

Bachelor's Thesis

Bachelor's Degree in Chemical Engineering

**DEVELOPMENT OF A SOFTWARE FOR THE DESIGN OF
STRIPPING TOWERS TO REMOVE TRIHALOMETHANES
FROM DISINFECTED WATER**

MEMORY AND ANNEXES

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“Engineering is not merely knowing and being knowledgeable, like a walking encyclopedia; engineering is not merely analysis; engineering is not merely the possession of the capacity to get elegant solutions to non-existent engineering problems...”

Engineering is practicing the art of the organizing forces of technological change; engineers operate at the interface between science and society.”

Gordon Stanley Brown, 2007



SUMMARY

The aim of this project is to develop a software (called STRIP) able to design how an stripping tower should be to remove components dissolved in a liquid. In special, after analysing technical and environmental sustainable alternatives, the aim is focused on removing trihalomethanes (THMs) from water putting the flow in contact with air along a stripping tower. Consequently, the idea is to reduce the potential carcinogenic risk associated to the THMs formed in the water after a disinfection process.

Accordingly to input parameters such as the initial and final concentrations and the flow desired to treat, STRIP calculates the most efficient features of the system to carry on the operation ensuring its correct performance. The software code is developed by Matlab as it is programming language widely used and known by scientists and engineers.

Therefore, a wide range of different topics are integrated in this project: from the calculation of the efficient size and features of the stripping tower depending on the input data to the study of legislation and cancer risk rates in order to analyse the effects of THMs on the potential consumers: humans.

After the complex methodology carried on, STRIP provides different information as results: On one hand, the indispensable values regarding on the stripping tower: its height, diameter, the best type of fillings, an approach of the investment required... plus the potential cancer risk of the water before and after its installation. On the other hand, it shows graphical representations of the equilibrium of the stripping system and the resistance of the liquid and gas streams against the mass transfer. In addition, a text file is created in the same folder where the software is executed with more detailed values: flows velocities, individual and overall mass transfer coefficients, molar fractions on the top and the bottom of the tower, features of the filling selected...

Finally, once STRIP is validated and checked it gets the best theoretical solution, it is purposed several proper applications for the stripping towers to remove THMs. Basically, using information from 2 different Drinking Water Treatment Plants (DWTPs) located in Spain and one city of Venezuela, it is studied the possibility to install a stripping tower in a certain point between the water disinfection treatment and the final users consumption point. In order to analyse the viability, health carcinogenic indexes are related with economical costs of the installation and the population to who the quality water is supplied to estimate how much costs to save a human life in each scenario.



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1. NOMENCLATURE

1.1. Latin alphabet

$A_{interphase}$: Interphase area [m^2]

AE : Absorption efficiency in alveoli [-]

AT : Average time [day]

BW : Body weight [kg]

C_0 : Design factor in Eq. 7.10. [-]

$C_{A,bottom}$: Concentration of component A at the bottom of the column [$\mu g/L$]

$C_{A,top}$: Concentration of component A at the top of the column [$\mu g/L$]

$C_{THM,air}$: Concentration of each THM species in the air [$\mu g/L$]

$C_{THM,w}$: Concentration of each THM species in the water [$\mu g/L$]

$C_{TTHMs,bottom}$: Total concentration of THMs at the bottom of the column [$\mu g/L$]

$C_{TTHMs,top}$: Total concentration of THMs at the top of the column [$\mu g/L$]

$C_v = 1,15$: Design factor in Eq. 8.11. [-]

$Coef_{\$ to \text{€}} = 0,92$: Coefficient to transform dollars into euros [€/\\$]

$Coef_{Gal to L} = 3,79$: Coefficient to transform gallons into liters [L/Gal]

$Cost_1$: Capital cost of project 1 with capacity S_1 [€]

$Cost_2$: Capital cost of project 2 with capacity S_2 [€]

$CF1$: Conversion factor number 1 [$mg/\mu g$] or [L/cm^3]

$CF2$: Conversion factor number 2 [cm^2/m^2]

$CF3$: Conversion factor number 3 [min/h]

$D_{A,g}$: Diffusion coefficient of component A on the gas phase [m^2/s]

$D_{A,l}$: Diffusion coefficient of component A on the liquid phase [m^2/s]

$D_{THM,air}$: Diffusion coefficient of each THM species on the air [m^2/s]

$D_{THM,w}$: Diffusion coefficient of each THM species on the water [m^2/s]

$D_{TTHMs,air}$: Total diffusion coefficient of THMs on the air [m^2/s]

$D_{TTHMs,w}$: Total diffusion coefficient of THMs on the water [m^2/s]

$D_{column} = D_i + th \cdot 10^{-3}/2$: Diameter of the stripping column [m]

D_i : Interior diameter of the stripping column [m]



DC: Direct (purchased) costs [€]

E: Chemical acceleration factor (mass transfer with chemical reaction) [–]

ED: Exposure duration [year]

EF: Exposure frequency [day/year]

ET: Exposure time [min/day]

F: Fraction of skin in contact with water [–]

F_{LG}: Design parameter defined by Eq. 8.8. [–]

F_{LG, flooding}: Design parameter defined by Eq. 8.8. when flooding occurs [–]

F_{LG, operating}: Design parameter defined by Eq. 8.8. in operating conditions [–]

F_P: Packing factor [m^{-1}]

G: Gas total flow [mol/s]

*G**: Gas molar flow rate per unit cross – section area [$mol/(m^2 \cdot s)$]

G_L: Gas total flow [L/min]

G_w: Gas total flow [kg/s]

*G_w** = $\rho_G \cdot v_G$: Gas mass flow rate per unit cross – section area [$kg/(m^2 \cdot s)$]

H_{A, atm}: Henry's law coefficient [$atm \cdot m^3/mol$]

H_{A, bar}: Henry's law coefficient [$bar \cdot m^3/mol$]

H_A: Henry's law coefficient [$Pa \cdot m^3/mol$]

H'_A: Henry's law coefficient [–]

H_G: Height of an overall mass transfer unit on the gas phase [m]

H_L: Height of an overall mass transfer unit on the liquid phase [m]

H_{THM, atm}: Henry's law coefficient of each THM species [$atm \cdot m^3/mol$]

H_{TTHMs, atm}: Total henry's law coefficient of THMs [$atm \cdot m^3/mol$]

H_{TTHMs, bar}: Total henry's law coefficient of THMs [$bar \cdot m^3/mol$]

H_{column}: Height of the stripping tower [m]

H_g: Height of an individual mass transfer unit on the gas phase [m]

H_l: Height of an individual mass transfer unit on the liquid phase [m]

H_a: Hatta modulus [–]

IC: Indirect costs [€]

IR: Ingestion rate [L/day]

K₄: Design parameter defined by Eq. 8.9. [–]

- $K_{4, flooding}$: Design parameter defined by Eq. 8.9. when flooding occurs [–]
- $K_{4, operating}$: Design parameter defined by Eq. 8.9. in operating conditions [–]
- K_G : Overall mass transfer coefficient on the gas phase [$\text{mol}/(\text{m}^2 \cdot \text{s} \cdot \text{Pa})$]
- $K_G \cdot a$: Volumetric overall mass transfer coeff. on the gas phase [$\text{mol}/(\text{s} \cdot \text{m}^3 \cdot \text{Pa})$]
- K_L : Overall mass transfer coefficient on the liquid phase [m/s]
- L : Liquid total flow [mol/s]
- L^* : Liquid molar flow rate per unit cross – section area [$\text{mol}/(\text{m}^2 \cdot \text{s})$]
- L_L : Liquid total flow [L/min]
- L_w : Liquid total flow [kg/s]
- $L_w^* = \rho_L \cdot v_L$: Liquid mass flow rate per unit cross – section area [$\text{kg}/(\text{m}^2 \cdot \text{s})$]
- M_A : Molar weight of component A [g/mol]
- M_G : Gas molar weight [g/mol]
- M_L : Liquid molar weight [g/mol]
- M_{THM} : Molar weight of each THM species [g/mol]
- M_{TTHMs} : Total molar weight of THMs [g/mol]
- N_A : Moles flow of component A [mol]
- N_G : Number of overall mass transfer units on the gas phase [–]
- N_L : Number of overall mass transfer units on the liquid phase [–]
- N_g : Number of individual mass transfer units on the gas phase [–]
- N_l : Number of individual mass transfer units on the liquid phase [–]
- $N_{sc,g} = \frac{\mu_G}{\rho_G \cdot D_{A,g}}$: Adimensional Schmitt number on the gas phase [–]
- $N_{sc,l} = \frac{\mu_L}{\rho_L \cdot D_{A,l}}$: Adimensional Schmitt number on the liquid phase [–]
- PC : Permeability coefficient [cm/h]
- Q_G : Gas volumetric flow rate [m^3/s]
- Q_L : Liquid volumetric flow rate [m^3/s]
- $R = 0,08314$: Ideal gases constant [$\text{bar} \cdot \text{m}^3 / (\text{kmol} \cdot \text{K})$]
- R_T : Total resistance for the mass transfer [$\text{h} \cdot \text{Pa} \cdot \text{m}^3 / \text{mol}$]
- R_G : Resistance of the gas phase for the mass transfer [%]
- R_L : Resistance of the liquid phase for the mass transfer [%]

S : Cross – section area of the stripping column [m^2]

S_1 : Size or capacity of production/treatment of project 1 [m^3], [kg/s], [L/min] ...

S_2 : Size or capacity of production/treatment of project 2 [m^3], [kg/s], [L/min] ...

$SF_{\text{exposure way}}$: Slope factor of a specific exposure way [$kg \cdot day/mg$]

SA : Skin surface area [m^2]

$T = 293,15$: Temperature [K]

TFC : Total fixed capital costs [€]

TI : Total investment costs [€]

V_{reactor} : Volume of the reactor [m^3]

VF : Volatilization factor [-]

VR : Ventilation rate [m^3/h]

W : Total weight of the stripping tower [kg]

W_p : Weight of the stripping tower excluding internal packing [kg]

WC : Working capital costs [€]

a : Effective interfacial area of packing in contact with liquid per unit volume [m^2/m^3]

a_p : Interfacial area of packing in contact with liquid per unit volume [m^2/m^3]

c_A : Concentration of component A [mol/m^3]

$c_{A,bottom}$: Concentration of component A at the bottom of the column [mol/m^3]

$c_{A,top}$: Concentration of component A at the top of the column [mol/m^3]

$c_{THMs,bottom}$: Total concentration of THMs at the bottom of the column [mol/m^3]

$c_{THMs,top}$: Total concentration of THMs at the top of the column [mol/m^3]

c_A^{eq} : Concentration of component A in equilibrium with the gas [mol/m^3]

c_A^i : Concentration of component A on the interphase [mol/m^3]

c_T : Total concentration of the liquid [mol/m^3]

d_N : Nominal diameter of packing [m]

$g = 9,81$: Gravitational acceleration [m/s^2]

k_g : Individual mass transfer coefficient on the gas phase [m/s]

k'_g : Individual mass transfer coefficient on the gas phase [$kmol/(m^2 \cdot s \cdot bar)$]

$k'_g \cdot a$: Volumetric mass transfer coefficient on the gas phase [$kmol/(m^3 \cdot s \cdot bar)$]

k''_g : Individual mass transfer coefficient on the gas phase [$mol/(m^2 \cdot s \cdot Pa)$]

$k_g'' \cdot a$: Volumetric mass transfer coefficient on the gas phase [$\text{mol}/(\text{m}^3 \cdot \text{s} \cdot \text{Pa})$]

k_l : Individual mass transfer coefficient on the liquid phase [m/s]

$k_l \cdot a$: Volumetric mass transfer coefficient on the liquid phase [$1/\text{s}$]

p_A : Partial pressure of component A [Pa]

$p_{A,bottom}$: Concentration of component A on the gas at the bottom of the column [$\mu\text{g}/\text{L}$]

$p_{A,bottom,Pa}$: Partial pressure of component A at the bottom of the column [Pa]

$p_{A,top}$: Concentration of component A on the gas at the top of the column [$\mu\text{g}/\text{L}$]

$p_{A,top,Pa}$: Partial pressure of component A at the top of the column [Pa]

$p_{TTHMs,bottom}$: Total partial pressure of THMs at the bottom of the column [Pa]

$p_{TTHMs,top}$: Total partial pressure of THMs at the top of the column [Pa]

p_A^{eq} : Partial pressure of component A in equilibrium with the liquid [Pa]

p_A^i : Partial pressure of component A on the interphase [Pa]

$p_T = 101325$: Atmospheric pressure [Pa]

$p_{T,bar}$: Atmospheric pressure [bar]

r_A : Mass transfer velocity (without chemical reaction) [$\text{mol}/(\text{m}^3 \cdot \text{s})$]

t : Time [s]

th : Wall thickness [mm]

$v_G = \frac{Q_G}{S}$: Gas velocity [m/s]

$v_{G,flooding}$: Gas velocity when flooding occurs [m/s]

$v_{G,operating}$: Gas velocity in operating conditions [m/s]

$v_L = \frac{Q_L}{S}$: Liquid velocity [m/s]

$v_{L,flooding}$: Liquid velocity when flooding occurs [m/s]

$v_{L,operating}$: Liquid velocity in operating conditions [m/s]

x : Distance from the interphase [m]

$x_{0,G}$: Gas film width [m]

$x_{0,L}$: Liquid film width [m]

x_A : Mole fraction of component A on the liquid [–]

$x_{A,bottom}$: Mole fraction of component A on the liquid at the bottom of the column [–]

$x_{A,top}$: Mole fraction of component A on the liquid at the top of the column [–]



- x_A^i : Mole fraction of component A on the liquid interphase [–]
- $x_{TTHMs,bottom}$: Total mole fraction of THMs on the liquid at the bottom of the column [–]
- $x_{TTHMs,top}$: Total mole fraction of THMs on the liquid at the top of the column [–]
- y_A : Mole fraction of component A on the gas [–]
- $y_{A,bottom}$: Mole fraction of component A on the gas at the bottom of the column [–]
- $y_{A,top}$: Mole fraction of component A on the gas at the top of the column [–]
- $y_{TTHMs,bottom}$: Total mole fraction of THMs on the gas at the bottom of the column [–]
- $y_{TTHMs,top}$: Total mole fraction of THMs on the gas at the top of the column [–]
- y_A^{eq} : Mole fraction of component A in equilibrium with the liquid [–]
- y_A^i : Mole fraction of component A on the gas interphase [–]
- z : Vertical distance [m]

1.2. Greek alphabet

- $\Delta C_{top\ to\ bottom}$: Concentration gradient between the top and the bottom of the column [$\mu\text{g/L}$]
- ΔP : Pressure drop [$\text{mmH}_2\text{O}/(\text{column m})$]
- ε : Void fraction of packing [–]
- ε_L : Retained liquid in the reactor [m^3/m^3]
- μ_G : Dynamic viscosity of the gas [$\text{kg}/(\text{s} \cdot \text{m})$]
- μ_L : Dynamic viscosity of the liquid [$\text{kg}/(\text{s} \cdot \text{m})$]
- ρ_G : Density of the gas [kg/m^3]
- ρ_L : Density of the liquid [kg/m^3]
- $\rho_{material}$: Density of the packing material [kg/m^3]
- ρ_{shell} : Density of stripping column shell [kg/m^3]
- σ_L : Liquid surface tension [kg/s^2]
- $\sigma_{c,material}$: Critic surface tension of a material [kg/s^2]
- σ_{circ} : Circumferential stress [N/mm^2]
- σ_{long} : Longitudinal stress [N/mm^2]
- σ_w : Dead – weight stress [N/mm^2]
- ϕ : Sphericity of packing [–]

2. PRESENTATION

2.1. Origin of the project

The initial idea comes from the need to remove trihalomethanes (THMs), chemical by-products, from disinfected water due to their potential carcinogenic risk. Although there are several techniques to do this, the aim of this project is to analyse an alternative: the stripping tower.

The main target of the project is to develop a software to get the basic data design of a stripping tower depending on each system. Furthermore, important improvements will apply to the standard methodology due to its current limitations.

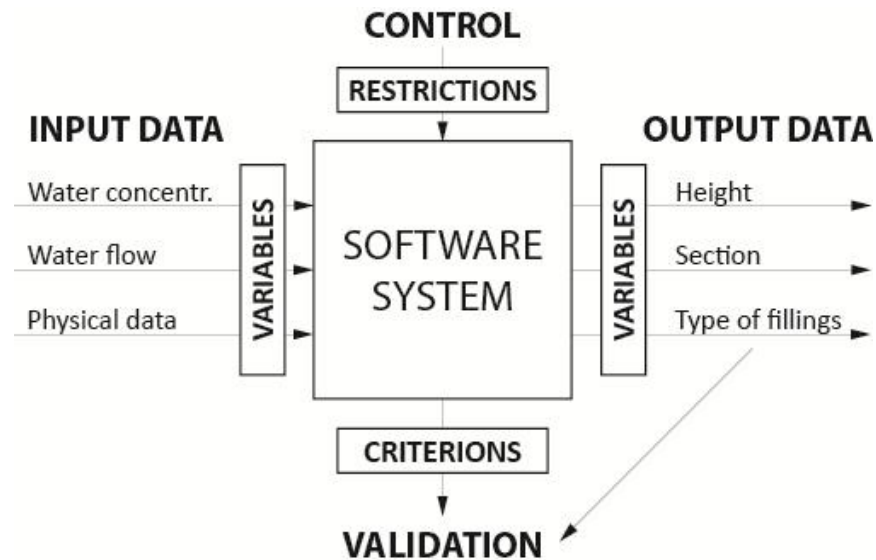


Figure 2.1. Black box scheme of the project.

2.2. Motivation

As an engineer student, the first aim is to solve a problem. In this case, it is to program a software to design installations of stripping towers to treat disinfected water in order to ensure its health quality.

There are other interests in this project like applying theoretical concepts acquired at university to a practical case, be competitive using programming skills to get better results with less time or combine and integrate different Chemical Engineering courses.

However, the 3 big axis over the project is turning around are the ones represented in Figure 2.2.:



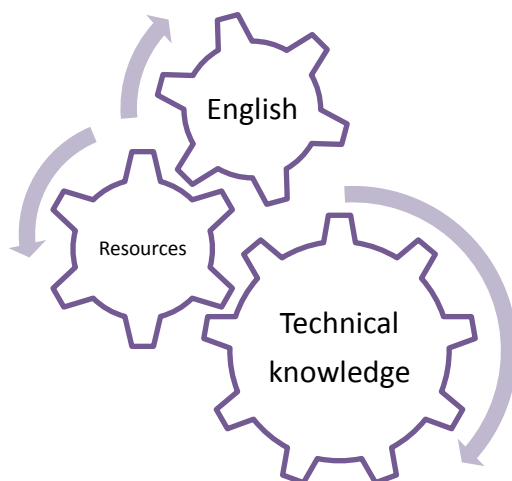


Figure 2.2. Main axis of the project.

The knowledge is situated on the base because it is the most important issue of any project. As Francis Bacon said in 1597:

“Knowledge is power”

Complementing it, other resources are indispensable: from the ability of using programs to represent a phenomenon or the bibliographic search until the experience or the psychological mentalities; all of them are essential to make thoughts be understood or stand difficult situations.

At the top there is the soul of the project. To be philosophic, everybody cannot succeed. To achieve it, something different is required, something else... Focusing on people, communication is essential and if it is wanted that a project can be potentially useful all over the world, it must be international. That is the reason why English is the language used on it: because it opens new doors and offers your vision to other perspectives.

2.3. Previous requirements

In general, to start any project, material, economical and human sources are required. On one hand, as it is a theoretical project (without laboratory or field experiences) it is mainly used books to search information and Matlab, a mathematic program, to develop the software to do all algorithm calculations. Then, besides other software are used:

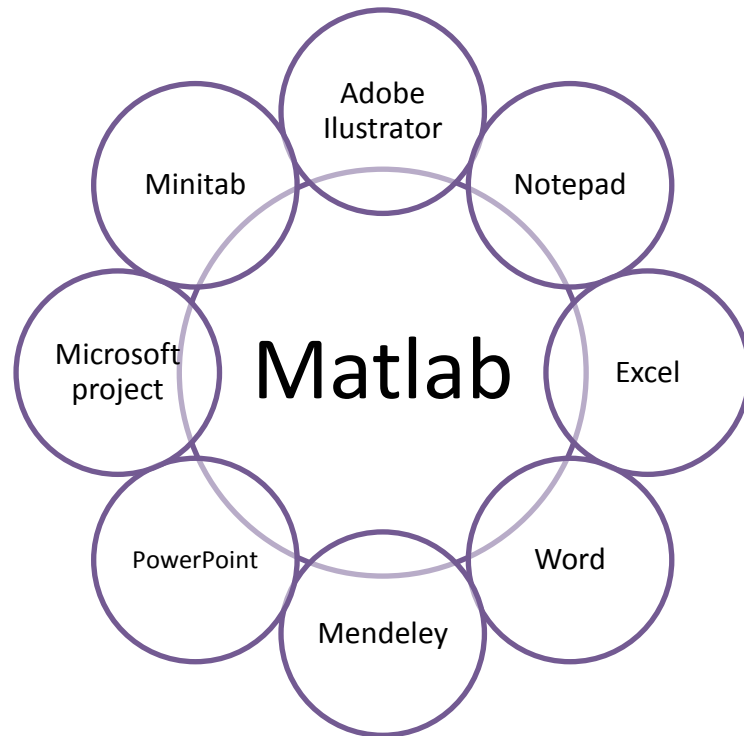


Figure 2.3. Software used along the project.

Any capital investment is demanded at the beginning of the project because all of them are free or available at Polytechnic University of Catalonia (UPC).

On the other hand, people implied to do it are the director of the project, Vicenç Martí Gregorio, and the student who carried on it, Joel Canosa Planes, the both mainly moved to acquire new knowledge and to apply concepts of the Bachelor's Degree in Chemical Engineering.

To conclude, just remark the wide range of concepts applied in this project and, consequently, the multiple disciplines involved on it:

- Industrial chemistry to contextualise the problematic of THMs.
- Unit operations to understand the design of a stripping system.
- Thermodynamics to know how streams must be considerate.
- Reactors to compare stripping towers with other technologies.
- Kinetics to demonstrate the mass transfer velocity equation.
- Programming and numeric methods to develop the software.
- Optimisation to validate the results of the software.
- Statistics to make regressions of bibliographic graphics.
- Science of materials to have an idea about the possible materials to use.

- Elasticity and resistance of materials to make approximations of the real installation.
- Economy to calculate an approach of the budget.
- Project management to organize the resources properly.
- Graphic design to illustrate the explanations.

This transversal behaviour implies a lot of effort to join these different concepts acquired along the engineer formation but, it is the reason that makes it worth it: because the complete and exhaustive analysis from different points of view.

Apart from its complexity, this project is made with the purpose to be understood for any person with a basic level of scientific knowledge. As one indirect intention is to increase its potential use as much as possible around all scientific community; the methodologies followed are detail explained since its initial theories and the procedures carried on are complemented with equations and draws. Moreover, for supplementary information, demonstrations and the software code can be found at the end of the document.

3. INTRODUCTION

This project can be assimilated to a basic engineering project of a stripping tower construction. It is situated between the preliminary study to know the installation viability and the detailed design done before its construction. In general, it pretends to identify and define the problem and develop a global solution until a subsystem level of detail.

3.1. Objectives of the project

Once the problematic is known and the final purpose understood, the final objective of the project is to help a hypothetical engineering team to decide if it is a clever option to install a stripping column to remove THMs from water in a specific situation.

As the software can also operate for a general case, a parallel objective is to determine the basic design parameters of how a stripping column should be to eliminate any specific compound from a liquid.

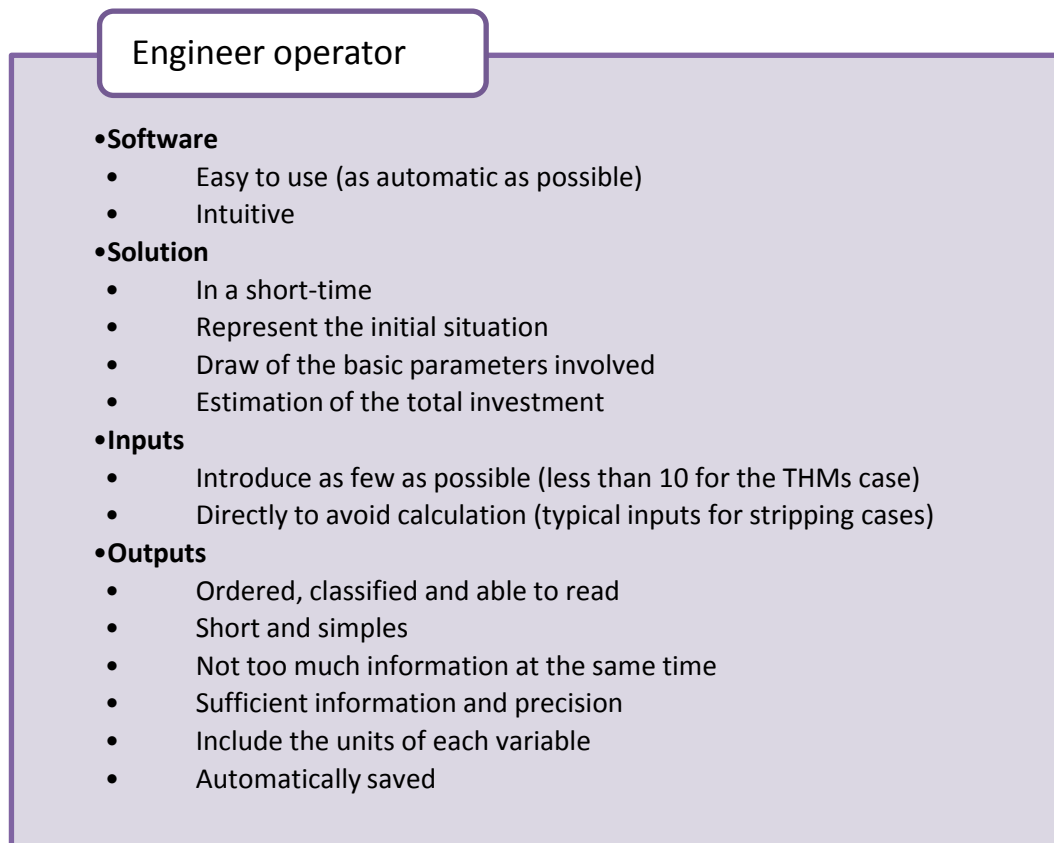


Figure 3.1. Technical specifications for the main user.

The success of any project is always directly dependent on their user satisfaction. For this kind of software, the engineer operator is who executes it and who treat its information (interpretation and evaluation). So, it is critical to contextualise the possible need of the most important user in order to achieve a good machine-person interaction (Figure 3.1.).

3.2. Project scope

Apart from the main aims of this project:

- Apply a new methodology for the design of stripping towers.
- Develop a software to get the basic parameters of a stripping tower accordingly to inputs of a specific system.

The scope of it is wider and it also involves:

- Preliminary study of THMs and its potential carcinogenic indexes.
- Comparison of similar technologies to remove unwanted components.
- Description of a general stripping system.
- Explanation of the mechanical design: basic parts of a stripping tower.
- Approach calculation of the budget for each case.
- Module validation of the software.
- Specific study of its application in real situations.

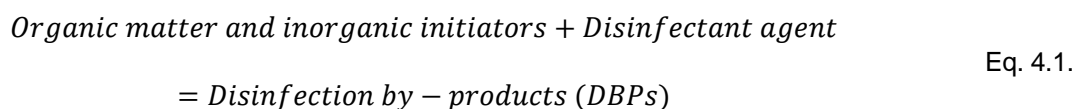
4. TRIHALOMETHANES (THMS)

4.1. Introduction

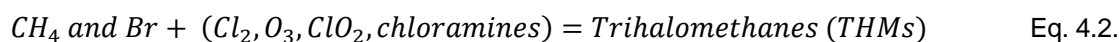
4.1.1. Origin

The origin of trihalomethanes (THMs) comes from the process of water disinfection. Once the water arrives at any Drinking Water Treatment Plant (DWTP) it has to go across different processes in order to minimise the presence of pathogenic microorganismes and be able to be used again for the human consumption without health problems.

There are different ways to get a good quality of the final water but, one indispensable step is the disinfection. In this treatment, the main drawback is the generation of harmful disinfection by-products (DBPs). The global reaction can be written as:



Although, the drinking water production involves the formation of unhealthy compounds, the risks for an inadequate disinfection are far greater than the potential risk for long-term exposure of DBPs. One common example are:



Consistent with previous studies (WHO¹ 2005), THMs are the most abundant DBPs whose presence in the drinking water involves a severe treatment due to its potential carcinogenicity. The most usual are the ones whose chemical formula is based on methane (CH₄):

- Chloroform or trichloromethane: CHCl_3
- Bromodichloromethane: CHCl_2Br
- Dibromochloromethane: CHClBr_2
- Bromoform or tribromomethane: CHBr_3

Their different proportions between concentrations are differently depending on factors such

¹ World Health Organisation (WHO) makes standard water plans as a measure of maintaining safe supply of drinking water to the public.

as: disinfectant product and concentration used, time since it is applied on the water, organic matter type and amount, water pH, temperature and presence of bromide and ammonia in the raw water. Normally, chloroform is the first THM formed, probably because its formation is faster or because it requires a lower disinfectant dose or organic matter.

Accordingly on Eq. 4.1., higher DBPs concentration is expected for the source water with higher natural organic matter (level of pathogens) or higher inorganic precursors (like bromide). For this reason, it is interesting to minimize them before chlorination.

4.2. Legislation

In the European Union (EU) the Drinking Water Directive 98/83/EC concerns the quality of water for human consumption. Accordingly to this legislation, apart from monitoring and testing parameters regularly, since 01/01/2009, the maximum concentration of THMs in drinking water is $100 \mu\text{g}/\text{L}$ in EU. In Spain, this directive is legislated by RD 140/2003.

In the United States (US) the Environmental Protection Agency (EPA) is the organization who regulates the acceptable levels for the most prevalent DBPs in chlorination process. About THMs, its maximum total concentration is $80 \mu\text{g}/\text{L}$ for drinking water.

These critic values are the current for the countries legislation nevertheless, they should be reviewed due to [1]:

- The risk for chemicals is just accounted for the oral ingestion while their exposure can also be from other pathways: dermal contact or inhalation.
- Quality standards regulate THMs in drinking water with the total concentration as the base and this is unsuitable because each one give different long-term carcinogenicities. They should not be treated equal and take into account the different risk resulting from each THM species. For example, if there is higher bromide in raw water, bromated-THMs will play a major role as by-products. Consequently, the lifetime cancer risk may even be reduced as they are less dangerous than chlorine but, ironically, total THMs concentration will increase because bromide has higher atomic weight. So, in contrast with the current legislation, higher THMs concentration does not necessarily introduce higher cancer risk.

4.3. Potentially carcinogenic risk

Assessing health consequence of chemicals in drinking water is a challenge: exposures are

long, via multiple routes and normally at low concentrations, measurements are typically insufficient and the magnitude of relative risks tends to be small.

RAIS² and WHO are the guidelines databases used to assess quantitatively the toxicity of THMs that can be found in the water. Despite there are several methods to apply, this project is focused on the individual carcinogenic effects which are only considered in RAIS [2].

The amount of data required is the biggest limitation of this methodology: monthly averages are needed, they are influenced by the time when they are taken and the number of analysis, analytical techniques have their own constrains as their sensible limit... Nevertheless, it is able to determine the evolution of chemical hazards of water when a change in the treatment line is introduced and estimate its potential health benefits [3].

In contrast with other studies, the aim of this project is not to evaluate from where the highest risk comes from (for example, the exposure to chloroform through oral ingestion) because more specific data must be needed for a complete study. The idea is to explain a pattern that can be followed to make a preliminary exposure assessment and calculate the potential risk for the following scenario; The receptor is an adult who:

- Ingest water which has THMs.
- Is in physical contact with the same type of water (dermal absorption).
- Inhales the same water once it is evaporated.

However, for these 2 pathways, the major exposure route is assumed during shower. So, the process to calculate the chronic daily intake is divided into the 3 main pathways and the data required is summarized on Table 4.1., Table 4.2., Table 4.3. and Table 4.4.. Its corresponding values are the ones used on the posterior cases of study:

4.3.1. Exposure assessment

- Oral ingestion:

INPUT PARAMETER – 3 pathways	VALUE
$C_{THM,w}$: Concentration of each THM species in the water [$\mu\text{g/L}$]	It depends on each case
IR: Ingestion rate [L/day]	2
EF: Exposure frequency [day/year]	365

² Risk Assessment Information System (RAIS).

ED: Exposure duration [year]	29
CF1: Conversion factor number 1 [mg/μg] or [L/cm ³]	10 ⁻³
BW: Body weight (for males) [kg]	64,8
AT: Average time [day]	70 · 365

Table 4.1. Input parameters to determine the exposure of THMs via the 3 pathways.

$$\text{Oral ingestion} \left[\frac{\text{mg}}{\text{kg} \cdot \text{day}} \right] = \frac{C_{THM,w} \cdot IR \cdot EF \cdot ED \cdot CF1}{BW \cdot AT} \quad \text{Eq. 4.3.}$$

- Dermal ingestion:

INPUT PARAMETER – Dermal absorption	VALUE			
SA: Skin surface area [m ²]	(4 · BW + 7)/(BW + 90)			
F: Fraction of skin in contact with water [–]	0,8			
ET: Exposure time [min/day]	18,9			
CF2: Conversion factor number 2 [cm ² /m ²]	10 ⁴			
CF3: Conversion factor number 4 [min/h]	60			
SPECIFIC INPUT PARAMETER	CHCl ₃	CHCl ₂ Br	CHClBr ₂	CHBr ₃
PC: Permeability coefficient (· 10 ³) [cm/h]	8,9	5,8	3,9	2,6

Table 4.2. Input parameters to determine the exposure of THMs via dermal ingestion.

$$\text{Dermal absorption} \left[\frac{\text{mg}}{\text{kg} \cdot \text{day}} \right] = \frac{C_{THM,w} \cdot SA \cdot F \cdot PC \cdot ET \cdot EF \cdot ED \cdot CF1^2 \cdot CF2}{BW \cdot AT \cdot CF3} \quad \text{Eq. 4.4.}$$

- Inhalation:

INPUT PARAMETER – Inhalation in shower	VALUE
C _{THM,air} : Concentration of each THM in the air [μg/L]	Eq. 4.6.
VR: Ventilation rate for males [m ³ /h]	0,84
AE: Absorption efficiency in alveoli [–]	0,5

Table 4.3. Input parameters to determine the exposure of THMs via inhalation.

$$\text{Inhalation intake} \left[\frac{\text{mg}}{\text{kg} \cdot \text{day}} \right] = \frac{C_{THM,air} \cdot VR \cdot AE \cdot ET \cdot EF \cdot ED}{BW \cdot AT \cdot CF3} \quad \text{Eq. 4.5.}$$

Normally, as THMs air content in the shower room ($C_{THM,air}$) depends on the time (t [min]) since the shower has opened, a procedure is followed to predict how a drop of water behaves using the water flow rate, the bathroom volume and other parameters ([1] or [4]). However, in this project, it is used the experimental indoor volatilization factors (VFs) of [5]. Their values come from a drop sphere model in a personal/domestic hygiene scenario (shower and hand cleaning) with chloroform as the most representative THM: $VF = (3,5 - 18) L/m^3$. So, taking the higher value as it is the most critical one, it is possible to get the air concentration using volatilization factor definition:

$$C_{THM,air} = VF \cdot C_{THM,w} \quad \text{Eq. 4.6.}$$

4.3.2. Toxicity

After to estimate the exposure of each substance, its health damage on the human organism (toxicity) is measured using the slope factors:

INPUT PARAMETER – Slope factors	$CHCl_3$	$CHCl_2Br$	$CHClBr_2$	$CHBr_3$
SF _{oral} [kg · day/mg]	$6,10 \cdot 10^{-3}$	$6,20 \cdot 10^{-2}$	$8,40 \cdot 10^{-2}$	$7,90 \cdot 10^{-2}$
SF _{dermal} [kg · day/mg]	$3,05 \cdot 10^{-2}$	$6,33 \cdot 10^{-2}$	$1,40 \cdot 10^{-1}$	$1,32 \cdot 10^{-2}$
SF _{inhalation} [kg · day/mg]	$8,05 \cdot 10^{-2}$	$6,20 \cdot 10^{-2}$	$8,40 \cdot 10^{-2}$	$3,85 \cdot 10^{-3}$

Table 4.4. Slope factors (toxicity values) for each THM to determine the potential carcinogenic risk.

For example, a guideline value of 10^{-5} means one additional cancer per 100.000 of the population ingesting drinking water containing the corresponding substance.

4.3.3. Risk evaluation

Finally, the total cancer risk is calculated by multiplying the estimated dose by the appropriate measure of carcinogenic potency. In other words, combining the exposure models with the slope factors (toxicity values) of each THM for the three exposure routes:

$$\text{Potential cancer risk} = \sum_{THM \text{ species}} \text{Daily THM intake} \cdot \text{THM slope factor} \quad \text{Eq. 4.7.}$$

Then, following the principal of additively, the global carcinogenic risk index for all

compounds is calculated like:

$$Total\ cancer\ risk = Risk_{oral\ ing.} + Risk_{inhalation} + Risk_{dermal\ abs.} \quad Eq. 4.8.$$

Normally, inhalation is the major exposure pathway, usually for chloroform because its easier volatilization and inhalation slope factor ($SF_{inhalation}$). In contrast, dermal absorption is not usually significant; 1 or 2 orders of magnitude lower.

This methodology is applied to determine the evolution of long-term cancer risk to get the right health quality water.

5. MEMORY SCHEME

Once the project has been introduced and it is contextualized the real problematic for the population (Sections 2 to 4), the solution is developed (Sections 6 to 11): At the beginning, different alternatives are analyzed and the best technical one chosen. In addition, the problematic is deeply investigated and quantified. Then, the procedure to solve it is studied since the microscopic point of view until the reality scales. Furthermore, the indispensable software is programmed (from a new methodology developed) and validated.

Next, real cases are used to apply the program and take advantages of its potential power to solve current situations related with the initial problematic (Section 12). Afterwards, additional considerations are shortly commented (Sections 13 and 14) and, finally, the memory ends with the conclusions (Section 15) of all the work done.

