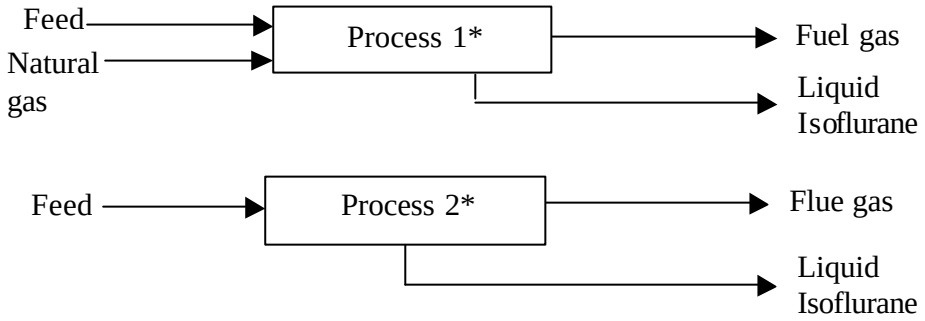


Fig. 7.1 In and Out flow scheme of a process

7.1 Volatile organic compound Separation and Recycle

In our process, we have approximately calculated the quantity of zeolite required for one day (app 8.1) .We have considered desorption and condensation will take place after the complete exhaustion of adsorber bed (approximately each day).

Mass balance

The separation is a physical process without chemical reactions. More than 99.98% of Isoflurane is adsorbed by high-sillica zeolites. N_2O and O_2 pass through the zeolites with tiny adsorption, and flow into the following process: decomposition.

The separated Isoflurane is then recovered by desorption and condensation. The overall efficiency of recovering is more than 90%. The remained gas phase in condenser are sent back prior to adsorption.

Heat balance

Separation section is composed by 3 main steps, which are adsorption & desorption of Isoflurane and condensation. Under low pressure, such as in our process, gases are considered as ideal gases and pressure effects on heat capacity coefficients can be neglected.

Note:

*****Process 1: separation of Isoflurane and thermal decomposition of N_2O

Process 2: separation of Isoflurane and catalytic decomposition of N_2O

The heat of each step is calculated

$$Q = m_j \cdot \int_{T_0}^{T_1} C_p dT$$

Table 7.1 Condition changes and the heat load in separation section:

Steps	inlet conditions		final conditions		? T	? P	kJ/day
	T °C	P atm	T °C	P atm			
Adsorption	25	0.2	25	0.2	~0	~0	~0
Desorption	25	0.2	130	0.01	105	0.2	354.019
Condensation	130	0.01	8	1	-122	1	-465.853*

It is obviously to see no energy produced or required for adsorption. In desorption step, microwave will cause the bonds of polar molecular vibrate to generate heat consequently. The energy for desorption is supplied by electricity, which is supposed to be available freely in hospitals (assignment description). NaCl Brine is used as cooling utilities for condensation.

7.2 Thermal decomposition

Mass Balance

In this section the mass balance of separation and N_2O thermal decomposition is mentioned. N_2O and O_2 from the separation unit directly go to the heating system, where the decomposition of N_2O takes place at high temperature. The temperature needed for 70%-80% conversion is around 700°C-800°C [8], but in reality the temperature is high i.e. around 1000°C-1200°C, so it is expected that the conversion will increase to more than 90%-95%, as the reaction is temperature dependent.

The conversion of natural gas is assumed to be 100%. All the data for heating system is taken as a reference from the heating system of TU Delft. The system provides hot water for some buildings, and the comparison is made for the hospitals and guesses are made. We were unfortunate, as the exactly required information cannot be received from the hospital.

The basic reactions for the N_2O decomposition and natural gas burning can be written as follows;

$$2N_2O \rightarrow 2N_2 + O_2 \text{ ----------(1)}$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \text{ ----------(2)}$$

Note: In Table 7.1
* including the heat of zeolites need to be removed.
+ means the system need heat supplying,
- means the system need heat removing.

The amount of oxygen from the separation section will be added in the first reaction and the total oxygen will be higher than the stochiometric balance. The oxygen will be 35% of the total stream, which is coming out from the separation unit.

There are assumptions for the natural gas flow rate, which are based on the comparison with the TU Delft's heating system.

Assumptions for Mass and Heat Balance:

- Natural gas flow rate: 200 m^3/hr = 6063.327 gm/min
- Airflow rate: 50% excess air is used for the safety purpose, as the operating temperature is very high.
- Oxygen = 36379.960 gm/min and Nitrogen = 11975.712 gm/min
- The temperature available in the heating system = 1000°C
- 100% methane conversion in a heating system
- The temperature of the vent gas is 110°C
- No heat loss in the system
- For the water, which is being heated in the heating system, is sent at a pressure of 3.5 bar_a and the pressure drop is assumed to be 1 bar.
- In the mixer unit natural gas at 1 bar_a is mixed with N_2O at 0.2 bar_a

All the mass and heat balance calculations are discussed in detail in the Appendix 7.3.

7.3 Catalytic decomposition

Mass Balance

External and internal mass transport:

Diffusion is one of the main transport mechanisms in heterogeneous reaction system. In the case of the monolith, where we have many small channels (fig. 7.1 in App. 7.4) the gas is flowing trough the small channel. The molecule has a convective transport in the axial direction. The flow in the channel is assumed laminar and the diffusion in the axial direction is negligible. Due to diffusion, the molecule travels in the radial direction to the wall of the monolith. Diffusion and reaction takes place simultaneously in the porous catalytic coating layer and the product diffuses back to the gas flow.

Mass balances for a monolith catalyst-reactor

The monolith reactor is treated as an ideal plug flow reactor. In a plug flow reactor the composition of the fluid varies from point to point along the flow path, consequently, the material balance for a reaction component must be made for a differential element of volume dV .

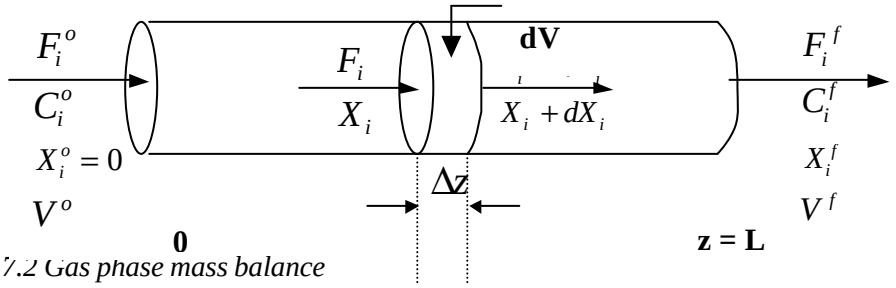


Figure 7.2 Gas phase mass balance

Consider a differential element of volume dV of the reactor (see figure 7.2). The mass/mole balance for component i for the gas phase is:

$$\begin{pmatrix} rate of \\ accumulation \\ of\ i \end{pmatrix} = \begin{pmatrix} rate\ of\ i \\ entering\ dV \\ by\ bulk\ flow \end{pmatrix} - \begin{pmatrix} rate of\ i \\ leaving\ dV \\ by\ bulk\ flow \end{pmatrix} - \begin{pmatrix} rate\ of\ i \\ leaving\ dV \\ by mass transfer \end{pmatrix} \text{-------} (1)$$

The derivation of this mass balance can be read in detail in appendix 7.4.1.
The design equation of this monolith reactor is:
Where $C_b = C_{A0} e^{-k_c a V / n_0}$

The reaction takes place at the surface of the catalysts. The correlation [18] to calculate the mass transfer coefficient is:

$$sh = \frac{k_f \cdot d_p}{D_{if}} \qquad Sc = \frac{m_f}{r_f \cdot D_{if}}$$

For monoliths reactor:

$$Sh = Nu_\infty (1 + B_1 \cdot \mathrm{Re} \cdot Sc \frac{d_H}{L})^{0.45}$$

In Appendix 1 the meaning of the symbols is reported.

Mass balance on the catalyst surface

The mass balanced for component i at the surface of the catalyst is given by:

$$\begin{pmatrix} rate of\ i \\ entering \\ by\ mass\ transfer \end{pmatrix} = \begin{pmatrix} rate of\ i \\ consumed\ by\ the \\ reaction at\ surface \end{pmatrix} \text{----------} \quad (2)$$

rate of 'i 'entering by mass transfer is : $k_{GS} a_{GS} (C_b - C_s)$

$$\begin{pmatrix} rate of\ i \\ consumed \\ by\ reaction \end{pmatrix} = \begin{pmatrix} catalyst \\ effectiveness \\ factor \end{pmatrix} \times \begin{pmatrix} rate \\ of \\ reaction \end{pmatrix} \times \begin{pmatrix} catalyst \\ density \end{pmatrix} \times \begin{pmatrix} catalyst \\ holdup \end{pmatrix}$$

$$= h\ e_s\ r_s\ v_i R \qquad \text{----------} \quad (3)$$

Equation (2) becomes

$$k_{GS} a_{GS} (C_b - C_s) = h\ e_s\ r_s\ v_i R \qquad \text{----------} \quad (4)$$

Table 7.3: Mass and energy balance of the adiabatic plug flow reactor from simulation output in Aspen.