The interesting point this structure is that the reader can easily jump from Section 4 until Section 12 without knowing how the problem has been solved to directly be focused on the final results.

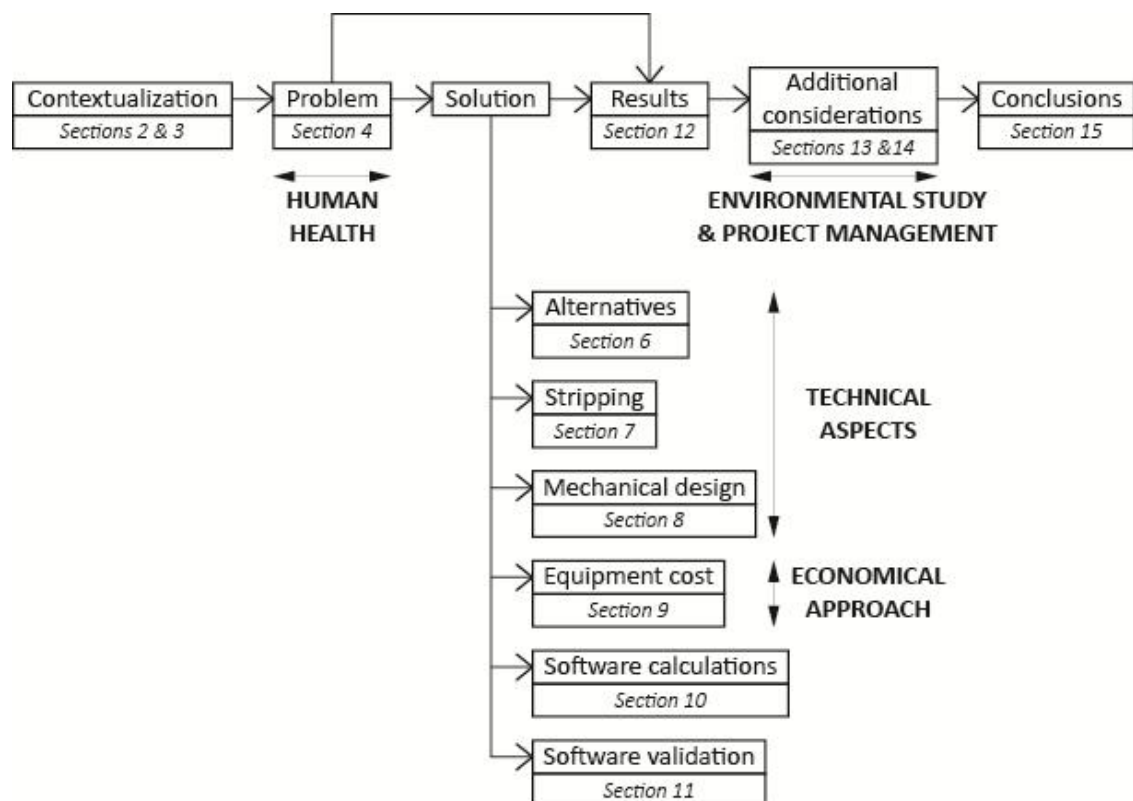


Figure 5.1. General structure of the memory.

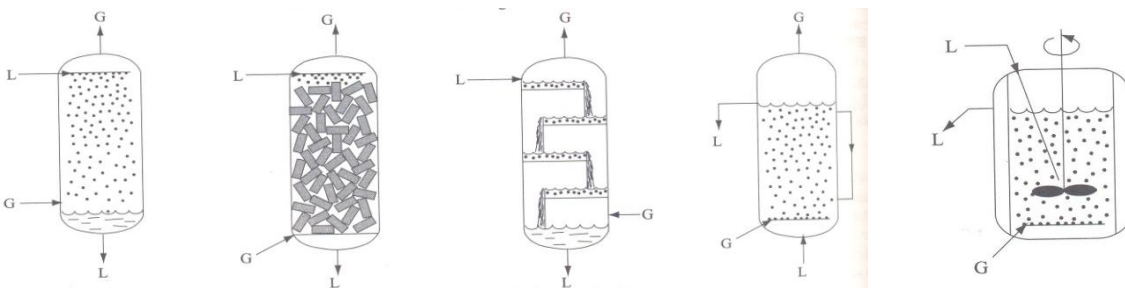
6. ALTERNATIVES

6.1. Introduction

A common procedure to remove components from a fluid is to provoke their movement to another fluid without these components. This theoretical idea is translated into engineering equipment with the gas-liquid reactors.

A huge number of industrial processes are based on gas-liquid interactions. Apart from the ones to eliminate an unwanted component (absorption and stripping cases), there are a lot of other operations between these two phases. For example, to achieve a certain product: organic compounds can be hydrogenated, chlorinated, halogenated, nitrated, oxidised by oxygen or air... some alcohols are typically sulphated by SO_3 , olefins are used to be polymerized in organic solutions...

This process implies detailed analyses of the simultaneous phenomenon that occur at the same time: diffusion and, possibly, chemical reactions. In addition, hydrodynamic conditions, that are difficult to define, influence a lot the reactor behavior. Apart from this complex characterization, accordingly to [6] and [7] the main features of different gas-liquid alternatives are:



Raining tower

Filling tower

Tower of plates

Bubble tower

Stirred tank

Figure 6.1. Types of gas-liquid equipment (Images based on [7]).

6.2. Raining tower

This equipment is practically empty and it is used when the gas flow has solids particles on it. On the top, the liquid is dispersed with little holes while the gas goes through the opposite direction. Normally, the amount of liquid retained is few and the gas phase is continuous.

Near the distributors it is created some big liquid interfacial areas but, when the drops

coalesce when going down, the area decreases quickly. For this reason, this equipment is just useful for cases where absorption (or stripping) occurs quickly.

6.3. Filling tower

In this case, the liquid and the gas circulate parallel or countercurrent through the empty spaces of the filling material. The liquid is distributed over the filling like a film while the gas forms a continuous phase. In general, the amount of liquid retained and the pressure drop are few. Consequently, filling towers are not suitable to treat big flows of gas commonly used to treat corrosive flows due to their easy construction and the possibility of material election.

6.4. Tower of plates

In contrast with the other equipments, the liquid and the gas are not interacting while they are flowing along the tower; they are only in contact in each plate and, it is during this time when the gas is dispersed in the liquid phase. There are different types of plates: perforated, with a bell of bubbles or with valves.

It can generally be said that the pressure drop in each plate is small and that the amount of liquid retained is bigger than in a filling tower. Mainly, they are suitable when an operation divided by stages is necessary, when there are big flows of liquid to be treated or if it is the case of slow reactions that need a big contact time.

6.5. Bubble tower

The main feature is the perforated ring on the base of the column to allow the entrance and dispersion of the gas flow while the column is full of liquid. The bubbles of gas go up through the liquid agitating and mixing themselves.

One of its disadvantages is the bubbles coalescence what causes the formation of big gas cavities and consequently, the gas-liquid contact efficiency decreases. Nevertheless, this problem can be solved putting fillings inside the column and operating in an inundation way knowing that the maximum gas surface velocity is not as big as in the normal column. In general, they are used for relatively slow reactions with the essential component in the liquid phase.

6.6. Stirred tank

On this vessel, the agitation is done mechanically and it is suitable for good gas dispersion in the liquid: perforate discs create small bubbles which increase the interphase areas between



the gas and liquid phases. However, it has some disadvantages when it works with corrosive substances or at high pressure or temperature. In general, they are suitable when big chemical heat is involved and, particularly, to carry on slow reactions which requires big liquid proportions.

6.7. Choice of the reactor

In a complete design of a gas-liquid reactor, a chemical exhaustive study should also be developed to check the possibility to use any kind of reaction in the system to promote the mass transfer. However, as THMs are not easy to react, expensive products like O_3 to oxidize them should be used. As this kind of reactions to make the process more efficient are not economically viable it is not considerate this possibility and air is selected as the other flow to transfer the undesired THMs on the water.

For a general case, some other criteria can be followed [7]:

- The driving force for the mass transfer is higher for towers than vessels.
- For droplets of liquid on the gas, gas mass transfer resistance is lower than liquid.
- For bubbles of gas on the liquid, gas mass transfer resistance is higher than liquid.
- If the liquid film is the controllable, avoid raining equipment.
- If the gas film is the controllable, avoid the bubble equipment.
- For insoluble gases avoid raining equipment.
- For soluble gases avoid bubble equipment.
- As chemical reactions decrease the resistance of the liquid film, it is useful for gases with few solubility.

On the other hand, although it is difficult to be exact and precise when parameters about reactors are calculated because they depend on each case, accordingly to [6], Table 6.1. and Table 6.2. contain some standard values that can be used to characterize different reactors:

TYPE OF REACTOR	$\frac{\text{Interface area}}{\text{Liquid volume}}$	a	ε_L	$\frac{\text{Liquid volume}}{\text{Film volume}}$
Raining tower	1.200	10-100; 60	0,05	2-10
Filling tower	1.200	10-350; 100	0,08	10-100
Tower of plates	1.000	100-200; 150	0,15	40-100

Bubble tower	200	50-600; 200	0,90	150-800
Stirred tank	20	100-2.000; 200	0,98	4.000-10.000

Table 6.1. Standard values of liquid-gas equipment (I).

TYPE OF REACTOR	$k'_g \cdot 10^{-1}$	$k'_g \cdot a \cdot 10^2$	$k_l \cdot 10^4$	$k_l \cdot a \cdot 10^2$
Raining tower	0,5-2	0,05-2	0,7-1,5	0,07-1,5
Filling tower	0,03-2	0,003-51	0,4-2	0,04-102
Tower of plates	0,5-6	0,5-12	1-20	1-40
Bubble tower	0,5-2	0,25-12	1-4	0,5-24
Stirred tank	-	-	0,3-4	0,3-80

Table 6.2. Standard values of liquid-gas equipment (II).

Analyzing them, filling towers looks the best option because, in spite of their volumetric mass transfer coefficients ($'k'_g \cdot a'$ and $'k_l \cdot a'$) are more variability, their positive extreme present a higher value. For this reason, as these parameters are finally used to dimension the filling tower, if it is well designed, this fact can compensate to do not have any chemical reaction involved and the normally small THMs concentration gradient between water and air.

6.7.1. Operation mode

Due to the nature of the flows involved, the most coherent option is to use a vertical, countercurrent filling towers to optimize the mechanical design: once a pump impulse the water until the top of the filling tower, it can easily go down because its density while a compressor gives to the air the enough pressure to go across the equipment from the bottom until the top.

7. STRIPPING

7.1. Definition

Stripping (or *desorption*) is a unit operation in which volatile components of a liquid mixture are transferred into a gas. The inverse operation is called *absorption* and it consists on dissolve soluble components of a gas mixture in a liquid.

To achieve the aim of both operations is necessary to use special equipment for bringing liquid and gas phases into intimate contact to transfer the components: gas-liquid reactors. They are usually carried out in vertical, cylindrical columns or towers in which devices such as plates or packing elements are placed inside to increase the contact between the fluids and improve the mass transfer that it takes place.

7.2. Stripping mechanism

7.2.1. Driving force

Besides there are several studies related on this concept, as this project is based on Chemical Engineering and its aim is to understand its procedure and apply it to develop a software, it is used the reference [8] to get the main idea of it:

- From the liquid phase point of view, the driving force is the difference between the concentration of the component A in the liquid and a theoretical concentration of the component A in the liquid if it was in equilibrium with the gas.
- From the gas phase point of view, the driving force is the difference between the partial pressure of the component A on the gas and a theoretical partial pressure of the component A on the gas if it was in equilibrium with the liquid.

It is essential to understand that this theoretical amount of component A of flow 1 in equilibrium with flow 2 is the *equivalent* amount of component A of flow 2 but in the same units as flow 1. This nomenclature is employed to be able to calculate the gradient amount of component A between flows. In the stripping case, always happens:

$$(c_A^{eq} - c_A) < 0 \quad \text{Eq. 7.1.}$$

$$(p_A^{eq} - p_A) > 0 \quad \text{Eq. 7.2.}$$

In general, it is defined as the different amount of component A on both phases that involves a movement of this component from the richest phase to the poorest phase.

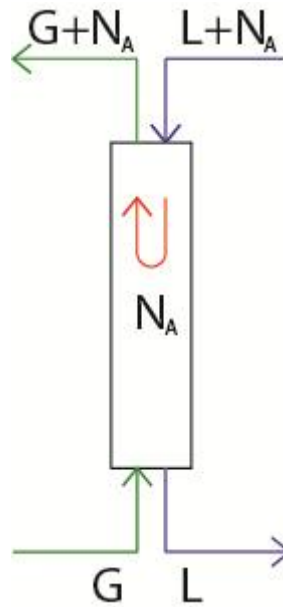


Figure 7.1. Driving force representation.

7.2.2. Double film theory

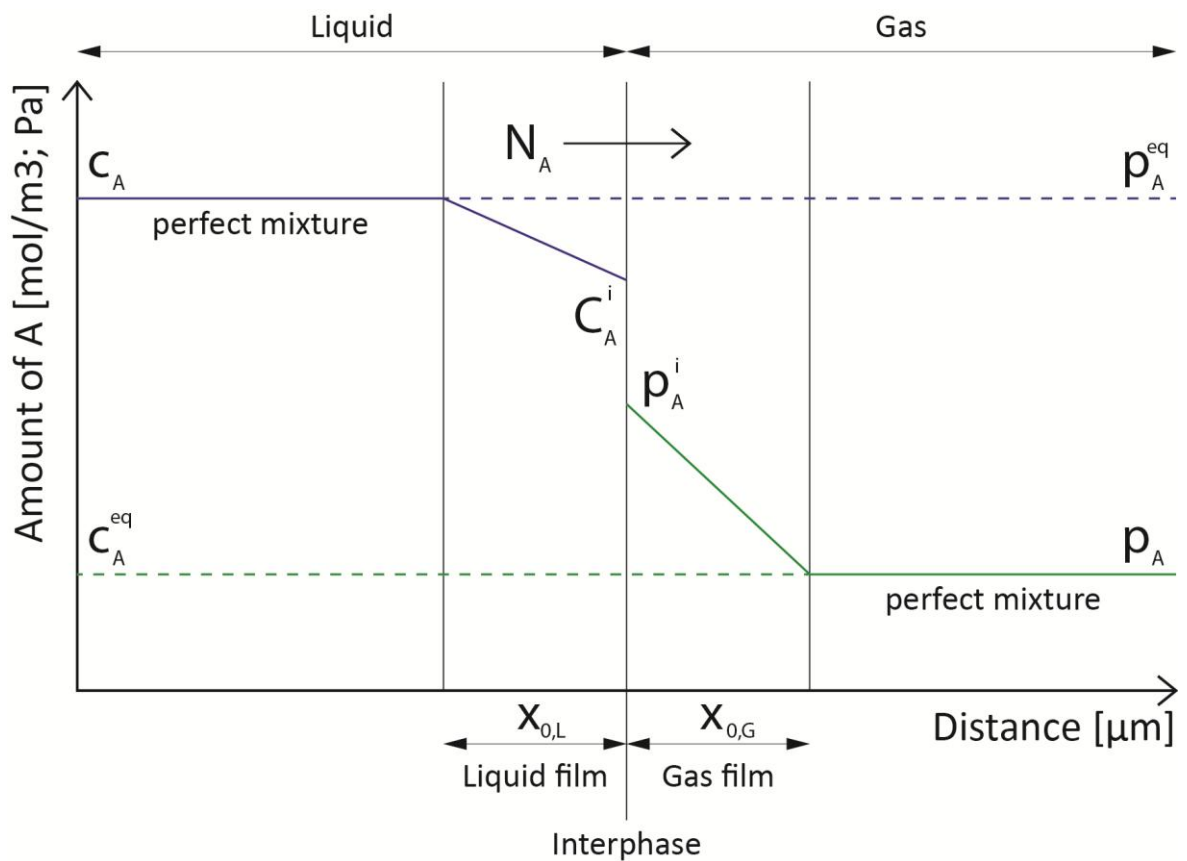


Figure 7.2. Double film theory scheme.

This physical phenomenon tries to describe the procedure that takes place when the driving force occurs. In the stripping case, at the beginning, the concentration of A on the liquid phase is greater than the partial pressure of A on the gas phase.

Far from the interphase ($x > x_0$) the mixture of the component A on each phase is perfect. However, once the component is closer to the other phase ($x < x_0$), the richest phase starts to interact with the poorest phase to search the equilibrium following the 2nd Thermodynamic Law or, equivalently, the minimum energy principal. For this reason, the amount of component A starts to move from one phase to the other until the equilibrium; the exact point where both mixtures are in perfect equilibrium (on the interphase) Henry's law is accomplished:

$$p_A^i = H_A \cdot c_A^i \quad \text{Eq. 7.3.}$$

Obviously, an ideal stripping system which wants to achieve the perfect equilibrium would need an infinitive tower to have an absolute contact of both phases. As it is not physically possible, the intention of this project is to achieve a great mass transfer of A until a close point from the equilibrium (indirectly imposed by the software input data).

7.2.3. Individual mass transfer coefficients (k_l and k_g)

It is possible to extract analytical equations from the double film theory: First of all, it is necessary to consider that there is a moles flow of component A (N_A) which goes from the liquid phase to the gas phase just because the different amount of A between them. Assuming that there is not longitudinal mixture and knowing the definition of diffusion³, both concepts can be easily associated and Fick's law of diffusion is able to be applied to develop the formula of the process which takes place on the double film region. Focusing the example of the liquid phase:

$$\frac{1}{A_{interphase}} \cdot \left(\frac{dN_A}{dt} \right) = D_{A,l} \cdot \frac{dc_A}{dx} \quad \text{Eq. 7.4.}$$

Then, accordingly to the nomenclature used on the Figure 7.2.:

³ Time-dependent physical process, that consists on an axial movement of molecules from a region of high concentration to a region of low concentration (mass redistribution).

$$\frac{1}{A_{interphase}} \cdot \left(\frac{dN_A}{dt} \right) \cdot \int_0^{x_{0,L}} dx = D_{A,l} \cdot \int_{c_A}^{c_A^i} dc_A \quad \text{Eq. 7.5.}$$

After, solving the equation:

$$\frac{1}{A_{interphase}} \cdot \left(\frac{dN_A}{dt} \right) \cdot (x_{0,L} - 0) = D_{A,l} \cdot (c_A^i - c_A) \quad \text{Eq. 7.6.}$$

Finally, reorganizing all the terms:

$$\frac{1}{A_{interphase}} \cdot \left(\frac{dN_A}{dt} \right) = \frac{D_{A,l}}{x_{0,L}} \cdot (c_A^i - c_A) \quad \text{Eq. 7.7.}$$

Commonly, as $\frac{D_{A,l}}{x_{0,L}}$ just depends on parameters related on the features of each process, it is called *individual mass transfer coefficient on the liquid phase* and is designed like k_l .

Carrying on the same procedure as before but on the gas phase result is the *individual mass transfer coefficient on the gas phase* (k_g):

$$\frac{1}{A_{interphase}} \cdot \left(\frac{dN_A}{dt} \right) = k_l \cdot (c_A^i - c_A) = k_g \cdot \left(\frac{p_A}{H_A} - \frac{p_A^i}{H_A} \right) \quad \text{Eq. 7.8.}$$

This general equation let indirectly know very useful information about how the stripping process behave:

- If the gas phase is very soluble for the component A (low H_A), the parameter k_l increases and the gas film is which controls the stripping system.
- If the gas phase is not very soluble for the component A (high H_A), the parameter k_g is considerably higher and the liquid film is which controls the stripping system.

7.2.4. Correlations of individual mass transfer coefficients (k_l and k'_g)

It is indispensable to estimate the *liquid* and *gas individual mass transfer coefficients* to be able to design the stripping column. It should be highlighted that there are several studies which allow approach them:

Accordingly to Wagner [9] there is a way based on the penetration model which can calculate k_l and k_g , but as it is developed across correlations over correlations and it is necessary to know very specific data about the system, it is not applied in the software.

Then, as it is ascribed by Piché in [10] and [11], there is another method based on the neuronal network which can completely characterise the operation inside the filling random

columns. Nevertheless, this procedure carries on a lot of iterative operations and, consequently, implies the use of powerful computers to execute it.

Finally, managing the compromise between the accuracy of results and the simplicity of the method, several books like [12] and [13] advice to use Onda correlations [14]:

$$k_l \cdot \left(\frac{\rho_L}{\mu_L \cdot g} \right)^{1/3} = 0,0051 \cdot \left(\frac{L_w^*}{a \cdot \mu_L} \right)^{2/3} \cdot N_{sc,l}^{-1/2} \cdot (a_p \cdot d_N)^{0,4} \quad \text{Eq. 7.9.}$$

$$k'_g \cdot \left(\frac{R \cdot T}{a_p \cdot D_{A,g}} \right) = C_0 \cdot \left(\frac{G_w^*}{a_p \cdot \mu_G} \right)^{0,7} \cdot N_{sc,g}^{1/3} \cdot (a_p \cdot d_N)^{-2} \quad \text{Eq. 7.10.}$$

$$C_0 = \{2 \text{ if } d_N \leq 15 \text{ mm or } 5,23 \text{ if } d_N > 15 \text{ mm}\}$$

$$\frac{a}{a_p} = 1 - \exp \left[-1,45 \cdot \left(\frac{\sigma_{c,material}}{\sigma_L} \right)^{3/4} \cdot \left(\frac{L_w^*}{a_p \cdot \mu_L} \right)^{0,1} \cdot \left(\frac{a_p \cdot L_w^{*2}}{\rho_L^2 \cdot g} \right)^{-0,05} \cdot \left(\frac{L_w^{*2}}{\rho_L \cdot a_p \cdot \sigma_L} \right)^{0,2} \right] \quad \text{Eq. 7.11.}$$

An important parameter is the relation between $\sigma_{c,material}$ and σ_L because it is proportionally with the resistance of the solid to be wet for the liquid.

7.2.5. Overall mass transfer coefficients (K_G and K_L)

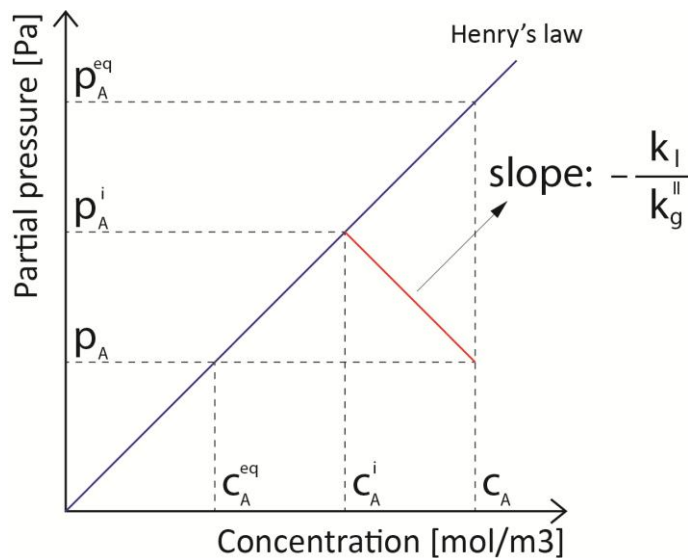


Figure 7.3. Graphical relationships of the double film theory parameters.

Representing the double film theory parameters in a concentration versus partial pressure diagram is useful to visualize the relation between the amount of component A and its

equilibrium. Moreover, representing Eq. 7.8. the interphase amount of component A of a certain point can also be related. As it can be seen, they are determined from c_A , p_A , the equilibrium curve and the relation k_l and k_g'' .

Additionally, the *equivalent concentration* (c_A^{eq}) and the *equivalent partial pressure* (p_A^{eq}) of the same point of the system are also represented. In this case, they are indirectly defined by c_A and p_A using the equilibrium curve. In terms of equations, it can be written as:

$$c_A^{eq} = p_A / H_A \quad \text{Eq. 7.12.}$$

$$p_A^{eq} = H_A \cdot c_A \quad \text{Eq. 7.13.}$$

To complement this information, carrying on the same procedure as on Section 7.2.3. but for the *equivalent* amount of component A, it is typical to use 2 other general equations regarding on the global mass transfer:

$$\frac{1}{A_{interphase}} \cdot \left(\frac{dN_A}{dt} \right) = K_L \cdot (c_A^{eq} - c_A) = K_G \cdot (p_A - p_A^{eq}) \quad \text{Eq. 7.14.}$$

Where K_G is the *overall mass transfer coefficient on the gas phase* and K_L is the *overall mass transfer coefficient on the liquid phase*.

Additionally, in spite of demonstration is done in Annexes (Section 18.1.), there is a double-relation between mass transfer coefficients:

$$\frac{1}{k_g''} + \frac{H_A}{k_l} = \frac{1}{K_G} = \frac{H_A}{K_L} \quad \text{Eq. 7.15.}$$

7.3. Design procedure of a stripping system

7.3.1. Mass transfer velocity equation (without reaction)

In general, the formula of the global velocity should consider the resistance of the mass transfer and of the reaction. Due to relative magnitude between these two resistances can widely vary; there are 8 special cases to consider between the extreme situations: when the reaction is infinite quickly (the mass transfer controls the velocity) and when the reaction is very slow (the chemical reaction has more influence on the mass transfer velocity). There are dimensionless numbers like chemical acceleration factor (E) or Hatta modulus (Ha) which are used to characterise each system. However, as the main aim of this project is to study the system water (with THMs) versus air, the development will be focused on the case of



mass transfer without reaction.

$$N_{A,(gas)} \xrightarrow{\text{Mass transfer}} N_{A,(liquid)}$$

The *double film theory* is the base to calculate the global mass transfer velocity; applying the definition of reaction velocity and complementing it with Eq. 7.8., it is possible to get the following expression:

$$r_A = \frac{1}{V_{reactor}} \cdot \frac{dN_A}{dt} = \frac{A_{interphase}}{V_{reactor}} \cdot k_l \cdot (c_A^i - c_A) = a \cdot k_l \cdot (c_A^i - c_A) \quad \text{Eq. 7.16.}$$

Or, equivalently:

$$r_A = a \cdot k_g \cdot \left(\frac{p_A}{H_A} - \frac{p_A^i}{H_A} \right) = a \cdot k_g'' \cdot (p_A - p_A^i) \quad \text{Eq. 7.17.}$$

Finally, combining Eq. 7.3., Eq. 7.21., Eq. 7.16. and Eq. 7.17., the interphase unknown parameters can be eliminated from the velocity expressions and, the global mass transfer velocity equation without chemical reaction at any point of the stripper is (check demonstration on Annexes; Section 18.2.):

$$r_A = \frac{1}{\left(\frac{1}{k_g''} + \frac{H_A}{k_l} \right)} \cdot a \cdot (p_A - H_A \cdot c_A) \quad \text{Eq. 7.18.}$$

The first term is assimilated with an expression of two resistances in series for the mass transfer. Obviously, as bigger this term is, more mass transfer will be across the fluids. Moreover, being more precise, it is possible to remark the importance of Henry constant value as a distribution coefficient between phases:

- The resistance of the gas film is the controllable for very soluble gases (small H_A).
- The resistance of the liquid film is the controllable for not very soluble gases (high H_A).

Linking this result with what is explained in Section 7.2.5., Eq. 7.18. can be rewritten as:

$$r_A = K_G \cdot a \cdot (p_A - p_A^{eq}) \quad \text{Eq. 7.19.}$$

7.3.2. Optimum solvent circulation rate

This information is essential in terms to determine the gas rate necessary to achieve the solute recovery demanded. Accordingly to [12] and [13], in order to ensure a correct

operation of the stripping column, the follow equation should be accomplished:

$$G = 0,75 \cdot L/H'_A \quad \text{Eq. 7.20.}$$

In this case, it is necessary to be aware that Henry's constant changes its dimensions due to the molar units of flows. Rewriting Eq. 7.3.:

$$y_A^i = H'_A \cdot x_A^i \quad \text{Eq. 7.21.}$$

So, the relation between both Henry's constant is:

$$H'_A = H_A \cdot (c_T/p_T) \quad \text{Eq. 7.22.}$$

Taking the standard value of p_T as the atmospheric pressure (101325 Pa) and c_T as:

$$c_T = (\rho_L/M_L) \cdot 10^3 \quad \text{Eq. 7.23.}$$

The final gas flow rate can be determined.

7.3.3. Column balance

First of all, due to flows are expressed in molar units, molar fractions are determined:

$$x_A = \frac{c_A}{c_T} \quad \text{Eq. 7.24.}$$

$$y_A = \frac{p_A}{p_T} \quad \text{Eq. 7.25.}$$

Since the beginning, all the data related to the liquid is known (flow, initial and final concentrations) and the gas flow rate recommended to use it is also limited by Eq. 7.20. Moreover, for the specific system of water with THMs, the normal air which initially circulates counter currently has approximately 0 Pa of THMs in its composition.

KNOWN TERMS	Comments
$x_{A,top}$	Initial concentration of the unwanted component in the liquid.
$x_{A,bottom}$	Final concentration desired of the unwanted component in the liquid. For THMs, it is legislated $< 100 \mu g/L$ in the European Union.
$y_{A,bottom}$	Initial partial pressure of the unwanted component in the gas. For THMs in the air, it is $\simeq 0$.
L	Amount of liquid desired to be treated.



G	Recommended gas flow used; Eq. 7.20..
-----	---------------------------------------

Table 7.1. Known terms of the stripping system.

In order to calculate the final amount of the unwanted component in the gas, it is done a global mass balance along the stripping column.

For THMs case, it can be thought that it does not make sense to remove unhealthy compounds from the water to the air because their presence is still in contact with people but in another fluid. However, the advantage to remove them by a stripping operation is that their total presence is the same while on the outlet gas, due to the bigger amount of it, THMs are more dilute and, consequently, their health potential risk is lower than initially.

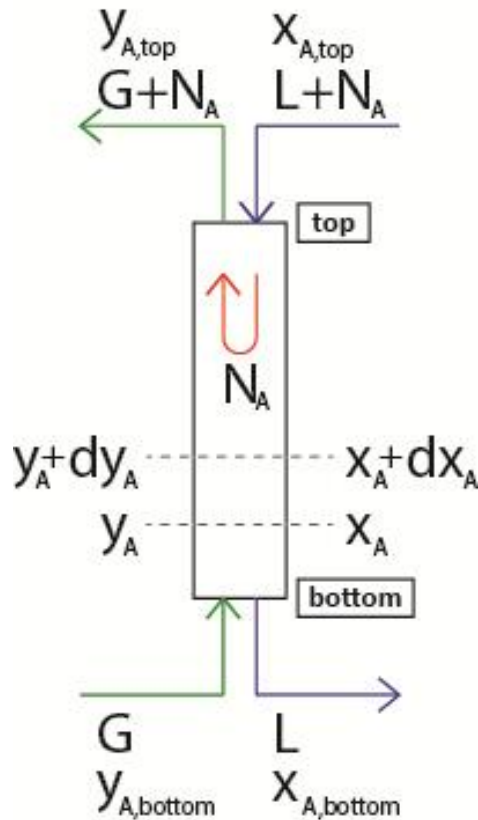


Figure 7.4. Stripping tower scheme.

Applying the mass conservation law to an infinitesimal section of the stripping tower, the following equation is obtained:

$$G \cdot dy_A = L \cdot dx_A \tag{Eq. 7.26.}$$

Then, looking the scheme from a certain point in the middle of the tower until the bottom, the infinitesimal part can be integrated:

$$G \cdot \int_{y_{A,bottom}}^{y_A} dy_A = L \cdot \int_{x_{A,bottom}}^{x_A} dx_A \quad \text{Eq. 7.27.}$$

After to solve these integrations, the *operation line* is deduced:

$$G \cdot (y_A - y_{A,bottom}) = L \cdot (x_A - x_{A,bottom}) \quad \text{Eq. 7.28.}$$

Finally, rearranging all the terms, the final concentration on the gas can be calculated at any point of the stripping tower:

$$y_A = \frac{L}{G} \cdot x_A + (y_{A,bottom} - \frac{L}{G} \cdot x_{A,bottom}) \quad \text{Eq. 7.29.}$$

Applying this expression at the top of the column, $y_{A,top}$ can be determined and, consequently, $p_{A,top}$.

As this expression reflects the behaviour of the stripping system, it is interesting to represent it in an axis diagram to understand better the patter it follows:

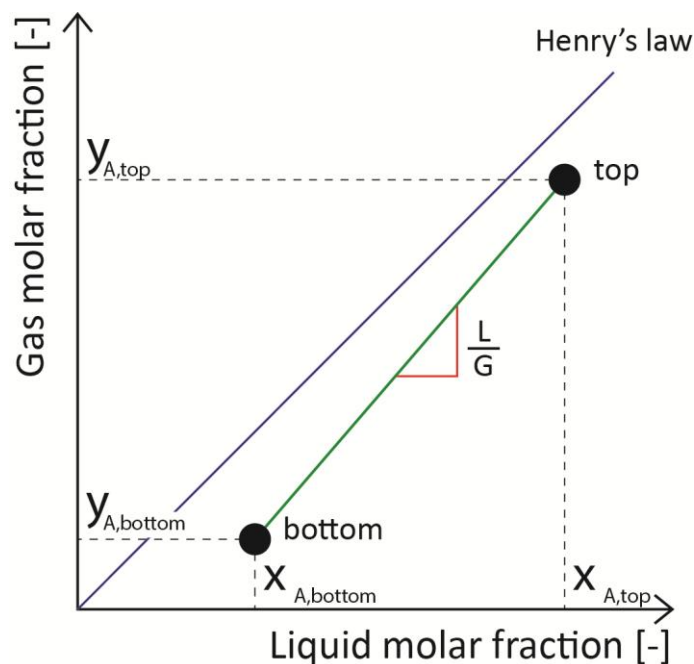


Figure 7.5. Graphical representation of a counter-current stripping system.

Once all molar fractions are known or calculated, the slope of the *operation line* is graphically determined as a function of other data; the molar flows:

$$\frac{L}{G} = \frac{y_{A,top} - y_{A,bottom}}{x_{A,top} - x_{A,bottom}} \quad \text{Eq. 7.30.}$$

Finally, comment that knowing the equilibrium between liquid and gas phases of a component is related on Henry's law, it is coherent that operation line is more close to equilibrium at the top of the stripping column than at the bottom: the higher concentrations gradient at the bottom of the column allows the pure inlet gas to take unwanted component until it arrives on the top where its amount increases until a closer value from equilibrium.

7.3.4. Assumptions

Along this project and on the software calculations, the following hypothesis are assumed:

- Steady-state
- There is not any chemical reaction during the operation.
- There is not longitudinal mixture of unwanted components between flows.
- There are not significant variations of pressure (1 atm) or temperature (20 °C).
- Henry's law is fulfilled in equilibrium.
- The solutions are dilute.
- Global mixture parameters (molar mass, Henry constant and diffusivities) are approached by the equivalent proportions between the initial species concentrations:

$$\overline{Property}_{TTHMs} = \frac{\sum (Property_{Each\ THM} \cdot c_{Each\ THM,top})}{\sum c_{Each\ THM,top}} \quad \text{Eq. 7.31.}$$

7.4. Methodology

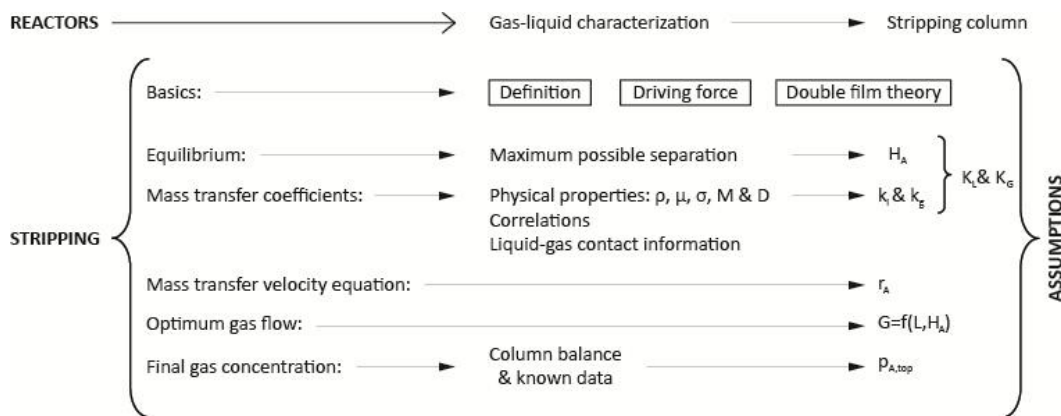


Figure 7.6. General stripping scheme.

7.5. Additional comments

7.5.1. Pressure and temperatures

Regarding on the operation conditions and on the streams which enter or leave the

equipment, this project considers the temperatures and pressures invariant. The main reason remains on the fact that the aim of a stripping column is to transfer mass from a stream to another in contrast than, for example, a heat exchanger, which pretends to maximise the heat transferred. So, the mass transfer is carried on without thermal effects involved or pressure changes (although the software calculates the pressure drop along the stripping column, it is considerate constant for the rest of calculations due to its normally small variation).

7.5.2. Solubility data

Commonly, chemical systems require specific models to describe their solubility models. However, Henry's law is a good approximation for physical systems. So, as it is the case of THMs, the solubility is defined knowing the value of the Henry's constant. It should be said that it can strongly vary with temperature in a nonlinear form. Otherwise, as it was clarified, there is not any heat transferred in the whole process.

7.5.3. Dilute solutions

This simplification is done in almost all the stripping cases because the few amount of unwanted component to remove. In special, for THMs case, the legislated maximum level is $100 \mu\text{g}/\text{L}$. This approach allows to consider the liquid and gas flows as constant without taking into account the small mass variations because the solutions of the unwanted components.

7.5.4. Selection of the best solvent

In any case, it is preferred a solvent with high solubility for the target solute and high selectivity over the other species in the liquid mixture. Otherwise, it is recommended that the solvent has additional advantages: low cost, low corrosion, high stability, low viscosity, low tendency to foam and low flammability.