Total	Unit	In	Out	Generated
Mol-flow	Mol/min	0.54988536	0.7129535	0.16306813
Mass-flow	Gm/min	21.5139	21.5139	0
Enthalpy	Watt (J/s)	524.845739	524.845739	0

8 Process and Equipment Design

8.1 Absorber

Properties of zeolite

Adsorption of inhalational anesthetics, by charcoal filters one of the options, but is not very economical as recycling of the Isoflurane (desorption process) is difficult.
We found a so-called "high-silica zeolite" adsorbent, which may adsorb Isoflurane at room temperature and desorption can happen at higher temperature (90-130 °C). [19]

High-silica zeolite is chosen as the adsorbent in our Isoflurane adsorption. Almost all (98%) Isoflurane existing in exhausted gas stream (inlet stream) is adsorbed completely by zeolite. Maximum amount of N_2O that can be adsorbed by 620gram zeolite is 9 gram, under the flow rate of 3L/min for 110minutes. In real life, N_2O can be replaced by pure oxygen or Isoflurane completely. [19] As in our process, the concentration of oxygen is not high (40% vol) and that of Isoflurane is only 2% vol, N_2O is more likely to be partially replaced by oxygen. The components remaining in gas phase in adsorption section are mainly N_2O and O_2, along with ppm% of Isoflurane. The gas mixture is send to N_2O removal section. After adsorbing a certain amount of Isoflurane (here we refer to the reference, 90 g desflurane/620 g zeolites, for Isoflurane and desflurane have similar structure and molecular weight), used zeolites are replaced by fresh zeolites and are sent to desorption section. In desorption section, temperature rise to 130 °C under vacuum and last for 1 hr. Isoflurane and N_2O is released to gas phase. This Isoflurane-rich gas mixture is sent for further treatment to condensation unit. Zeolites can be recovered and reused.
Adsorption capacity of zeolite is given in Appendix figure 1

Adsorber bed

We have considered the hydrophobic zeolite, which normally absorbs organic gases. The zeolite bed is completely enclosed except the space for inlet and outlet tubes. From the calculation we obtained the amount of zeolite required for one day is 4.092 kg. The height/ diameter of bed is assumed as 1. Each adsorber bed can be used for 6 hours at the average flow rate of 55 L/min. In general one zeolite bed will adsorb 594 gm of Isoflurane. Depending upon the different flow rates in the hospital, the zeolite usage time is tabulated below. The detailed calculations for the adsorber bed specifications are shown in [App 8.1]

Table 8.1 Zeolite usage time under cases:

Cases	Volumetric Flow rate	Zeolite Usage Time
Average case	55 L/min	100 min
Worst case	80 L/min	68.75 min
Least case	20 L/min	275 min

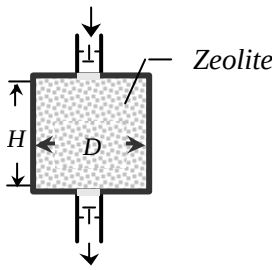


Fig. 8.1 Adsorber

Table8.2 Adsorber designed Parameters:

Zeolite bed	Values
Zeolite bed weight (kg)	4.092
Diameter (m)	0.202
Height (m)	0.302
Area (m^2)	0.256
Volume (m^3)	$6.43*10^{-3}$

To prevent mixing with air outside the adsorber, we have a totally innovative design:
The inlet and outlet tubes are both fail-to-close designed. Only when the adsorber is settled in process and connected with other tubes, these two ends will be open (as shown in Fig. 8.1).

8.2 Condenser

We have considered a vertical shell and tube condensers for condensation of vapor gases from desorbing system to obtain liquid Isoflurane. The condenser is a single pass unit and coolant and vapor will flow in counter current way. The vapor condenses inside tubes and flows from top to bottom and the coolant flows through the shell side. The bottom head of the condenser acts as settler to separate incondensable gases and liquid Isoflurane. The coolant that we have used is NaCl brine solution. The heat transfer coefficient between the vapor and coolant gas is considered as 40 $J/m^2/s$ / ^oC and the total heat transfer area calculated is 0.017 m^2. The total amount of coolant required for year is 3.075 ton/yr for the basic assumed situations. The calculations are shown in [App 8.1]

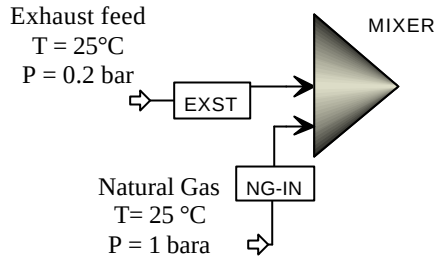
8.3 Microwave Oven

The microwave equipment supplies the heat for desorption. Heating the zeolite by means of air or hot gas is not possible, as it will cause the low purity of product Isoflurane and also increase condensation energy cost. So heating by means of microwaves is chose as one of the option. As well as the electricity for the microwave heating is the best and easy utility available in hospitals.

Microwave equipment is provided with a tube at the top connecting to condenser so that the desorbed gas can go directly into the condensation section. The temperature of the desorbed gas controls the microwave heating.

8.4 Mixer

Injection of nitrous oxide can increase the power of the car engine by 25% - 30%. Nitrous oxide is a power increasing modification. The higher content of oxygen than air and higher density than air makes it a favorite choice as a fuel combustion enhancer. Appropriate control of air during combustion and use of specific amount of N_2O can be used as a power enhancer [20]. We have no intension to increase the power of the heating system, but this information is very interesting as we also have N_2O in the system. The addition of N_2O and natural gas in the system will make the system more cautious, as far as the process controls are concerned. The ratio of flow rate of natural gas and N_2O in the system can act as a set point for a natural gas flow rate set point. This is explained in detail in process control section [Ref. Chapter 6.4]. For gas mixing, inline-mixing unit is used and most of the times it is not difficult, as the less viscosities make them mix easily. Sometimes baffles, orifices are also used to increase the rate of mixing.



EXST = Exhaust Gas
NG-IN = Natural Gas In

Fig. 8.2 Mixer Unit for N_2O and Natural Gas

The exhaust gas stream is not 24 hrs a day, but there is a separate transport line for this stream. This streamline has an inline mixing connection of natural gas, which is fed to the heating system at 2 $bar_{a.}$ Exhaust gas will be at 1 bar_a from the venting system. Exhaust gas and natural gas can be mixed together, but the possible pressure difference can make the mixing difficult. The natural gas is at 1 bar_a and this will be compressed to 2 $bar_{a.}$ The exhaust gas is mixed with the natural gas in an inline mixer and it is possible, as the pressure difference will make it possible. Even if the exhaust stream has no N_2O in it and there is no gas in the exhaust stream, natural gas will always be transported through the inline connection [Ref Fig 8.3] as the heating system is constantly in use.

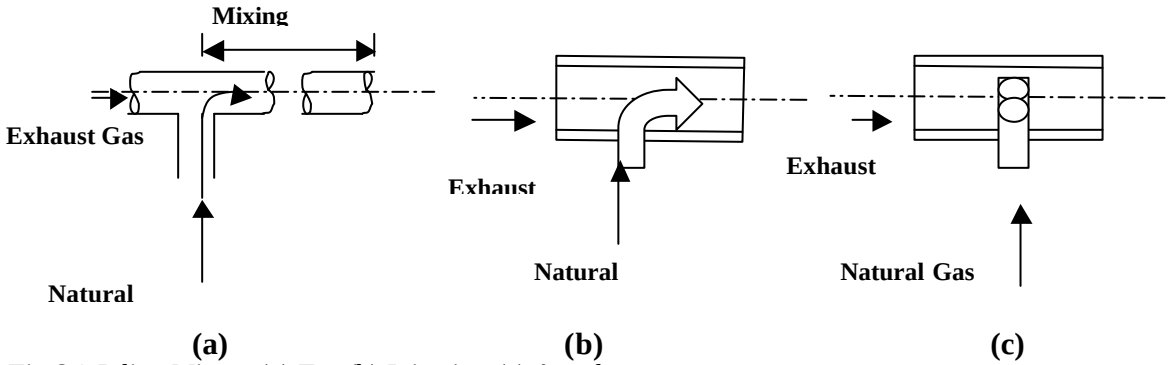


Fig 8.3 Inline Mixers (a) Tee (b) Injection (c) Annular

8.5 Heating System:

The storage and handling of methane is outside the battery limit, as the heating system is the existing system, but the explosion hazard analysis has been studied for this system as we have decided to use natural gas heating system [App 10.3.1].

The outlet mixture from the compressor is 116.8°C and it is fed to the combustion section of the heating system. The temperature of the combustion zone is around 1500°C-1600°C, but the reaction temperature is assumed to be approximately 1000°C. The radiation section temperature is always higher than that of the convection section temperature. This temperature is enough for N_2O for decomposition. The circulating water for warming uses the heat. There is a pressure loss between radiation and convection zone of the heating system. A cooler is placed after the heating system to make sure that the vent temperature is around 110 – 120 °C, and the pressure is around or greater than atmospheric pressure to release all the gases in the atmosphere. As shown in Fig. 8.4 heating system and a cooler is a combined unit in reality.