Solvents are distinguished between physical which just have weaker interactions with the solute (diffusion) and chemical which forms complexes and chemical compound with the solute. In general, chemical solvents are chosen when the solute must be reduced to very low levels and when the solute concentration is low (high selectivity is needed). However as in case of study of this project the components removed from the water are THMs and there are not easy to chemically react (maybe, just a strong and uneconomic oxidation could be possible), the interaction will be physical. Accordingly to the cheapest option over any other type of gas, atmospheric air moved by a compressor is selected as the best solvent.



8. MECHANICAL DESIGN OF EQUIPMENT

The gas-liquid contact in a stripping column is continuous and not stage-wise as in a plate column. The liquid flows down the column over the packing surface and the gas counter-currently, up the column. Apart from this general description, there are other indispensable complements that ensure an optimal performance of the whole process. In order to complement the theoretical calculations, it is interesting to know the basics about how to design a stripping column and which factors and needs must be taken into account.

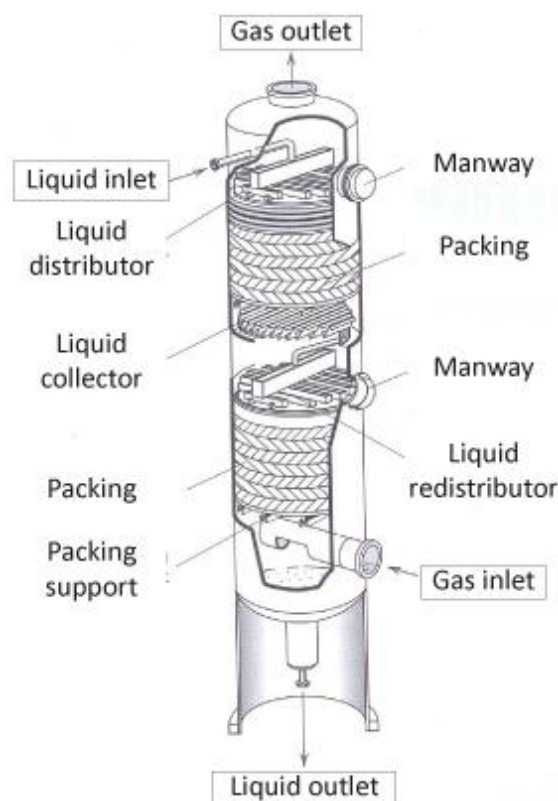


Figure 8.1. Illustrative cutaway of a packed tower, depicting structured packing (Image based on [15]).

8.1. Height of the column

The main aim of Section 8.1. is to develop the procedure to be able to calculate the most important feature of a column: its height. The methodology can be focused since different perspective as there are 2 different phases (liquid and gas) and, additionally, individual and overall mass transfer coefficients can be calculated for both. To standardize the procedure, it is taken as base the *overall mass transfer coefficient on the gas phase* (K_G) because, as Eq. 7.19. demonstrate, it is directly proportional to the global mass transfer velocity.

First, considering that at the same time the liquid removes the unwanted component, the gas

increases its amount on its flow: $(r_A)_{liquid} = (-r_A)_{gas}$. Then, retaking Eq. 7.19. and complementing it with Eq. 7.25. it can be written:

$$(-r_A) = K_G \cdot a \cdot (p_A^{eq} - p_A) = K_G \cdot a \cdot p_T \cdot (y_A^{eq} - y_A) \quad \text{Eq. 8.1.}$$

Next, knowing that there is an axial mass transfer velocity and, at the same time, a moles flow across the constant section of the stripping tower; being consistent with Eq. 7.26.:

$$(-r_A) \cdot dV_{reactor} = (-r_A) \cdot S \cdot dz = G \cdot dy_A \quad \text{Eq. 8.2.}$$

Then, if the last two equations are combined:

$$(K_G \cdot a) \cdot (S \cdot dz) \cdot p_T \cdot (y_A^{eq} - y_A) = G \cdot dy_A \quad \text{Eq. 8.3.}$$

In order to get the height of the vessel:

$$\int_0^{H_{column}} dz = H_{column} = \int_{y_{A,bottom}}^{y_{A,top}} \frac{G}{S \cdot (K_G \cdot a) \cdot p_T \cdot (y_A^{eq} - y_A)} dy_A \quad \text{Eq. 8.4.}$$

In spite of it looks complicated to solve, the Eq. 8.4. can be easily simplified because some terms are constant because their initial value is known (p_T), because they are calculated by the stripping methodology (K_G , a and G) or by the mechanical design (S):

$$H_{column} = \frac{G/S}{(K_G \cdot a) \cdot p_T} \cdot \int_{p_{A,bottom,Pa}}^{p_{A,top,Pa}} \frac{dp_A}{(p_A^{eq} - p_A)} \quad \text{Eq. 8.5.}$$

Commonly, this specific expression is summarized as:

$$H_{column} = H_G \cdot N_G \quad \text{Eq. 8.6.}$$

Where H_G is known as the *height of an overall mass transfer unit on the gas phase* and N_G is the *number of overall mass transfer units on the gas phase*.

Obviously, if instead the global case gas phase, the procedure is developed for the liquid or the individual cases with the interphase parameter, there are other equivalences:

$$H_{column} = H_l \cdot N_l = H_g \cdot N_g = H_L \cdot N_L \quad \text{Eq. 8.7.}$$

As it can be seen in Figure 8.1., apart from the mass transfer height (H_{column}), there is an extra height on the top and on the bottom of the column for other mechanical equipments. However, due to its lower value in comparison with the rest of the column, it is usually neglected.



8.2. Internal packing members

Basically, the main aim of putting fillings inside a stripping column is to increase the surface area in order to improve the contact between the gas and the liquid. Even though, there are some requirements that should be taken into account:

- Have an open structure to achieve a low gas flow resistance.
- Ensure a uniform liquid distribution on the packing surface.
- Promote uniform gas flow on the column cross-section.

In recent decades, many types and shapes of packing have been developed to satisfy these requirements:

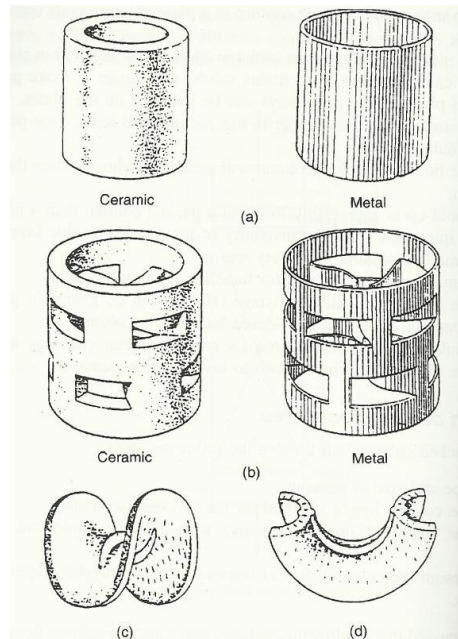


Figure 8.2. Shapes of different random packing: (a) Raschig rings. (b) Pall rings. (c) Berl saddle ceramic. (d) Intalox saddle ceramic [12].

They can be divided into two classes:

- Structured packing
- Random packing

The material of the first type of packing is folded and arranged with a regular geometry to give a high surface area with a high void fraction. Its advantages over the random packing are the lower pressure drop and the higher efficiency. On the other hand, justified by the fact that the cost per cubic meter is significantly higher, in this project it is selected the random packing for the stripping column filling.

The next step is to decide the material which will be used to fill the column. In order to make the correct choice, some bibliographic references like [16], [17] and [18] are essential however, for a general performance, it can be said:

- Ceramic packing will be the first choice for corrosive liquids but, they are unsuitable for use with strong alkaline dilutions.
- Metal packing should be specified when the column operation is likely to be unstable because ceramic packing is easily broken.
- Plastic packing are attacked by some organic solvents and can only be used up to moderate temperatures.

The special feature of each filling material is the critical surface tension ($\sigma_{c,material}$), information required on *individual mass transfers* correlations (Section 7.2.4.). Acquiring this information from several literature sources ([19] and [12]), these are the values that will be used for the software calculations:

Surface tension	$\sigma_{c,ceramic}$	$\sigma_{c,metal(steel)}$	$\sigma_{c,plastic(polyethylene)}$
Value	0,061	0,075	0,033

Table 8.1. Surface tension values of the typical filling materials of stripping towers.

8.2.1. Installation of the packing

In the case of metal and ceramic packing, they are fitted inside the column while it is partially filled with water (always, above the packing) to ensure a random distribution and, mainly, to prevent their damage. Then, the column is drained opening the tap or valve situated on the bottom. Even though, if the column must be packed dry (for example, to avoid contamination with water), the packing can be introduced using buckets or containers from the manways (check Figure 8.1.).

8.3. Pressure drop

Normally, a stripping column will be designed to operate in a way to achieve a low pressure drop for satisfactory liquid distribution. For random packing the pressure drop is usually $\Delta P < 50 \text{ mmH}_2\text{O}/(\text{column } m)$ and it is not recommended that this value exceeds $80 \text{ mmH}_2\text{O}/(\text{column } m)$.

Nevertheless, the biggest difficulty to get the pressure drop is that the literature correlations are graphical. In other words, knowing the terms:



$$F_{LG} = \frac{L_W^*}{G_W^*} \cdot \sqrt{\frac{\rho_G}{\rho_L}} \quad \text{Eq. 8.8.}$$

$$K_4 = \frac{13.1 \cdot (G_W^*)^2 \cdot F_P \cdot \left(\frac{\mu_L}{\rho_L}\right)^{0.1}}{\rho_G \cdot (\rho_L - \rho_G)} \quad \text{Eq. 8.9.}$$

$$\text{Limits: } 0,02 \leq F_{LG} \leq 4 \text{ and } 0,07 \leq K_4 \leq 6$$

It is possible to eye-determine the pressure drop of a stripping column, evaluating them in a diagram:

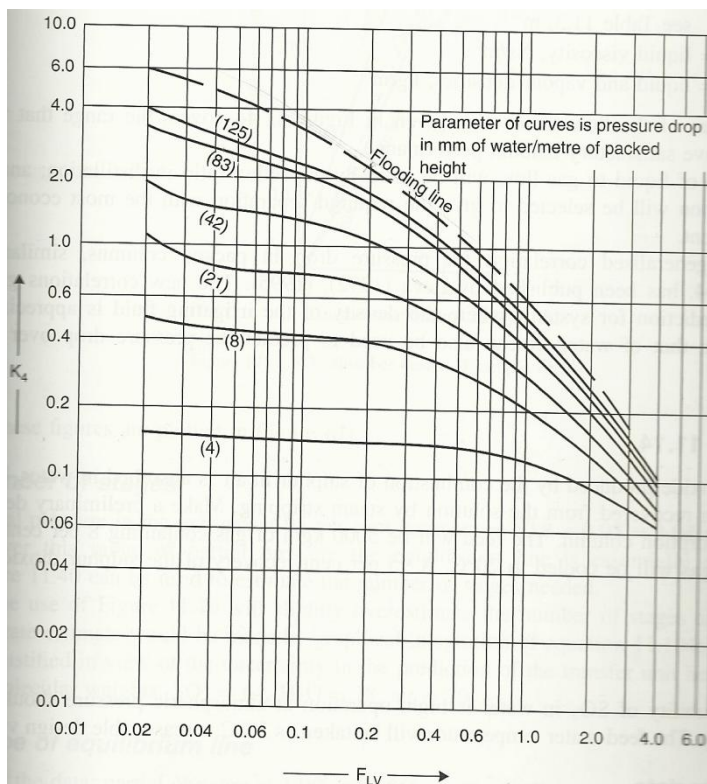


Figure 8.3. Pressure drop diagram.

8.4. Thickness of the walls

Due to the fact that the pressure is considerate constant on the whole process because the few value of the pressure drop, the column cannot be considered as a pressure vessel because there is not a pressure difference greater than 0,5 bars. Thus, involves that it is not possible to apply the design methodology for pressure vessels to determine the thickness of the walls.

For this reason, standard values depending on the diameter are taken as the minimum

thickness required to ensure that any vessel is sufficiently rigid to withstand its own weight and any accidental load (including corrosion allowance of 2 mm):

D_i	< 1	1 – 2	2 – 2,5	2,5 – 3	3 – 3,5
th	5	7	9	10	12

Table 8.2. Thickness minimum value of a vessel depending on its diameter ([12]).

Alternatively, it is also possible to add stiffening rings or longitudinal strips to keep the system rigid enough.

8.5. Column internals

8.5.1. Packing supports

In order to support the small size of the random packing, at the bottom of the stripping column it is putted a stacked packing on a wide-spaced grid. Its principal function is to carry the weight of the wet packing but, at the same time, it allows the gas and the liquid to pass through it while it also avoids local flooding caused by a high pressure drop.

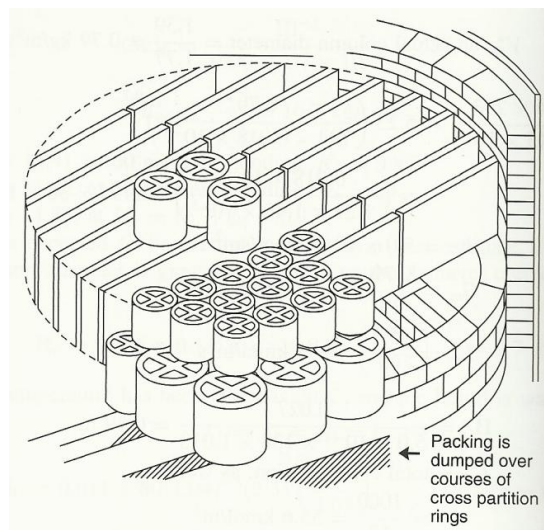
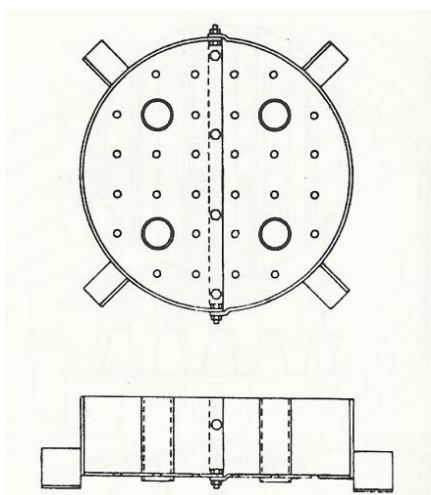


Figure 8.4. Structured packing used to support random packing [12].

8.5.2. Liquid distributors and redistributors

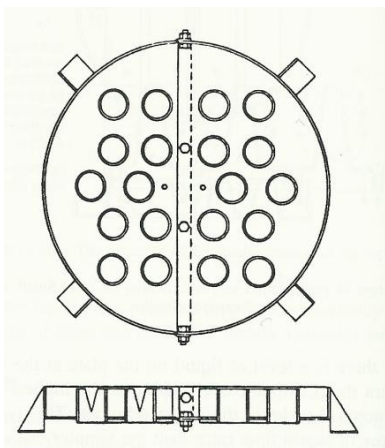
The correct performance of a packed column is very dependent on the maintenance of good liquid and gas distribution through the fillings. In fact, this is the main reason to put liquid distributors on the top of strippers:



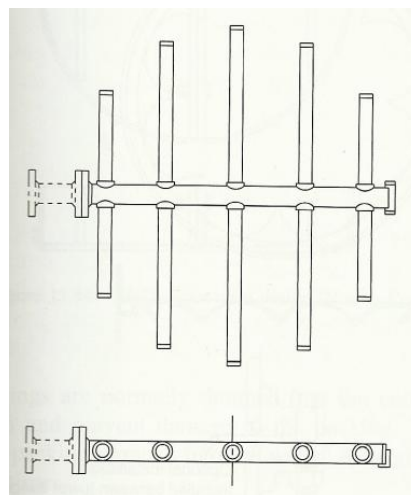
Orifice-type distributor



Weir-trough distributor



Weir-type distributor



Pipe distributor

Figure 8.5. Different types of distributors [12].

It is very important the size of the holes: not big enough can cause overflowing when liquid rate is big and not small enough cannot ensure that there is level of liquid on the column when liquid rate is small.

It should also be highlighted the importance of redistributors to collect liquid that has migrated to the column walls and redistribute it again over the packing. Furthermore, it can also help packing supports and column walls to support the weight of the packing. About when it is necessary to put them, there is not an exact answer because it depends on the type and on the weight of packing however, for large-diameter columns it is around 5 m.

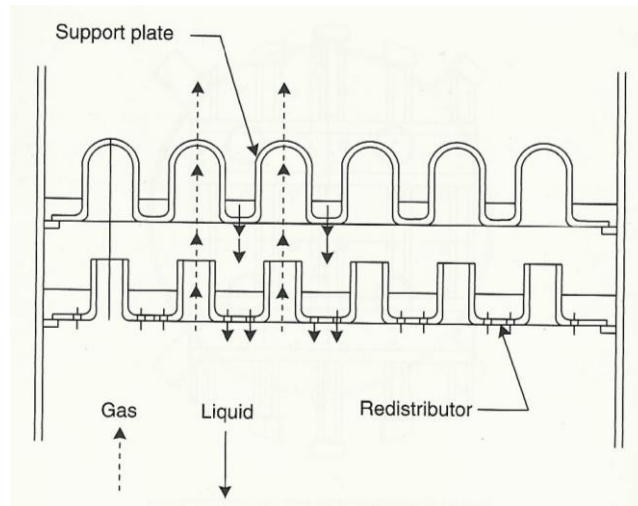


Figure 8.6. Redistributor performance [12].

8.5.3. Hold-down plates and bed-limiters

One of the most important considerations needed to take into account when a stripper is designed is to keep all the packing pieces inside the column in the case of miss-operation. On one hand, if the top layers are fluidised, the ceramic packing can break up and the small pieces filter down the column so, hold-down plates are installed on the top of the column to prevent this effect. On the other hand, if the bed suffers an expansion, the metal and plastic packing can be blown out of the column and to retain these packing is common to use bed-limiters. Obviously, the openings of this complements should be smaller enough to keep the packing inside the column but without avoiding the pass of gas and liquid.

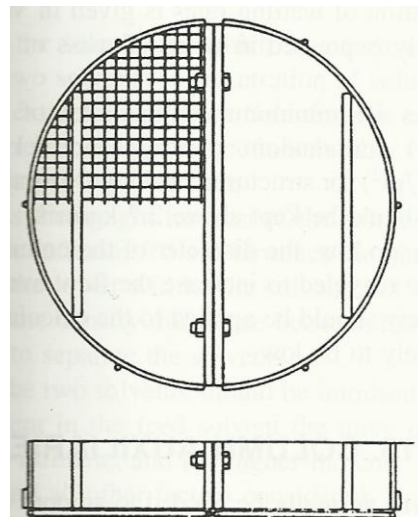


Figure 8.7. Hold-down plate [12].

8.6. System auxiliaries

In order to smooth out fluctuations and process upsets, it is normally needed an intermediate storage tank. The most critical value of this type of accumulators is the time when it is needed to feed the column because it must be between when the level of the normal operating falls and when the minimum operating level is reached.

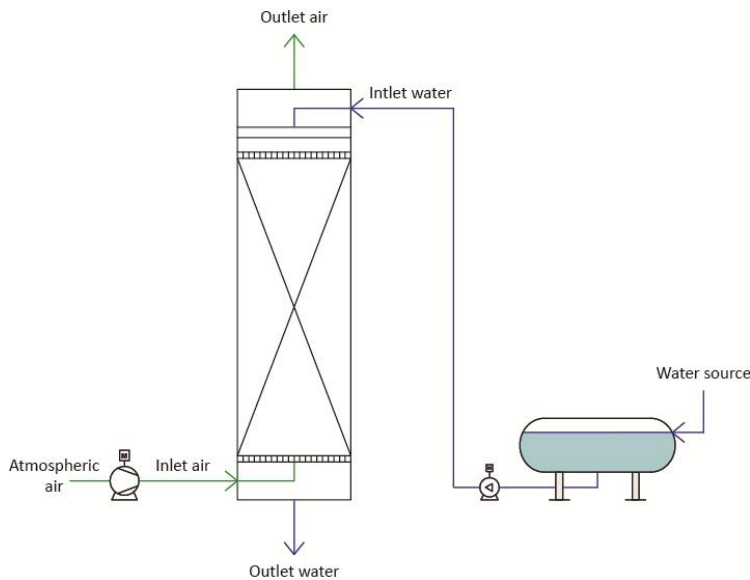


Figure 8.8. Auxiliary equipments of a stripping tower.

8.7. Loads to consider

In theory, the first source of load to pay attention is the pressure. However, as it is considerate constant along the equipment, it does not involve any other longitudinal (σ_{long}) or circumferential (σ_{circ}) stress.

Otherwise, due to the weight of the column, its content and any attachments, there is a dead-weight stress (σ_w) along the vertical axis. Accordingly to [12], it can be calculated like:

$$\sigma_w = \frac{W \cdot g}{\pi \cdot (D_i \cdot 10^3 + th) \cdot th} \quad \text{Eq. 8.10.}$$

In addition, other types of loads like bending stresses can also occur over the system caused by wind, seismic (earthquake) loads or because other equipment attached to the column.

8.7.1. Weight of the stripper

For preliminary calculations, instead it is not the exact case of a stripping column, the formula to estimate the weight (without internal fillings) can be approximated by how [12] calculate

the weight of cylindrical vessels with domed ends and uniform thickness:

$$W_v = C_v \cdot \pi \cdot \rho_{shell} \cdot D_{column} \cdot (H_{column} + 0,8 \cdot D_{column}) \cdot th \cdot 10^{-3} \quad \text{Eq. 8.11.}$$

Furthermore, the total weight of the stripping column can be calculated like:

$$W = W_v + \rho_{material} \cdot H_{column} \cdot S \cdot \varepsilon \quad \text{Eq. 8.12.}$$

8.8. Materials

8.8.1. Common industrial materials

In a general way, it can be said that a stripping column must be designed to withstand the worst combination of loading without failure. In other words, it means that the maximum allowable stress intensity is not exceeded at any point. Due to the main load in the stripping case is compressive, the vessel may fail by elastic instability (buckling or wrinkling the shell) along the vertical axis. So, making an approach, a column design must be checked to ensure that the maximum value of the resultant axial stress does not exceed the critical value.

Many factors have to be considerate when selecting engineering materials: strength, ability to be worked, maintenance, costs over the working life... However, in the stripping case, the overriding consideration is usually the feature to resist corrosion ([20] and [21]) caused by the chemicals carried on by the fluids.

Taking into account all of these facts, it is interesting to analyse the usual material for equipment construction:

- Iron and steel: Low carbon steel is the most commonly used engineering material because it is cheap, it can be easily worked and welded and it has good tensile strength and ductility. However, iron and low carbon steels are not resistant to corrosion so, they are suitable for organic solvents.
- Stainless steel: It is the most frequently used corrosion resistant material due to the formation of a thin oxide film. The higher content of chromium, the higher the cost and the better the corrosion resistance (especially when chromium content is above 12% and nickel is added). Between their microstructure classes, the uniform structure of austenite (FCC) is the most suitable for corrosion resistance. To be sure in which situation it is possible to use it, some sources like [22] and [23] should be consulted. This material has other good properties like high strength, not brittle at low temperatures, not high thermal conductivity and non-magnetic behaviour. On the

other hand, there are some disadvantages: possibility of intergranular corrosion and stress corrosion cracking, the last one, caused by few ppm of chloride ions; fact that reflects that this material is not suitable for a THMs dilution (species structural formed by chlorides that can be diluted in the water like chloride ions).

- **Plastics:** They are being increasingly used as corrosion-resistant materials, mainly for piping and lining vessels. Their lower mechanical strength and operating temperature (than metals) provoke that they are usually reinforced with glass or carbon fibres. Normally, they can be used for pressure vessels but, there are some disadvantage like flammability level and degradation with some organic solvents.

In general, they are considerate to complement metals as corrosion-resistant materials of construction being conscious that, unlike metals, plastics can absorb solvents, causing swelling and softening. Although they are not perfect for all applications, they are suitable for the water with THMs treatment because they can resist the corrosion power of the solvent while solute does not cause any damage on its structure.

- **Others:** There are a lot of possible materials to use in construction of industrial equipment like carbon, ceramics or alloys (with nickel, molybdenum, copper, zinc, aluminium, monel...) however, as they are less common, their characterisations are out of the boundaries of this project.

To sum up, the material of the fillings recommended for the 'water with THMs vs. air' case is plastic because its structural properties and its low price. However, for the shell, as it is the main part of the stripping column, the strength of the stainless steel is more important than the plastic non-intergranular corrosion.

8.8.2. Compensation for openings, branches and connections

As a result of openings and branches for connections and instrument fittings, the shell of the stripper is weaker in certain points because stresses are concentrated (for example, in a edge of a hole). To compensate this effect, the wall thickness is increased in the region adjacent to the opening but, being careful that over-reinforcement can reduce the flexibility of the wall and secondary stresses can appear. There are several methods like welded pad, inset nozzle, forged ring... to solve this problem. Instead it is an over-estimation guide, it is advisable to follow the 'equal area method of compensation' to calculate the amount of extra material required. Curiously, there is not a single value of effective area; it depends on the standards (like British Standard or European Standard) or codes (like ASME) applied.

9. STRIPPING COLUMN COST

9.1. Introduction

When it is talking about industrial equipment, the economic factor is one of the most relevant parameters for the viability of its execution. So, the investment and production costs are needed to estimate to be aware about the profitability of the project.

The accuracy of the approach depends on the project stage, the cost data available and the time spent on preparing it. As this is just a preliminary design of a stripping column a big approximation is enough. Accordingly to [12], for basic budget estimations, the typical accuracy obtained is around $\pm 15\%$ and it is mainly used to proceed with the design until the next point where more accurate approximation can be made.

In the software implementation, one hypothesis is the non-existence of inflation. In other words, as all cost-estimating methods use historical data and are themselves forecasts of future costs, it should be necessary to upload this data because the escalation of costs in markets. To achieve this purpose, published costs indexes are the tools to relate present costs to past costs and are based on data for labour, material and energy costs published in government statistical digests. However, as it is not a detailed study, this information will be mistaken.

9.2. Estimation of total investment

In a general way, the total investment needed for a project can be defined as the sum of the fixed and working capital. On one hand, the first term is the cost paid to the contractors; being more precise, it is the total cost of the plant ready for start-up and it includes the design, engineering, construction supervision, civil engineering work, control systems, equipments and its installation. On the other hand, the second term is the additional investment needed to start the plant up and operate it and, mainly, it consists of initial charges, raw materials and intermediates in the process.

9.2.1. Direct costs

The fact to acquire new equipment is the equivalence of the direct costs. In order to make a quick and rough cost estimation of the capital cost of a project it is possible to use information from earlier projects with the same manufacturing process (historical data of costs). So, to get an approach about the investment required, it is useful to apply the well-



known six-tenths rule [24] for industrial equipment and processes:

$$Cost_2 = Cost_1 \cdot \left(\frac{S_2}{S_1}\right)^{0,6} \quad \text{Eq. 9.1.}$$

Be noted that this relationship between size (or capacity of production/treatment) and cost can be used for projects and for equipment of similar features.

Alternatively, there are graphical drawings relating sizes of equipment with its cost which can be also used as a base. However, due the fact that these curves must be parameterised to be input in the software code and their values are not updated, the six-tenths rule is a better option.

9.2.2. Indirect costs

Complementing the direct costs of purchasing and installing the equipment, the capital cost of a project also includes the indirect costs which can be estimated as a function of the direct costs:

TYPE OF INDIRECT COSTS	% of DIRECT COSTS
Design and engineering costs	20% to 30%
Contractor's fees	5% to 10%
Contingency allowance for unforeseen circumstances	5% to 10%

Table 9.1. Relation between direct and indirect costs.

9.2.3. Working capital

Previous studies ([25], [26] and [27]) have suggested that working capital can vary around 5% of the fixed capital costs for a simple and single-product process with little storage as a complement. As this description perfectly fits in the studied case of this project (stripping column and maybe an auxiliary storage), it will be the percentage used to calculate its value.

9.2.4. Cost estimation methodology

Finally, after characterise the main factors that have to be included in a quick approach of the total investment required, it is added a table to get the idea of how the software gets the different parameters involved in the economical study of the design and installation of a stripping tower:

ECONOMICAL FACTOR	CALCULATION
<i>DC</i> : Direct (purchased) costs	Eq. 9.1.
<i>IC</i> : Indirect costs	$IC = 0,4 \cdot DC$
<i>TFC</i> : Total fixed capital	$TFC = DC + IC$
<i>WC</i> : Working capital	$WC = 0,05 \cdot TFC$
<i>TI</i> : Total investment	$TI = TFC + WC$

Table 9.2. Economical procedure to calculate the total investment needed for chemical equipment.

9.3. Operating costs

Apart from the initial investment needed to start a project, it is also important to know the costs required to produce the final product or, in the case of this project, to treat the disinfected water to remove THMs. Obviously, these costs are essential to be evaluated to study the viability of the installation. Even though, as the data required is extremely related on each situation, they are just ascribed and their features are not calculated on the software. The process/treatment costs are divided into three groups:

9.3.1. Fixed operating costs

These costs don't vary with production rate because they have to be paid whatever the quantity produced is. Some examples are: maintenance, operating labour, supervision, capital charges, insurance, taxes...

9.3.2. Variable operating costs

In contrast, the variable costs are dependent on the amount of product produced like the raw material, the utilities (power, steam, etc.) and services, the machines used...

9.3.3. General operating expenses

Apart from the direct costs related with the final product, there are other costs like general overheads, research and development, reserves... that add around 25% to the total operating costs.

9.4. Economic evaluation of the project

Usually, the purpose of investing money in an industrial plant is to earn money however, in this case the purpose is not to make any product or produce goods for sale; the final aim is to



remove a chemical unhealthy compound from disinfected water.

In a complete economical evaluation, it makes sense the calculations of the equipment economical behaviour using variables like cash-flow, pay-back time, break-even point, rate of return, profit, time-value of money... but in this specific situation it is just considerate the investment required to start-up as the only economic criteria. Once the project is contextualized in a certain scenario, it is when the advantages and disadvantages assuming risk in forecast have to be evaluated.

Moreover, as a general rule, it can be said that anybody cannot know how good will be to take one investment opportunity because there are a lot of uncertainties about plant performance, market, government policy... that can completely change the economic evaluation plan.

10. SOFTWARE CALCULATIONS

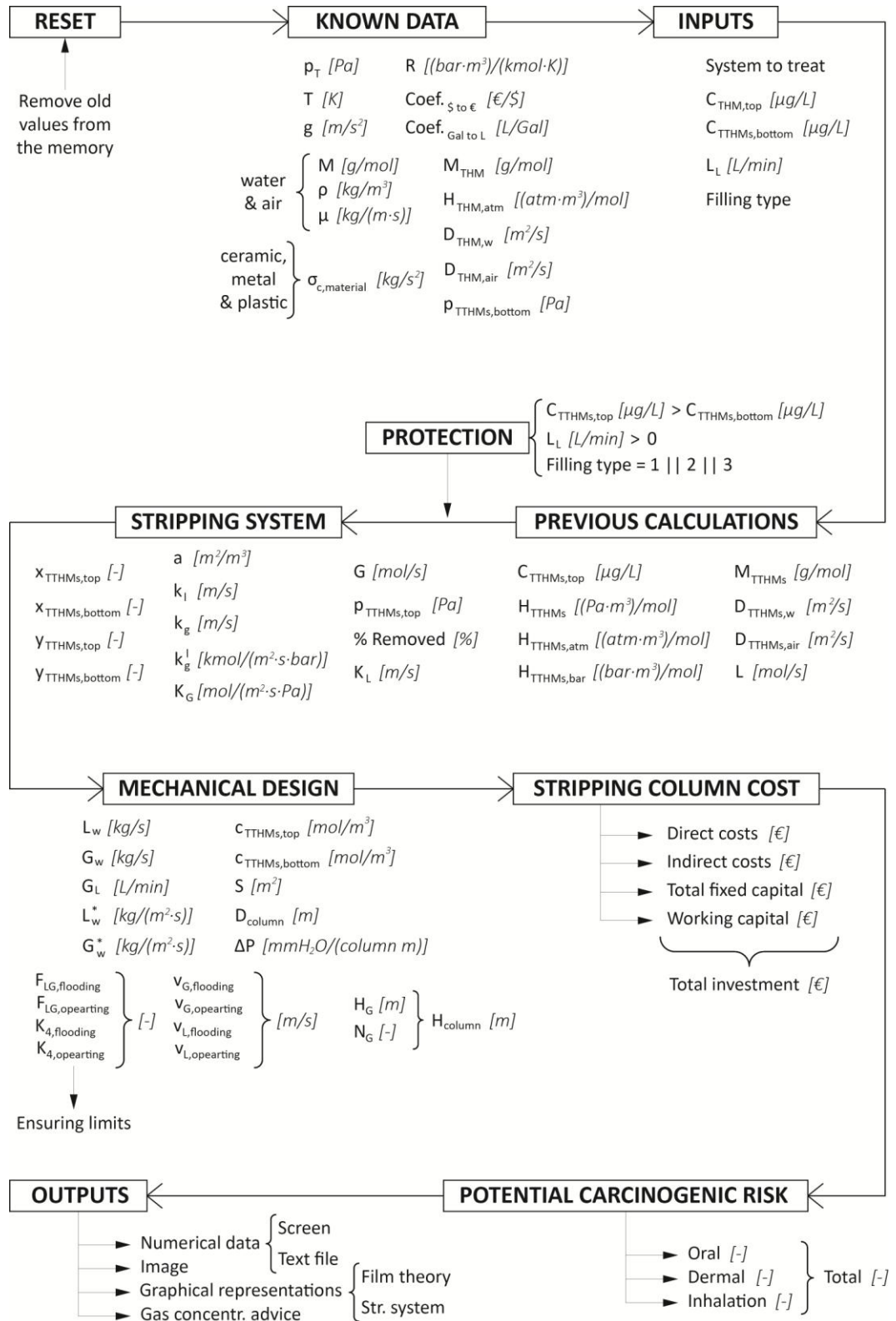


Figure 10.1. General scheme of calculations done by STRIP.



This Section pretends to be a summary of all the concepts explained and, at the same time, be useful to understand how the software does the calculations to determine the best design of a stripping column for each specific case. In order to avoid repetitions, visual diagrams and tables are used to follow the methodologies in order to link the knowledge with the procedure carried on.

10.1. Inputs

First of all, to contextualise how the software is implemented, it is extremely necessary to know the logic information available for the user at the beginning: the initial concentrations of the unwanted component in the liquid and in the gas and, of course, the amount of liquid it is wanted to treat. Moreover, it is also coherent to be able to choose the final concentration of the unwanted component in the liquid due to it can vary depending on each situation:

$C_{A,top}$	$p_{A,bottom}$	L_L	$C_{A,bottom}$
-------------	----------------	-------	----------------

Table 10.1. General input data.

However, as the user will be previously asked to specify if it is a *general* case or the *water with THMs versus air* case there are 2 important aspects to clarify about these parameters:

Firstly, for the THMs stripping system, the initial concentration of THMs in the air ($p_{THMs,bottom}$) is approximately 0 due to the composition of air is almost 79%_V of N_2 and 21%_V of O_2 . So, for THMs case, this value is not asked and it is internally approximated by $\epsilon ps (= 2,22 \cdot 10^{-22})$; the minimum accepted value for the software different than 0 (to avoid possible mathematical operation problems).

Secondly, although it is more complex to introduce each THM at the beginning instead a global THMs value (equivalent than $C_{A,top}$ in the *general* case), it is more coherent because in a hypothetical water analysis, each compound concentration will be found individually:

$C_{CHCl_3,top}$	$C_{CHCl_2Br,top}$	$C_{CHClBr_2,top}$	$C_{CHBr_3,top}$
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Table 10.2. Equivalent $C_{A,top}$ input data for THMs case.

Apart from these logic parameters, as THMs system is deeply studied along this project, the physical and chemical data regarding on it is already introduced in the software. In contrast, as these parameters are not valid for any other general situation, the user has to externally provide them:

ρ_L	ρ_G	μ_L	μ_G	σ_L	$H_{A,atm}$
$D_{A,l}$	$D_{A,g}$	M_L	M_G	M_A	

Table 10.3. Additional input data required for the general case.

Just comparing both tables, it is easy to conclude that this software is optimised for the THMs problematic because some extra data is required for any other case.

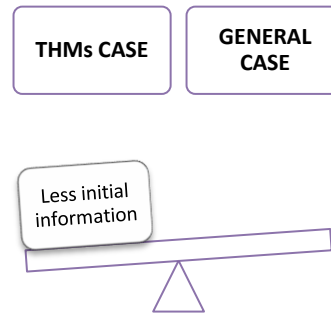


Figure 10.2. Schematic balance between software operating alternatives.

After introducing these inputs, the user is also available to choose the type of filling: ceramic, metal or plastic. It is an interesting parameter to be chosen externally because the user can have its own preferences, for example, due to the maximum weight of the stripping tower desired.

10.2. Known data

In line with what has been explained, there are supplementary known data already introduced in the software before its execution for the *water with THMs versus air* case. Mainly, the information sources are [12] and [2]:

M_{CHCl_3}	119	$D_{CHCl_3,air}$	$7,69 \cdot 10^{-6}$
M_{CHCl_2Br}	164	$D_{CHCl_2Br,air}$	$5,63 \cdot 10^{-6}$
M_{CHClBr_2}	208	$D_{CHClBr_2,air}$	$3,66 \cdot 10^{-6}$
M_{CHBr_3}	253	$D_{CHBr_3,air}$	$3,57 \cdot 10^{-6}$
$H_{CHCl_3,atm}$	$3,67 \cdot 10^{-3}$	M_{water}	18,02
$H_{CHCl_2Br,atm}$	$2,12 \cdot 10^{-3}$	M_{air}	28,96
$H_{CHClBr_2,atm}$	$7,83 \cdot 10^{-4}$	ρ_{water}	998

$H_{CHBr_3,atm}$	$5,35 \cdot 10^{-4}$	ρ_{air}	1
$D_{CHCl_3,water}$	$1,09 \cdot 10^{-9}$	μ_{water}	$1002 \cdot 10^{-6}$
$D_{CHCl_2Br,water}$	$1,07 \cdot 10^{-9}$	μ_{air}	$17,40 \cdot 10^{-6}$
$D_{CHClBr_2,water}$	$1,06 \cdot 10^{-9}$	σ_{water}	$7,20 \cdot 10^{-2}$
$D_{CHBr_3,water}$	$1,04 \cdot 10^{-9}$		

Table 10.4. Data introduced in the software to optimize the execution of THMs case.