Heating system:

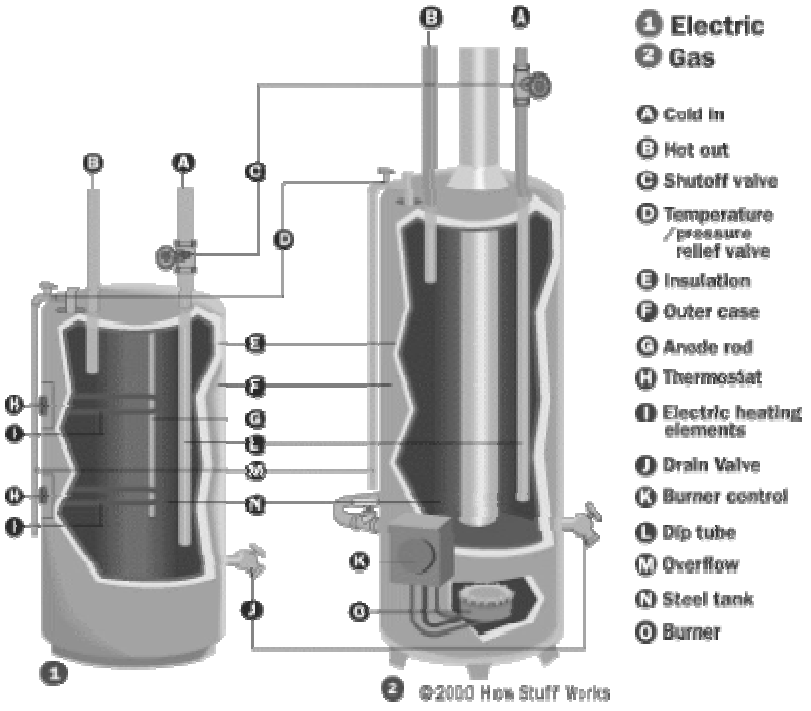


Fig. 8.4 Internals of a Heating system (Electrical and Natural gas heating system) [21]

Thermal decomposition of N_2O:

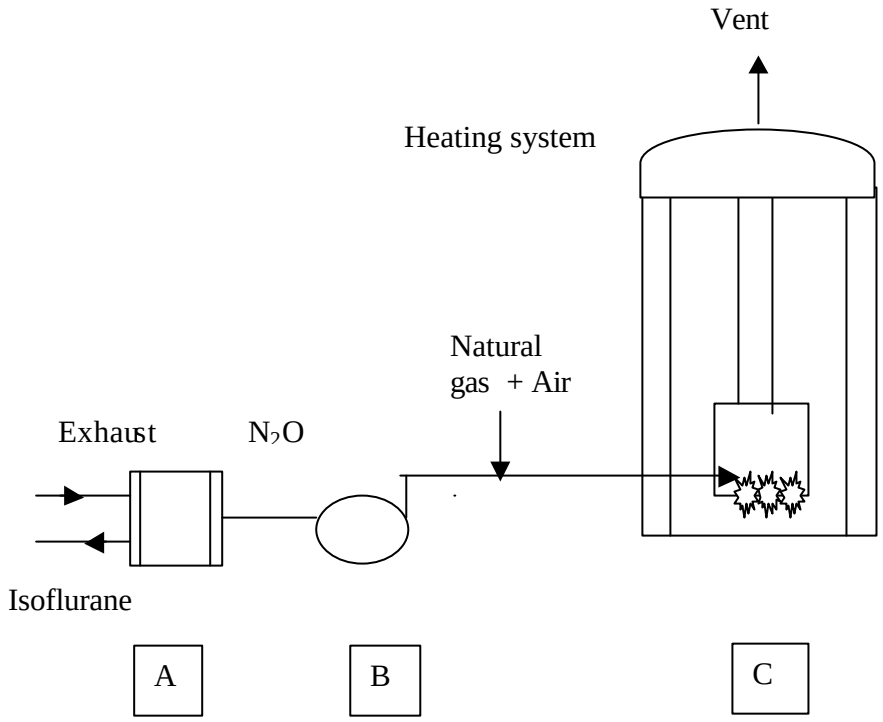


Fig. 8.5 Conceptual layout of Thermal Decomposition

A	Volatile compound separation unit	B	Suction pump of ventilation system
C	Centralized water heater (Natural gas burner)		

The conceptual layout is drawn here to show the idea behind using the heating system for the thermal decomposition. The heating system internals are not discussed in detail here. There is a radiation section and a convection section in the heating system. The radiation section is approximately 1200°C-1500°C and the vent temperature is approximately 110°C-120°C. If economical, a preheater can be used to preheat the exhaust feed from the separation section to the heating system. We don't think that for a hospital they need a preheater as the vast temperature in the heating system can handle the low exhaust feed temperature, if its less than room temperature, especially in winter. The insulation for the pipes outside the hospital will help to maintain temperature and leak prevention of the exhaust gas.

Advantages of centralized Gas fired water heater:

1. Clean operation
2. Inexpensive to operate
3. Fast recovery

4. High conversion rate
5. Available in many sizes
6. Low maintenance and high durability

The idea behind using the heating system is to use the high temperature only, as the use of heating system will prohibit the hospital to spend much more money on the investment, which will be required for the catalytic process. The concern behind this concept is not to design the heating system, as this is out of our objective, but the heat balance of the system and the change in flow rate of natural gas or water circulation in the heating system has to be studied.
When high temperatures and high flow rates are required, fired heating systems are used. The direct heat from the combustion gases is used as a heating source. The capacity ranges from 3 to 100 MW.

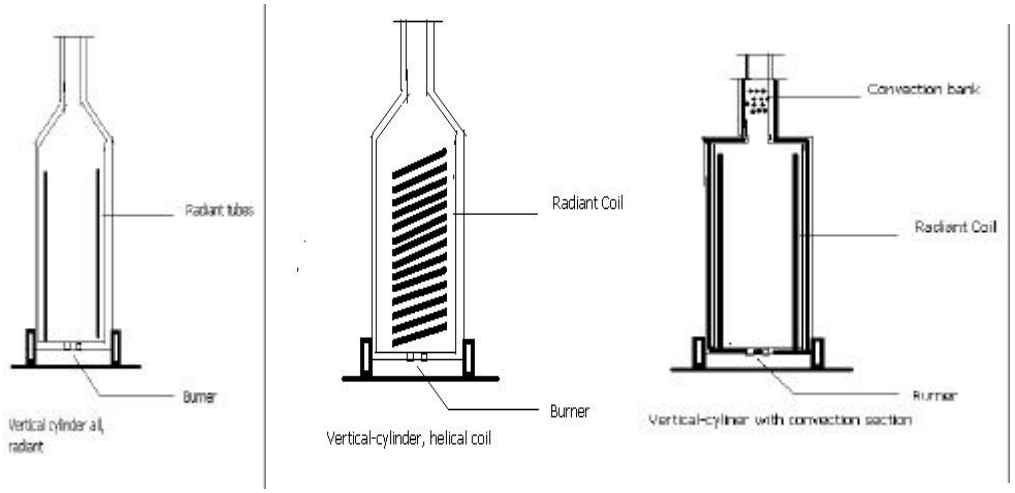


Fig 8.6 Different types of heating systems [22]

Basic Construction:

There are many different deigns available for fired heating systems. The basic construction consists of a rectangular or cylindrical steel chamber lined with refractory bricks. The arrangement of the tubes can be different viz. horizontal or vertical. The fluid that has to be heated is passed through the tubes and the combustion gases used as a heating source.
There are two sections in the heating system, one is where the heat is produced and the other is where it is conveyed by convection. Extended surface are used in the convection section to improve the heat transfer from the combustion gases.
In modern designs a smaller section surmounts the radiant section in which the combustion gases flow over the banks of tubes and transfer heat by convection.

8.6 Compressor:

The pressure of the exhaust gas stream from the adsorption unit is 0.2 bar_a and this has to be fed to the heating system. The natural gas pressure is 2 bar_a and an equal or more pressure of the exhaust stream has to be maintained if the destination of the exhaust gas stream is a heating system. A compressor is needed in the flow scheme for this purpose that can compress the exhaust stream from 1 bar_a to 2 bar_a. The compression will cause the temperature rise of the outlet exhaust stream around 116.8°C. The compressor of natural gas is used for the purpose of compression, as the natural gas is also compressed to 2 bar_a. A mixer unit is used to mix the two gases and the combined flow is passed to the heating system. The exhaust gas temperature is around 25°C and the pressure is also low. High insulation has to be used to maintain the temperature, as the use of a preheater is not a feasible idea. This will increase the operating cost and will not serve any special purpose in the system, but if the insulation is not trusted, then of course, a preheater is needed.

8.7 Blower

First of all the blower design is outside the battery limit, but it is taken into account for the thermal decomposition process. The blower is already present in the vent system of the operation theatre and we don't have to build a new one for our proposed designs. A blower is placed in the outlet of the vent system, which creates a vacuum in the vent system the operation theatre. The vent system pressure is expected to be 0.2 bar_a. The out let from the blower is assumed to be 1 bar_a, which is connected with the inline mixer for the Thermal Decomposition process. For the Catalytic Decomposition process the blower is placed after the monolith reactor and there won't be any pressure drop in the monolith reactor. Some of the blower design considerations are mentioned in the [App 8.2]

8.8 Monolith Reactor

In chapter 7 the mass balance equations are given. More details of the mass transfer and reaction is given in [23]. To use the catalytic layer effectively it is important to match the diffusion distance and the reaction rate with the thickness of the layer. If we do not consider this point and we fix a thickness than we might not use the catalyst effectively. So the thickness of the catalyst layer has been calculated using some assumptions. The thickness 20 ~ 200 nm [App Fig 8.3.1]
We assume, for a steady state situation that the mass transfer to the surface equals the reaction rate on the surface of the catalyst, see equation 5 [App 8.3]. The reaction is then mass transfer limited. A high contact area is needed to reduce the effect of diffusion-limited reactions. A monolith reactor gives very high contact area per volume reactor [App Table 8.2]. The design volume of the reactor is 1.22 e-4 (m3), length is 7.08 e-3 (m).
In the simulation in Aspen a length of 1 m is used to be sure that the reactor can handle wide range of flow rate (30-85 g/min).

For the reactor design the maximum flow rate of 85 g/min is used to be sure that the process can handle the flow rate range.

8.9 Heat Exchanger

The disadvantage in this idea is not considered in the design. The heat of the outlet gas can be partly used to preheat the feed gas. Only the startup of the process needs to be considered to heat the feed stream to 250 ^{o}C. This can be for example electrically heated.

To preheat the feed stream of the reactor with the outlet stream of the reactor a heat exchanger is designed. The procedure described in Coulson and Richardson [24] is used. Designed value for a tube and shell heat exchanger is: Area of tube is: 0.0222 m2, length is: 0.045 m, shell diameter is 17.6 mm.
Design details is given in [App 8.5]

All the equipments design specifications are shown in tables in Appendix 8.6 to 8.9.

9 Wastes

Basically our process is dealing with wastes from a hospital. The output from the process consists of components, which have less environmental effect when compared to the feed to the process.

9.1 Direct waste: Volatile Organic Compound separation and recycle

9.1.1 Stream - zeolite

Zeolite used for adsorption of Isoflurane can be used for many years. But for the better purity and yield of Isoflurane, zeolite bed is replaced once in a year. For about 8.184 kg of zeolite is treated as waste if at least two adsorber beds are used in series throughout the year. The used zeolite should be safely dumped as landfill waste.

9.1.2 Stream- NaCl Brine

The cooling agent for the condensation of Isoflurane mixture is NaCl Brine. Nearly 3.075 ton of NaCl Brine is required for one year. The outlet stream form condenser leaves at 0^{o}C so this stream still has an option to cooling utility for some other streams in the hospital if necessary, or else, this brine stream can be dumped as waste from the process.

9.2 Direct waste: N_2O Removal

9.2.1 Stream – Flue gas<11>* (Thermal decomposition)

The flue gas stream, leaving the Furnace, contains mainly CO_2, NOx, O_2 and some steam. The CO_2 vapor stream is formed by oxidation of methane present in the feed stream. The CO_2 is a green house gas and for that reason must be minimized. The new process uses comparatively less natural gas as a fuel because of N_2O gas, and no CO_2 is produced in the N_2O decomposition and thus creating less greenhouse gas. In this process principal, the N_2O decomposition replaces the Natural gas burning. The amount of CO_2 formed will always be dependent on the incoming natural gas.

The estimation of NO_X formed in the furnace at the operating temperature is highly complicated. The values of TU Delft University's heating system are referenced. In this process, while the temperature and resistance time of the furnace stays equal to the current heating system. The actual NO_x values for a furnace additive natural gas: 18.9mg/Nm^3 burning in the emission air. With a total ingoing air stream of 7689.642m^3/hr air (air density is 1.225kg/m^3), the total amount of formed NO_x is 0.318 tons/yr. The maximum emission according to government regulations of NO_x is 200mg/Nm^3 in the emission air. Hence, the produced emissions are significantly lower. [25]

9.2.2 Stream – Outlet gas<10 >*(Catalytic decomposition)

During start up of the process there is no reaction till the temperature inside reactor increases to 255 ^{o}C. At that time N_2O will be not converted and this will pass the reactor into environment as waste. We can ignore this waste because the reactor will reach 255^{o}C in 0.98s (App 9.1) after N_2O is feed in.

9.2.3 Catalyst and monolith reactor (Catalytic decomposition)

After 4 years the catalyst and monolith reactor have to be replace by a new one. The exhaust catalyst can be regenerated by producer or be land filled along with monolith reactor. We have no harmful, toxic and hazardous component, so our process is very safe.

Note:
* <11>, <10> are the stream numbers referred from the stream summary i.e. Appendix 5.3

10 Safety

10.1 Toxicity

Isoflurane and N_2O in the process are poisonous. The toxicity hazard of the whole process is leakage of these gases in the transport part. N_2O is the anesthetic gas in hospital, but chronic exposure to this agent, a common anesthetic, has been linked to various nervous system disorders only at very high levels [27]. The PVC pipes used in the hospitals for the gas transferring are also a good preventive material to gas leakage.

10.2 HAZOP Analysis [28]

To get the qualitative analysis for the process, a HAZOP study is performed on the furnace, which is the most hazardous equipment of the process. A HAZOP study is a procedure for the systematic, critical, examination of the operability of a process. When applied to a process design or operating plant, it indicates potential hazards that may arise from deviations from the intended design conditions. The seven "guide words" recommended in the CIA booklet are given in [App Table 10.2.2] and to help generate thought about the way deviations from the intended operating conditions can cause hazardous situations.

The result from the HAZOP analysis are utilized to formulate recommendations for improved process safety for the N_2O removal

Table 10.2.1 HAZOP study for the word NO or NOT

Stream number	Hazard	Measure
Gas desorbed (4)	• Low temperature • High temperature	• Low temperature alarm TC1 controls electricity supply; • High temperature alarm TC1 controls electricity supply;
Natural Gas flow (8)	• Low temperature in Heating system F01 • Low pressure in the F01	• Low temperature alarm controls valve V5 • Low pressure controls blower rotation
Coolant flow	• Low temperature in the condenser	• Low temperature alarm controls valve V2
Condenser C01	• High pressure	• Open Valve 03
Reactor Feed (7) (catalytic process)	• Low temperature	• Low temperature alarm controls switch and electric heater starts heating

Table 10.2.2 HAZOP study for the word MORE or LESS

Stream number	Hazard	Measure
Natural Gas flow (8)	• Too Low temperature in Heating system F01 • Too Low pressure in the F01 • Too High temperature in F01 • Too High pressure in F01	• Low temperature alarm controls valve V5 • Low pressure alarm controls blower rotation • High temperature alarm controls valve V5 • High pressure alarm controls valve V7
Coolant flow	• Low temperature in the condenser	• Low temperature alarm controls valve V2
Reactor Feed (7) (catalytic process)	• Too high temperature	• High temperature alarm controls switch and signal is given to valve V7 or V6

Table 10.2.3 HAZOP study for the word REVERSE

Stream number	Hazard	Measure
Natural Gas flow (8)	• Too High temperature in F01 • Too High pressure in F01	• High temperature alarm controls valve V5 • High pressure alarm controls valve V7
Coolant flow	• Low temperature in the condenser • High temperature in C01	• Low temperature alarm controls valve V2 • High temperature alarm controls valve V2
Exhaust flow (1)	• Too high temperature in R01	• High temperature alarm controls switch and signal is given to valve V7or V6

Table 10.2.4 HAZOP study for the word OTHER THAN

Stream number	Hazard	Measure
Natural Gas flow (8)	• Explosion of natural gas and air mixture • Too high pressure in F01	• Stream # must be closed (shut down) • High pressure alarm controls Safety relief valve
Coolant flow (Condenser failure)	• Low temperature in the condenser • High temperature in C01	• Low temperature alarm controls valve V2 • High temperature alarm controls valve V2

10.3 Dow Fire & Explosion Index

The Dow Fire & Explosion Index indicates the potential hazard of equipment and thus of the process, in term of reactivity, flammability and explosiveness. Guideline for the hazard indications is the Dow Fire & Explosion Index Hazard Classification Guide [29]. A numerical "Fire & Explosion Index (F&EI)" is calculated, based on the nature of the process and the properties of the process material. The larger the value of the F&EI more hazardous the process. The absorber of separate Isoflurane, in principle, do not show any hazard concerning fire and explosion through chemicals, which have the property to explode or cause fire. Hence, it is not analyzed.