Furthermore, other general parameters are needed to be introduced in the software because there are some complementary operations: unit transformation of some variables, to calculate the individual mass transfer coefficients, to estimate the project evaluation...

p_T	101325	$Coef_{\$ to €}$	0,92
T	293,15	$\sigma_{ceramic}$	$61 \cdot 10^{-3}$
R	0,08314	σ_{metal}	$75 \cdot 10^{-3}$
g	9,81	$\sigma_{plastic}$	$33 \cdot 10^{-3}$
$Coef_{Gal to L}$	3,79		

Table 10.5. General data introduced in the software.

It should also be taken into account that there are some of these properties that depend on the temperature and pressure of the environment. Instead there are some studies to recalculate them (for example: [28] or [29]), due to the hypothesis of this project, they remind constant along all the stripping operation (1 atm and 20 °C).

10.3. Initial reset

Additionally, as the software is implemented to do all the calculations just with the initial data introduced in each case, without taking into account any another execution, it is conceptually interesting to remove from the memory all the previous values to ensure that the software does not keep old unnecessary information.

10.4. Previous calculations

For THMs case, some initial data must be converted from individual values of each THM into a total value of THMs. At the beginning, it is necessary to sum the input concentrations to get

the total THMs concentration on the top of the stripping column:

$$C_{TTHMs,top} = C_{CHCl_3,top} + C_{CHCl_2Br,top} + C_{CHClBr_2,top} + C_{CHBr_3,top} \quad \text{Eq. 10.1.}$$

Then, as every physical property depends on each compound and on its each concentration, it is also necessary to get global mixture properties. So, using the initial concentrations to make the right proportions, the molar weight, the Henry's constant and the diffusivities of THMs on the air and on the water are determined (as Eq. 7.31.). For example:

$$M_{TTHMs} = \frac{\sum M_{Each\ THM} \cdot C_{Each\ THM,top}}{\sum C_{TTHMs,top}} \quad \text{Eq. 10.2.}$$

This assumption is critical because, in a real case, as the concentrations vary from the top until the bottom of the column, the mixture physical properties should also change. However, it is not coherent to know each THM concentration at the bottom of the column because, in terms of legislation, the total THMs concentration is the final parameter to take into account for the health quality. For this reason, the initial concentrations are the alternative chosen to calculate the proportions of each species in the total physical properties. This kind of approach is justified by the fact the species proportions between the initial and final concentrations are sustainable to change because the different Henry's constant but, at the same time, due to its values because their organic structure, there is not a significant variation.

Obviously, these recalculations are not necessary if the software executes the general case.

10.4.1. Unit transformation

Units of variables must be transformed during the software calculations to adapt them in all equations. To get a general idea, Figure 10.1. can be followed. For further detail, software code can be found on Annexes (Section 18.5.) with all the equivalences noted on the right of each expression.

10.5. Protections

A good programming code should avoid as unnecessary operations as possible when a calculation does not make sense. For this reason, some protections are implemented at the beginning to break the iterations if the user introduces non coherent values:

- When there is not concentration gradient between the top and the bottom of the column: $\Delta C_{top\ to\ bottom} > 0$.



- When there is not flow of liquid to treat: $L_L > 0$.
- When the user does not choose any type of filling (1 = *ceramic*, 2 = *metal* and 3 = *plastic*).

10.6. Stripping system

As it is detailed in Section 7., the main goals of the stripping system is to determine the following parameters:

- An optimal gas flow to treat the liquid (G_L).
- The final gas concentration of the unwanted component ($p_{A,top}$).
- The total amount of the unwanted component that has been removed (*% Removed*).

But, as initially some variables are given in other unit, previous conversions are required at the same time that intermediate parameters (like molar fractions) are calculated to get the final results.

10.7. Mechanical design

10.7.1. Fillings data base

Matlab software also interacts with other software for different purposes. For the mechanical design, as one of the aims is to select the best type of filling for each stripping system, it is needed a big data base of packing. The one that this project uses is based on [19] and it consists on an Excel file called 'FeaturesOfFillings.xlsx' classified into 3 different sections (ceramic, metal and plastic fillings) where there are data for different types of fillings. For example:

Filling name	$d_N (\cdot 10^3)$	a_p	ε	ϕ	F_p
BERL SADDLE (Ceramic - 1/2 in.)	12,7	510	0,670	0,440	788
BERL SADDLE (Ceramic - 3/4 in.)	19,1	280	0,650	0,420	588

Table 10.6. Part of the ceramic fillings data base.

So, depending on the material selected by the user for the packing, the software imports this file and it saves on its internal memory the numeric and text data of the selected type of fillings. Moreover, it also updates the value of the surface tension of the material ($\sigma_{c,material}$).

For the system *water with THMs versus air*, the software also allows the user to choose the fillings material however, as it is explained in Section 8.8.1., it is recommended to operate

with the cheapest and corrosion-resistance: plastic.

Before to continue, it is interesting to clarify that all the methodology is developed taken into account that if the data base is increased or modified, it is possible to carry on the same iterative calculations without reprogramming the code at any point.

10.7.2. Iterative procedure

As it is explained in Section 8, the main mechanical parameter to determine is the height of the column but, accordingly to Eq. 8.5. to achieve this, it is necessary to know other features of the tower; the most difficult is to specify the size of the section. Firstly, because it has to be indirectly calculated from the gas flow rate or the gas velocity:

$$S = G_w / G_w^* = G_w / (\rho_G \cdot v_G) \quad \text{Eq. 10.3.}$$

And, secondly, because, accordingly to Figure 8.3., v_G depends on the packing factor of the filling (F_p). Normally, the packing is fixed and since this point, the other parameters can be easily calculated. However, as the aim of this project is further and it searches the best packing for each case, the process considerably increases its level of complexity.

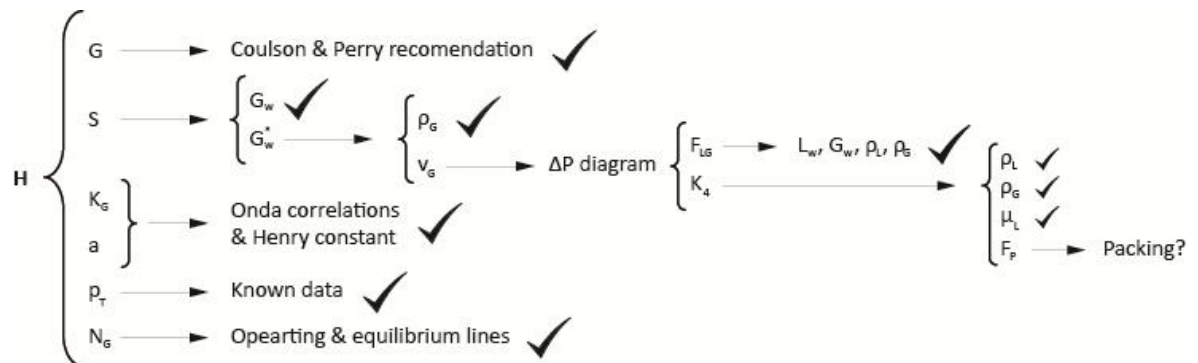


Figure 10.3. Initial design problem of the stripping column.

Operating logically, it is better to ensure a safety operation along all the process than chose a certain packing since the beginning. For this reason, the software iterative procedure is different and based on the criteria that the gas operating velocity must be around 70% of the gas velocity which causes flooding ([12]).

$$v_{G,operating} = 0,7 \cdot v_{G,flooding} \quad \text{Eq. 10.4.}$$

As to apply this condition the pressure drop diagram (Figure 8.3.) plays an important role, some aspects should be commented:

- The axis parameter can be calculated with mass flow values:

$$F_{LG} = (L_w^* / G_w^*) \cdot \sqrt{\rho_L / \rho_G} = (L_w / G_w) \cdot \sqrt{\rho_L / \rho_G} \quad \text{Eq. 10.5.}$$

- The gas velocity is possible to be determined by:

$$v_G = \sqrt{\frac{K_4 \cdot (\rho_L - \rho_G)}{13,1 \cdot \rho_G \cdot F_p \cdot (\mu_L / \rho_L)^{0,1}}} \quad \text{Eq. 10.6.}$$

- The ordinate value when flooding occurs can be calculated with a regression of the corresponding curve of Figure 8.3. (done by Matlab). It just depends of F_{LG} :

$$K_{4,flooding} = 0,3359 - 1,889 \cdot e^{-F_{LG}} + 4,939 \cdot (e^{-F_{LG}})^2 \quad \text{Eq. 10.7.}$$

- It is important to take into account the limits of the diagram to avoid extrapolations. Being more precise, if F_{LG} is lower than 0,02 or higher than 3, F_{LG} is taken as the limit value and G_w and G_w^* are recalculated. Operating in this way, the gas flow is determined with the suggestion of [12] and [13] if only if, the result allows F_{LG} to be between the interval (0,02-3).

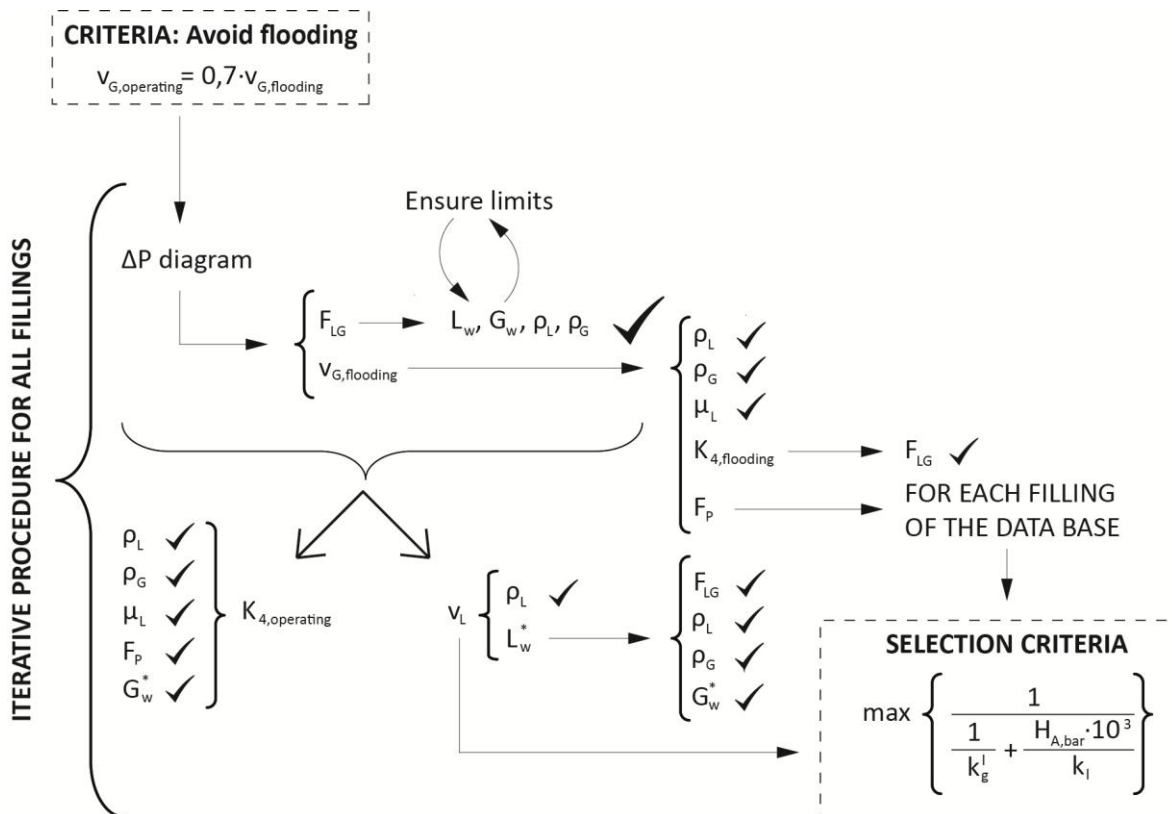


Figure 10.4. Calculations iterative procedure.

Apart from the theoretical way to operate, what the software does is: It creates a big matrix

formed by the features of the type of fillings selected (5 columns) and it adds on it 10 extra columns full of zeros (15 columns in total). In general, it can be said that the purpose is to store the different partial results in each empty column. And, once the row of the best type of filling (the one that maximise the mass transfer from the liquid phase to the gas phase) is known, all the columns are checked again to find the corresponding values of all the parameters of the final mechanical design.

Filling features		$v_{G,flooding}$	$v_{G,operating}$	G_w^*	$K_{4,operating}$
1 st to 5 th columns		6 th column	7 th column	8 th column	9 th column
L_w^*	$v_{L,operating}$	k_l	k_g	k'_g	$\frac{1}{\left(\frac{1}{k'_g} + \frac{H_{A,bar} \cdot 10^3}{k_l}\right)}$
10 th column	11 th column	12 th column	13 th column	14 th column	15 th column

Table 10.7. Big matrix scheme.

At the end of this complex but smart method to operate correctly, the section of the stripping column can be calculated (Eq. 10.3.). From a wider point of view, this iterative procedure demonstrates how useful can be to know programming in order to do a lot of calculations in short time in order to get accurate results.

10.7.3. Calculation of the height

At this point, as the *height of a unit transfer* (check Section 8.1.) is possible to calculate because the data is known directly or indirectly, the main question is how the *number of transfer units* can be determined. There are different methods to be applied:

- Geometrical calculation of N_G

As equilibrium and operation lines are straight, it is possible to calculate the value of *number of transfer units* (N_G) with the arithmetic mean between the gradient $p_A^{eq} - p_A$ at the top and the bottom of the column. This procedure is just possible due to the geometry of the stripping system:



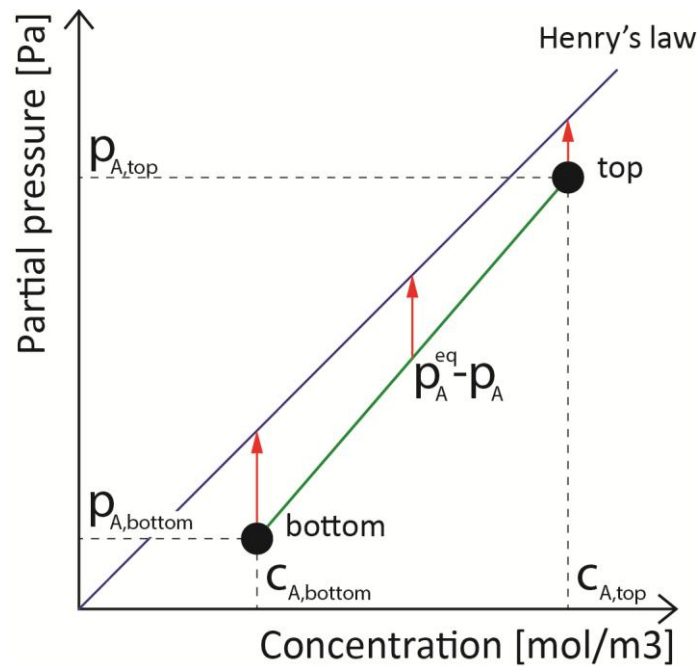


Figure 10.5. Geometrical N_G calculation.

There are alternative methods to calculate N_G however, the software does not calculate them in order to take advantage of the stripping system geometry.

- Numerical or graphical integration

It involves successive, complex and precise calculations just recommended to do when it is possible to use a software. Mainly, it consists on relating the infinite points between the operation line and the equilibrium line by its equivalent or interphase points. In each iteration the parameters have to be actualized by analytic formulas deduced from stripping concepts.

It should be noted that this method can also be carried on graphically. For example, in a plot diagram: reading the values in the equilibrium line following the slope previously determined with the *individual mass transfer coefficients*.

- Analytical integration or average driving force method

In this case, there are some bibliographic sources that define analytical equivalent expressions than the integral. For example, one of the most usually applied is the equation deduced from the driving force which corresponds to the logarithmic mean between the top and the bottom of the column using their respective equivalent points.

- Empirical formulas

Another option is to use empirical expressions got experimentally under different conditions.

Although there are several scientists who validate these sources, each case must be suitable for the specific dynamic characterisation and the experimental boundaries. Moreover, it is usually demanded a lot and precise data to get values from these deduced expressions.

10.7.4. Calculation of the pressure drop (ΔP)

Accordingly to [12], apart from specify a certain packing of the column since the beginning, it is typical to choose the pressure drop and then, calculate the column cross-section area and diameter. However, as it is more interesting to determine this parameter once the mechanical design is optimised, the calculations are done inversely.

So, following what is explained on Section 8.3., from data of the stripping system and the mechanical design of the column, the pressure drop is approached with graphical diagrams (Figure 8.3.). As Matlab does not have any function to numerically interact with a picture, the graphic curves must be parameterized. Due to it is a long development because it consists on several mathematical stages, the detailed explanation can be followed in Annexes (Section 18.3.). The final equations implemented are:

<i>Pressure drop (ΔP) curve</i>	<i>Regression equation</i>
125 mmH ₂ O/(column m)	$K_4 = 0,3359 - 1,889 \cdot e^{-F_{LG}} + 4,939 \cdot (e^{-F_{LG}})^2$
83 mmH ₂ O/(column m)	$K_4 = 0,3072 - 1,792 \cdot e^{-F_{LG}} + 4,551 \cdot (e^{-F_{LG}})^2$
42 mmH ₂ O/(column m)	$K_4 = 0,1585 - 0,228 \cdot e^{-F_{LG}} + 1,760 \cdot (e^{-F_{LG}})^2$
21 mmH ₂ O/(column m)	$K_4 = 0,1001 + 0,318 \cdot e^{-F_{LG}} + 0,504 \cdot (e^{-F_{LG}})^2$
8 mmH ₂ O/(column m)	$K_4 = 0,0772 + 0,354 \cdot e^{-F_{LG}} + 0,037 \cdot (e^{-F_{LG}})^2$
4 mmH ₂ O/(column m)	$K_4 = 0,0675 + 0,204 \cdot e^{-F_{LG}} - 0,121 \cdot (e^{-F_{LG}})^2$

Table 10.8. Parameterization of the pressure drop curves.

To sum up, as F_{LG} value is calculated for the software, it is evaluated in all the curves parameterized to get the corresponding K_4 value. From another side, K_4 is also calculated in the operating conditions. So, both curves with the closest value of the real K_4 are used to calculate the final pressure drop interpolating their values between these 3 points.

10.8. Project evaluation

As it is explained in Section 9.2.1., it is necessary again to operate with other updated sources of data. In this case, [30] presents some direct costs of stripping towers depending



on its flow available to treat (L_L) and on the percentage removed of the unwanted component (high efficiency: $> 90\%$). Reorganizing those parameters, depending on the flow (2nd row of Figure 10.6.) and on its efficiency (3rd row), it is possible to compare each case with a similar one and approximate the direct cost.

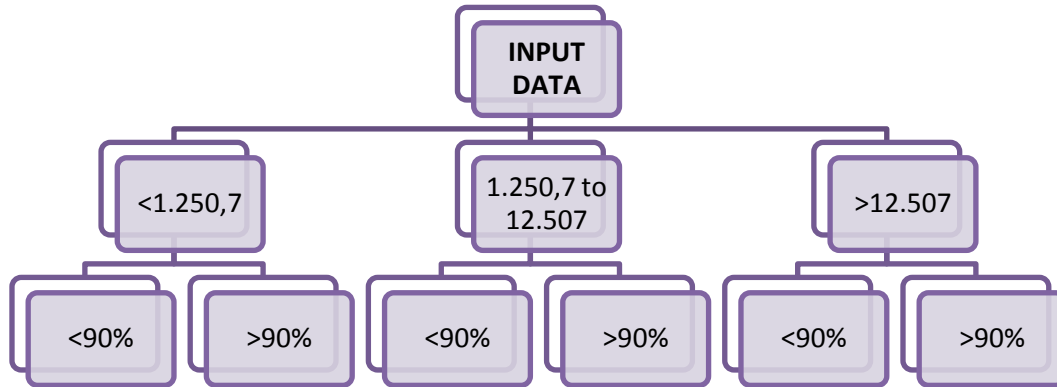


Figure 10.6. Scheme of the classification used in the project evaluation.

Once the comparison is done, the purchased equipment cost is determined. Then, complementing it with the economical procedure (Table 9.2.), the total investment cost is calculated.

10.9. Outputs

10.9.1. Numerical data

- Command Window:

At the end of software execution, it shows on the *Command Window* of Matlab the final results of the stripping column design:

$\% \text{ Removed}$	H_{column}	S	D_i
<i>Fillings name</i>	G_L	v_G	v_L
ΔP	<i>Investment</i>	$Risk_{initial}$	$Risk_{final}$

Table 10.9. Numerical output parameters shown on *Command Window*.

In addition, if any of the initial protections are used, the software displays and advice to make the user aware some non coherent values are introduced.

- Notepad:

Furthermore, the software also creates a *Notepad file* called 'StrippingTowerResults.txt'

where, apart from the results of Table 10.9., more detailed information is written.

L_w^*	G_w^*	K_G	K_L
k_l	k_g	k'_g	a
$v_{L, flooding}$	$v_{G, flooding}$	Number of liquid distributors	

Table 10.10. Some of the numerical outputs written on the *Notepad* file.

This file is saved in the *Current Folder* and it can be extremely useful to avoid rewriting all the results. However, it is important to be aware that after every simulation, the results are overwritten. So, if the user wants to keep them, it is recommended to resave the file with another name.

Obviously, if the user is interested in any other parameter like the features of fillings, the indirect costs... they can also be found in the *Workspace* of Matlab after its execution.

10.9.2. Graphical representations

Apart from the numerical outputs, taking profits from the potential that offers Matlab, some complementing visual information is possible to get. On one hand, it is useful for the user to contextualise which kind of stripping system is treated. To be more precise, the software draws a diagram as an output, similar as Figure 7.5., with:

- Equilibrium line: Continuous and blue line.
- Operating line: Discontinuous and green line.
- Top and bottom points: Small red circles.
- Title, legend and axis information.

Furthermore, a scheme of the double-film theory is also displayed as it is very illustrative to visualise which phase controls the mass transfer. Finally, complementing the results shown on the screen by the *Command Window*, an image of a stripping tower is also projected to contextualise the basic mechanical features of the stripping tower.

11. BLOCKS VALIDATION

As the final software use several models, it is essential to check that each part is implemented correctly and that the partial results are accurate approximations. For this reason, this Section pretends to corroborate that the main blocks, considerate like the structure of the software, obtain similar results as bibliographic sources and, consequently, theoretically validate the design of the stripping column.

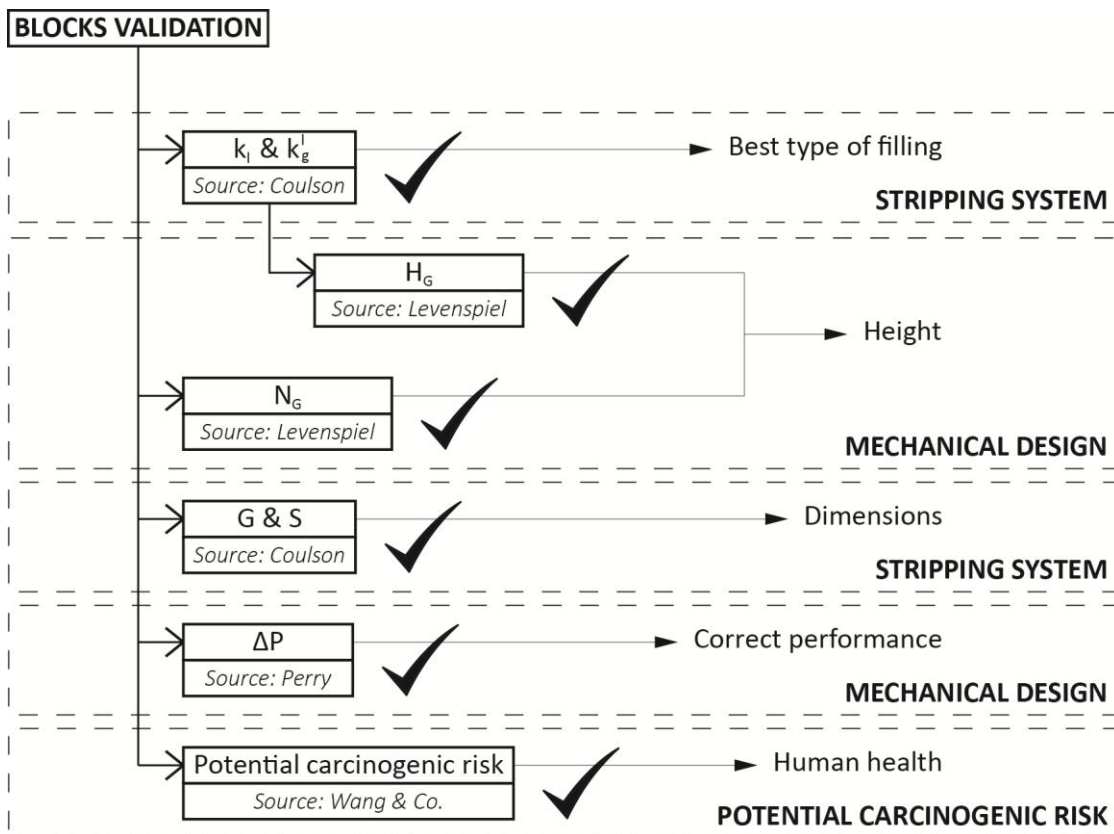


Figure 11.1. General validation scheme.

In order to adapt each validation example with the corresponding part of the software some specific operations and transformations are required in order to initialize both cases equal or to get the results in the same dimensions. These details can be found on Annexes (Section 18.6.) along the software validation codes and in the rest of this Section, the results are presented:

11.1. Individual mass transfer coefficients (k_l and k'_g)

There are 2 different possibilities to validate the correct performance of the software about k_l and k'_g calculations. The first option is to introduce the same input data than the bibliographic

source and compare the results. So, on Coulson's book [12] from page 605 until 609, there is an example where water is used in order to remove sulphure dioxide (SO_2) produced by the combustion of sulphur (S) in the air. It is an absorption case but, as Onda's correlation formulas do not have any specification about the operation mode, they are also valid for stripping. So, its input data are:

$p_{T,bar}$	1	ρ_L	10^3	$v_{L,operating}$	0,018	$D_{SO_2,w}$	$1,7 \cdot 10^{-9}$
T	293,15	ρ_G	1,21	$v_{G,operating}$	0,719	$D_{SO_2,air}$	$1,45 \cdot 10^{-5}$
R	0,08314	μ_L	10^{-3}	$p_{SO_2,bottom,Pa}$	60,8	σ_L	$70 \cdot 10^{-3}$
g	9,81	μ_G	$18 \cdot 10^{-6}$	$p_{SO_2,top,Pa}$	3,04	$\sigma_{c,material}$	$61 \cdot 10^{-3}$

Table 11.1. Input data of individual mass transfer coefficients validation.

After to do the suitable previous calculations to get the same variables as the ones the software use, it is possible to compare its values with the results of the bibliographic source:

Indiv. mass transfer coeff.	Coulson's book [12]	Software	Relative error [%]
k_l	$2,5 \cdot 10^{-4}$	$2,566 \cdot 10^{-4}$	2,64
k'_g	$5 \cdot 10^{-4}$	$5,331 \cdot 10^{-4}$	6,62
a_w	138	138,67	0,49

Table 11.2. Comparison between software and Coulson's book values of k_l and k'_g .

Evaluating the results, due to the almost equal values (few relative error), it is possible to conclude that the short differences mainly come from the hand-made calculation versus the software precision.

The second option is to check if the results are similar than general values. Being conscious that individual mass transfer coefficients depend on each case, accordingly to [6], they can be properly approached by standard values of Table 6.2.. So, for the filling tower reactor:

Volumetric mass transf. coeff.	Filling tower	Software
$k_l \cdot a$	$(0,04 - 102) \cdot 10^{-2}$	$3,56 \cdot 10^{-2}$
$k'_g \cdot a$	$(0,003 - 51) \cdot 10^{-2}$	$7,39 \cdot 10^{-2}$

Table 11.3. Comparison between software and standard values of k_l and k'_g .

Logically, this validation is not as precise as the first one but, as the order of magnitude is the same and the numbers are inside the intervals, it also indirectly justifies the good approach of the software.

11.2. Height of an overall mass transfer unit on the gas phase (H_G)

The height of an overall mass transfer unit on the gas phase validation is based on an example of Levenspiel's book [7] from page 551 to page 553 where it is pretended to remove an impurity of the air. This situation also corresponds to an absorption case where the gas is the flow which initially carries on the unwanted component. Nevertheless, accordingly to Eq. 8.5., the expression is also valid. So, the final result is calculated with these input data:

p_T	10^5	L^*	$7 \cdot 10^5 \cdot 3600$	$k_g'' \cdot a$	0,32/3600
G^*	$10^5 \cdot 3600$	H_A	12,5	$k_l \cdot a$	0,1 \cdot 3600

Table 11.4. Input data of the height of an overall mass transfer unit on the gas phase validation.

After the particular variable transformations, it can be said that software values are exactly the same than Levenspiel results (0% of relative error):

Parameters	Levenspiel's book [7]	Software
R_T	128,125	128,125
R_G	2,439	2,439
R_L	97,561	97,561
$K_G \cdot a$	$7,8 \cdot 10^{-3} \cdot 3600$	$7,8 \cdot 10^{-3} \cdot 3600$
H_G	128,125	128,125

Table 11.5. Comparison between software and Levenspiel's book values of H_G validation.

Although the final values are correct and, consequently, the software performance checked. It is interesting to analyze the uncommon number calculated: 128,125 meters of height of each unit what implies an unacceptable enormous tower. As the main resistance belongs to the liquid film (> 95%), one possible solution could be to add another component in the water to provoke a chemical reaction and increase the mass transfer velocity.

11.3. Number of overall mass transfer units on the gas film (N_G)

Taking the same example as the validation of the height of an overall mass transfer unit on the gas phase (Section 11.2.), doing a simple modification to calculate the partial pressure gradient, it is possible to apply this absorption case to validate the number of overall mass transfer units on the gas phase. Apart from the data of Table 11.4., some additional information is needed:

$p_{A,bottom,Pa}$	100	$c_{A,top}$	0
$p_{A,top,Pa}$	20	c_T	56.000

Table 11.6. Additional input data of number of overall mass transfer units on the gas phase validation.

Then, equal values of Levenspiel's book are calculated for the software:

Parameters	Levenspiel's book [7]	Software
$c_{A,bottom}$	6,4	6,4
$p_A - p_A^{eq}$	20	20
N_G	4	4

Table 11.7. Comparison between software and Levenspiel's book values of N_G validation.

At this point, once the correct performance of the number of overall mass transfer units on the gas phase validation is checked, it should be noted that as lower the final results is, as lower the height of the column is. In terms of equipment it is interesting to minimize this parameter to reduce the cost and difficulty of the stripping tower construction. For this reason, increasing the difference between the partial pressure at the bottom or at the top of the column (p_A) and its equilibrium pressure (p_A^{eq}) causes that N_G value decreases thanks to the bigger gradient that allows a higher mass transfer velocity between both phases.

11.4. Gas flow (G_w^*) and section (S)

The block that pretends to validate the correct performance of the software regarding on the calculation of the gas mass flow rate over the cross-section of the column (G_w^*) and the section (S) calculations is based on the same Coulson's book example as k_l and k'_g validation. So, the results are calculated from the same initial values of ρ_L , ρ_G and μ_L and the following extra data:



M_L	18	L_w	29,5	K_4	0,35	$K_{4, flooding}$	0,8
M_G	29	H'_A	27,4	F_P	170		

Table 11.8. Input data of gas flow rate and section validation.

The software gets small relative errors between software and Coulson's book results:

	Coulson's book [12]	Software	Relative error [%]
Gas flow rate (G_w^*)	1,39	1,388	0,14
Section (S)	1,6	1,599	0,06
Diameter (D_i)	1,43	1,427	0,21

Table 11.9. Comparison between software and Coulson's values of G_w^* and S validation.

In conclusion, it can be assumed that the block of the software whose aim is to calculate the gas amount necessary to remove the unwanted components and determines the right section of the stripping column gets accurate results.

11.5. Pressure drop (ΔP)

In order to check if the pressure drop calculation with sufficient precision, it is selected an example of Perry's book [13] from page 293 to page 294 where air and water are flowing counter-currently through a packed column. Its initial data is:

L^*	$40,67 \cdot 1000 / 3600$	ρ_L	999,57	μ_L	10^{-3}
G^*	$4,2 \cdot 1000 / 3600$	ρ_G	1,19	F_P	88,58

Table 11.10. Input data of pressure drop validation.

As it is explained on Section 8.3., all the methodologies to determine the pressure drop along the column are graphical. In this case, 2 of them are approached on the bibliographic source and they are almost equivalent than the results got for the software parameterizations:

ΔP	Perry's book [13]	Software	Relative error [%]
Robbins method	33,33	36,11	8,34
GPDC method	31,67		14,02

Table 11.11. Comparison between software and Perry's values of ΔP validation.

After applying the complex equations of the pressure drop curves deduced from the statistical regressions done by Minitab, the software results are very similar as the eye-graphical methods. For this reason, it can be concluded that the precision for this calculation is very satisfactory.

11.6. Potential carcinogenic risk

For the human health validation, it is used an study of the carcinogenic risk associated with THMs carried on in Taiwan, specifically, on Taipei City [1]. All the input data required is already introduced in Section 4.3. in Table 4.1., Table 4.2., Table 4.3. and Table 4.4.. Moreover, the initial concentrations are also extracted from [1] (Table 3):

<i>THM species</i>	$CHCl_3$	$CHCl_2Br$	$CHClBr_2$	$CHBr_3$
$C_{THM,w}$	5,9	4,3	2,8	1,9

Table 11.12. Input data of carcinogenic risk validation.

Comparing both results for the different pathways:

<i>Lifetime cancer risk</i>	<i>Accordingly to [1]</i>	<i>Software results</i>
<i>Ingestion</i>	$0,66 \cdot 10^{-5}$	$0,88 \cdot 10^{-5}$
<i>Dermal</i>	$0,01 \cdot 10^{-5}$	$0,01 \cdot 10^{-5}$
<i>Inhalation</i>	$1,22 \cdot 10^{-5}$	$1,50 \cdot 10^{-5}$

Table 11.13. Comparison between software and [1] (Table 4) values of carcinogenic risk validation.

Even though the software results are not equal than the base source, it cannot be considerate as a big error due to: On one hand, because the lack of precision in the input data (small initial concentrations; there is just 1 decimal) and, on the other hand, as the concentration determined in all the samples are not the same, in [1] a log-normal distribution is assumed for the input data of exposure as well as risk assessment. However, the software is just based on the mean values without taking into account the standard deviation of them.

For these reasons, it can be said that the software calculations approach cancer risk values sufficiently to be able to assess if there is any probability that a big carcinogenic risk exists.

12. CASES OF STUDY

12.1. Sant Joan Despí DWTP (Spain)

12.1.1. Site considerations

BARCELONA METROPOLITAN AREA (BMA)	
Size [km ²]	635
Population [million inhabitants]	4,5
Drinking water supply network based on	<i>Llobregat and Ter Rivers</i>
LLOBREGAT RIVER	
Waste Water Treatment Plants (WWTPs) [units]	30
SANT JOAN DESPÍ DWTP	
Maximum treatment capacity [m ³ /s]; [L/min]	5,5; 330.000
Drinking water provided to BMA [%]	50

Table 12.1. General data of the case of study.

The water supplied in Barcelona Metropolitan Area (BMA) comes mainly from the surface water resources from Llobregat and Ter Rivers. They are constantly suffering the effects of industrial discharges of urban and industrial wastewater mixtures so, it is crucial the role WWTPs play to remove contaminants. However, it is Sant Joan Despí DWTP, situated at the lower part of Llobregat River, which provides almost the 50% of the annual drinking water in BMA (see Figure 12.1.). Accordingly to [3] its main water treatment line is:

Pre-oxidation with chlorine dioxide (ClO_2) as a primary disinfectant because its low cost.
Pre-treated water is clarified in flow solid contact clarifiers with previous addition of chemical species to promote sedimentation (coagulation and flocculation).
Clarified water is passed through sand filters and ground water is added.
Ozonisation (O_3) and granular activated carbon (GAC) filtration.
Finally, the water is further disinfected with chlorine (Cl_2).

Table 12.2. Water treatment process steps.

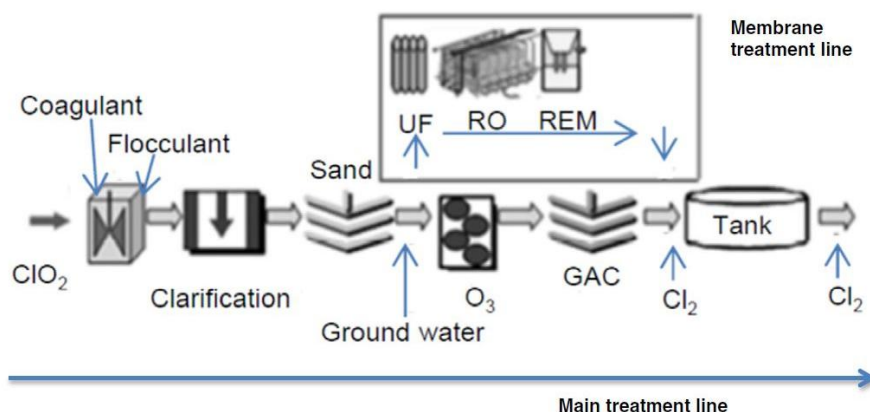


Figure 12.1. Main lines of Sant Joan Despí DWTP.

In 2009, a membrane treatment line began its operation. It is placed after the sand bed filtration where the flow is splitted and the 50% is treated in the new process. The main step in the new implementation is the reverse osmosis (RO) which carries on a concentration reduction of the DBPs precursors (bromide, iodide and organic matter). Before, the flow is pre-treated via ultrafiltration (UF) and micro-coagulation as a protection for the RO step. Finally, the water is remineralised (REM) and mixed with water from the conventional process.