Furthermore, the Furnace in heating system, which is used to decompose the N_2O, will only be analyzed for the thermo decomposition process. The differences in properties of the chemicals that affect the Dow Fire & Explosion Index of the streams are negligible. The Appendix 10.3.1 shows the analysis undertaken for the Furnace. From the sheets, the Dow Fire & Explosion Index can be estimated. From that index, the hazard according to Dow can be estimated. The material Factors on which that index are based on can find in the Appendix Table 10.1

The degree of the Furnace (Heating system) to N_2O decomposed is moderately heavy. Hence, the Furnace requires extra attention with regards to safety measures. Moderately hazardous processes and units need extra safety measures. Although N_2O is non-flammable gas, it can help combustion. However, the heating system already exits in the hospital. The safety measures have already been taken into consideration. The hazard of the Furnace (Heating system) is only the burning of natural gas in heating system. The degree of the N_2O decomposition is lower, because the CO_2 that the natural gas burning produced is an extinguisher gas for N_2O. The recycled cooling water system also takes a lot of heat that the N_2O decomposition produces. The safety aspects of the heating system are considered in Appendix 10.

10.4 Explosion limits

The explosion limits, as defined in literature, from the boundary conditions for a mixture of oxygen and a combustible component to react and explode. The boundary conditions are the amount of oxygen and a combustible component to react and explode. The boundary conditions are the amount of oxygen relative to the amount of combustible species. In general the values are given in the volumetric fractions of the substance in air. There are two boundaries defined: the Lower Explosion Limit (LEL) and the Upper Explosion Limit (UEL).

In the N_2O removal process with thermal decomposition, the natural gas has the LEL and UEL. The values for the LEL and UEL are show in Appendix 10.5 (Table 10.5.1). N_2O itself is a nonflammable gas, but the gas air mixture can be explosive. The flammable limits for N_2O are not available.

The explosion limits are vital to the thermal process design. The operating conditions must be outside the boundary conditions for explosion. Hence, the operating conditions must be below or above the LEL or UEL value for the stream mixture, containing methane as the combustible compounds. Since the furnace must burn all the natural gas, an excess of air has to be present, thus, the LEL value is of importance for explosion hazard and the Furnace must operate below this boundary value. The concentration of oxygen required for the complete combustion of a combustible component is the Minimum Oxygen Concentration. Only purging will not guarantee the safe level of oxygen in the system. There are some dilution methods, which can dilute the oxygen concentration in the system. The Required Minimum Oxygen Content (RMOC) is 8%. See in Appendix 10.5. If according to the assumption there is 100% conversion of natural gas. In reality may be it is not possible and some of the methane may be 2% - 3% will enter in the heating system and comes in contact with the 35%- 40% oxygen, so the safety aspect has to be studied for a real life situation, and this proves that even if the conversion is not 100 % this will not be dangerous for the process.

10.5 Safety aspects of a monolithic reactor

Consider the safety of a monolithic reactor is very important. For the monolith reactor we have negligible pressure drop, we don't have toxicity component in raw material and product. The only thing we need to consider is the temperature of the outlet and inside reactor temperature. The temperature is nearly 1127 °C of outlet from the monolithic reactor but after that we will use a heat exchanger to cool it down and send that mixture gas back to reactor as recycle, so not only the outlet is being cool down, but also inside temperature of the reactor.
Actually 1127 °C is quiet safe for monolithic reactor, it can withstand in this temperature for few hours safely. Necessary controls must be placed in the system e.g. temperature control.

11 Economy

11.1 Separation and Thermal Decomposition Process

From the two mentioned processes of Catalytic and Thermal decomposition, in this section of economics Thermal decomposition process will be discussed. All the necessary formulas are mentioned in the Appendix 11.1

Capital Cost summary: (Total Purchased Equipment Costs) @ 2003

Table 11.1.1 Capital Cost summary [Ref. App 8 Theory]

Adsorbers	Costs (Euros)
Column1 (A01)	1,080
Column2 (A02)	1,080
Total	2,160

Table 11.1.2 Capital Cost summary

Compressors and Blowers	Costs (Euros)
Compressor 1	2,146
Blower1	1,200
Total	3,346

Utility and Raw materials costs Per Unit

Table 11.1.3 Utility costs [(b)]

Utility Costs Per Unit (Dfl)		
Utility	Unit	Costs per Unit (Euros)
Electricity	kWh	0.1016
Boiler feed Water	Ton	1.50
Cooling Water	Ton	0.05
Brine	Ton	300[(c)]
Natural Gas	Ton	205.00

Table 11.1.4 Raw Materials

Raw Materials Cost Per Unit (Euros) [(a)]		
Raw Material	Unit	Costs per unit (Euros)
Isoflurane	Ton	0
Nitrous oxide	Ton	0
Oxygen	Ton	0

Note:
[(a)] No raw material cost, as all these gases are waste gases that are coming out from the vent system of the operating room in the hospitals.
[(b)] Utility values are referred from CPD manual
[(c)] Brine value is assumed

Table 11.1.5 Product income

Gross Income (Euro)			
Product	Flow (t/a)	Sales (Euros/t)	Costs (Euros/a)
Recycled Isoflurane	0.219	825,600	180,806.40
Natural Gas saved	0.22	205	46.47
Total			180,852.87

1. Capital Investment Costs

From the attached Purchased Equipment Cost (PEC) summary we can get the values of;

- Direct Capital Cost
- Indirect Capital Cost
- Fixed Capital Cost

Lang factor method:

It uses a factorial estimation, which is accurate and the cost factors are compounded into the Lang factor are considered individually.

Direct Capital Cost (DCC) representation;

$$PPC = PEC(1 + f_1 + f_2 + ... + f_9)$$

Where, PPC = Physical Plant Cost or Direct Capital Cost with direct cost items that are incurred in the construction of a plant, in addition to the cost of the equipment.

Indirect Capital Cost takes into account:

a. Design and engineering costs, which are 20-30% of DCC
b. Contractor's fee 5%-10% DCC
c. Contingency allowance 5%-10% DCC

Fixed Capital Cost = PPC (1+ a + b + c)

Direct Capital Cost, Indirect Capital Cost, Fixed capital by escalating given totals @ 2003.

Table 11.1.6 Escalation from year 1989 to 2003

Year			2003
			Rate=7%
Equipment	*Price (Euros)*		*Price (Euros)*
Microwave Oven			500.00
Condenser			840.00
Adsorbers			2160.00
Compressor	In 1993	1050.00	2065.50
Blowers	In 1989	1200.00	3094.24
PEC			8659.74
PPC			24247.29

2. Total Investment Costs and Working Capital

Table 11.1.7 Total Investment and working Capital

Type	Relation	Cost (Euros)
Fixed Capital Cost		42432.77
Working	5% FCC	1697.31
Total Investment	FCC+WC	42432.276

License fees has to be paid if the process used by the company is not exclusively developed by the company it self. Working Capital is the additional investment needed over and above the fixed capital, to start the plant and operate it to the point when income is earned. This includes the cost of:

a. Start up
b. Initial catalyst charges
c. Raw materials and intermediates
d. Finished product inventories etc.

3. Total production costs

Table 11.1.8 Production Costs

Raw Material	Stream nr.	Flows (ton/a)
Isoflurane	1	0.219
Nitrous oxide	1	7.544
Oxygen	1,8	3.759
Total		11.523

Table 11.1.9 Utility costs

Utilities	Flows (ton/a)	Cost Per Unit (Euro/t)	Cost (Euro/a)
Brine	3.07	200.00	614.00
Electricity	417960 (kWh/a)	0.1016 (Euros/kWh)	42465.74
Total			43078.74

Natural gas cost and boiler feed water cost is not taken into consideration because it is outside the battery limit.

Table 11.1.10 Zeolite Cost

Item	Flows (ton/a)	Cost Per Unit (Euro/t)	Cost (Euro/a)
Zeolite	0.016	66666.66	1566.66

Table 11.1.11 The lay out of the production cost

Cost Type			Euros/a
Direct			
	Variable		
		1.Raw materials	0
		2.Miscellaneous materials	170
		3.Utilities	43,079
		4.Shipping & packaging	0
		Sub-total	*43,248*
	Fixed		
		5.Maintenance	1,697
		6.Operating labour	20,000
		7.Laboratory	0
		8.Supervision	6,789
		9.Plant overhead	10,000
		10.Capital charges	5,092
		11.Insurance	339
		12.Local taxes	0
		13.Royalties	0
		Sub-total	*43,918*
	Total		*87,166*
Other			
		14.Sales expenses	
		15.General overhead	*NA*
		16.Research & Dev.	
Total Production Costs			
	Annual		
	[Euros/a]		**87,166**
	Per ton Isoflurane [Euros/t]		398,020

4. Economic criteria on an annual basis

(a). Net Cash Flow (NCF)

It is the cash, which remains when a total investment is subtracted from gross income. The way you handle your cash flow makes a difference to your investment scene. Making money is the prime objective of both profit making and non-profit making firms. It is very important to handle the cash in an efficient way to make all the payments to the vendors and employees.

Tax and depreciation factors are excluded.

Table 11.1.12 Net cash flow calculation

Item	Euros/a
Gross Income	180,852
Total Production Costs	87,166
Net Cash Flow	**93,686**

(b). Rate of Return (ROR), Pay Out (Back) Time (POT)

Table 11.1.13 Rate of return [Fig. 11.1.1]

Item	Unit	Value
Pay-Out Time, *Before Tax*	Years	3.2
Rate of Return, *Before Tax*	%	31.25

$$ROR = \frac{1}{3.2} * 100 = 31.25\%$$

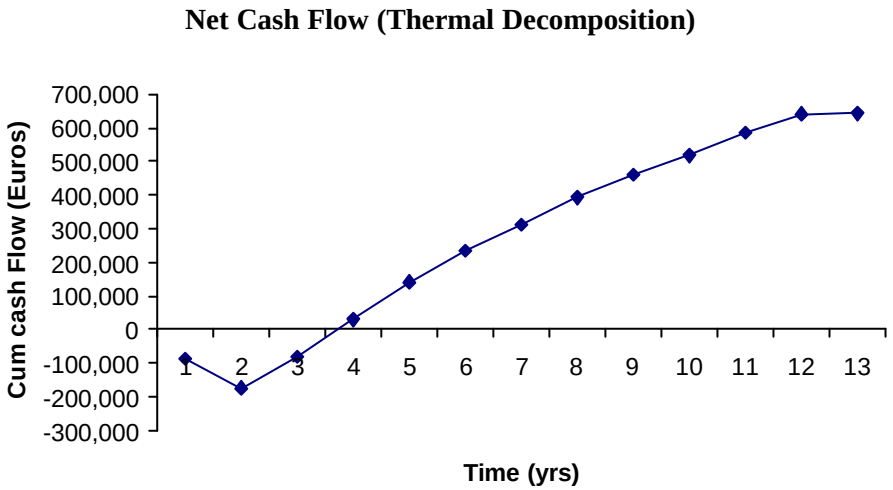


Fig 11.1.1 Net Cash flow diagram [Ref. App 11, Table 11.1]

From the fig 11.1.1 it is shown that the pay back time is around three years. This looks logical, as the equipments used for this process are small, but the layout and piping of the process is expected to take this much time for the process to operate. Natural gas usage consideration is not taken into account, as this is outside battery limit.

(c). Discounted cash Flow Rate of Return (DCFRR), Net Future Value (NFV), Net Present Value (NPV)

DCFRR is found by trial and error method. By trail and error we have to calculate the rate to give the zero present worth. This is basically the amount of interest we can afford to pay if we borrowed the money and the project would just break even.

Table 11.1.14 DCFRR calculation [Ref. App 11, Table 11.1.2]

DCFRR (%)	NPV (Euro)
8.0	335,191
44	0

The process is highly profitable, as the DCFRR is 44%.

11.2 Separation and Catalytic Decomposition Process

From the two mentioned processes of Catalytic and Thermal decomposition, in this section of economics Catalytic Decomposition process will be discussed.

Capital Cost summary: (Total Purchased Equipment Costs) @ 2003

Table 11.2.1 Capital Cost summary

Adsorbers	Costs (Euros)
Column1 (A01)	1,080
Column2 (A02)	1,080
Total	2,160

Table 11.2.2 Capital Cost summary

Reactor and Blowers	Costs (Euros)
Reactor 1	500*
Blower1	1,200
Total	1,700

Utility and Raw materials costs Per Unit

Table 11.2.3 Utility costs [b]

Utility Costs Per Unit (Euros)		
Utility	Unit	Costs per Unit (Euros)
Electricity	kWh	0.1016
Boiler feed Water	Ton	1.50
Cooling Water	Ton	0.05
Brine	Ton	300[c]
Natural Gas	Ton	205.00

Table 11.2.4 Raw Materials Cost

Raw Materials Cost Per Unit (Euros) [a]		
Raw Material	Unit	Costs per unit (Euros)
Isoflurane	Ton	0
Nitrous oxide	Ton	0
Oxygen	Ton	0

Note:
[a] No raw material cost, as all these gases are waste gases that are coming out from the vent system of the operating room in the hospitals.
[b] Utility values are referred from CPD manual
[c] Brine value is assumed
* Referred from www.mathche.com

Table 11.2.5 Product income

Gross Income (Euro)			
Product	Flow (t/a)	Sales (Euros/t)	Costs (Euros/a)
Recycled Isoflurane	0.219	825,600	180,806.40
Total			180,806.40

1. Capital Investment Costs

From the attached Purchased Equipment Cost (PEC) summary we can get the values of;

- Direct Capital Cost
- Indirect Capital Cost
- Fixed Capital Cost

Lang factor method:

It uses a factorial estimation, which is accurate and the cost factors are compounded into the Lang factor are considered individually.

Direct Capital Cost (DCC) representation;

$$PPC = PCE(1 + f_1 + f_2 + ... + f_9)$$

Where, PPC = Physical Plant Cost or Direct Capital Cost with direct cost items that are incurred in the construction of a plant, in addition to the cost of the equipment.

Indirect Capital Cost takes into account:

d. Design and engineering costs, which are 20-30% of DCC
e. Contractor's fee 5%-10% DCC
f. Contingency allowance 5%-10% DCC

Fixed Capital Cost = PPC (1+ a + b + c)

Direct Capital Cost, Indirect Capital Cost, Fixed capital by escalating given totals @ 2003.

Table 11.2.6 Escalation from year 1989 to 2003

Year		2003
		Rate=7%
Equipment	*Price (Euros)*	*Price (Euros)*
Reactor		500.00
Microwave oven		500.00
Condenser		840.00
Adsorbers		2160.00
Blowers	In 1989 1200.00	3094.24
PCE		7094.24
PPC		19863.87

2. Total Investment Costs and Working Capital

Table 11.2.7 Total Investment Costs and Working Capital

Type	Relation	Cost (Euros)
Fixed Capital Cost		27809.420
Working	5% FCC	1390.471
Total Investment	FCC+WC	34761.776

License fees has to be paid if the process used by the company is not exclusively developed by the company it self. Working Capital is the additional investment needed over and above the fixed capital, to start the plant and operate it to the point when income is earned. This includes the cost of:

e. Start up
f. Initial catalyst charges
g. Raw materials and intermediates
h. Finished product inventories etc.

3. Total production costs

Table 11.2.8 Production Costs

Raw Material	Stream nr.	Flows (ton/a)
Isoflurane	1	0.219
Nitrous oxide	1	7.544
Oxygen	1,8	3.759
Total		11.523

Table 11.2.9 Utility costs

Utilities	Flows (ton/a)	Cost Per Unit (Euro/t)	Cost (Euro/a)
Brine	3.07	200.00	614.00
Electricity	376.71 (kWh/a)	0.1016 (Euros/kWh)	38.61
Total			652.61

Natural gas cost and boiler feed water cost is not taken into consideration because it is outside the battery limit.

*Table 11.2.10 Catalyst Cost**

Item	Cost (Euro/a)
Catalyst	600

Note:
* Catalyst cost depends on the volume of the reactor and a wash-coated monolith catalyst is used in the process, which is rather cheap. For coating of Rhodium i.e.25 gm costs approximately 100 euros, and assumption has been made to use approximate 150 gm of rhodium coating on the monolith. The cost of catalyst would be 150*100/25 = 600 Euros

Table 11.2.11 The lay out of the production cost

Cost Type			Euros/a
Direct			
	Variable		
		1.Raw materials	0
		2.Miscellaneous materials	278
		3.Utilities	652
		4.Shipping & packaging	0
		Sub-total	*930*
	Fixed		
		Catalyst*	600
		5.Maintenance	2,781
		6.Operating labour	40,000
		7.Laboratory	0
		8.Supervision	5,562
		9.Plant overhead	13,905
		10.Capital cha rges	4,171
		11.Insurance	278
		12.Local taxes	0
		13.Royalties	0
		Sub-total	*67,297*
	Total		*68,227*
Other			
		14.Sales expenses	
		15.General overhead	*NA*
		16.Research & Dev.	
Total Production Costs			
	Annual		
	[Euros/a]		**68,227**
	Per ton Isoflurane [Euros/t]		311,539

4. Economic criteria on an annual basis

(a). Net Cash Flow (NCF)

It is the cash, which remains when a total investment is subtracted from gross income. The way you handle your cash flow makes a difference to your investment scene.
Making money is the prime objective of both profit making and non-profit making firms. It is very important to handle the cash in an efficient way to make all the payments to the vendors and employees. Tax and depreciation factors are excluded.