12.1.2. Software input data

In this case of study, the idea is to compare the membrane treatment line (50% of the water flow) with the possibility to install a stripping column at the end of the conventional process (100% of the water flow) to remove part of the THMs formed and reduce the risk associated.

At the inlet of the DWTP, there is not any appreciable risk index associated with THMs because raw water normally does not carry on them (in general, there are organic matter and some THMs precursors). It is at the outlet of the DWTP, after the disinfection process takes place, when their presence can be detected.

Comparing THMs species evolution before and after the implementation of the new membrane treatment line, a reduction of them is noticed:

$C_{THM,w}$	$CHCl_3$	$CHCl_2Br$	$CHClBr_2$	$CHBr_3$
Year: 2008	9,37	18,65	28,84	39,65
Year: 2012	0,62	0,63	4,28	16,13

Table 12.3. Annual average concentration [$\mu g/L$] of THMs at the outlet of the DWTP.

So, the total THMs concentration at the outlet stream in 2012 is the equivalent software input parameter necessary to obtain the same outlet health risk: $C_{THMs,bottom} = 21,66 \mu\text{g/L}$.

It should be highlighted that, when the new EU law was applied (1st of January of 2009), in order to force Sant Joan Despí DWTP to follow the legislation, the membrane treatment line was installed and began its operation to reduce the total THMs concentration level.

12.1.3. Software results

With the aim to obtain the same water quality and treat the equivalent quantity (330.000 L/min) of the current DWTP (with membrane technologies), this project pretends to evaluate the possibility to install a stripping column taking the same concentrations data:

- At the top of the stripping column: $C_{THM,w}$ of 2008.
- At the bottom of the stripping column: $C_{THMs,bottom} = 21,66 \mu\text{g/L}$ of 2012.

```
>> STRIP
Which is the system you want to treat: WATER(THMs)-AIR (Input: 1) or GENERIC SYSTEM (Input: 2)? 1
Which is the initial concentration of CHCl3 dissolved in the water [microg/L]? 9.37
Which is the initial concentration of CHCl2Br dissolved in the water [microg/L]? 18.65
Which is the initial concentration of CHClBr2 dissolved in the water [microg/L]? 28.84
Which is the initial concentration of CHBr3 dissolved in the water [microg/L]? 39.65
Which is the final desired concentration of THMs in the water [microg/L]? 21.66
Which is the flow of liquid needed to treat [L/min]? 330000
Which type of filling do you want: CERAMIC (Input: 1), METAL (Input: 2) or PLASTIC (Input: 3)? 3
```

Figure 12.2. Software input data to treat all the water flow of Sant Joan Despí DWTP.

So, using the software, the parameters related with the stripping tower are determined:

Initial risk	$1,483 \cdot 10^{-4}$	Final risk	$3,327 \cdot 10^{-5}$
% Removed	77,56	G_L	$4,84 \cdot 10^6$
H_{column}	17,43	D_i	10,95
ΔP	4,03	Investment	13,54 M€
Filling type	ENVIPAC RING (Plastic – $3\frac{1}{8}$ in.)		

Table 12.4. Mechanical parameters of a single stripping column that treats all the DWTP flow.

Accordingly to [12], there are some limitations of a stripping column dimensions that come from the standard values between they should vary:

- H_{column} : 1 – 15 m.
- D_i : 0,5 – 3 m.
- ΔP : < 50 mmH₂O/(column m).

Obviously, due to the enormous amount of liquid needed to treat, this column is almost 4 times wider than a normal one.

A possible solution is to divide the flow at the outlet of the conventional treatment of the DWTP in different columns. Consequently, while the rest of parameters remain constant due to the species and its concentrations do not change, the new diameter of each column and the required gas can be deduced from the number of stripping columns needed to treat all the water flow:

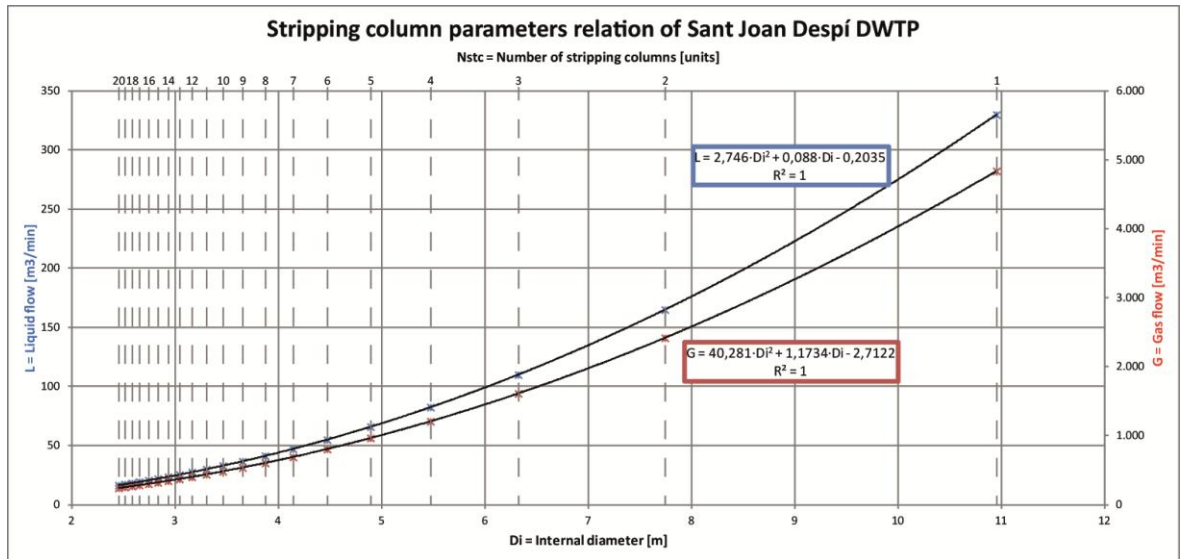


Figure 12.3. Stripping column parameters of Sant Joan Despí DWTP.

Analysing Figure 12.3., the blue point at the top on the right, represents the data introduced in the software to treat all the water flow with just one column. Splitting several times (number of stripping columns) the total flow needed to treat and calculating the diameter and the gas flow required for each case with the software, the rest of the diagram can be drawn.

Consequently, to fulfil the diameter restriction ($\leq 3\text{ m}$), using the regression curve, the most suitable stripping tower that should be used can be designed by:

$$L = 2,746 \cdot D_i^2 + 0,088 \cdot D_i - 0,2035; D_i \leq 3\text{ m} \quad \text{Eq. 12.1.}$$

So, the maximum water flow able to treat for a single column with a diameter of 3 m for Sant Joan Despí DWTP case is: $L_{max} = 24,775\text{ m}^3/\text{min}$. However, accordingly to Figure 12.4., between 13 and 14 stripping columns are required for this limit conditions. As the number of stripping columns must be integer, the maximum number of those two is selected: 14 (see Figure 12.5. to understand the final configuration).

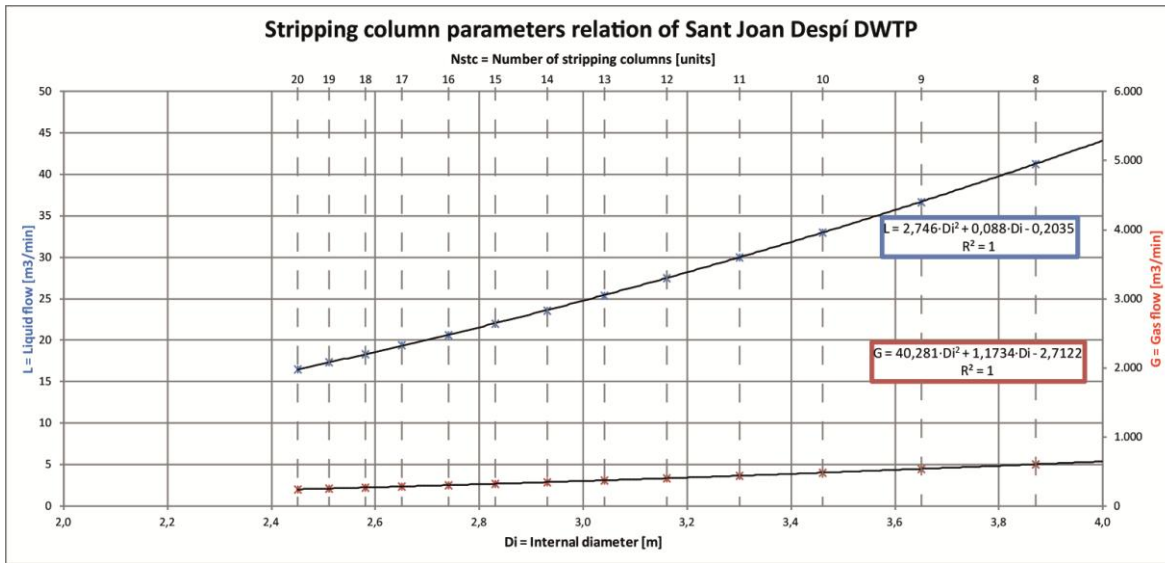


Figure 12.4. Zoom of Figure 12.3..

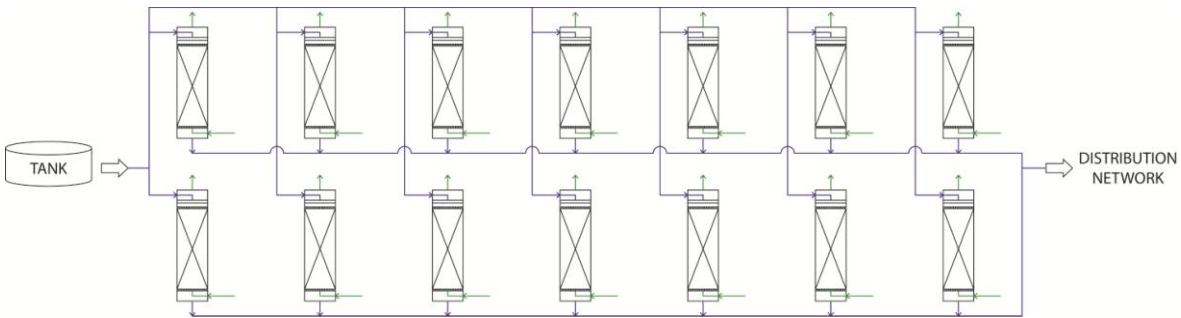


Figure 12.5. Stripping columns combination to treat all the water flow of the conventional line.

In addition, studying each column as an independent part of the whole system:

```
>> STRIP
Which is the system you want to treat: WATER(THMs)-AIR (Input: 1) or GENERIC SYSTEM (Input: 2)? 1
Which is the initial concentration of CHCl3 dissolved in the water [microg/L]? 9.37
Which is the initial concentration of CHCl2Br dissolved in the water [microg/L]? 18.65
Which is the initial concentration of CHClBr2 dissolved in the water [microg/L]? 28.84
Which is the initial concentration of CHBr3 dissolved in the water [microg/L]? 39.65
Which is the final desired concentration of THMs in the water [microg/L]? 21.66
Which is the flow of liquid needed to treat [L/min]? 23571
Which type of filling do you want: CERAMIC (Input: 1), METAL (Input: 2) or PLASTIC (Input: 3)? 3
```

Figure 12.6. Software input data for each single column purposed for Sant Joan Despí DWTP.

Initial risk	$1,483 \cdot 10^{-4}$	Final risk	$3,327 \cdot 10^{-5}$
% Removed	77,56	G_L	$0,35 \cdot 10^6$
H_{column}	17,43	D_i	2,93
ΔP	4,03	Investment	2,78 M€

Filling type	<i>ENVIPAC RING (Plastic – $3\frac{1}{8}$ in.)</i>
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Table 12.5. Basic parameters of each stripping column.

The resultant graphics the software show as outputs are:

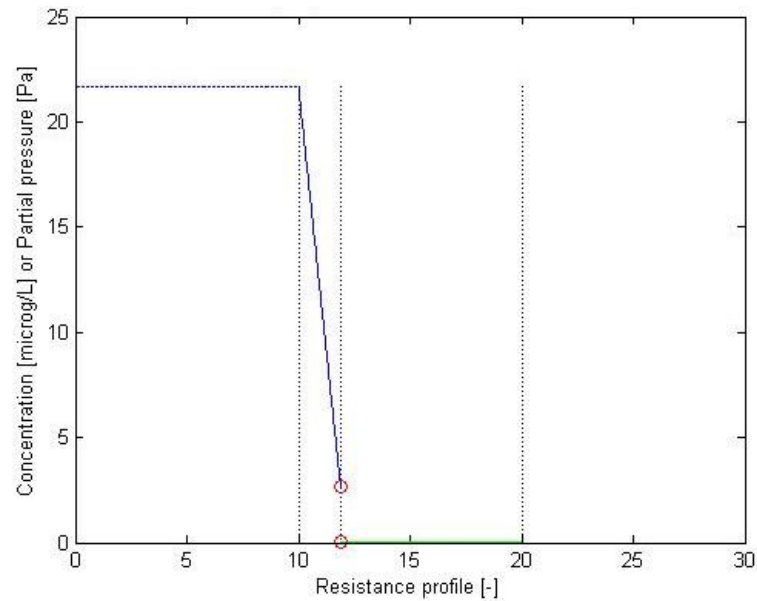


Figure 12.7. Double film theory representation at the bottom of the column.

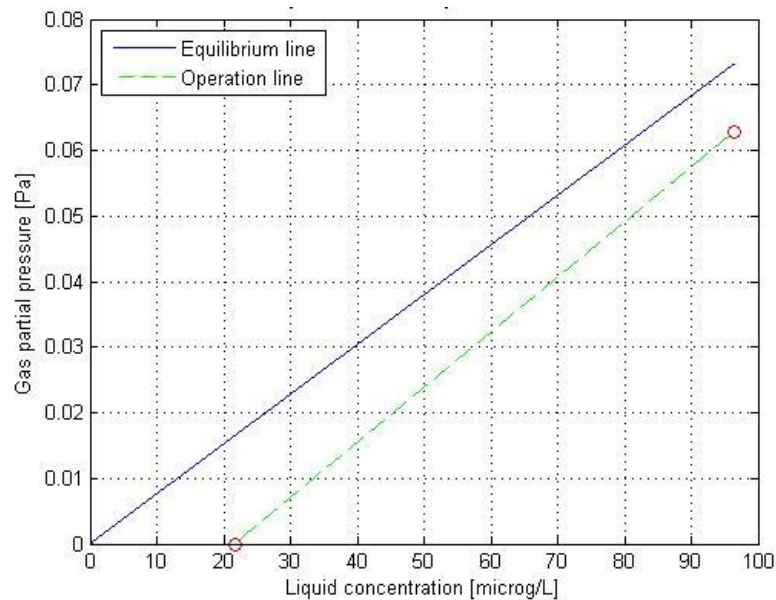


Figure 12.8. Equilibrium and operation lines of the stripping system.

More precise and detailed numerical data results can be found on Annexes (Section 18.7.).

As in the case of study, it is searched to maintain the quality of the final drinking water, the



same human health risk indexes ($3,327 \cdot 10^{-5}$), once the technical details between the current technology and the stripping tower are compared, the economical factor must be taken into account for the viability of the project.

Although the economical budget of the membrane technology is not available and the cost comparison impossible, installing each stripping column to get similar health result costs around 2,78 M€. Proportionally, the economical approach of the whole system is 38,92 M€.

Finally, comment that this pattern can be followed in other studies, apart from the THMs case, to compare the viability of installing a stripping column as an alternative.

12.2. Hypothetical neighbourhood

12.2.1. Site considerations

In contrast with Section 12.1. where the aim is to study the possibility to implement a stripping column technology in a big scale (a DWTP), in this small scale scenario, it is analysed the option to install this equipment in an hypothetical neighbourhood. The data used is extracted from another DWTP in Spain:

GUADALMELLATO RESERVOIR	
Total water volume [hm ³]	145
Medium pluviometry [mm/year]	575
Tributary rivers	Guadalbarbo, Cuzna, Matapuercas and Varas
CÓRDOBA DWTP	
Maximum treatment capacity [m ³ /day]	180.000
Population supplied [inhabitants]	300.000

Table 12.6. General data of the case of study.

Accordingly to [31], THMs concentrations were determined using accurate and sensitive methods at 7 different points in the DWTP and its distribution network collecting samples in the four seasons of the year. In general, the plant uses chlorine dioxide (ClO_2) and chloramines (NH_2Cl) as disinfectants and its main scheme from the raw water until the distribution network is:

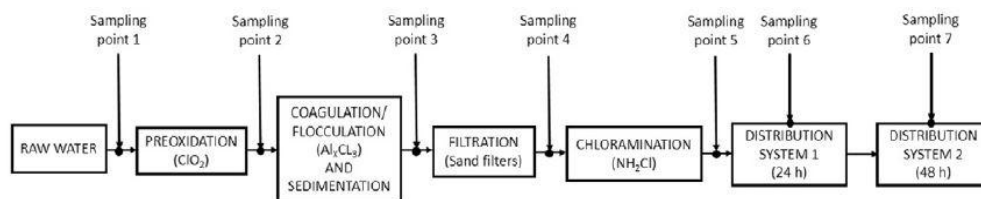


Figure 12.9. Principal steps of the water treatment process and location of the 7 sampling points.

DWTP steps
Pump high quality water (without direct input of wastewater) from the reservoir.
Pre-oxidation with chlorine dioxide (ClO_2).
Coagulation, flocculation (Al_xCl_3) and sedimentation: pre-treated water in flow solid contact clarifiers with addition of aluminium polychloride.
Filtration: clarified water is passed through sand filters.
The water is further disinfected with chloramines (NH_2Cl).
Extra additions of ammonia and free chlorine separately and chloramines are formed in situ.
The water circulates in the distribution systems after 24h and 48h from the DWTP exit.

Table 12.7. Water treatment process details.

12.2.2. Spatial and seasonal variability of THMs concentrations

From Figure 12.9., the results of THMs concentrations obtained by sampling at points 1-7 during the 4 seasons are:

Season	Water T average	SP1	SP2	SP3	SP4	SP5	SP6	SP7
Spring	22	0	0,44	2,0	3,0	10,0	12,0	15,0
Summer	29	0	0,32	1,4	2,4	7,9	13,0	22,0
Autumn	19	0	0,17	0,6	1,7	5,8	7,1	8,4
Winter	12	0	0,12	0,4	1,2	4,0	5,0	5,7

Table 12.8. THMs concentration [$\mu g/L$] depending on the seasons and the sampling points.

As can be seen from Table 12.8., important facts are deduced:

- None of the 4 main THMs was found in raw water at any time. Therefore, their presence on the treated water can be exclusively ascribed to the process of

disinfection.

- The concentration of THMs in the finished water (SP5) change between months: spring>summer>autumn>winter.
- No sample presented total THM concentrations above the levels allowed by US EPA (80 $\mu\text{g/L}$) or EU (100 $\mu\text{g/L}$) legislations even in the worst case.

$SP_{initial}$	SP_{final}	$\%(\Delta C_{THMs})$	<i>Results explanation</i>
SP1	SP2	–	Reaction of ClO_2 with organic matter and precursors.
SP2	SP3	230 – 350	Coagulation, flocculation and sedimentation.
SP3	SP4	50 – 200	Filtration does not remove THMs.
SP4	SP5	230 – 240	Reaction of NH_2Cl with organic matter and precursors.
SP5	SP6	20 – 65	Residual disinfectant reacting with organic matter.
SP6	SP7	230 – 240	

Table 12.9. THMs concentrations evolutions along the sampling points (SPs).

12.2.3. Software input data and results

In this scenario, the idea is to focalise the case of study in a small scale to check the viability of installing a single stripping column in order to improve the quality of the water for a part of the population, for example, for a neighbourhood.

Accordingly to the information of Table 12.6., the ratio water flow – inhabitants is:

$$\frac{180.000 \text{ m}^3/\text{day}}{300.000 \text{ inhabitants}} = 0,6 \frac{\text{m}^3/\text{day}}{\text{inhabitants}} = 0,42 \frac{\text{L}/\text{min}}{\text{inhabitants}} \quad \text{Eq. 12.2.}$$

Then, assuming that almost all the THMs concentration is due to chloroform ($CHCl_3$) and studying the worst case between the spatial and seasonal variability (22 $\mu\text{g/L}$ at SP7 in the summer), the height and the diameter of the stripping column, depending on the outlet $CHCl_3$ concentration, are:

$H_{column}; D_i$		$C_{THMs,bottom}$		
<i>Inhabitants</i>	L_L	15	10	5
1.000	420	2,07; 0,29	5,55; 0,29	18,01; 0,29
3.000	1.260	2,07; 0,50	5,55; 0,50	18,01; 0,50

100.000	42.000	2,07; 2,89	5,55; 2,89	18,01; 2,89
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Table 12.10. Stripping column dimensions depending on neighbourhood conditions and targets.

Consistent with Table 12.10., it can be said that, for these specific conditions, a single stripping column can treat $1.260 L/min - 42.000 L/min$ accordingly to the standard diameter values (it should not be lower than $0,5 m$ or greater than $3 m$ [12]). Then, Eq. 12.2. allows to relate these amounts to the water supplied to $3.000 - 100.000$ inhabitants of Córdoba..

For example, for an hypothetical case, it could be interesting to supply water to around 3.000 inhabitants of a neighbourhood with a potential carcinogenic risk improved more than 50% :

```
>> STRIP
Which is the system you want to treat: WATER(THMs)-AIR (Input: 1) or GENERIC SYSTEM (Input: 2)? 1
Which is the initial concentration of CHCl3 dissolved in the water [microg/L]? 22
Which is the initial concentration of CHCl2Br dissolved in the water [microg/L]? 0
Which is the initial concentration of CHClBr2 dissolved in the water [microg/L]? 0
Which is the initial concentration of CHBr3 dissolved in the water [microg/L]? 0
Which is the final desired concentration of THMs in the water [microg/L]? 10
Which is the flow of liquid needed to treat [L/min]? 1260
Which type of filling do you want: CERAMIC (Input: 1), METAL (Input: 2) or PLASTIC (Input: 3)? 3
```

Figure 12.10. Software input data for each a hypothetical neighbourhood of 3.000 inhabitants.

The stripping column designed by the software (check Annexes; Section 18.8.) is:

Initial risk	$2,596 \cdot 10^{-5}$	Final risk	$1,180 \cdot 10^{-5}$
% Removed	54,55	G_L	7.457
H_{column}	5,55	D_i	0,5
ΔP	25,48	Investment	0,22 M€
Filling type	HIFLOW RING (Plastic - $3\frac{1}{2}$ in.)		

Table 12.11. Basic parameters of the stripping column.

12.3. San Diego, Carabobo region (Venezuela)

12.3.1. Site considerations

Once extreme scenarios have been studied on Section 12.1. and Section 12.2., a 3rd intermediate case of study is selected to combine their positive features.

Carabobo region is located in the central part of Venezuela and it has a population of almost 2 million inhabitants. The water distribution is done by 2 different pumped systems known as 'Sistema Regional del Centro I' (SRC-I) and 'Sistema Regional del Centro II' (SRC-II). The



first one is constituted by ‘embalse Pao-Cachinche’ and ‘Alejo Zuloaga’ DWTP. On the other hand, SRC-II consists of ‘embalse Pao-La Balsa’ and ‘Lucio Baldo Soules’ DWTP.

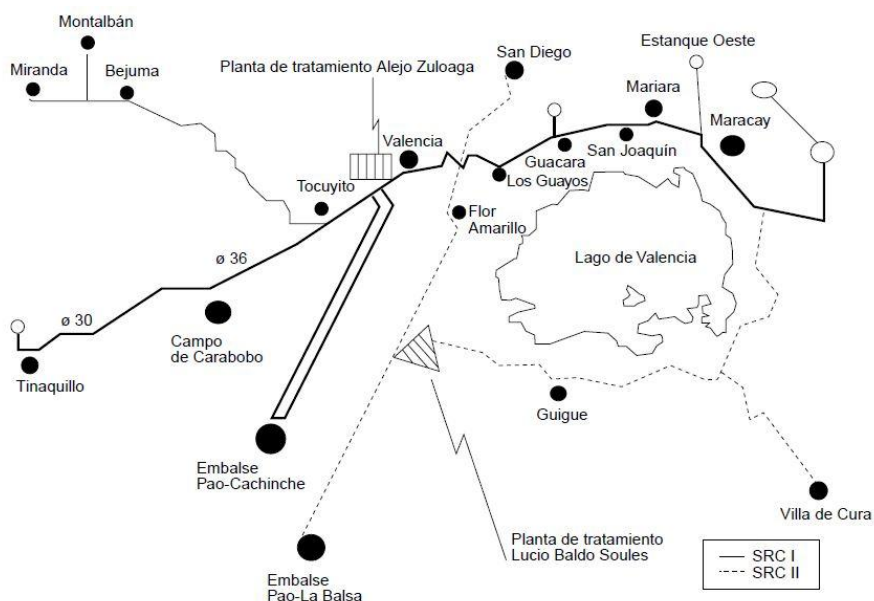


Figure 12.11. Distribution of the drinking water systems.

The interesting point is that due to the high organic matter accumulated on ‘embalse Pao-Cachinche’, high doses of chlorine are required to disinfect the water. Accordingly to [32], probably as a consequence of the sun exposure (higher temperature), THMs concentrations are above Environmental Protection Agency (EPA) limits $80 \mu\text{g}/\text{L}$ in San Diego water. This fact can provoke important negative health effects on the population supplied.

12.3.2. Software input data

Assuming that the normal San Diego water consumption ratio is $180 \text{ L}/(\text{day} \cdot \text{inhabitant})$ and that there are around 120.000 people living in that city, the water flow needed to treat for the stripping tower (input of the software) is $15.000 \text{ L}/\text{min}$. Moreover, the corresponding concentrations determined by [32] are:

CHCl_3	CHCl_2Br	CHClBr_2	CHBr_3
70	10	2	0

Table 12.12. Annual average concentration of THMs [$\mu\text{g}/\text{L}$] at the outlet of the DWTP.

12.3.3. Software results

Representing the relation between the stripping column height and the final carcinogenic risk depending on the final THMs concentration ($C_{\text{THMs}, \text{bottom}}$) introduced in the software:

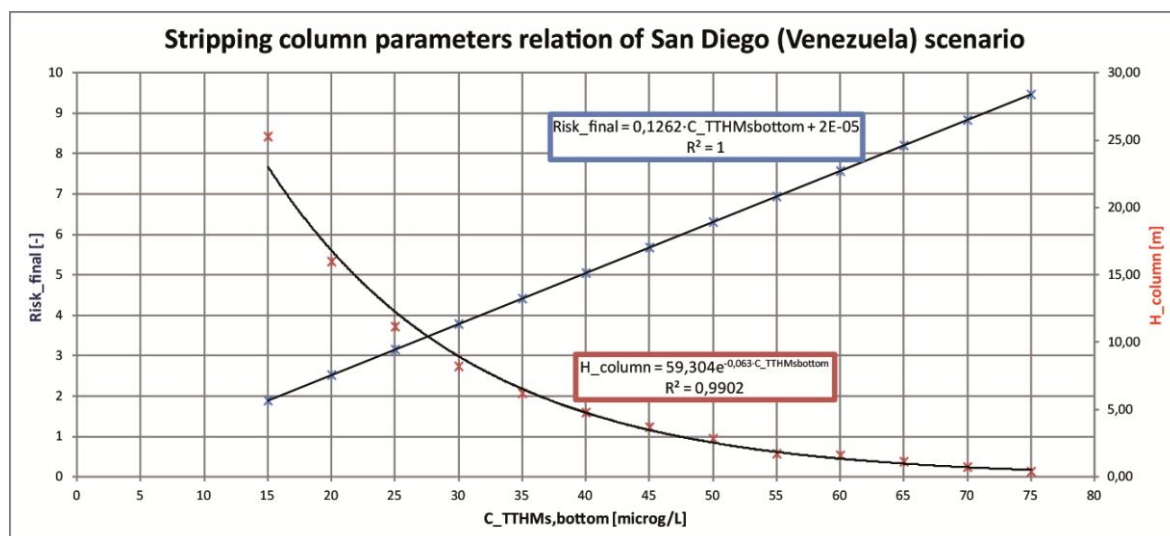


Figure 12.12. Stripping column parameters of San Diego scenario.

Following the same pattern as the other studied cases, as the standard values of the stripping column height varies between 1 to 15 meters, the range of the $C_{TTHMs,bottom}$ is: $64,8 \mu\text{g}/\text{L} - 21,8$. Obviously, due to the fact that the stripping column would be located after Carabobo distribution system and before all the water is supplied to the population, it is wanted the smallest value as possible due to the lower health risk associated. So:

```
>> STRIP
Which is the system you want to treat: WATER (THMs)-AIR (Input: 1) or GENERIC SYSTEM (Input: 2)? 1
Which is the initial concentration of CHCl3 dissolved in the water [microg/L]? 70
Which is the initial concentration of CHCl2Br dissolved in the water [microg/L]? 10
Which is the initial concentration of CHClBr2 dissolved in the water [microg/L]? 2
Which is the initial concentration of CHBr3 dissolved in the water [microg/L]? 0
Which is the final desired concentration of THMs in the water [microg/L]? 21.8
Which is the flow of liquid needed to treat [L/min]? 15000
Which type of filling do you want: CERAMIC (Input: 1), METAL (Input: 2) or PLASTIC (Input: 3)? 3
```

Figure 12.13. Software input data of San Diego scenario.

Initial risk	$1,035 \cdot 10^{-4}$	Final risk	$2,752 \cdot 10^{-5}$
% Removed	73,41	G_L	93.502
H_{column}	13,95	D_i	1,73
ΔP	25,48	Investment	0,22 M€
Filling type	HIFLOW RING (Plastic - $3\frac{1}{2}$ in.)		

Table 12.13. Basic parameters of the stripping column.

For further details of this case, check Annexes; Section 18.9..



12.4. Cases of study comparison

The idea of Sant Joan Despí DWTP and San Diego studies is to fulfil the legislation and, consequently, indirectly reduce the carcinogenic potential risk of the final water. In contrast, the aim of installing a stripping column in a hypothetical neighbourhood is to improve the water consumption quality. This fact can also be justified by the higher order of risk indexes on the 1st and 3rd cases than on the 2nd one.

On one hand, whereas in all the cases the initial potential carcinogenic risk is exactly calculated due to each THM specie concentration is known, the risk at the end is just approached because it is known the total (instead the individual) THMs concentration. This fact is because it is not logic to introduce each final concentration desired while in the legislation it is taken into account the sum of THMs. Therefore, the health risk improved is exactly the same than the percentage of THMs removed due to the direct proportion between THMs concentration and risk indexes (maintaining the rest of scenario parameters constant). So, the health risk enhancement on the 3 studies can be approached into 77,56%, 54,55% and 73,41% respectively.

On the other hand, once the inlet and outlet risk of the stripping column are numerically calculated and the cost of the equipment approached, as the population of each case of study is known, it is possible to quantify *how much costs to save a human life*:

$$Ratio_{cost/life} = \frac{Investment}{(Initial\ risk - final\ risk) \cdot Population} \quad \text{Eq. 12.3.}$$

	Case 1	Case 2	Case 3
Initial risk	$1,483 \cdot 10^{-4}$	$2,596 \cdot 10^{-5}$	$1,035 \cdot 10^{-4}$
Final risk	$3,327 \cdot 10^{-5}$	$1,180 \cdot 10^{-5}$	$2,752 \cdot 10^{-5}$
Population	2.250.000	3.000	120.000
Investment [M€]	38,92	0,22	0,22
Number of stripping columns	14	1	1
Ratio cost/life [€/life]	150.000	5.180.000	24.000

Table 12.14. Health risk versus economical comparison for each case of study.

Being conscious the hypothesis taken into account, the 3rd case of study is the most suitable scenario where a stripping column should be used. Firstly, justified by the fact that this current scenario does not fulfil the legislation and, secondly, because the cost to save a human life is just 24.000 €; 6 and 216 times cheaper than the other cases.

13. PROJECT MANAGEMENT

13.1. Time programming

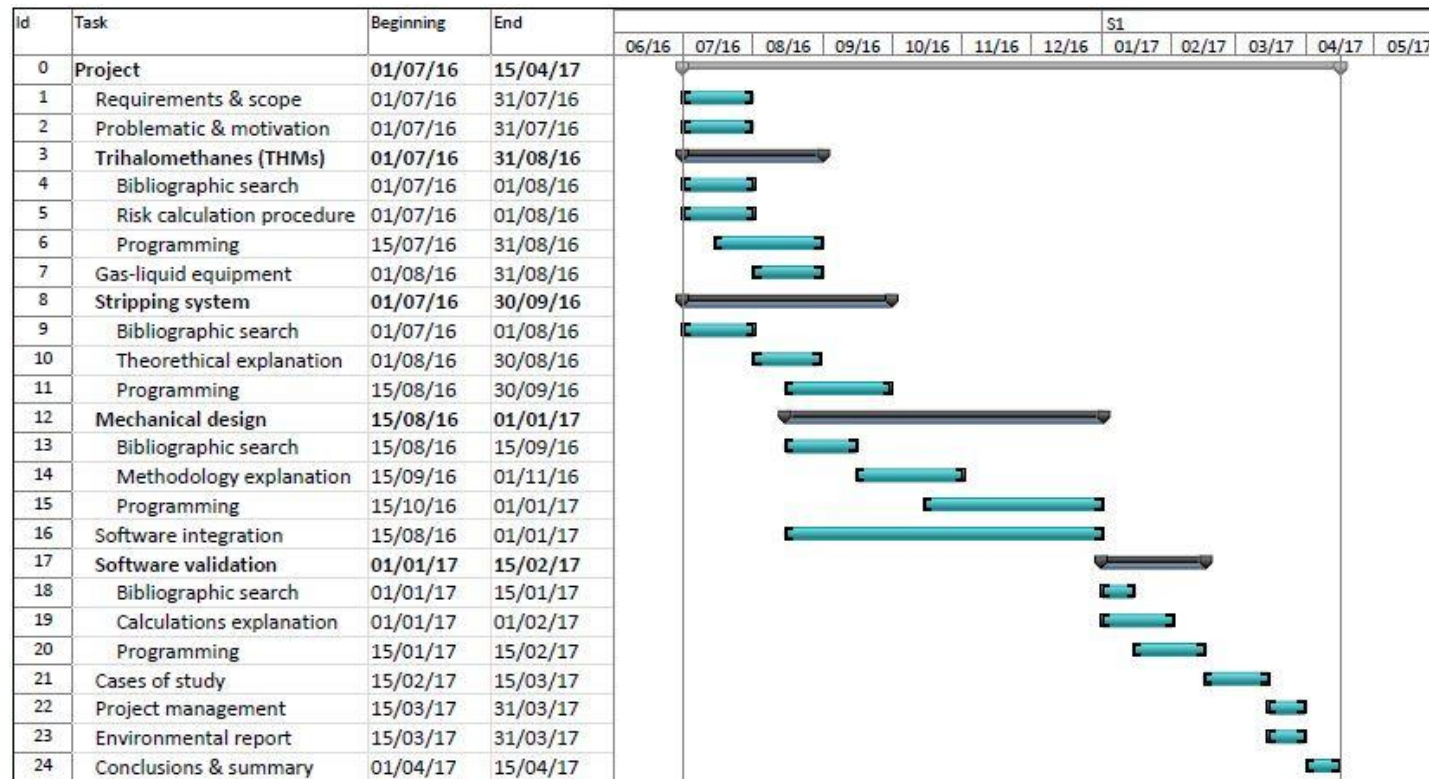


Figure 13.1. Gantt diagram.



13.2. Total cost of the project

The total cost is divided into economic evaluation of the human resources employed and the material needed to do the project. On one hand, about the first item, it is considerate that a junior engineer carried on the whole parts of the project. Accordingly to Gantt diagram, the project is developed along 9 months with a load of work per week of 20 hours. As a result, in total, the project needs around 700 hours for its execution. In addition, the council taxes applied on its salary are already considerate in the fix cost.

On the other hand, about the second item, there is a single concept included where some non-quantifiable costs are approach as a proportion of the direct costs.

Human resources	Quantity [h]	Fix cost [€/h]	Cost [€]
Design	250	20	5.000
Memory elaboration	250	15	3.750
Software development	200	15	3.750
Material resources			Cost [€]
Computer, mouse, keyword...			400
Software licences			350
Office material (scan, paper, calculator...)			50
Costs			13.300
Indirect costs (electricity consumption, internet, taxes...) = 10%			1.330
Total costs of the project			14.630

Table 13.1. Calculation of the total costs of the project.

14. ENVIRONMENTAL REPORT

14.1. Introduction

To achieve a successful project, it is extremely important to take into account the balance between the following points of view:



Figure 14.1. Common impacts studied in any project.

Although they are independently studied, each of them depends on the other ones. For example, an improvement in drinking water quality increases the need of energy and material resources and, consequently, the overall environmental impact of the system becomes bigger. Or, when a high efficient technology is used to improve the quality of the water, the economical costs rises exponentially. Nevertheless, the most difficulty is to extrapolate the data and evaluate the cost/benefit of each part of the system and choose the best solution over another technology.

14.2. Environmental effects

In general, the influence of this project on the environment can be almost neglected because it consists on the design of a software which involves relatively little computer and calculator energy consumptions, paper, ink and complementary office materials (similar than [33]).

On the other hand, the project can indirectly have a big impact if its installation is implemented in reality as a pilot plant or in an industrial context. The environmental benefit criteria evaluating the new process should be particularized, what makes necessary to specify data of each situation: electricity consumption, materials, machines, chemicals... during the construction stage, its cleaning, and while it is operating (producing drinking water). For example, if the stripping technology pretends to replace another process, both installations needs environmental studies to be compared.

Then, once the necessary information is recollected, specific software (like Simapro v7.3.3.) is normally used to evaluate different environmental impacts categories such as [3]:

- Climate change
- Human toxicity
- Fossil depletion
- Ozone depletion
- Freshwater eutrophication
- Metal depletion

So, in order to select the most environmental friendly technology for drinking water production, detailed information of each situation is necessary. Due to the information limited access, this project just introduces what must be taken into account for a detailed study if exists any plan to continue the construction of a stripping column.

14.3. Alternatives to minimize by-products concentration

Since the beginning, the development of the software is focused on the final user: the operator engineer. However, its origin comes from to reduce the potential carcinogenic risk of disinfected water to achieve benefits on population health. The fact that users will consume the water treated for this installation is the first motion of the stripping columns design. In contrast, there are other strategies to improve the drinking water quality:

- Change the origin of the water (less organic matter or initiators).
- Change the disinfection product or products.
- Change the filter process: active carbon instead sand (reduce organic matter).
- Minimize doses of disinfectant and contact time.
- Optimization of reuses of disinfectant products in the network.
- Use membrane technologies: reverse osmosis (RO), nanofiltration (NF) and reverse electrodialysis (RED).

Once the alternatives are defined, the next step is to select the suitable water treatment process depending on each particular case. Around Europe, there are different Drinking Water Treatment Plants (DWTPs) that tries to apply these methodologies to improve the quality of the water. So, this project studies the stripping columns as another option justified by the fact that it is not normally taken into account despite the economical and technical limitation of the current processes.

14.4. Evaluation

The main conclusion of the environmental report is that the development of this project is green-friendly due to the few impact on nature it involves as it is based on a theoretical study and a software development. At the same time, if a hypothetical construction of the installation occurs, it also suggests the necessity of a more detailed study about the impacts: control, eventual difficulties plan, measures of correction, prevention and minimisation for significant effects... In addition, accordingly on its features (permanent or temporal, short or long, along the construction, operation and abandon...) the best technology and the most suitable location must be chosen searching the minimum impact.

15. CONCLUSIONS

This bachelor's thesis mainly consists on the development of a software, called STRIP, for the design of stripping columns to remove trihalomethanes (THMs) species formed in the water by disinfection treatments. Justified by the fact that THMs are risky for human health, their concentration must be reduced below certain legislated levels to prevent negative health impacts on population.

The first conclusion is the technical viability of stripping columns when little concentrations of the THMs are involved. In other words, although normally there are just parts per billion (ppb) or equivalently, $\mu\text{g}/\text{L}$, of THMs in the water, there is not necessary an enormous height of the equipment to achieve a correct mass transfer from the water to the gas.

Analyzing the results the software calculates from real studied cases (Sant Joan Despí DWTP, hypothetical neighbourhood and San Diego), interesting conclusions are highlighted:

	Case 1	Case 2	Case 3
Initial risk	$1,483 \cdot 10^{-4}$	$2,596 \cdot 10^{-5}$	$1,035 \cdot 10^{-4}$
Final risk	$3,327 \cdot 10^{-5}$	$1,180 \cdot 10^{-5}$	$2,752 \cdot 10^{-5}$
L_L	23.571	1.260	15.000
% Removed	77,56	54,55	73,41
H_{column}	17,43	5,55	13,95
D_i	2,93	0,50	1,73
Number of stripping columns	14	1	1
Investment [M€]	38,92	0,22	0,22
Ratio cost – life [€/life]	150.000	5.180.000	24.000

Table 15.1. Cases of study comparison.

Regarding on the initial investment and their direct proportion on the water flow treated, the rough estimations for each case of study are 38,92 M€ for the 1st case and 0,22 M€ for the 2nd and 3rd cases. Be noticed that any of them are not affected by the efficiency because their value is lower than 90%. Being conscious the big estimation done, the most viable situation looks San Diego scenario due to the relation between the investment and the people affected is more satisfactory: relatively low technological cost (24.000 €) allows to save a human life between the users population. Moreover, it is the only case where the legislation is not fulfilled and the carcinogenic risk more potential for the human health.



Apart from these general facts, there is a positive linear tendency between the percentage removed of THMs and the risk associated: it is because the direct proportion between the initial and final species concentrations and risk indexes.

Furthermore, there is another relation between the elimination ratio and the height of the stripping column. Accordingly to Table 15.1., as much THMs are removed, as higher the tower must be. In the 3rd case of study, this tendency is a positive exponential. Following the same patten, if more water is needed to treat, more counter-currently gas flow is required and a greater diameter of the stripping tower is necessary (wider section). In the 1st case of study, both correlations are quadratic. Apart from that, the wall thickness also increases. Although depending on the features of each situation, the relation can differ, be noticed about the potential tendencies between the stripping system and the mechanical design of the stripper:

- When the percentage removed increases, the height of the stripping column also increases although the biggest concentration gradient between the top and the bottom of the tower. Specifically, if the species and the filling type selected are the same, k_l and k_g remain constant and, consequently, H_G doesn't change while N_G varies due to the concentrations variation.
- When the liquid flow increases, the diameter of the stripping column and the gas flow required also increase while the height remains constant.

Additionally, in order to ensure a correct performance of the stripping column, it is useful to check that the pressure drop is below the normal limits ($\Delta P < 50 \text{ mmH}_2\text{O}/(\text{column } m)$) in all cases. In fact, its value is always around $25 \text{ mmH}_2\text{O}/(\text{column } m)$ and flooding is further to occur. This right behaviour is justified by the limitation of the gas operating velocity and the buckle done by STRIP to check the limits of the pressure drop diagram. For this reason, other input parameters like the properties of the species involved or concentrations gradient have relative influence on the final design because the software is optimised to design a column able to perform correctly as its priority over the possibility to achieve big mass transfer without safety operations.

Furthermore, as a result of the low final concentration of THMs at the top of the stripping column on the outlet gas on the 3 cases of study ($5,10 \mu\text{g}/\text{L}$, $2,03 \mu\text{g}/\text{L}$ and $9,60 \mu\text{g}/\text{L}$, respectively), it can also be thought that in any of them the resultant gas carries on considerable toxicity doses of THMs before human consumption: because their first dilution on the big amount of air used and a their second dilution at the top of the column with the environmental air.

Regarding on the mass transfer, the corresponding volumetric coefficients on the liquid phase ($k_l \cdot a$) and on the gas phase ($k'_g \cdot a$) are between $(6,30 \cdot 10^{-2} - 9,08 \cdot 10^{-2})$ 1/s and $(9,71 \cdot 10^{-3} - 1,63 \cdot 10^{-2})$ kmol/(m³ · s · bar) respectively for the 3 cases of study. At the same time, as the standard values of filling towers are usually inside the range $(4 \cdot 10^{-4} - 1,02)$ 1/s and $(3 \cdot 10^{-5} - 5,10 \cdot 10^{-1})$ kmol/(m³ · s · bar), it can be said that the designed columns for STRIP achieve a normal mass transfer on the liquid phase and a quick kinetic on the gas phase. Probably as a result the software selects the best type of filling (depending on the flows treated and on the species involved) to promote the mass transfer, the term related with the gas volumetric coefficient is relatively near the highest extreme of the typical values for filling reactors.

Complementing this information, in the double film representations (at the bottom of the stripping column) it can be seen that the gas film is the dominant phase. Consequently, as $R_G > R_L$, any reactant added in the water to chemically interact with THMs would not highly increase the mass transfer between phases due to the liquid film is not the controllable. In addition, in the stripping system diagrams it is very visual to relate what in reality happens: since the gas perspective, as its content in THMs at the bottom of column is almost zero, it tends to the equilibrium until the top of the column because the existing concentrations gradient. So, the operation line goes from the left to the right for the gas phase. On the other hand, the liquid follows the opposite tendency because it transfers part of THMs concentration. Therefore, taking the process in its globalism, the top of the stripping column is closer to the equilibrium than the bottom because the higher THMs content. This point can be assimilated to the 'concentrations pinch point' of any particular installation.

In fact, cycle of deep thinking should be analysis if more data was available. Even though, to experimentally validate the theoretical calculations, pilot plant studies should carried on to assess the performance of the stripping column in any global process. As a consequence of the wide initial idea, limitations are necessary to contextualise the project and focus its real purpose. In contrast, it can also be executed from other perspectives: For example, from a certain stripping column (H_{column} , S , filling features...) designed by STRIP, develop an alternative branch able to simulate its behaviour from a specific input. In other words, analyse the stability and sensibility of the system versus changes on the operating conditions and determine which factors (for example, $C_{A,top}$) affects which results (as $p_{A,top}$) to adjust them.



16. ACKNOWLEDGMENTS

Personally, I consider the family the most important what a person has. So, the first thought is always for them. Especially for my mother, the person who always takes care of me and who is always next to me in the difficult moments. As Kelly Clarkson said:

“My family and friends are my support system. They tell me what I need to hear, not what I want to hear, and they are there for me in good and bad times. [...] Their love for me is what’s keeping my head above the water.”

Then, I would like to appreciate the brilliant idea that Vicenç Martí, the director of this project, had. Apart from the interesting programming application, it is extremely pedagogic to relate these amounts of theoretical concepts in order to fulfill a need of a real case. At the same time, it is a pleasure to work with someone who is flexible, knows how to adapt and understands other points of view.

Especially for this project, the help of Toni Dalmases, Adrián López and Judit Duaigües was indispensable because their knowledge about the others software used.

Finally, to close this period of my life, I also want to say thank you to all the people who I met during these years. From all the classmates until the teachers going through the people who I met during the Erasmus program in Sweden. They are part of my life forever.

Since the first day, the academic level was extremely high and it was not any gift to arrive until here. Lots of effort, lot of suffering and a lot of sacrifice. However, all what I am today, as an engineer, is thanks to this. I consider that I am finishing the Bachelor’s Degree in Chemical Engineering with a level of knowledge, abilities and skills I could never imagine before starting. To be honest, I am proud of this experience, of being able to come to ETSEIB!

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18. ANNEXES

18.1. Deduction of Eq. 7.15.

The aim of this mathematical development (based on [15]) is to achieve:

$$\frac{1}{k_g''} + \frac{H_A}{k_l} = \frac{1}{K_G} = \frac{H_A}{K_L} \quad \text{Eq. 18.1.}$$

First of all, using Figure 7.3. it is possible to write:

$$H_A = \frac{p_A^{eq} - p_A^i}{c_A - c_A^i} \quad \text{Eq. 18.2.}$$

Then, Eq. 7.14. can be rewritten as:

$$K_G \cdot (p_A - p_A^{eq}) = K_G \cdot [(p_A - p_A^i) + (p_A^i - p_A^{eq})] \quad \text{Eq. 18.3.}$$

Complementing these expressions with Eq. 7.8.:

$$\frac{1}{K_G} = \frac{(p_A - p_A^i) + (p_A^i - p_A^{eq})}{k_l \cdot (c_A^i - c_A)} \quad \text{Eq. 18.4.}$$

Finally, accordingly to Figure 7.3 and combining Eq. 18.2. and Eq. 18.4, the first part of Eq. 18.1. is obtained:

$$\frac{1}{K_G} = \frac{1}{k_g''} + \frac{H_A}{k_l} \quad \text{Eq. 18.5.}$$

Carrying on a similar procedure, it is possible to get the second part of Eq. 18.1.:

$$H_A = \frac{p_A^{eq} - p_A}{c_A - c_A^{eq}} \quad \text{Eq. 18.6.}$$

At the end, joining all the expressions:

$$\frac{1}{K_G} = \frac{p_A - p_A^{eq}}{K_L \cdot (c_A^{eq} - c_A)} = \frac{H_A}{K_L} \quad \text{Eq. 18.7.}$$

18.2. Deduction of Eq. 7.18.

Starting with:



$$p_A^i = H_A \cdot c_A^i \quad \text{Eq. 18.8.}$$

$$r_A = a \cdot k_g'' \cdot (p_A - p_A^i) \quad \text{Eq. 18.9.}$$

$$r_A = a \cdot k_l \cdot (c_A^i - c_A) \quad \text{Eq. 18.10.}$$

The aim is to arrive at:

$$r_A = \frac{1}{\left(\frac{1}{k_g''} + \frac{H_A}{k_l}\right)} \cdot a \cdot (p_A - H_A \cdot c_A) \quad \text{Eq. 18.11.}$$

First, Eq. 18.10. can be rewritten as:

$$c_A^i = \frac{r_A}{a \cdot k_l} + c_A \quad \text{Eq. 18.12.}$$

Then, substituting Eq. 18.8. on Eq. 18.9.:

$$r_A = a \cdot k_g'' \cdot (p_A - H_A \cdot c_A^i) \quad \text{Eq. 18.13.}$$

Next, combining Eq. 18.12. and Eq. 18.13. and developing the result:

$$r_A = a \cdot k_g'' \cdot \left(p_A - H_A \cdot \left(\frac{r_A}{a \cdot k_l} + c_A \right) \right) = a \cdot k_g'' \cdot p_A - \frac{k_g'' \cdot H_A \cdot r_A}{k_l} - a \cdot k_g'' \cdot H_A \cdot c_A \quad \text{Eq. 18.14.}$$

Later, rearranging terms:

$$r_A \cdot \left(1 + \frac{k_g'' \cdot H_A}{k_l} \right) = a \cdot k_g'' \cdot (p_A - H_A \cdot c_A) \quad \text{Eq. 18.15.}$$

Afterwards, isolating the velocity term:

$$r_A = \frac{a \cdot k_g''}{\left(1 + \frac{k_g'' \cdot H_A}{k_l} \right)} \cdot (p_A - H_A \cdot c_A) \quad \text{Eq. 18.16.}$$

Finally, operating the terms of the first part of Eq. 18.16.:

$$r_A = \frac{a}{\left(\frac{1}{k_g''} + \frac{H_A}{k_l} \right)} \cdot (p_A - H_A \cdot c_A) \quad \text{Eq. 18.17.}$$

Obviously, at the end, it can be checked that Eq. 18.17. is equal to the initial goal: Eq. 18.11..

18.3. Parameterization of pressure drop curve

In order to calculate the pressure drop value, it is necessary to introduce the curves of Figure 8.3. in the software. To parameterize each line with an equation, it is used the statistical software Minitab.

At the beginning, it is good to analyze bivariant diagrams to detect possible non-common values and the possible relationships between the variables. For example for the flooding line ($125 \text{ mmH}_2\text{O}/(\text{column } m)$):

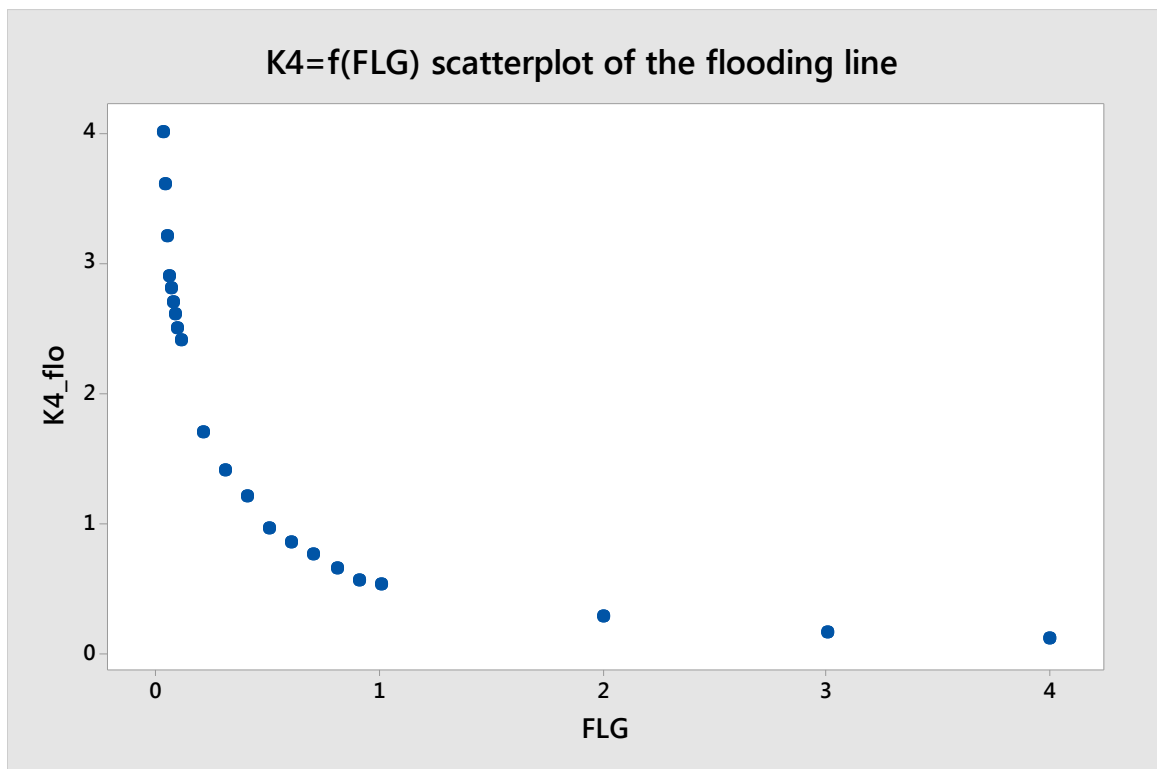


Figure 18.1. Bivariant diagram of the flooding line.

As it can be seen, it is necessary to transform the variable F_{LG} . Because its relation with K_4 , a negative exponential transformation should be done. Furthermore, due to the relation between the regression and the single values, it is interesting to improve it with a quadratic regression:

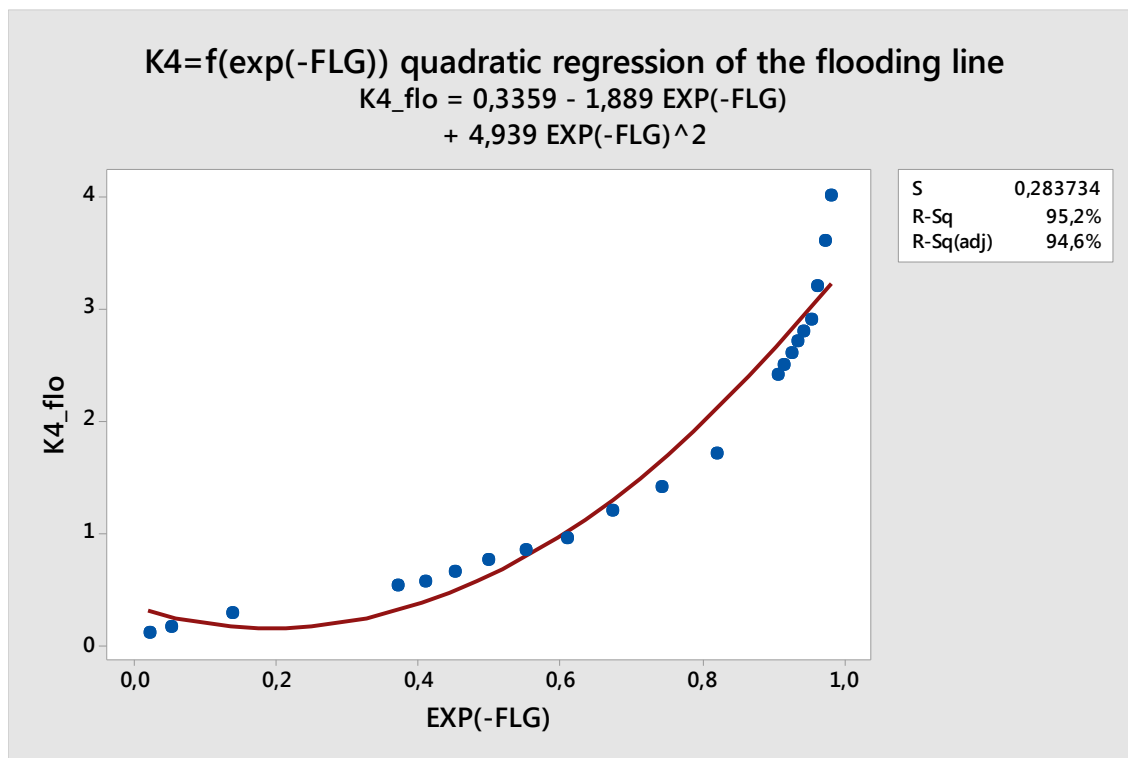


Figure 18.2. Quadratic regression of the flooding line after the exponential.

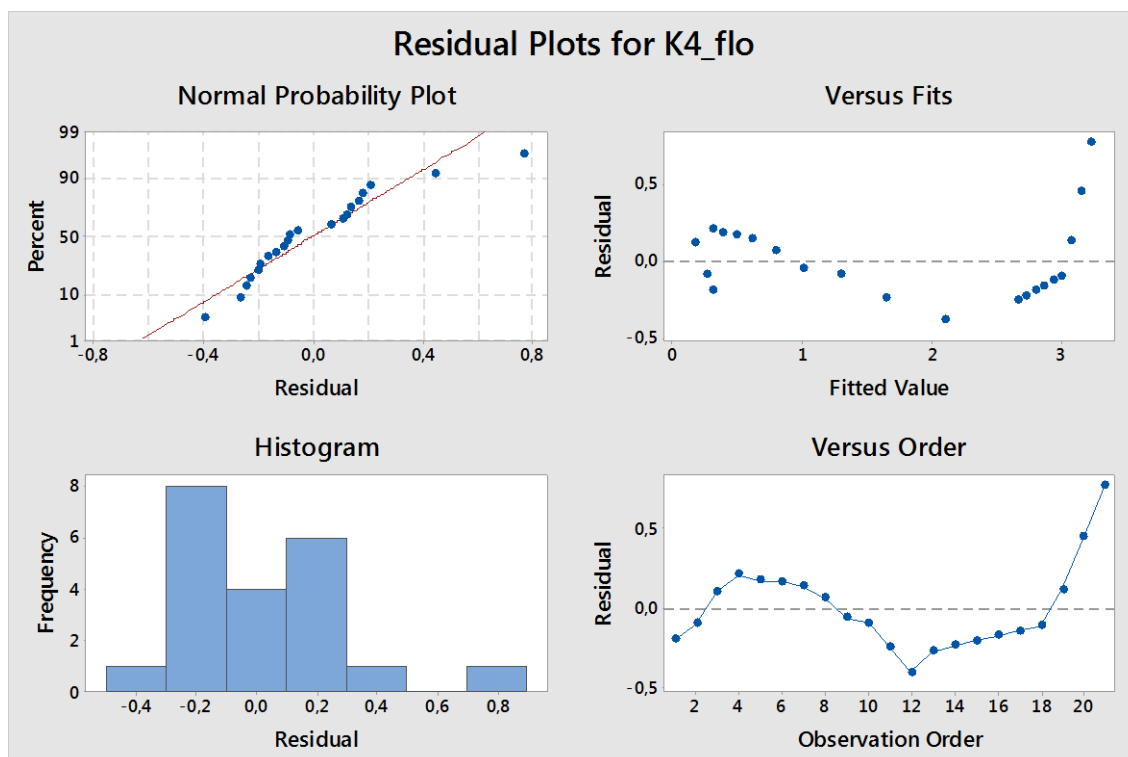


Figure 18.3. Residual study of the flooding line after the quadratic regression.

Examine the behaviour of the residual values (diagram at the top on the right), it can be seen that it is still following a tendency. It indirectly suggests that there is the possibility to continue improving the result. However, as the $R - sq$ value is higher enough ($> 90\%$) and the regression equation is quite difficult, the balance between precision and complexity recommends that it is a suitable parameterization.

Finally, after to carry on this procedure for all the pressure drop curves, the final regressions calculated by Matlab are:

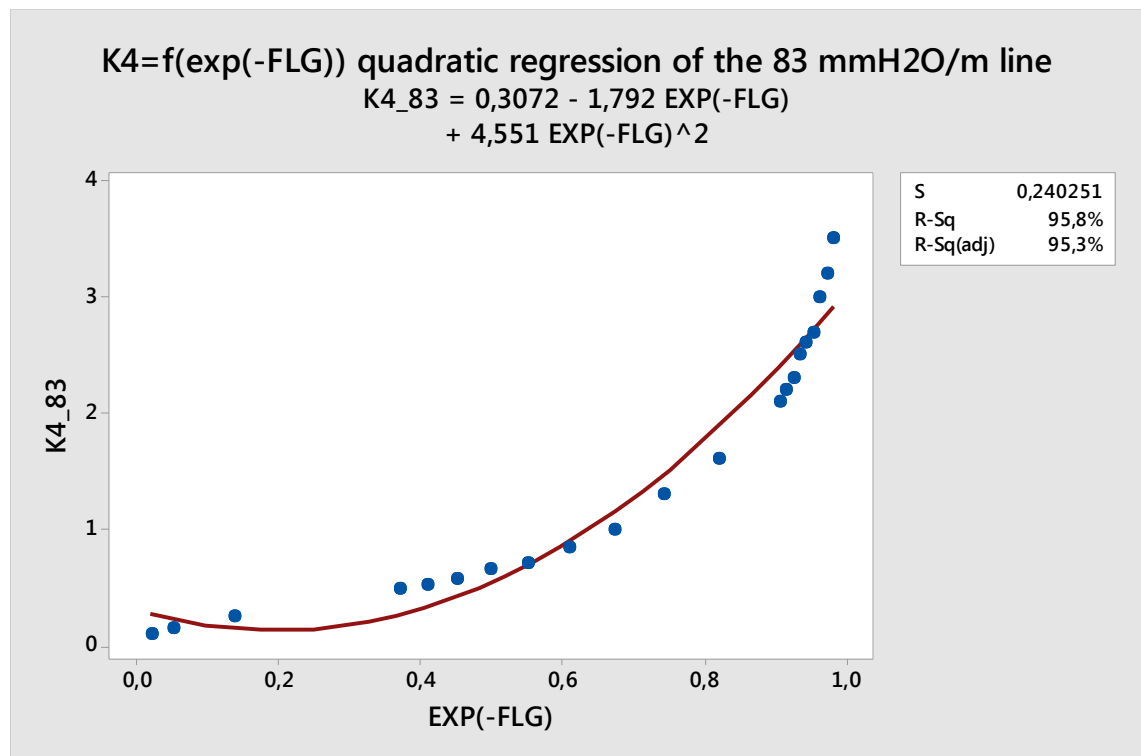


Figure 18.4. Quadratic regression of the 83 mmH₂O/m line after the exponential transformation.

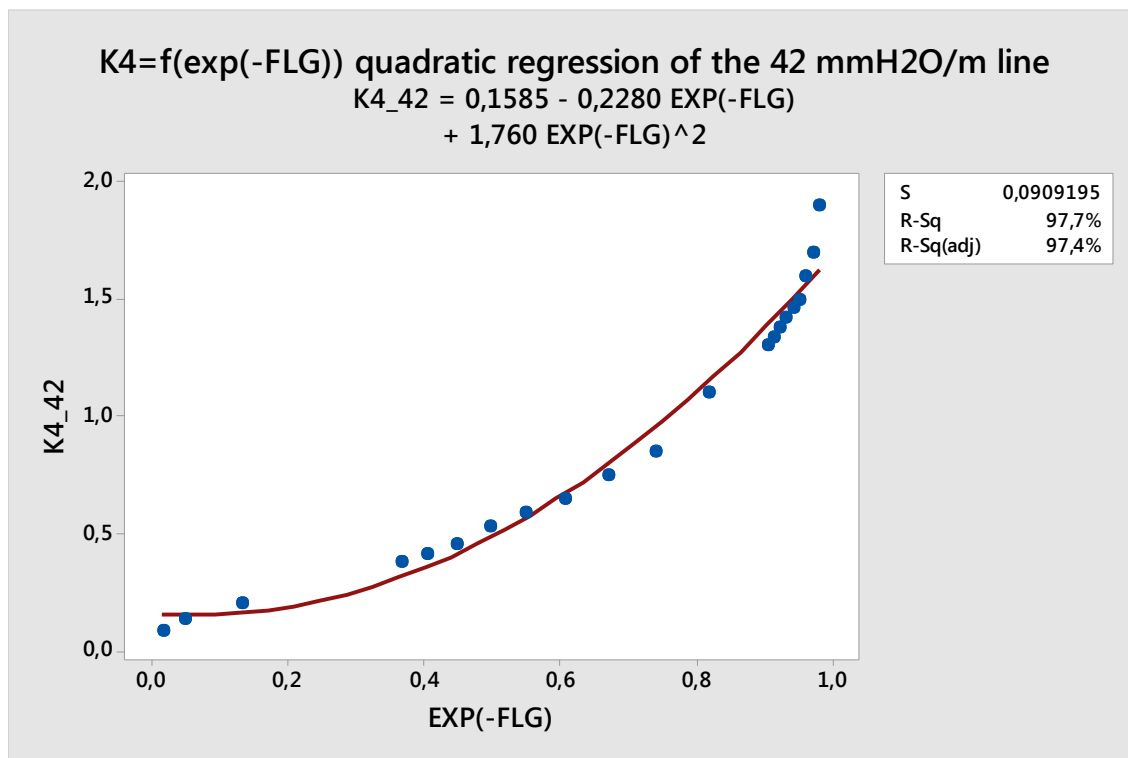


Figure 18.5. Quadratic regression of the 42 mmH₂O/m line after the exponential transformation.

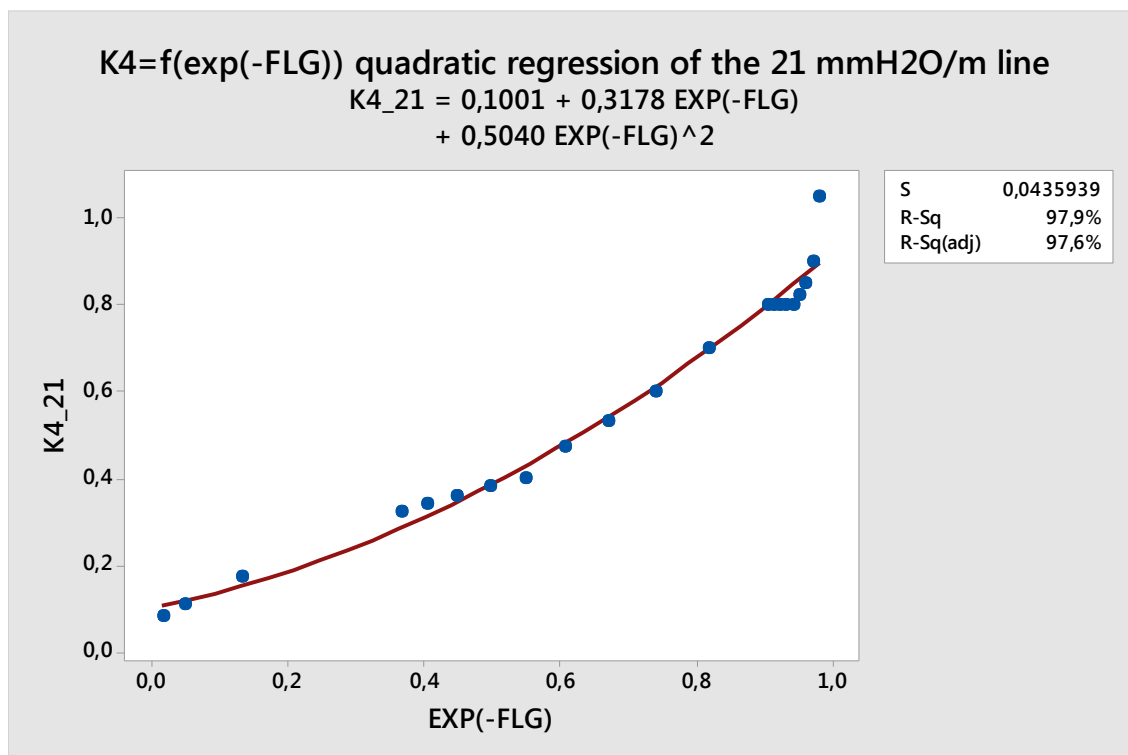
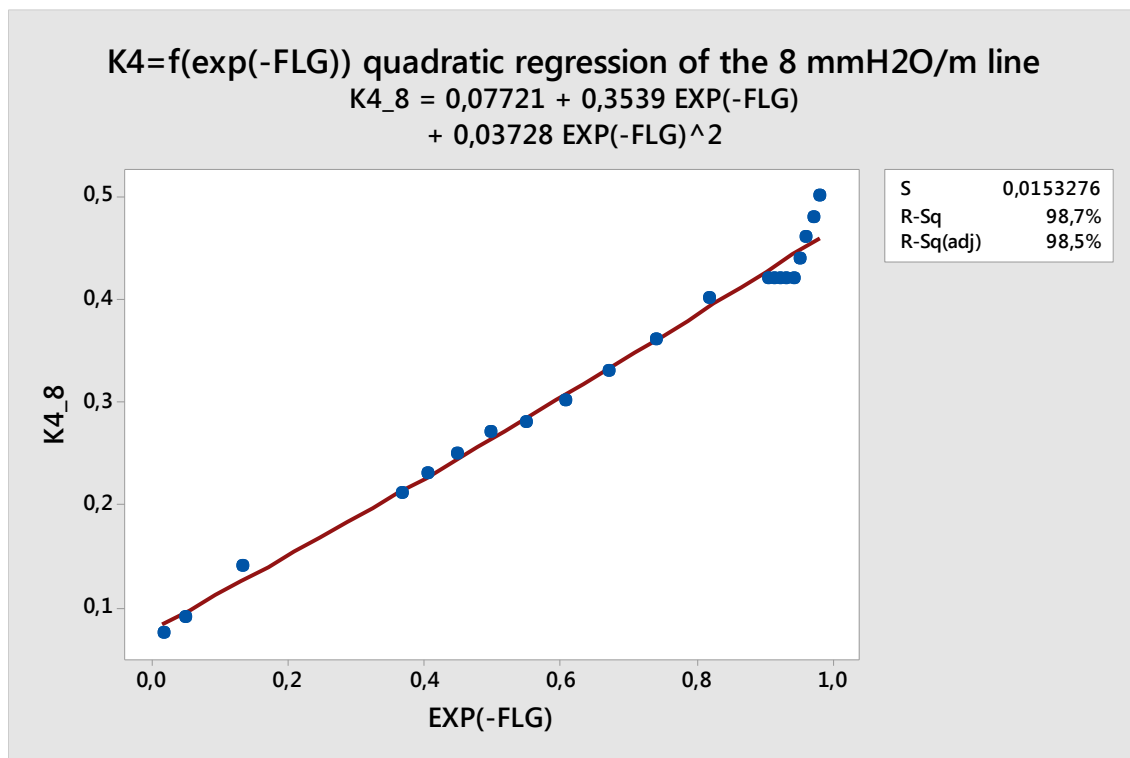
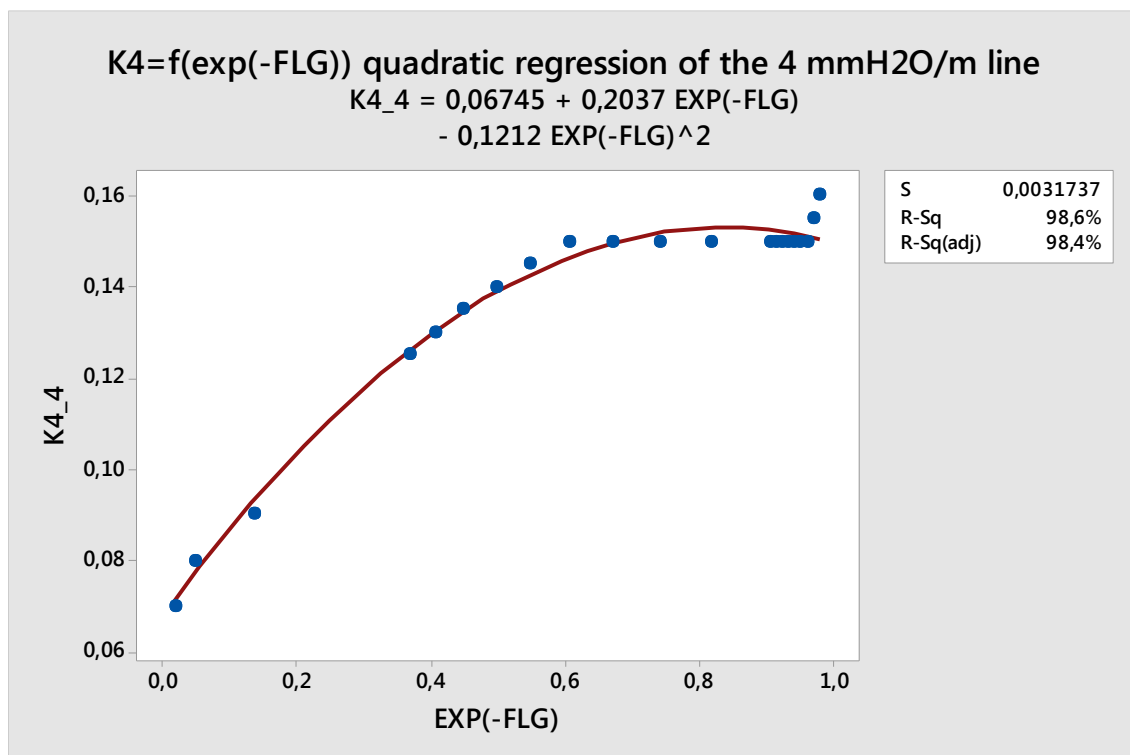


Figure 18.6. Quadratic regression of the 21 mmH₂O/m after the exponential transformation.

Figure 18.7. Quadratic regression of the 8 mmH₂O/m after the exponential transformation.Figure 18.8. Quadratic regression of the 4 mmH₂O/m after the exponential transformation.