Table 11.1.12 Net cash flow calculation

Item	Euros/a
Gross Income	180,852
Total Production Costs	68,227
Net Cash Flow	**112,625**

(b). Rate of Return (ROR), Pay Out (Back) Time (POT)

Table 11.1.13 Rate of return [Fig. 11.2.1]

Item	Unit	Value
Pay-Out Time, *Before Tax*	Years	2.5
Rate of Return, *Before Tax*	%	40.00

$$ROR = {}^{1}\!/_{2.5} * 100 = 40.00\%$$

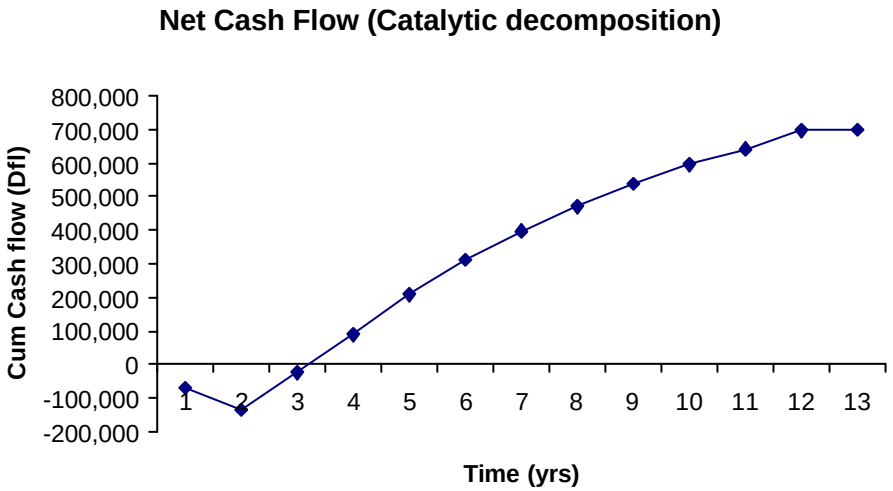


Fig 11.2.1 Net Cash flow diagram [Ref. App 11.2, Table 11.2.1]

From the fig 11.1.1 it is shown that the pay back time is around two years. This looks logical, as the equipments used for this process are small, but the piping and the commissioning of the plant takes some time, and it is expected that more than two years are needed for the process to operate.

(c). Discounted cash Flow Rate of Return (DCFRR), Net Future Value (NFV), Net Present Value (NPV)

DCFRR is found by trial and error method. By trail and error we have to calculate the rate to give the zero present worth. This is basically the amount of interest we can afford to pay if we borrowed the money and the project would just break even.

Table 11.1.14 DCFRR Calculation [Ref. App 11, Table 11.2.2]

DCFRR (%)	NPV (Euro)
8.0	389,856
60	0

The process is highly profitable, as the DCFRR is more than 50%.

12 Creativity and Group Process Tools

12.1 Creativity Method

Creativity is the ability to see connections and relationships where others have not. The ability to think in intuitive, non-verbal, and visual terms has been shown to enhance creativity in all disciplines. It has also been shown that the creative process is very similar in all fields. Essentially the design process is a problem-solving process. The designer, just like the engineer will be most successful if the problem is approached in a systematic manner.

The KJ Method was developed by Jiro Kawakita as a means of organizing diverse observations and qualitative information into useful documented facts. It is fundamentally similar to the *Snowball Technique*. Introduced by the Japanese, it has become one of the 'Seven management (New) tools' of modern Japanese quality management and uses values of Buddhism intended as structured meditation.

The basic cycle of this method is consisting of six parts.

- Problem identification
- Defining the circumstances
- Diagnosis and problem-formulation
- Solutions and working hypotheses
- Activation of solutions
- Programmed application of solutions.

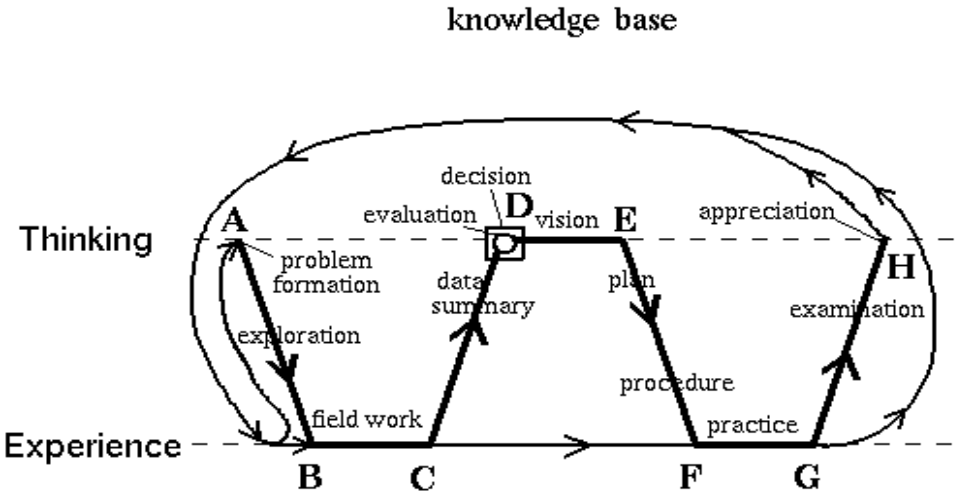


Fig 12.1 basic cycle of KJ method

The benefits of using the KJ method are:

- It helps separate facts from opinions.
- It is an efficient way of organizing seemingly unknown facts.
- It means thoughts are expressed rarified summarized and prioritized in a non-confrontational manner.
- It promotes effective teamwork.

It reduces the dominance of a vocal or strong individual on the conclusion of the team.
Initially the researcher or designer will tend to experiment in a rather random manner, collecting ideas and skills through reading or experimentation. Gradually a particular issue or question will become the focus of the reading and experimentation. The next step is to formulate a tentative problem, and begin to explore that topic. Eventually the problem is refined into a research question or design problem that the person will then pursue through repeated experimentation. In design or fine arts production, this takes the form of works created in a series. Each effort solves certain problems, and suggests issues to be dealt with in the next work (or experiment). Working in a series is the most important stage of the design process. The ability to experiment, to value and learn from mistakes, and build on the experience achieved is the hallmark of a truly successful and creative individual, whatever the field. The table that follows outlines the parallels between design process and classic scientific method. Table 12.2 gives list of creative ideas for CPD project of all group members.

Table 12.1 outlines of design process and classic scientific method

	Research method	Design process
Preparation for research	Literature review	Study historic and contemporary examples, media
Information gathering. Goal: to limit variables and identify problem	Collection of preliminary field data	Experimentation with materials and visual ideas
Identification of problem and hypothesis	Information correlated; problem defined; educated guesses made; hypotheses stated; research design prepared	Design problem identified through visual analysis and recognition
Exposition of facts and interpretation	Research plan is carried out; results are analyzed, plan is modified as necessary based on results; experiments are replicated	Work is created in a series, with each work suggesting problems to explore in subsequent work
Presentation of results and findings	Publication of findings	Exhibition of work or production of design

12.2 Creative idea for CPD Project

Table 12.2 List of Creative Ideas

Date	Creative idea
22/10/03	Anesthetic gases are not be used continuously for 24 hours a day, 365 days a year, so we can consider batch process as option, we can store the exhaust gases first and then process altogether. We can save energy, time and cost but the main drawback will be collection and storage .
22/10/03	As the input for out process is gas. We can think of separation step similar to which are used for air, gas separations and also in waste incineration plants.
23/10/03	As the large difference in the boiling points. There is a chance for separation by heat effects, may be mainly by condensation.
25/10/03	And also membrane separation can be a possibility as there are some membranes for the separation of volatile compounds (as seen in air separation)
25/10/03	Adsorption of Isoflurane on charcoal is old process .we can improve this one by checking for improved adsorbent which can desorbs gases easily
25/10/03	N_2O can be decomposed in high amount of heat. Effective use of the natural gas water heaters for a high amount of heat could be possible.
25/10/03	The corona pulse reactor can decompose N_2O. Corona pulse is an electrical reactor.
25/10/03	The effective heat integration by the catalytic Reverse Flow Regenerative Reactor will require less amount of heat and can give high conversion.
25/10/03 27/10/03	Use of methane for N_2O reduction. Burning of N_2O in methane using Selective Catalytic Reactor requires low temperature and atmospheric pressure Use of mobile chillers, which uses ethylene glycol as a coolant for onsite condensation of Isoflurane
27/10/03	Because of the small amount of the exhaust gas can we collect all the stream of hospitals in a big region to put it in a big flow and then further process it? This will save some equipment.
28/10/03	CO_2 and H_2O are impurities in Anesthetic gases and difficult to separate them by condensation or adsorption. Soda lime is then considered to remove CO_2
29/10/03	High-silica zeolites are good adsorbent to Isoflurane. Isoflurane can be recovered by desorption at 130 centigrade

12.3 Creative Project Plant layout

The purpose behind drawing a layout of our system is because the piping system and the proposed design approach can be well defined. The exhaust from all the operating rooms will be combined and, then it is sent to the atmosphere via main exhaust stream. The main exhaust stream doesn't contain CO_2, as CO_2 is removed in the operating room by CO_2 absorber. The operating vent and exhaust stream of patient are two separate streams.