18.4. Types of fillings taken into account

18.4.1. Ceramic

Filling_name	Nominal_size, dN [mm]	Specific_surface_area, ap [m ² /m ³]	Void_fraction, eps [-]	Sphericity, phi [-]	Packing_factor, Fp [1/m]
BERL SADDLE (Ceramic - 1/2 in.)	12,7	510,0	0,670	0,440	788,0
BERL SADDLE (Ceramic - 3/4 in.)	19,1	280,0	0,650	0,420	588,0
BERL SADDLE (Ceramic - 1 in.)	25,4	255,0	0,685	0,410	361,0
BERL SADDLE (Ceramic - 1 1/2 in.)	38,1	160,0	0,715	0,405	225,0
BERL SADDLE (Ceramic - 2 in.)	50,8	110,0	0,730	0,390	148,0
CERAPAC (Ceramic - 1 1/2 in.)	38,1	167,0	0,760	0,350	131,0
CERAPAC (Ceramic - 2 in.)	50,8	118,0	0,787	0,340	98,0
CERAPAC (Ceramic - 3 in.)	76,2	79,0	0,795	0,320	59,0
HIFLOW RING (Ceramic - 13/16 in.)	20,0	280,0	0,720	0,325	200,0
HIFLOW RING (Ceramic - 1 1/2 in.)	38,1	128,0	0,760	0,355	121,0
HIFLOW RING (Ceramic - 2 in.)	50,8	102,0	0,780	0,308	85,0
HIFLOW RING (Ceramic - 3 in.)	76,2	70,0	0,800	0,288	49,0
INTALOX SADDLE (Ceramic - 1/2 in.)	12,7	550,0	0,745	0,254	660,0
INTALOX SADDLE (Ceramic - 1 in.)	25,4	256,0	0,733	0,334	302,0
INTALOX SADDLE (Ceramic - 1 1/2 in.)	38,1	195,0	0,760	0,337	230,0
INTALOX SADDLE (Ceramic - 2 in.)	50,4	118,0	0,765	0,342	159,0
LANTEC SADDLE (Ceramic - 1 in.)	25,4	253,0	0,772	0,316	280,0
LANTEC SADDLE (Ceramic - 1 1/2 in.)	38,1	164,0	0,780	0,308	164,0
LANTEC SADDLE (Ceramic - 2 in.)	50,8	115,0	0,791	0,298	121,0
LANTEC SADDLE (Ceramic - 3 in.)	76,2	92,0	0,752	0,336	79,0
NOVALOX SADDLE (Ceramic - 1 in.)	25,4	256,0	0,740	0,320	318,0
NOVALOX SADDLE (Ceramic - 2 in.)	50,8	121,0	0,770	0,310	131,0
NOVALOX SADDLE (Ceramic - 3 in.)	76,2	92,0	0,770	0,300	72,0
PALL RING (Ceramic - 1 in.)	25,4	213,0	0,741	0,306	351,0
PALL RING (Ceramic - 1 3/8 in.)	35,0	139,0	0,773	0,271	164,0
PALL RING (Ceramic - 1 1/2 in.)	38,1	154,0	0,760	0,321	181,0
PALL RING (Ceramic - 2 in.)	50,8	119,0	0,778	0,273	141,0
RASCHIG RING (Ceramic - 3/8 in.)	9,5	475,0	0,624	0,467	3280,0
RASCHIG RING (Ceramic - 1/2 in.)	12,7	368,0	0,640	0,488	1980,0
RASCHIG RING (Ceramic - 5/8 in.)	15,9	310,0	0,675	0,434	1250,0
RASCHIG RING (Ceramic - 3/4 in.)	19,1	266,0	0,733	0,374	840,0
RASCHIG RING (Ceramic - 1 in.)	25,4	188,0	0,740	0,400	525,0
RASCHIG RING (Ceramic - 1 1/2 in.)	38,1	119,0	0,750	0,438	310,0
RASCHIG RING (Ceramic - 2 in.)	50,8	92,0	0,755	0,334	215,0
RASCHIG RING (Ceramic - 3 in.)	76,2	62,0	0,765	0,369	120,0
SUPER INTALOX SADDLE (Ceramic - 1 in.)	25,4	249,0	0,790	0,257	197,0
SUPER INTALOX SADDLE (Ceramic - 2 in.)	50,8	105,0	0,810	0,282	98,0

Table 18.1. Database of ceramic fillings.

18.4.2. Metal

Filling_name	Nominal_size, dp [m]	Specific_surface_area, ap [m ² /m ³]	Void_fraction, eps [-]	Sphericity, phi [-]	Packing_factor, Fp [1/m]
BIALECKI RING (Metal - 1/2 in.)	12,7	340,0	0,932	0,072	250,0
BIALECKI RING (Metal - 1 in.)	25,4	220,0	0,947	0,110	215,0
BIALECKI RING (Metal - 1 3/8 in.)	35,0	155,0	0,959	0,099	200,0
BIALECKI RING (Metal - 2 in.)	50,8	116,0	0,966	0,083	175,0
CASCADE MINI-RING (Metal - 1/2 in.)	12,7	356,0	0,952	0,150	300,0
CASCADE MINI-RING (Metal - 5/8 in.)	15,9	357,0	0,955	0,141	287,0
CASCADE MINI-RING (Metal - 1 in.)	25,4	235,0	0,962	0,110	95,0
CASCADE MINI-RING (Metal - 1 1/2 in.)	38,1	175,0	0,974	0,095	95,0
CASCADE MINI-RING (Metal - 2 in.)	50,8	155,0	0,969	0,093	72,0
CASCADE MINI-RING (Metal - 2 1/2 in.)	63,5	110,0	0,987	0,090	62,0
CASCADE MINI-RING (Metal - 3 in.)	76,2	105,0	0,970	0,088	46,0
FLEXIRING (Metal - 5/8 in.)	15,9	340,0	0,930	0,144	230,0
FLEXIRING (Metal - 1 in.)	25,4	208,0	0,940	0,131	157,0
FLEXIRING (Metal - 1 1/2 in.)	38,1	128,0	0,950	0,121	92,0
FLEXIRING (Metal - 2 in.)	50,8	102,0	0,960	0,101	66,0
FLEXIRING (Metal - 3 3/8 in.)	88,9	65,0	0,970	0,163	53,0
GLITSCH 30P RING (Metal - 1 3/16 in.)	30,0	164,0	0,959	0,110	152,0
GLITSCH 30Pmk RING (Metal - 1 3/16 in.)	30,0	181,0	0,975	0,070	124,0
HIFLOW RING (Metal - 1 in.)	25,4	185,0	0,964	0,093	165,0
HIFLOW RING (Metal - 2 in.)	50,8	95,0	0,977	0,071	52,0
HY-PAK RING (Metal - 1 in.)	25,4	183,0	0,961	0,094	148,0
HY-PAK RING (Metal - 1 1/2 in.)	38,1	122,0	0,965	0,090	85,0
HY-PAK RING (Metal - 2 in.)	50,8	88,0	0,971	0,080	85,0
HY-PAK RING (Metal - 3 in.)	76,2	60,0	0,973	0,075	62,0
IMTP RING (Metal - 1 in.)	25,4	207,0	0,962	0,101	135,0
IMTP RING (Metal - 1 3/5 in.)	40,6	151,0	0,971	0,087	79,0
IMTP RING (Metal - 2 in.)	50,8	98,0	0,977	0,078	59,0
IMTP RING (Metal - 2 4/5 in.)	71,1	70,0	0,982	0,070	39,0
INTERPAK (Metal - 3/8 in.)	9,5	620,0	0,900	0,200	800,0
INTERPAK (Metal - 5/8 in.)	15,9	361,0	0,940	0,180	400,0
INTERPAK (Metal - 3/4 in.)	19,1	261,0	0,960	0,160	240,0
NOR-PAK or NSW RING (Metal - 1 in.)	25,4	203,0	0,962	0,093	145,0
NOR-PAK or NSW RING (Metal - 2 in.)	50,8	92,0	0,977	0,073	60,0
NUTTER RING (Metal - 3/4 in.)	19,1	226,0	0,978	0,093	128,0
NUTTER RING (Metal - 1 in.)	25,4	168,0	0,977	0,093	98,0
NUTTER RING (Metal - 1 1/2 in.)	38,1	124,0	0,978	0,092	66,0
NUTTER RING (Metal - 2 in.)	50,8	96,0	0,978	0,093	56,0
NUTTER RING (Metal - 2 1/2 in.)	63,5	82,0	0,982	0,084	49,0
NUTTER RING (Metal - 3 in.)	76,2	66,0	0,984	0,075	36,0
PALL RING (Metal - 5/8 in.)	15,9	348,0	0,931	0,139	242,0
PALL RING (Metal - 1 in.)	25,4	210,0	0,943	0,126	167,0
PALL RING (Metal - 1 3/8 in.)	35,0	140,0	0,956	0,108	130,0
PALL RING (Metal - 1 1/2 in.)	38,1	137,0	0,951	0,115	112,0
PALL RING (Metal - 2 in.)	50,8	105,0	0,956	0,104	76,0
PALL RING (Metal - 3 in.)	76,2	71,0	0,965	0,080	65,0
PALL RING (Metal - 3 1/2 in.)	88,9	66,0	0,970	0,075	59,0
RALU RING (Metal - 1 in.)	25,4	215,0	0,960	0,098	160,0
RALU RING (Metal - 1 1/2 in.)	38,1	135,0	0,965	0,093	92,0
RALU RING (Metal - 2 in.)	50,8	105,0	0,975	0,073	66,0
RASCHIG RING (Metal - 1/4 in.)	6,4	717,0	0,721	0,422	2300,0
RASCHIG RING (Metal - 1/2 in.)	12,7	420,0	0,850	0,200	985,0
RASCHIG RING (Metal - 5/8 in.)	15,9	332,0	0,870	0,199	975,0
RASCHIG RING (Metal - 1 in.)	25,4	197,0	0,884	0,227	437,0
RASCHIG RING (Metal - 1 1/2 in.)	38,1	131,0	0,900	0,193	272,0
RASCHIG RING (Metal - 2 in.)	50,8	102,0	0,929	0,157	187,0
RASCHIG RING (Metal - 3 in.)	76,4	69,0	0,950	0,116	104,0
RASCHIG SUPER-RING (Metal - 1/2 in.)	12,7	250,0	0,975	0,087	235,0
RASCHIG SUPER-RING (Metal - 1 in.)	25,4	160,0	0,980	0,071	105,0
RASCHIG SUPER-RING (Metal - 2 in.)	50,8	98,0	0,985	0,064	85,0
RASCHIG SUPER-RING (Metal - 3 in.)	76,2	80,0	0,982	0,068	53,0
TRI-PAK or TOP-PAK RING (Metal - 1 1/4 in.)	31,8	200,0	0,972	0,072	120,0
TRI-PAK or TOP-PAK RING (Metal - 2 in.)	50,8	105,0	0,972	0,081	85,0
TRI-PAK or TOP-PAK RING (Metal - 3 in.)	76,2	75,0	0,980	0,067	53,0
VSP RING (Metal - 1 in.)	25,4	204,0	0,975	0,067	105,0
VSP RING (Metal - 1 1/2 in.)	38,1	112,0	0,980	0,073	69,0
VSP RING (Metal - 2 in.)	50,8	105,0	0,980	0,067	66,0

Table 18.2. Database of metal fillings.



18.4.3. Plastic

Filling_name	Nominal_size, dp [m]	Specific_surface_area, ap [m ² /m ³]	Void_fraction, eps [-]	Sphericity, phi [-]	Packing_factor, Fp [1/m]
BIALECKI RING (Plastic - 2 in.)	50,8	100,0	0,972	0,070	160,0
CASCADE MINI-RING (Plastic - 1 in.)	25,4	212,0	0,920	0,220	98,0
CASCADE MINI-RING (Plastic - 2 in.)	50,8	118,0	0,930	0,204	49,0
CASCADE MINI-RING (Plastic - 3 in.)	76,2	79,0	0,940	0,179	26,0
ENVIPAC RING (Plastic 1 1/4 in.)	31,8	138,0	0,936	0,209	79,0
ENVIPAC RING (Plastic 2 3/8 in.)	60,0	98,0	0,961	0,108	40,0
ENVIPAC RING (Plastic - 3 1/8 in.)	28,6	80,0	0,955	0,128	37,0
FLEXIRING (Plastic - 5/8 in.)	15,9	341,0	0,870	0,217	318,0
FLEXIRING (Plastic - 1 in.)	25,4	207,0	0,900	0,186	171,0
FLEXIRING (Plastic - 1 1/2 in.)	38,1	128,0	0,910	0,182	131,0
FLEXIRING (Plastic - 2 in.)	50,8	102,0	0,920	0,163	82,0
FLEXIRING (Plastic - 3 1/2 in.)	88,9	85,0	0,920	0,111	52,0
HIFLOW RING (Plastic - 5/8 in.)	15,9	313,0	0,910	0,172	175,0
HIFLOW RING (Plastic - 1 in.)	25,4	214,0	0,919	0,165	125,0
HIFLOW RING (Plastic - 1 1/2 in.)	38,1	125,0	0,940	0,144	75,0
HIFLOW RING (Plastic - 2 in.)	50,8	110,0	0,940	0,141	49,0
HIFLOW RING (Plastic - 3 1/2 in.)	88,9	66,0	0,958	0,086	30,0
IMPAC (Plastic - 3 5/16 in.)	83,8	213,0	0,914	0,056	49,0
IMPAC (Plastic - 5 1/2 in.)	139,7	108,0	0,950	0,038	20,0
INTALOX SADDLE (Plastic - 1 in.)	25,4	222,0	0,907	0,180	105,0
INTALOX SADDLE (Plastic - 1 1/2 in.)	38,1	170,0	0,910	0,169	85,0
INTALOX SADDLE (Plastic - 2 in.)	50,8	116,0	0,917	0,160	69,0
INTALOX SADDLE (Plastic - 3 in.)	76,2	88,0	0,940	0,097	45,0
JAEGER RING (Plastic - 5/8 in.)	15,9	354,0	0,860	0,180	318,0
JAEGER RING (Plastic - 1 in.)	25,4	210,0	0,900	0,170	170,0
JAEGER RING (Plastic - 1 1/2 in.)	38,1	144,0	0,910	0,140	105,0
JAEGER RING (Plastic - 2 in.)	50,8	108,0	0,920	0,130	82,0
JAEGER RING (Plastic - 3 1/2 in.)	88,9	72,0	0,930	0,120	53,0
JAEGER SADDLE (Plastic - 1 in.)	25,4	197,0	0,910	0,150	108,0
JAEGER SADDLE (Plastic - 2 in.)	50,8	98,0	0,940	0,110	69,0
JAEGER SADDLE (Plastic - 3 in.)	76,2	66,0	0,950	0,095	52,0
LANPAC (Plastic - 2 5/16 in.)	58,4	223,0	0,890	0,096	69,0
LANPAC (Plastic - 3 1/2 in.)	88,9	144,0	0,925	0,072	46,0
NOR-PAK or NSW RING (Plastic - 5/8 in.)	15,9	300,0	0,890	0,216	275,0
NOR-PAK or NSW RING (Plastic - 1 in.)	25,4	202,0	0,953	0,115	125,0
NOR-PAK or NSW RING (Plastic - 1 3/8 in.)	35,0	142,0	0,944	0,129	85,0
NOR-PAK or NSW RING (Plastic - 1 1/2 in.)	38,1	122,0	0,940	0,159	69,0
NOR-PAK or NSW RING (Plastic - 2 in.)	50,8	90,0	0,952	0,138	46,0
NUPAC (Plastic - 2 1/2 in.)	63,5	180,0	0,909	0,089	49,0
NUPAC (Plastic - 4 1/2 in.)	114,3	125,0	0,942	0,053	26,0
PALL RING (Plastic - 5/8 in.)	15,9	350,0	0,870	0,218	316,0
PALL RING (Plastic - 1 in.)	25,4	212,0	0,897	0,187	174,0
PALL RING (Plastic - 1 3/8 in.)	35,0	156,0	0,906	0,170	154,0
PALL RING (Plastic - 1 1/2 in.)	38,1	128,0	0,910	0,182	131,0
PALL RING (Plastic - 2 in.)	50,8	107,0	0,920	0,159	83,0
PALL RING (Plastic - 3 1/2 in.)	88,9	80,0	0,930	0,111	56,0
RALU RING (Plastic - 1 in.)	25,4	190,0	0,940	0,129	135,0
RALU RING (Plastic - 1 1/2 in.)	38,1	150,0	0,942	0,110	79,0
RALU RING (Plastic - 2 in.)	50,8	103,0	0,941	0,128	56,0
RALU RING (Plastic - 3 1/2 in.)	88,9	75,0	0,960	0,075	39,0
RASCHIG RING (Plastic - 3/8 in.)	9,5	550,0	0,880	0,207	625,0
RASCHIG RING (Plastic - 5/8 in.)	15,9	336,0	0,870	0,218	375,0
RASCHIG RING (Plastic - 1 in.)	25,4	198,0	0,853	0,220	170,0
RASCHIG SUPER-RING (Plastic - 2 in.)	50,8	100,0	0,960	0,118	65,0
SNOWFLAKE (Plastic - 3 11/16 in.)	94,0	92,0	0,951	0,120	43,0
SUPER INTALOX SADDLE (Plastic - 1 in.)	25,4	202,0	0,900	0,199	108,0
SUPER INTALOX SADDLE (Plastic - 2 in.)	50,8	108,0	0,930	0,143	92,0
SUPER INTALOX SADDLE (Plastic - 3 in.)	76,2	89,0	0,940	0,095	59,0
SUPER TORUS SADDLE (Plastic - 1 in.)	25,4	240,0	0,900	0,148	164,0
SUPER TORUS SADDLE (Plastic - 2 in.)	50,8	110,0	0,940	0,120	105,0
SUPER TORUS SADDLE (Plastic - 3 in.)	76,2	90,0	0,955	0,073	49,0
TELLERETTE (Plastic - 1 in.)	25,4	210,0	0,865	0,183	117,0
TELLERETTE (Plastic - 2 in.)	50,8	184,0	0,930	0,142	75,0
TELLERETTE (Plastic - 3 in.)	76,2	104,0	0,925	0,171	46,0
TRI-PAK or HACKETTES (Plastic - 1 in.)	25,4	279,0	0,900	0,200	92,0
TRI-PAK or HACKETTES (Plastic - 1 1/4 in.)	31,8	230,0	0,920	0,190	82,0
TRI-PAK or HACKETTES (Plastic - 2 in.)	50,8	157,0	0,930	0,180	57,0
TRI-PAK or HACKETTES (Plastic - 3 1/2 in.)	88,9	125,0	0,950	0,150	39,0

Table 18.3. Database of plastic fillings.

18.5. Software code

```

%%% DESIGN OF STRIPPING COLUMNS %%%

%RESET
clear all

%KNOWN DATA
p_T=101325; %[Pa]; Pressure
p_Tatm=1; %[atm]
p_Tbar=1.01325; %[bar]
T=20+273.15; %[K]; Temperature
R_J=8.3145; %[J/(K*mol)]; Ideal gas constant
R_atm=0.082; %[atm*L/(K*mol)]
R_bar=0.08314; %[bar*m3/(K*kmol)]
g=9.81; %[m/S_2]; Gravitational acceleration

M_CHCl3=119; %[g/mol]; RAIS
M_CHCl2Br=164; %[g/mol]
M_CHClBr2=208; %[g/mol]
M_CHBr3=253; %[g/mol]

H_CHCl3atm=0.00367; %[atm*m3/mol]; 1.5e-1 [-]; RAIS
H_CHCl2Bratm=0.00212; %[atm*m3/mol]; 8.67e-2 [-]
H_CHClBr2atm=0.000783; %[atm*m3/mol]; 3.2e-2 [-]
H_CHBr3atm=0.000535; %[atm*m3/mol]; 2.19e-2 [-]

D_CHCl3water=1.09e-9; %[m2/s]; RAIS
D_CHCl2Brwater=1.07e-9; %[m2/s]
D_CHClBr2water=1.06e-9; %[m2/s]
D_CHBr3water=1.04e-9; %[m2/s]

D_CHCl3air=7.69e-6; %[m2/s]; RAIS
D_CHCl2Brair=5.63e-6; %[m2/s]
D_CHClBr2air=3.66e-6; %[m2/s]
D_CHBr3air=3.57e-6; %[m2/s]

M_H2O=18.02; %[g/mol]; Molar weight
M_air=28.96; %[g/mol]
rho_H2O=998; %[kg/m3]; Density
rho_air=1; %[kg/m3]
mu_H2O=1002e-6; %[kg/(m*s)]; Viscosity
mu_air=17.4e-6; %[kg/(m/s)]
sigma_H2O=0.072; %[kg/S_2]; Surface tension

sigma_ceramic=61e-3; %[kg/S_2]
sigma_metal=75e-3; %[kg/S_2]
sigma_plastic=33e-3; %[kg/S_2]
rho_StainlessSteel=7500; %[kg/m3]

Coef_DollarToEuro=0.92; %1 US dollar = 0.9211 €
Coef_GallonToLiter=3.79; %1 US gallon = 3.7854 liters

%INPUTS

```



```

Question=input('Which is the system you want to treat: WATER(THMs)-AIR
(Input: 1) or GENERIC SYSTEM (Input: 2)? ');
if Question ~= 1 && Question ~= 2
    display('Remember to introduce the STRIPPING system; execute again
and press 1 or 2 depending on the case');
end
if Question == 1
    C_CHCl3w=input('Which is the initial concentration of CHCl3 dissolved
in the water [microg/L]? ');
    C_CHCl2Brw=input('Which is the initial concentration of CHCl2Br
dissolved in the water [microg/L]? ');
    C_CHClBr2w=input('Which is the initial concentration of CHClBr2
dissolved in the water [microg/L]? ');
    C_CHBr3w=input('Which is the initial concentration of CHBr3 dissolved
in the water [microg/L]? ');
    C_TTHMstop=C_CHCl3w+C_CHCl2Brw+C_CHClBr2w+C_CHBr3w; %[microg/L]
    c_CHCl3top=C_CHCl3w/(M_CHCl3*1e6); %[kmol/m3]
    c_CHCl2Brtop=C_CHCl2Brw/(M_CHCl2Br*1e6); %[kmol/m3]
    c_CHClBr2top=C_CHClBr2w/(M_CHClBr2*1e6); %[kmol/m3]
    c_CHBr3top=C_CHBr3w/(M_CHBr3*1e6); %[kmol/m3]

M=(M_CHCl3*c_CHCl3top+M_CHCl2Br*c_CHCl2Brtop+M_CHClBr2*c_CHClBr2top+M_CHBr3*c_CHBr3top)/(c_CHCl3top+c_CHCl2Brtop+c_CHClBr2top+c_CHBr3top);
%[g/mol]

H_atm=(H_CHCl3atm*c_CHCl3top+H_CHCl2Bratm*c_CHCl2Brtop+H_CHClBr2atm*c_CHClBr2top+H_CHBr3atm*c_CHBr3top)/(c_CHCl3top+c_CHCl2Brtop+c_CHClBr2top+c_CHBr3top); %[atm*m3/mol]
    C_TTHMsbottom=input('Which is the final desired concentration of THMs
in the water [microg/L]? '); %[microg/L]
    p_TTHMsbottom=eps; %[microg/L]; In general, there are not THMs in the
air
    p_TTHMsbottomPa=p_TTHMsbottom*R_J*T/(M*1e3); %[Pa]
    M_L=M_H2O; %[g/mol]
    M_G=M_air; %[g/mol]
    rho_L=rho_H2O; %[kg/m3]
    rho_G=rho_air; %[kg/m3]
    mu_L=mu_H2O; %[kg/(m/s)]
    mu_G=mu_air; %[kg/(m/s)]

D_L=(D_CHCl3water*c_CHCl3top+D_CHCl2Brwater*c_CHCl2Brtop+D_CHClBr2water*c_CHClBr2top+D_CHBr3water*c_CHBr3top)/(c_CHCl3top+c_CHCl2Brtop+c_CHClBr2top+c_CHBr3top); %[m2/s]; Diffusivity of THMs in the water

D_G=(D_CHCl3air*c_CHCl3top+D_CHCl2Brair*c_CHCl2Brtop+D_CHClBr2air*c_CHClBr2top+D_CHBr3air*c_CHBr3top)/(c_CHCl3top+c_CHCl2Brtop+c_CHClBr2top+c_CHBr3top); %[m2/s]; Diffusivity of THMs in the air
    sigma_L=sigma_H2O; %[kg/S_2]
elseif Question == 2
    C_TTHMstop=input('Which is the initial concentration of the unwanted
component dissolved in the liquid [microg/L]? ');
    C_TTHMsbottom=input('Which is the final concentration of the unwanted
component in the liquid [microg/L]? ');
    p_TTHMsbottom=input('Which is the initial concentration of the
unwanted component in the air [microg/L]? ');
    M=input('Which is the molecular weight of the unwanted component
dissolved in the liquid [g/mol]? ');

```



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p_TTHMsbottomPa=p_TTHMsbottom*R_J*T/(M*1e3); %[Pa]
H_atm=input('Which is the Henry constant of the unwanted component
[atm*m3/mol]? ');
M_L=input('Which is the molecular weight of the liquid [g/mol]? ');
M_G=input('Which is the molecular weight of the gas [g/mol]? ');
rho_L=input('Which is the density of the liquid [kg/m3]? ');
rho_G=input('Which is the density of the gas [kg/m3]? ');
mu_L=input('Which is the viscosity of the liquid [kg/(m*s)]? ');
mu_G=input('Which is the viscosity of the gas [kg/(m*s)]? ');
D_L=input('Which is the diffusivity of the solute in the liquid
[m2/s]? ');
D_G=input('Which is the diffusivity of the solute in the gas [m2/s]?
');
sigma_L=input('Which is the surface tension of the liquid [kg/S_2]?
');
else
    break
end
L_L=input('Which is the flow of liquid needed to treat [L/min]? ');
TypeOfFilling=input('Which type of filling do you want: CERAMIC (Input:
1), METAL (Input: 2) or PLASTIC (Input: 3)? ');

%PROTECTION for coherent operation
if C_TTHMstop<=C_TTHMsbottom %[microg/L]
    display('The initial liquid concentration is lower or equal than the
final desired concentration');
    break
elseif L_L<0 %[L/min]
    display('The liquid flow to treat must be greater than zero');
    break
elseif TypeOfFilling~=1 && TypeOfFilling~=2 && TypeOfFilling~=3 %[-]
    display('The type of fillin_G must be ceramic (press 1), metallic
(press 2) or plastic (press 3)');
    break
else
    t_ini=cputime; %To know the calculations time
    %PREVIOUS CALCULATIONS
    C_TTHMs=(C_TTHMstop+C_TTHMsbottom)/2; %[microg/L]
    c_TTHMs=C_TTHMs/(M*1e6); %[kmol/m3]
    L=L_L*rho_L/(M_L*1e3*60); %[kmol/s]
    H_Pa=H_atm*p_T; %[Pa*m3/mol]
    H_bar=H_atm*p_Tbar; %[bar*m3/mol]
    H_microg=H_atm*p_T/(M*1e3); %[Pa*L/microg]

    %STRIPPING SYSTEM
    x_top=C_TTHMstop*M_L/(M*rho_L*10^(6)); %[liquid molar fraction]; At
the top of the tower
    x_bottom=C_TTHMsbottom*M_L/(M*rho_L*10^(6)); %[liquid molar
fraction]; At the bottom of the tower
    y_bottom=p_TTHMsbottom*M_G/(M*rho_G*10^(6)); %[gas molar fraction];
At the bottom of the tower
    m=H_atm*rho_L*1e3/(M_L*p_Tatm); %[-]; Slope of equilibrium curve with
molar fractions on axis (equivalent than H)
    G_L=0.75*L/m; %[kmol/s]; Suggestion of Coulson (Colburn 1939) and
Perry
    y_top=y_bottom+L*(x_top-x_bottom)/G_L; %[gas molar fraction];
Operation line

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p_TTHMstop=y_top*M*rho_G*10^(6)/M_G; %[microg/L]
p_TTHMstopPa=p_TTHMstop*R_J*T/(M*1e3); %[Pa]
PercentageRemoved=((C_TTHMstop-C_TTHMsbottom)/C_TTHMstop)*100; [%]

%MECHANICAL DESIGN
FillingGeneralData=importdata('FeaturesOfFillings.xlsx');
if TypeOfFilling == 1
    Features=FillingGeneralData.data.CERAMIC;
    Names=FillingGeneralData.textdata.CERAMIC;
    sigma_c=sigma_ceramic;
    rho_material=650; %[kg/m3]; To adjust depending on the filling
elseif TypeOfFilling == 2
    Features=FillingGeneralData.data.METAL;
    Names=FillingGeneralData.textdata.METAL;
    sigma_c=sigma_metal;
    rho_material=8000; %[kg/m3]; To adjust depending on the filling
elseif TypeOfFilling == 3
    Features=FillingGeneralData.data.PLASTIC;
    Names=FillingGeneralData.textdata.PLASTIC;
    sigma_c=sigma_plastic;
    rho_material=950; %[kg/m3]; To adjust depending on the filling
end
L_w=L*M_L; %[kg/s]
G_w=G_L*M_G; %[kg/s]
F_LG=L_w*sqrt(rho_G/rho_L)/G_w; %[-]; Equal than
Lw'*sqrt(rho_G/rho_L)/Gw' with Lw' & Gw' [kg/(s*m2)]
%In order to ensure F_LG is in the correct interval:
if F_LG<0.02
    F_LG=0.02; %[-]
    G_w=L_w*sqrt(rho_G/rho_L)/F_LG; %[kg/s]
elseif F_LG>3
    F_LG=3; %[-]
    G_w=L_w*sqrt(rho_G/rho_L)/F_LG; %[kg/s]
elseif 0.02<F_LG || F_LG>3
    G_L=G_w/M_G; %[kmol/s]; It substitutes the suggestion of Coulson
and Perry
end
G_L=G_L*M_G*60*1e3/rho_G; %[L/min]
K4_125=0.3359-1.889*exp(-F_LG)+4.939*(exp(-F_LG)^2); %[-]; Flooding
line regression from the pressure drop diagram
Names=Names(2:end,1); %Just names of fillings, without the 1st
explanation row
rows=size(Features,1); %Number of rows
MechanicalDesignMatrix=[Features zeros(rows,10)]; %Big matrix of
features + 10 new columns full of 0
N_scL=mu_L/(rho_L*D_L); %[-]; Schmitt adimensional number
N_scG=mu_G/(rho_G*D_G); %[-]
for i=1:rows %For each filliN_G... (1 by 1)
    Fp=Features(i,5); %[1/m]; Fp value of the data base
    v_Gflooding=sqrt(K4_125*rho_G*(rho_L-
rho_G)/(13.1*rho_G^(2)*Fp*(mu_L/rho_L)^(0.1))); %[m/s]
    MechanicalDesignMatrix(i,6)=v_Gflooding; %v_Gflooding stored in
the 6th column
    v_Goperating=0.7*v_Gflooding; %[m/s]
    MechanicalDesignMatrix(i,7)=v_Goperating; %v_Goperating stored in
the 7th column
    G_wS=rho_G*v_Goperating; %[kg/(m2*s)]

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    MechanicalDesignMatrix(i,8)=G_ws; %G_ws stored in the 8th column
    K4_operating=(13.1*G_ws^(2)*Fp*(mu_L/rho_L)^(0.1))/(rho_G*(rho_L-
rho_G)); %[-]
    MechanicalDesignMatrix(i,9)=K4_operating; %K4_operating stored in
the 9th column
    L_ws=F_LG*G_ws*sqrt(rho_L/rho_G); %[kg/(m2*s)]; Because F_LG
remains constant
    MechanicalDesignMatrix(i,10)=L_ws; %L_ws stored in the 10th
column
    v_Loperating=L_ws/rho_L; %[m/s]
    MechanicalDesignMatrix(i,11)=v_Loperating; %v_Loperating stored
in the 11th column
    dN=Features(i,1); %[mm]; Take dN value of the data base
    dN=dN*1e-3; %[m]
    ap=Features(i,2); %[m2/m3]; Take ap value of the data base
    if dN>=15e-3 %[m]
        A=5.23;
    else
        A=2;
    end
    a=ap*(1-exp(-
1.45*(sigma_c/sigma_L)^(0.75)*((rho_L*v_Loperating/(ap*mu_L))^(0.1))*((v
_Loperating^2)*ap/g)^(0.05))*(rho_L*(v_Loperating^2)/(ap*sigma_L))^(0.2))); %[m2/m3]

    k_l=((mu_L*g/rho_L)^(1/3))*0.0051*(rho_L*v_Loperating/(a*mu_L))^(2/3)*N_s
cL^(-1/2)*(ap*dN)^(0.4); %[m/s]
    MechanicalDesignMatrix(i,12)=k_l; %k_l stored in the 12th column

    k_g_2=D_G*ap/(R_bar*T)*A*(rho_G*v_Goperating/(ap*mu_G))^(0.7)*(N_scG^(1/3
))*(ap*dN)^(-2)); %[kmol/(s*m2*bar)]
    MechanicalDesignMatrix(i,14)=k_g_2; %k_g_2 stored in the 14th
column
    k_g=k_g_2*p_Tbar/c_TTHMs; %[m/s]
    MechanicalDesignMatrix(i,13)=k_g; %k_g stored in the 13th column
    k_l_a=k_l*a; %[1/s]
    k_g_2_a=k_g_2*a; %[kmol/(s*m3*bar)]
    k_g_a=k_g*a; %[1/s]; (additional information)
    MassTransferVelocityConstant=1/(1/(k_g_2)+H_bar*1e3/k_l);
%[kmol/(s*m2*bar)]
    MechanicalDesignMatrix(i,15)=MassTransferVelocityConstant;
%MassTransferVelocityConstant stored in the 15th (last) column
end
[BetterFilliN_G, index]=max(MechanicalDesignMatrix(:,15)); %Maximum
value of constant -> maximum mass transfer velocity (NO reaction)

%RESULTS OF MECHANICAL DESIGN
Filling_name=Names(index,1); %[-]
Filling_dN=MechanicalDesignMatrix(index,1); %[mm]; Nominal size
Filling_ap=MechanicalDesignMatrix(index,2); %[m2/m3]; Specific
surface area
Filling_eps=MechanicalDesignMatrix(index,3); %[-]; Void fraction
Filling_phi=MechanicalDesignMatrix(index,4); %[-]; Sphericity
Filling_Fp=MechanicalDesignMatrix(index,5); %[1/m]; Packing factor
v_Gflooding=MechanicalDesignMatrix(index,6); %[m/s]
v_Goperating=MechanicalDesignMatrix(index,7); %[m/s]
G_ws=MechanicalDesignMatrix(index,8); %[kg/(m2*s)]

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K4_operating=MechanicalDesignMatrix(index,9); %[-]
L_wS=MechanicalDesignMatrix(index,10); %[kg/(m2*s)]
v_Loperating=MechanicalDesignMatrix(index,11); %[m/s]
k_l=MechanicalDesignMatrix(index,12); %[m/s]
k_g=MechanicalDesignMatrix(index,13); %[m/s]
k_g_2=MechanicalDesignMatrix(index,14); %[kmol/(s*m2*bar)]
MassTransferVelocityConstant=MechanicalDesignMatrix(i,15);
%[kmol/(s*m2*bar)]
S=G_w/G_wS; %[m2]
D_i=sqrt(4*S/pi); %[m]
K_G=MassTransferVelocityConstant; %[kmol/(s*m2*bar)]
K_L=K_G*H_bar*1e3; %[m/s]; (additional information)

%H_column
%H_G calculation
kl_a=k_l_a*3600; %[1/h]
kg_a=k_g_2_a*1e3*3600*p_Tbar/p_T; %[mol/(h*m3*Pa)]
R_T=1/kg_a+H_Pa/kl_a; %[h*m3*Pa/mol]
R_G=(1/kg_a)*100/R_T; %[%]
R_L=(H_Pa/kl_a)*100/R_T; %[%]; =100-R_G
KG_a=1/R_T; %[mol/(h*Pa*m3)]
G_S=G_wS*1e3*3600/M_G; %[mol/(h*m2)]
L_S=L_wS*1e3*3600/M_L; %[mol/(h*m2)]; (additional information)
H_G=G_S/(p_T*KG_a); %[m/unit]
%N_G calculation
c_TTHMstop=C_TTHMstop/(M*1e3); %[mol/m3]
c_TTHMsbottom=C_TTHMsbottom/(1e3*M); %[mol/m3]
Incr_p_peq_top=H_Pa*c_TTHMstop-p_TTHMstopPa; %[Pa]; Operating line
below equilibrium line
Incr_p_peq_bottom=H_Pa*c_TTHMsbottom-p_TTHMsbottomPa; %[Pa]
Incr_p_peq=(Incr_p_peq_top+Incr_p_peq_bottom)/2; %[Pa]
N_G=(p_TTHMstopPa-p_TTHMsbottomPa)/Incr_p_peq; %[-]
%H_column
H_column=H_G*N_G; %[m]

%PRESSURE DROP
F_LG=L_wS*sqrt(rho_G/rho_L)/G_wS; %[-]
K4=13.1*(G_wS^2)*Filling_Fp*((mu_L/rho_L)^0.1)/(rho_G*(rho_L-rho_G));
K4_125=0.3359-1.889*exp(-F_LG)+4.939*(exp(-F_LG)^2);
K4_83=0.3072-1.792*exp(-F_LG)+4.551*(exp(-F_LG)^2);
K4_42=0.1585-0.228*exp(-F_LG)+1.76*(exp(-F_LG)^2);
K4_21=0.1001+0.318*exp(-F_LG)+0.504*(exp(-F_LG)^2);
K4_8=0.0772+0.354*exp(-F_LG)+0.037*(exp(-F_LG)^2);
K4_4=0.0675+0.204*exp(-F_LG)-0.121*(exp(-F_LG)^2);

Dif_125=abs(K4-K4_125);
Dif_83=abs(K4-K4_83);
Dif_42=abs(K4-K4_42);
Dif_21=abs(K4-K4_21);
Dif_8=abs(K4-K4_8);
Dif_4=abs(K4-K4_4);
Dif=[Dif_125 Dif_83 Dif_42 Dif_21 Dif_8 Dif_4];

[Ordered, InitialPosition]=sort(Dif);
Dif_min_1=Ordered(:,1);
Dif_min_2=Ordered(:,2);
if InitialPosition(:,1) == 1

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```

        min_1 = 125;
    elseif InitialPosition(:,1) == 2
        min_1 = 83;
    elseif InitialPosition(:,1) == 3
        min_1 = 42;
    elseif InitialPosition(:,1) == 4
        min_1 = 21;
    elseif InitialPosition(:,1) == 5
        min_1 = 8;
    else
        min_1 = 4;
    end
    if InitialPosition(:,2) == 1
        min_2 = 125;
    elseif InitialPosition(:,2) == 2
        min_2 = 83;
    elseif InitialPosition(:,2) == 3
        min_2 = 42;
    elseif InitialPosition(:,2) == 4
        min_2 = 21;
    elseif InitialPosition(:,2) == 5
        min_2 = 8;
    else
        min_2 = 4;
    end

    PressureDrop=min_1-Dif_min_1*(min_1-min_2)/(Dif_min_1+Dif_min_2);
    %[mmH2O/(column m)]; Interpolation