Separation:

The separation process will be semi-batch, as the separation of Isoflurane with adsorption is a continuous process, but the desorption and condensation process is a batch process. The adsorber will be connected to the main exhaust line. The amount of adsorber needed is approximately 4.16 kg. The adsorber will act as a fixed bed in the main exhaust pipeline. It has to be changed each day and desorption & condensation can be done batch wise to get the Isoflurane back. The separation process layout is not drawn here in this section.

Thermal:

For Thermal process, the heating system is used. The location of the heating system is outside of the hospital for safety reasons. The piping has to be done according to that, but the distance won't be very long and the cost of the piping can be a reasonable amount.

Catalytic:

For catalytic process, there are two options. The reactor can be placed in the building itself [App 12.2 side view (1)] or can be mounted on the roof of the hospital [App 12.2 side view (2)]. The flow rates are not high, so the reactor is also small and needs less area for the set up.

Consideration for Thermal / Catalytic part:

The weather conditions can make a difference during winter and summer conditions. If the pipeline is outside the building, then the consideration has to be given to the fact the temperature will be different in summer and winter.

Thick insulation can be done on the pipeline. The insulation will take care of the leak and the temperature of the exhaust stream during winter. The process of N2O decomposition will be a continuous process, so there won't be any storage facility for the exhaust gas.

13 Conclusion and Recommendations

13.1 Conclusion

Anesthetic gas recycle is very interesting idea and to maintain the purity after recycle is even difficult task. Adsorption and batch-wise desorption of the Isoflurane is considered as an option. If maximum possible amount of Isoflurane is recycled each time, then large amount of money income is expected. Though after every year 10% of less income is expected due to purity problems of the anesthetic gas.

Two designs for N_2O removal have been considered in the report i.e. Thermal Decomposition and Catalytic Decomposition. The section of Isoflurane recycle remains the same for both the processes. The feasibility and economics of both the processes are complementary. If the economics is considered, then for thermal decomposition ROR is 31.25% and for catalytic decomposition it is 40.00%. DCFRR for thermal is 44 % and for catalytic it is 60%. Both the processes are highly profitable and the low flow rate and standard conditions help the economics of the processes.

Thermal process could be comparatively economic for the countries like Netherlands or any country where the climate is mostly cold and heaters are needed to keep the rooms warm. For the developing countries or the countries where there is not much cold climate round the year, they have to invest into the furnace or a heating system for a thermal decomposition. The idea of pursuing the thermal decomposition route depended mainly on the weather. Catalytic decomposition is highly profitable, though the maintenance cost is higher. The monoliths are cheap and they can be replaced in three to four years.

Developing countries can always opt the catalytic decomposition route, as the natural gas is not always easily available and the safety aspects need to be followed strictly. There is not much difference in the economics of the two processes, so even a developing country can opt thermal process, but the operating cost (electricity) is very high for the thermal process.

13.2 Recommendation

13.2.1 Separate adsorption units in an operation theatre

There is not only one anesthetic gas used in an operation theatre but it can be more than one i.e. Isoflurane and Sevoflurane. If there are two different anesthetic gases used in two different operations, then the idea of combining the exhaust gas for adsorption is no more possible, as there will be a mixture of gases. The solution for this kind of problem could be to use an adsorption unit in each room and that will be used separately for desorption. In such a way we will make each operation room independently operated.

13.2.2 To overcome the rapid heat simulation in Catalytic Decomposition

Reaction complete step by step:

An assumption that is made is the homogenous distribution of the wash-coated catalyst. Simulation shows that the reaction is already done at 0.1 m of the length of the reactor. The temperature rises very rapidly (1100- 1400 ^{o}C), [Appendix 5.4.2]

To avoid very rapid temperature rising inside the reactor, a solution is applied on a series of active position on different locations of a very long tube. The reaction will then happen only on these active positions and conversion will not be hundred percent, for catalysts in one active position is insufficient. During the gas transferring in the long tube, heat generated by reaction is distributed to tube. The heat is generated and removed continuously till a hundred percent conversion is reached.

A creative option for the fixed bed reactor is to dilute the catalyst with an inert material in such a way that there is no bypass of the gas. The heat per volume of reactor is decreasing and also the temperature.

Reversible control on monolith reactor

Temperature control inside the reactor is a difficult task, and two temperature sensors are mounted at the top and bottom of the monolith. Reverse flow reactor is an option to maintain the temperature within limit. Change the feed flow rate with respect to the temperature rise at top or bottom. The temperature rise gives a signal to the switch, which changes the flow direction. High select will give the signal to change the flow direction only when the temperature is higher than the set point.

13.2.3 Combination of the exhaust streams and decomposition

In the future if there are more than one hospital in a specified premise, then the combination of the waste gases from the operation theaters can be passed to a large reactor or to a furnace for a catalytic or thermal decomposition. The combined effort of the hospitals will distribute the investment and this kind of joined venture will be help other intended activities of the hospitals as well. The piping and the area of the decomposition unit should be a prime concern.

EU regulations are expected to become stricter and stricter in the future, so the maximum possible decomposition of N_2O is very necessary to reduce the environmental impacts.

14 Hospital Visits

Three hospital visits were planned during the completion of the assignment . Ziekenhuis Leyenburg(Den Haag), Rotterdam Erasmus hospital (Rotterdam), Leiden University Medical Hospital (Leiden) were the selected hospitals. The objective of all th evisits was to get exposed to the process and to interact with the experts. The hospitals were selected according to their area and size, so that maximum information can be obtained. Lot of information was achieved from the visits and especially the visits to the operation theatres helped us to see and observe the anesthesia procedure in reality. All the hospital reports are mentioned in the Appendix 14.

15 Learning from CPD

N D Shindgikar

It was like rafting in a strong water flow currents with the force hard enough to overcome and you never know where you will land, but the will to reach to the destination and the desire to succeed is very important. All the team members were very eager to solve the assignment creatively. It was more of a challenge, as all the team members took the remark very seriously of generalization about all Asian people of not doing something creative and reluctant to use new techniques. Working together with different cultures was a nice and learning experience, but some of the group members had some conflicts between them for some time and there was an immediate attention given by all the team members. Cultural and thinking difference is always a challenge and in a group everyone should not forget the golden rule. *" Treat the person the way he likes to be treated."* The straightforwardness of one of the team members and introversion of the other caused a bit tension, but finally with the discussion with coach and team everything was solved. Of course, this was also a learning experience. Everybody has some qualities and it is always nice to share your thoughts and interest with other person.

D Kisoen

The knowledge of all the courses putting together for one course was very challenging this. The use of the basic concept to achieve complex result was very interesting. It was not only the technical learning but also it helped to improve the socialism. The tension in the group or with someone can always be solved easily when you forget your ego and take the initiative to talk. Discussions are always useful doesn't matter if they are technical, social or of any topic.

Y (Sarah) Zhao

CPD asks for the fully understand of much knowledge, i.e. process control, thermodynamics. During these 3 months, I read lots books, literatures to deepen my knowledge. Since it is a heavy work for all students, CPD occupied my main time. Hence, I also learned how to arrange my life reasonable, to have enough rest, to work efficiently. Working in a group is the rehearsal of working in a company. Once some persons get into troubles, the rest will come to help them out. We get to be aware that each team members shall take responsibility to the project. The last but never to be the least, different persons and cultures need us have more understandings to each other. I learned to be a good listener and a good leader as well.

Max Ma

Things learn from CPD is not only accumulate of techniques but practice communication and cooperation, what I am not good at before, need improve in the future,

Communication of sciences has always been seen by many as a threatening and sometimes impossibility, especially to a diverse group with diverse interest. So how can one communicate complex technology to diverse interest people is a very attractive question. But as everybody can see we made it.

Vani Chilukuri

In the beginning, the topic seemed to be really exciting as well as original because this appears to be a totally different for a bio/chemical engineering student. We had to study lot for gaining the clear idea behind the project. It's nice that we have visited some hospitals for practical information.
I learnt the use of my basic technical skills as the primary material, which helped me to stimulate my creativity. I enjoyed the diversity of our team but it sometimes it seemed too difficult at times due to our different schedule, lifestyle habits, backgrounds, strengths and weaknesses, etc. however, the overall team dynamics worked well toward building a good product on schedule. We were able to use different member's unique strengths such as speaking, planning, innovation, scheduling, and organization, report writing etc. in addition to this the weekly meetings with Coach, we used to share our problems and future planning, which helped us a lot in the group organization.
I learnt lot of things like different ways of thinking about work and time management for doing certain tasks as a group and also communication skills. In end, the project brought us closer than before

YiLing Liu

It is the first time for me to do the CPD projects that need all the courses know ledges putting together. Using the basic things to get the complex results is a very big challenge. It is totally different way that I used before. Not only learn the knowledge, but also how to use it in practice. Working with a group for three month just like really work with a company. Working together with different cultures was a nice experiment. From that I have learnt how to meet with people who have different think ways and explains ways with myself or I met before. I learn how to communicate with them and work with them. For CPD, my big harvest is not only for my technical knowledge, but also for the socialism knowledge. Don't afraid to show yourself, you are always good.

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