    %THICKNESS OF THE WALLS
    if D_i<1 %[m]
        th=5; %[mm]
    elseif D_i<2 && D_i>=1 %[m]
        th=7; %[mm]
    elseif D_i<2.5 && D_i>=2 %[m]
        th=9; %[mm]
    elseif D_i<3 && D_i>=2.5 %[m]
        th=10; %[mm]
    elseif D_i<3.5 && D_i>=3 %[m]
        th=12; %[mm]
    else
        th=15; %[mm]
    end

    %NUMBER OF DISTRIBUTORS
    NumberOfDistributors=round(H_column/5)-1;

    %WEIGHT
    D_column=D_i+th*10^(-3)/2; %[m]
    C_v=1.15; %[-]

    W_v=C_v*pi*rho_StainlessSteel*D_column*(H_column+0.8*D_column)*th*10^(-
3); %[kg]
    W_Filling=rho_material*H_column*S*Filling_eps; %[kg]
    W=W_v+W_Filling; %[kg]

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%DEAD-WEIGHT STRESS
sigma_w=W*g/(pi*(D_i*1000+th)*th); %[N/mm]

%STRIPPING COLUMN COST
if L_L<330*Coef_GallonToLiter
    S_1=60*Coef_GallonToLiter; %[L/min]
    if PercentageRemoved<=90
        Cost_1=66654*Coef_DollarToEuro; %[€]
    else
        Cost_1=99981*Coef_DollarToEuro; %[€]
    end
elseif L_L>3300*Coef_GallonToLiter
    S_1=6000*Coef_GallonToLiter; %[L/min]
    if PercentageRemoved<=90
        Cost_1=2010729*Coef_DollarToEuro; %[€]
    else
        Cost_1=2514337*Coef_DollarToEuro; %[€]
    end
else
    S_1=600*Coef_GallonToLiter; %[L/min]
    if PercentageRemoved<=90
        Cost_1=227735*Coef_DollarToEuro; %[€]
    else
        Cost_1=288834*Coef_DollarToEuro; %[€]
    end
end
S_2=L_L; %[L/min]
Cost_2=Cost_1*(S_2/S_1)^(0.6); %[€]
DirectCosts=Cost_2; %[€]
IndirectCosts=0.4*DirectCosts; %[€]
TotalFixedCapital=DirectCosts+IndirectCosts; %[€]
WorkingCapital=0.05*TotalFixedCapital; %[€]
TotalInvestment=TotalFixedCapital+WorkingCapital; %[€]

%POTENTIALLY CARCINOGENIC RISK
IR=2; %[L/day]
EF=365; %[day/year]
ED=29; %[year]
CF1=1e-3; %[mg/microg] or [L/cm3]
BW=64.8; %[kg] Male
AT=70*365; %[day]

OralIngestion_CHCl3=C_CHCl3w*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
OralIngestion_CHCl2Br=C_CHCl2Brw*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
OralIngestion_CHClBr2=C_CHClBr2w*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
OralIngestion_CHBr3=C_CHBr3w*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]

SA=(4*BW+7)/(BW+90); %[m2]
F=0.8; %[-]
ET=18.9; %[min/day]
CF2=1e4; %[cm2/m2]
CF3=60; %[min/h]

PC_CHCl3=8.9e-3; %[cm/h]
PC_CHCl2Br=5.8e-3; %[cm/h]
PC_CHClBr2=3.9e-3; %[cm/h]

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PC_CHBr3=2.6e-3; %[cm/h]

DermalAbsorption_CHCl3=C_CHCl3w*SA*F*PC_CHCl3*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]

DermalAbsorption_CHCl2Br=C_CHCl2Brw*SA*F*PC_CHCl2Br*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]

DermalAbsorption_CHClBr2=C_CHClBr2w*SA*F*PC_CHClBr2*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]

DermalAbsorption_CHBr3=C_CHBr3w*SA*F*PC_CHBr3*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]

VR=(0.84+0.66)/2; %[m3/h]; Algebraic mean between male and female

AE=0.5; %[-]

VF=18e-3; %[-]

InhalationIntake_CHCl3=VF*C_CHCl3w*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]

InhalationIntake_CHCl2Br=VF*C_CHCl2Brw*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]

InhalationIntake_CHClBr2=VF*C_CHClBr2w*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]

InhalationIntake_CHBr3=VF*C_CHBr3w*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]

SF_oralCHCl3=6.1e-3; %[kg*day/mg]

SF_oralCHCl2Br=6.2e-2; %[kg*day/mg]

SF_oralCHClBr2=8.4e-2; %[kg*day/mg]

SF_oralCHBr3=7.9e-2; %[kg*day/mg]

SF_dermalCHCl3=3.05e-2; %[kg*day/mg]

SF_dermalCHCl2Br=6.33e-2; %[kg*day/mg]

SF_dermalCHClBr2=1.4e-1; %[kg*day/mg]

SF_dermalCHBr3=1.32e-2; %[kg*day/mg]

SF_inhalationCHCl3=8.05e-2; %[kg*day/mg]

SF_inhalationCHCl2Br=6.2e-2; %[kg*day/mg]

SF_inhalationCHClBr2=8.4e-2; %[kg*day/mg]

SF_inhalationCHBr3=3.85e-3; %[kg*day/mg]

OralCancerRisk_CHCl3=OralIngestion_CHCl3*SF_oralCHCl3; %[-]

OralCancerRisk_CHCl2Br=OralIngestion_CHCl2Br*SF_oralCHCl2Br; %[-]

OralCancerRisk_CHClBr2=OralIngestion_CHClBr2*SF_oralCHClBr2; %[-]

OralCancerRisk_CHBr3=OralIngestion_CHBr3*SF_oralCHBr3; %[-]

OralCancerRisk=OralCancerRisk_CHCl3+OralCancerRisk_CHCl2Br+OralCancerRisk_CHClBr2+OralCancerRisk_CHBr3; %[-]

DermalCancerRisk_CHCl3=DermalAbsorption_CHCl3*SF_dermalCHCl3; %[-]

DermalCancerRisk_CHCl2Br=DermalAbsorption_CHCl2Br*SF_dermalCHCl2Br;
%[-]

DermalCancerRisk_CHClBr2=DermalAbsorption_CHClBr2*SF_dermalCHClBr2;
%[-]



```

DermalCancerRisk_CHBr3=DermalAbsorption_CHBr3*SF_dermalCHBr3; %[-]

DermalCancerRisk=DermalCancerRisk_CHCl3+DermalCancerRisk_CHCl2Br+DermalCa
ncerRisk_CHClBr2+DermalCancerRisk_CHBr3; %[-]

InhalationCancerRisk_CHCl3=InhalationIntake_CHCl3*SF_inhalationCHCl3;
%[-]

InhalationCancerRisk_CHCl2Br=InhalationIntake_CHCl2Br*SF_inhalationCHCl2B
r; %[-]

InhalationCancerRisk_CHClBr2=InhalationIntake_CHClBr2*SF_inhalationCHClBr
2; %[-]
InhalationCancerRisk_CHBr3=InhalationIntake_CHBr3*SF_inhalationCHBr3;
%[-]

InhalationCancerRisk=InhalationCancerRisk_CHCl3+InhalationCancerRisk_CHCl
2Br+InhalationCancerRisk_CHClBr2+InhalationCancerRisk_CHBr3; %[-]

TotalCancerRisk_initial=OralCancerRisk+DermalCancerRisk+InhalationCancerR
isk; %[-]
TotalCancerRisk_final=TotalCancerRisk_initial*(100-
PercentageRemoved)/100; %[-]; Directly dependent on concentration
reduction

CancerRisk_CHCl3=OralCancerRisk_CHCl3+DermalCancerRisk_CHCl3+InhalationCa
ncerRisk_CHCl3; %[-] Specific cancer risks for each THM species

CancerRisk_CHCl2Br=OralCancerRisk_CHCl2Br+DermalCancerRisk_CHCl2Br+Inhala
tionCancerRisk_CHCl2Br; %[-]

CancerRisk_CHClBr2=OralCancerRisk_CHClBr2+DermalCancerRisk_CHClBr2+Inhala
tionCancerRisk_CHClBr2; %[-]

CancerRisk_CHBr3=OralCancerRisk_CHBr3+DermalCancerRisk_CHBr3+InhalationCa
ncerRisk_CHBr3; %[-]

t_fin=cputime-t_ini; %Total calculations time

%OUTPUTS
%STRIPPING SYSTEM REPRESENTATION
C_eqaxis=linspace(eps,C_TTHMstop,1e6); %[microg/L]
p_eqaxis=H_microg*C_eqaxis; %[Pa]
plot(C_eqaxis,p_eqaxis,'b-'),grid %Equilibrium line
hold on
C_opaxis=linspace(C_TTHMsbottom,C_TTHMstop,1e6); %[microg/L]
p_opaxis=linspace(p_TTHMsbottomPa,p_TTHMstopPa,1e6); %[Pa]
plot(C_opaxis,p_opaxis,'g--') %Operation line
plot(C_TTHMstop,p_TTHMstopPa,'ro') %Top point
plot(C_TTHMsbottom,p_TTHMsbottomPa,'ro') %Bottom point
title('Equilibrium and operation lines','FontWeight','bold')
xlabel('Liquid concentration [microg/L]')
ylabel('Gas partial pressure [Pa]')
legend('Equilibrium line','Operation line',2)

```



```

hold off
figure()

%DOUBLE FILM THEORY REPRESENTATION at the BOTTOM of the column
%Outside the double film
LiquidRange=linspace(0,10); %10 is a number to see the diagram
properly
GasRange=linspace(20,30);
plot(LiquidRange,C_TTHMsbottom,'b-'); %[microg/L]
hold on
plot(GasRange,p_TTHMsbottomPa,'g-'); %[Pa]
%Liquid film
slope=k_g_2*M*1e6*p_Tbar/(k_l*p_T); %[microg/(Pa*L)]
C_i=(p_TTHMsbottomPa*slope+C_TTHMsbottom)/(1+H_microg*slope);
%[microg/L]
LiquidSlope=(C_TTHMsbottom-C_i)/(R_L/10);
LiquidInterphaseRange=linspace(10,10+R_L/10);
C_interphase=linspace(C_TTHMsbottom,C_i); %[microg/L]
plot(LiquidInterphaseRange,C_interphase,'b-')
%Gas film
p_i=H_microg*C_i; %[Pa]
Gas_slope=(p_i-p_TTHMsbottomPa)/(R_G/10);
GasInterphaseRange=linspace(10+R_L/10,10+R_L/10+R_G/10);
p_interphase=linspace(p_i,p_TTHMsbottomPa); %[Pa]
plot(GasInterphaseRange,p_interphase,'g-')
%Information
plot(10+R_L/10,C_i,'ro'); %Interphase point
plot(10+R_L/10,p_i,'ro');
plot(10,linspace(0,C_TTHMsbottom),'k');
plot(10+R_L/10,linspace(0,C_TTHMsbottom),'k');
plot(20,linspace(0,C_TTHMsbottom),'k');
title('Double film theory representation at the bottom of the
column','FontWeight','bold')
xlabel('Resistance profile [-]')
ylabel('Concentration [microg/L] or Partial pressure [Pa]')
hold off
figure()

%STRIPPING COLUMN IMAGE
imshow('Output_image.tif','InitialMagnification',29);

%NUMERIC DATA
%ADVICE
if v_Loperating*rho_L*S/(a*mu_L)<4 ||
v_Loperating*rho_L*S/(a*mu_L)>400 %correlations limits
display('Onda correlation used to estimate k_l is extrapolated');
elseif v_Goperating*rho_G*S/(a*mu_G)<5 ||
v_Goperating*rho_G*S/(a*mu_G)>1000
display('Onda correlation used to estimate k_g is extrapolated');
end

%DATA PRINTED ON THE SCREEN
Results=fopen('StrippingTowerResults.txt','w');
fprintf(Results,'BASIC STRIPPING COLUMN DESIGN DATA\r\n\r\n');
fprintf(Results,'The percentage removed is: %4.2f\r\n',
PercentageRemoved);
fprintf(Results,'The height [m] of the column is: %4.2f\r\n',
H_column);

```



```

    fprintf(Results, 'The section [m2] of the column is: %4.2f\r\n', S);
    fprintf(Results, 'The diameter [m] of the column is: %4.2f\r\n',
D_i);
    Filling_name=cell2mat(Filling_name);
    Filling_name=mat2str(Filling_name);
    fprintf(Results, 'The best type of filling is: %s\r\n',
Filling_name);
    fprintf(Results, 'The flow of gas [L/min] required is: %4.2f\r\n',
G_L);
    fprintf(Results, 'The gas operating velocity [m/s] is: %4.2f\r\n',
v_Goperating);
    fprintf(Results, 'The liquid operating velocity [m/s] is: %4.2f\r\n',
v_Loperating);
    fprintf(Results, 'The total pressure drop [mmH2O/(column m)] is:
%4.2f\r\n', PressureDrop);
    fprintf(Results, 'An approach of the total investment [€] required
is: %4.0f\r\n', TotalInvestment);
    fprintf(Results, 'The total initial potential carcinogenic risk [-]
is: %3e\r\n', TotalCancerRisk_initial);
    fprintf(Results, 'The total final potential carcinogenic risk [-] is:
%3e\r\n', TotalCancerRisk_final);
    type StrippingTowerResults.txt
        %DATA SAVED ON THE NOTEPAD
    fprintf(Results, '\r\n');
    fprintf(Results, 'DETAIL STRIPPING COLUMN DESIGN DATA\r\n\r\n');
    fprintf(Results, 'TRIHALOMETHANES POTENTIAL RISK\r\n');
    fprintf(Results, 'The initial oral potential carcinogenic risk [-]
is: %3e\r\n', OralCancerRisk);
    fprintf(Results, 'The initial dermal potential carcinogenic risk [-]
is: %3e\r\n', DermalCancerRisk);
    fprintf(Results, 'The initial inhalation potential carcinogenic risk
[-] is: %3e\r\n', InhalationCancerRisk);
    fprintf(Results, 'The initial potential carcinogenic risk [-] of
CHCl3 is: %3e\r\n', CancerRisk_CHCl3);
    fprintf(Results, 'The initial potential carcinogenic risk [-] of
CHCl2Br is: %3e\r\n', CancerRisk_CHCl2Br);
    fprintf(Results, 'The initial potential carcinogenic risk [-] of
CHClBr2 is: %3e\r\n', CancerRisk_CHClBr2);
    fprintf(Results, 'The initial potential carcinogenic risk [-] of
CHBr3 is: %3e\r\n', CancerRisk_CHBr3);
    fprintf(Results, 'STRIPPING SYSTEM\r\n');
    fprintf(Results, 'The constant temperature [K] of the whole system
is: %0f\r\n', T);
    fprintf(Results, 'The constant pressure [Pa] of the whole system is:
%0f\r\n', p_T);
    fprintf(Results, 'The concentration [microg/L] of the gas at the top
of the column is: %4.2f\r\n', p_TTHMstop);
    fprintf(Results, 'The partial pressure [Pa] at the top of the column
is: %4.2f\r\n', p_TTHMstopPa);
    fprintf(Results, 'The concentration [microg/L] on the interphase is:
%4.4f\r\n', C_i);
    fprintf(Results, 'The partial pressure [Pa] on the interphase is:
%4.4f\r\n', p_i);
    fprintf(Results, 'The Henry constant [atm/(m3·mol)] on the whole
system is: %4.4f\r\n', H_atm);
    fprintf(Results, 'The liquid mass flow over the column section
[kg/(m2·s)] is: %4.2f\r\n', L_wS);

```

```

fprintf(Results, 'The gas mass flow over the column section
[kg/(m2·s)] is: %4.2f\r\n', G_wS);
fprintf(Results, 'The effective interfacial area of the filling
[m2/m3] is: %3e\r\n', a);
fprintf(Results, 'The individual mass transfer coefficient on the
liquid phase [m/s] is: %3e\r\n', k_l);
fprintf(Results, 'The individual mass transfer coefficient on the gas
phase [m/s] is: %3e\r\n', k_g);
fprintf(Results, 'The individual mass transfer coefficient on the gas
phase [kmol/(s·m2·bar)] is: %3e\r\n', k_g_2);
fprintf(Results, 'The overall mass transfer coefficient on the liquid
phase [m/s] is: %3e\r\n', K_L);
fprintf(Results, 'The overall mass transfer coefficient on the gas
phase [m/s] is: %3e\r\n', K_G);
fprintf(Results, 'The volumetric mass transfer coefficient on the
liquid phase [1/s] is: %3e\r\n', k_l_a);
fprintf(Results, 'The volumetric mass transfer coefficient on the gas
phase [kmol/(s·m3·bar)] is: %3e\r\n', k_g_2_a);
fprintf(Results, 'The total mass transfer resistance [h/(m3·Pa·mol)]
is: %4.2f\r\n', R_T);
fprintf(Results, 'The mass transfer resistance of the liquid phase
[percentage] is: %4.2f\r\n', R_L);
fprintf(Results, 'The mass transfer resistance of the gas phase
[percentage] is: %4.2f\r\n', R_G);
fprintf(Results, 'COLUMN MECHANICAL DESIGN\r\n');
fprintf(Results, 'The height of one transfer unit [m] on the overall
gas phase is: %4.2f\r\n', H_G);
fprintf(Results, 'The number of transfer units [-] on the overall gas
phase is: %4.2f\r\n', N_G);
fprintf(Results, 'The nominal size of the filling [mm] is:
%4.2f\r\n', Filling_dN);
fprintf(Results, 'The specific surface are of the filling [m2/m3] is:
%4.2f\r\n', Filling_ap);
fprintf(Results, 'The void fraction of the filling [-] is:
%4.3f\r\n', Filling_eps);
fprintf(Results, 'The sphericity of the filling [-] is: %4.3f\r\n',
Filling_phi);
fprintf(Results, 'The packing factor of the filling [1/m] is:
%4.2f\r\n', Filling_Fp);
fprintf(Results, 'K4 coefficient in operating conditions [-] is:
%4.3f\r\n', K4_operating);
fprintf(Results, 'K4 coefficient when flooding occurs [-] is:
%4.3f\r\n', K4_125);
fprintf(Results, 'FLG parameter is [-] is: %4.2f\r\n', F_LG);
fprintf(Results, 'The thickness of the column wall [mm] is:
%.0f\r\n', th);
fprintf(Results, 'The number of the liquid distributors needed is:
%.0f\r\n', NumberOfDistributors);
fprintf(Results, 'The weight [kg] of the empty column is: %4.2f\r\n',
W_v);
fprintf(Results, 'The weight [kg] of the fillings is: %4.2f\r\n',
W_Filling);
fprintf(Results, 'The total weight [kg] of the column is: %4.2f\r\n',
W);
fprintf(Results, 'The material of the column shell is stainless
steel\r\n');
fprintf(Results, 'COLUMN COST ESTIMATION\r\n');

```



```

    fprintf(Results, 'An approach of the direct costs [€] is: %4.0f\r\n',
DirectCosts);
    fprintf(Results, 'An approach of the indirect costs [€] is:
%4.0f\r\n', IndirectCosts);
    fprintf(Results, 'An approach of the total fixed capital costs [€]
is: %4.0f\r\n', TotalFixedCapital);
    fprintf(Results, 'An approach of the working capital [€] is:
%4.0f\r\n', WorkingCapital);
    fclose(Results);

```

```
end
```

18.6. Validations codes

18.6.1. k_l and k'_g validation

```

%% k_l & k_g_2 validations
%Coulson pages 608 and 609
%Onda's method: a=138 [m2/m3], k_l=2.5e-4 [m/s], k_g_2=5e-4
[kmol/(s*m2*bar)]

%RESET
clear all

%KNOWN & INPUT DATA
p_T=1; %[bar]
T=20+273.15; %[K]
R_bar=0.08314; %[bar*m3/(K*kmol)]
g=9.81; %[m/s2]

rho_L=1e3; %[kg/m3]
rho_G=1.21; %[kg/m3]
mu_L=1e-3; %[kg/(m*s)]
mu_G=0.018e-3; %[kg/(m*s)]
D_L=1.7e-9; %[m2/s]
D_G=1.45e-5; %[m2/s]
sigma_L=70e-3; %[kg/s2] or [N/m]
sigma_c=61e-3; %[kg/s2] or [N/m]

v_Loperating=0.018; %[m/s]; Gw_Section/rhoL=17.6/1e3
v_Goperating=0.719; %[m/s]; Gw_Section/rhoL=0.87/1.21

%PREVIOUS CALCULATIONS
p_bottom=60.8*760; %[bar]; Absorption case
p_top=3.04*760; %[bar]
p=(p_top+p_bottom)/2; %[bar]
C=p/(R_bar*T); %[kmol/m3]

%SOFTWARE CALCULATIONS
N_scL=mu_L/(rho_L*D_L); %[-]
N_scG=mu_G/(rho_G*D_G); %[-]
dN=38e-3; %[m];
ap=194; %[m2/m3];
if dN>=15e-3 %[m]
    A=5.23;

```

```

else
    A=2;
end
a=ap*(1-exp(-
1.45*(sigma_c/sigma_L)^(0.75)*((rho_L*v_Loperating/(ap*mu_L))^(0.1))*((v
_Loperating^2)*ap/g)^(-
0.05))*(rho_L*(v_Loperating^2)/(ap*sigma_L))^(0.2))) %[m2/m3]
k_l=((mu_L*g/rho_L)^(1/3))*0.0051*(rho_L*v_Loperating/(a*mu_L))^(2/3)*N_s
cL^(-1/2)*(ap*dN)^(0.4) %[m/s]
k_g_2=D_G*ap/(R_bar*T)*A*(rho_G*v_Goperating/(ap*mu_G))^(0.7)*(N_scG^(1/3
))*(ap*dN)^(-2) %[kmol/(s*m2*bar)]
k_g=k_g_2*p/C; %[m/s]
k_l_a=k_l*a %[1/s]
k_g_2_a=k_g_2*a %[kmol/(s*m2*bar)]

```

18.6.2. H_G validation

```

%% H_G validation
%%Levenspiel from page 551 to page 553
    %H_G=128.125 [m]

```

```

%RESET
clear all

```

```

%KNOWN & INPUT DATA
p_T=1e5; %[Pa]
G_S=1e5; %[mol/(m2*h)]
L_S=7*1e5; %[mol/(m2*h)]
k_g_2_a=0.32; %[mol/(m3*h*Pa)]
k_l_a=0.1; %[1/h]
H_Pa=12.5; %[Pa*m3/mol]

```

```

%SOFTWARE CALCULATIONS
R_T=1/k_g_2_a+H_Pa/k_l_a; %[h*Pa*m3/mol]
R_G=(1/k_g_2_a)*100/R_T; [%]
R_L=(H_Pa/k_l_a)*100/R_T; [%]
k_g_2_a=1/R_T; %[mol/(h*Pa*m3)]
H_G=G_S/(p_T*k_g_2_a) %[m]

```

18.6.3. N_G validation

```

%% N_G validation
%%Levenspiel from page 551 to page 553
    %N_G=4 [-]

```

```

%RESET
clear all

```

```

%INPUT DATA
G_S=1e5; %[mol/(h*m2)]
L_S=7*1e5; %[mol/(h*m2)]
k_g_a=0.32; %[mol/(m3*h*Pa)]
k_l_a=0.1; %[1/h]
R_L=97.6; %[-]
R_G=2.4; %[-]
H_Pa=12.5; %[Pa*m3/mol]

```



```

p_bottom=100; %[Pa]
p_top=20; %[Pa]
p=1e5; %[Pa]

c_top=0; %[mol/m3]
c=56000; %[mol/m3]

%SOFTWARE CALCULATIONS
c_bottom=(p_bottom-p_top)*G_S*c/(L_S*p)+c_top; %[mol/m3]; Operation line
Incr_p_peq_top=p_top-H_Pa*(G_S*(p_top-p_top)*c/(L_S*p)+c_top); %[-]
Incr_p_peq_bottom=p_bottom-H_Pa*(G_S*c*(p_bottom-p_top)/(L_S*p)+c_top);
%[-]
Incr_p_peq=(Incr_p_peq_top+Incr_p_peq_bottom)/2; %[-]
N_G=(p_bottom-p_top)/Incr_p_peq

```

18.6.4. G_w^* and S validation

```

%% G_wS & S validations
%Coulson pages 604 and 607
    %G_w=1.39 [kg/s], S=1.6 [m2], D_i=1.43 [m]

%RESET
clear all

%KNOWN DATA
rho_L=1e3; %[kg/m3]
rho_G=1.21; %[kg/m3]
mu_L=1e-3; %[kg/(m*s)]
M_L=18; %[g/mol]
M_G=29; %[g/mol]

%INPUT DATA
L_w=29.5; %[kg/s]
K4=0.35;
K4_125=0.8;
Fp=170; %[1/m]
m=27.4; %[-]; Slope of equilibrium curve with molar fractions on axis
(equivalent than H)

%PREVIOUS CALCULATIONS
L=L_w/M_L; %[kmol/s]

%SOFTWARE CALCULATIONS
G=0.8*L/m; %[kmol/s]; Normally: 0.75
G_w=G*M_G %[kg/s]

F_LG=L_w*sqrt(rho_G/rho_L)/G_w; %[-]
if F_LG<0.02
    F_LG=0.02; %[-]
    G_w=L_w*sqrt(rho_G/rho_L)/F_LG; %[kg/s]
elseif F_LG>3
    F_LG=3; %[-]
    G_w=L_w*sqrt(rho_G/rho_L)/F_LG; %[kg/s]
elseif 0.02<F_LG || F_LG>3
    G=G_w/M_G; %[kmol/s]

```



```
end
```

```
v_Gflooding=sqrt(K4_125*rho_G*(rho_L-
rho_G)/(13.1*rho_G^(2)*Fp*(mu_L/rho_L)^(0.1))); %[m/s]
v_Goperating=0.66*v_Gflooding; %[m/s]; Normally: 0.7
G_ws=rho_G*v_Goperating; %[kg/(m2*s)]
S=G_w/G_ws %[m2]
D_i=sqrt(4*S/pi) %[m]
```

18.6.5. ΔP validation

```
%% Pressure_drop_validation
%%Perry from page 293 to page 294
    %Robbins method=0.38 [mmHg]=31.67 [mmH2O/(column m)]
    %GPDC method=0.4 [mmHg]=33.33 [mmH2O/(column m)]

%RESET
clear all

%INPUT DATA
G_ws=2.03; %[kg/(m2*s)]
L_ws=12.2; %[kg/(m2*s)]
Fp=88.58; %[1/m]
rho_L=999.57; %[kg/m3]
rho_G=1.19; %[kg/m3]
mu_L=1e-3; %[kg/(m*s)]

%SOFTWARE CALCULATIONS
F_LG=L_ws*sqrt(rho_G/rho_L)/G_ws; %[-]
K4=13.1*(G_ws^2)*Fp*((mu_L/rho_L)^0.1)/(rho_G*(rho_L-rho_G));

K4_125=0.3359-1.889*exp(-F_LG)+4.939*(exp(-F_LG)^2);
K4_83=0.3072-1.792*exp(-F_LG)+4.551*(exp(-F_LG)^2);
K4_42=0.1585-0.228*exp(-F_LG)+1.76*(exp(-F_LG)^2);
K4_21=0.1001+0.318*exp(-F_LG)+0.504*(exp(-F_LG)^2);
K4_8=0.0772+0.354*exp(-F_LG)+0.037*(exp(-F_LG)^2);
K4_4=0.0675+0.204*exp(-F_LG)-0.121*(exp(-F_LG)^2);

Dif_125=abs(K4-K4_125);
Dif_83=abs(K4-K4_83);
Dif_42=abs(K4-K4_42);
Dif_21=abs(K4-K4_21);
Dif_8=abs(K4-K4_8);
Dif_4=abs(K4-K4_4);
Dif=[Dif_125 Dif_83 Dif_42 Dif_21 Dif_8 Dif_4];

[Ordered, InitialPosition]=sort(Dif);
Dif_min_1=Ordered(:,1);
Dif_min_2=Ordered(:,2);
if InitialPosition(:,1) == 1
    min_1 = 125;
elseif InitialPosition(:,1) == 2
    min_1 = 83;
elseif InitialPosition(:,1) == 3
    min_1 = 42;
elseif InitialPosition(:,1) == 4
```



```

    min_1 = 21;
elseif InitialPosition(:,1) == 5
    min_1 = 8;
else
    min_1 = 4;
end
if InitialPosition(:,2) == 1
    min_2 = 125;
elseif InitialPosition(:,2) == 2
    min_2 = 83;
elseif InitialPosition(:,2) == 3
    min_2 = 42;
elseif InitialPosition(:,2) == 4
    min_2 = 21;
elseif InitialPosition(:,2) == 5
    min_2 = 8;
else
    min_2 = 4;
end

PressureDrop=min_1-Dif_min_1*(min_1-min_2)/(Dif_min_1+Dif_min_2)
%[mmH2O/(column m)]

```

18.6.6. Potential carcinogenic risk validation

```

%% Potentially_carginogenic_risk_validation
%ScienceDirect: Cancer risk assessment from THMs in drinking water, Table
4
    %1st column: Lifetime cancer risk in Taipei City for males
        %Routes      Lifetime cancer risks 10(-5)
        %Ingestion    0.66
        %Dermal       0.01
        %Inhalation   1.22

%RESET
clear all

%INPUT DATA
    %4.3.1.
C_CHCl3w=5.9; %[microg/L] Taipei City
C_CHCl2Brw=4.3; %[microg/L]
C_CHClBr2w=2.8; %[microg/L]
C_CHBr3w=1.9; %[microg/L]

IR=2; %[L/day]
EF=365; %[day/year]
ED=29; %[year]
CF1=1e-3; %[mg/microg] or [L/cm3]
BW=64.8; %[kg] Male
AT=70*365; %[day]

OralIngestion_CHCl3=C_CHCl3w*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
OralIngestion_CHCl2Br=C_CHCl2Brw*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
OralIngestion_CHClBr2=C_CHClBr2w*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
OralIngestion_CHBr3=C_CHBr3w*IR*EF*ED*CF1/(BW*AT); %[mg/(kg*day)]
    %4.3.2.

```



```

SA=(4*BW+7)/(BW+90); %[m2]
F=0.8; %[-]
ET=18.9; %[min/day]
CF2=1e4; %[cm2/m2]
CF3=60; %[min/h]

PC_CHCl3=8.9e-3; %[cm/h]
PC_CHCl2Br=5.8e-3; %[cm/h]
PC_CHClBr2=3.9e-3; %[cm/h]
PC_CHBr3=2.6e-3; %[cm/h]

DermalAbsorption_CHCl3=C_CHCl3w*SA*F*PC_CHCl3*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]
DermalAbsorption_CHCl2Br=C_CHCl2Brw*SA*F*PC_CHCl2Br*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]
DermalAbsorption_CHClBr2=C_CHClBr2w*SA*F*PC_CHClBr2*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]
DermalAbsorption_CHBr3=C_CHBr3w*SA*F*PC_CHBr3*ET*EF*ED*CF1^2*CF2/(BW*AT*CF3); %[mg/(kg*day)]
    %4.3.3.
%CAir=Cwater
VR=0.84; %[m3/h] Male
AE=0.5; %[-]
VF=18e-3; %[-]

InhalationIntake_CHCl3=VF*C_CHCl3w*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]
InhalationIntake_CHCl2Br=VF*C_CHCl2Brw*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]
InhalationIntake_CHClBr2=VF*C_CHClBr2w*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]
InhalationIntake_CHBr3=VF*C_CHBr3w*VR*AE*ET*EF*ED/(BW*AT*CF3);
%[mg/(kg*day)]
    %4.3.4.
SF_oralCHCl3=6.1e-3; %[kg*day/mg]
SF_oralCHCl2Br=6.2e-2; %[kg*day/mg]
SF_oralCHClBr2=8.4e-2; %[kg*day/mg]
SF_oralCHBr3=7.9e-2; %[kg*day/mg]

SF_dermalCHCl3=3.05e-2; %[kg*day/mg]
SF_dermalCHCl2Br=6.33e-2; %[kg*day/mg]
SF_dermalCHClBr2=1.4e-1; %[kg*day/mg]
SF_dermalCHBr3=1.32e-2; %[kg*day/mg]

SF_inhalationCHCl3=8.05e-2; %[kg*day/mg]
SF_inhalationCHCl2Br=6.2e-2; %[kg*day/mg]
SF_inhalationCHClBr2=8.4e-2; %[kg*day/mg]
SF_inhalationCHBr3=3.85e-3; %[kg*day/mg]

%SOFTWARE CALCULATIONS

OralCancerRisk_CHCl3=OralIngestion_CHCl3*SF_oralCHCl3; %[-]
OralCancerRisk_CHCl2Br=OralIngestion_CHCl2Br*SF_oralCHCl2Br; %[-]
OralCancerRisk_CHClBr2=OralIngestion_CHClBr2*SF_oralCHClBr2; %[-]
OralCancerRisk_CHBr3=OralIngestion_CHBr3*SF_oralCHBr3; %[-]

```



$$\text{OralCancerRisk} = \text{OralCancerRisk_CHCl3} + \text{OralCancerRisk_CHCl2Br} + \text{OralCancerRisk_CHClBr2} + \text{OralCancerRisk_CHBr3} \quad \%[-]$$

$$\begin{aligned} \text{DermalCancerRisk_CHCl3} &= \text{DermalAbsorption_CHCl3} * \text{SF_dermalCHCl3}; \quad \%[-] \\ \text{DermalCancerRisk_CHCl2Br} &= \text{DermalAbsorption_CHCl2Br} * \text{SF_dermalCHCl2Br}; \quad \%[-] \\ \text{DermalCancerRisk_CHClBr2} &= \text{DermalAbsorption_CHClBr2} * \text{SF_dermalCHClBr2}; \quad \%[-] \\ \text{DermalCancerRisk_CHBr3} &= \text{DermalAbsorption_CHBr3} * \text{SF_dermalCHBr3}; \quad \%[-] \\ \text{DermalCancerRisk} &= \text{DermalCancerRisk_CHCl3} + \text{DermalCancerRisk_CHCl2Br} + \text{DermalCancerRisk_CHClBr2} + \text{DermalCancerRisk_CHBr3} \quad \%[-] \end{aligned}$$

$$\begin{aligned} \text{InhalationCancerRisk_CHCl3} &= \text{InhalationIntake_CHCl3} * \text{SF_inhalationCHCl3}; \quad \%[-] \\ \text{InhalationCancerRisk_CHCl2Br} &= \text{InhalationIntake_CHCl2Br} * \text{SF_inhalationCHCl2Br}; \quad \%[-] \\ \text{InhalationCancerRisk_CHClBr2} &= \text{InhalationIntake_CHClBr2} * \text{SF_inhalationCHClBr2}; \quad \%[-] \\ \text{InhalationCancerRisk_CHBr3} &= \text{InhalationIntake_CHBr3} * \text{SF_inhalationCHBr3}; \quad \%[-] \\ \text{InhalationCancerRisk} &= \text{InhalationCancerRisk_CHCl3} + \text{InhalationCancerRisk_CHCl2Br} + \text{InhalationCancerRisk_CHClBr2} + \text{InhalationCancerRisk_CHBr3} \quad \%[-] \end{aligned}$$

$$\text{TotalCancerRisk_initial} = \text{OralCancerRisk} + \text{DermalCancerRisk} + \text{InhalationCancerRisk}; \quad \%[-]$$

$$\begin{aligned} \text{CancerRisk_CHCl3} &= \text{OralCancerRisk_CHCl3} + \text{DermalCancerRisk_CHCl3} + \text{InhalationCancerRisk_CHCl3}; \quad \%[-] \quad \text{Specific cancer risks for each THM species} \\ \text{CancerRisk_CHCl2Br} &= \text{OralCancerRisk_CHCl2Br} + \text{DermalCancerRisk_CHCl2Br} + \text{InhalationCancerRisk_CHCl2Br}; \quad \%[-] \\ \text{CancerRisk_CHClBr2} &= \text{OralCancerRisk_CHClBr2} + \text{DermalCancerRisk_CHClBr2} + \text{InhalationCancerRisk_CHClBr2}; \quad \%[-] \\ \text{CancerRisk_CHBr3} &= \text{OralCancerRisk_CHBr3} + \text{DermalCancerRisk_CHBr3} + \text{InhalationCancerRisk_CHBr3}; \quad \%[-] \end{aligned}$$

18.7. Complementary data of Sant Joan Despí DWTP study

18.7.1. Numerical data

BASIC STRIPPING COLUMN DESIGN DATA

The percentage removed is: 77.56

The height [m] of the column is: 17.43

The section [m²] of the column is: 6.72

The diameter [m] of the column is: 2.93

The best type of filling is: 'ENVIPAC RING (Plastic - 3 1/8 in.)'

The flow of gas [L/min] required is: 345691.27

The gas operating velocity [m/s] is: 0.86

The liquid operating velocity [m/s] is: 0.06

The total pressure drop [mmH₂O/(column m)] is: 4.03

An approach of the total investment [€] required is: 2778505



The total initial potential carcinogenic risk [-] is: 1.483e-004

The total final potential carcinogenic risk [-] is: 3.327e-005

DETAIL STRIPPING COLUMN DESIGN DATA

TRIHALOMETHANES POTENTIAL RISK

The initial oral potential carcinogenic risk [-] is: 8.654e-005

The initial dermal potential carcinogenic risk [-] is: 7.341e-007

The initial inhalation potential carcinogenic risk [-] is: 6.098e-005

The initial potential carcinogenic risk [-] of CHCl_3 is: 1.105e-005

The initial potential carcinogenic risk [-] of CHCl_2Br is: 3.069e-005

The initial potential carcinogenic risk [-] of CHClBr_2 is: 6.434e-005

The initial potential carcinogenic risk [-] of CHBr_3 is: 4.216e-005

STRIPPING SYSTEM

The constant temperature [K] of the whole system is: 293

The constant pressure [Pa] of the whole system is: 101325

The concentration [microg/L] of the gas at the top of the column is: 5.10

The partial pressure [Pa] at the top of the column is: 0.06

The concentration [microg/L] on the interphase is: 2.6986

The partial pressure [Pa] on the interphase is: 0.0020

The Henry constant [atm/(m³·mol)] on the whole system is: 0.0015

The liquid mass flow over the column section [kg/(m²·s)] is: 58.34

The gas mass flow over the column section [kg/(m²·s)] is: 0.86

The effective interfacial area of the filling [m²/m³] is: 9.488e+001

The individual mass transfer coefficient on the liquid phase [m/s] is: 4.592e-004

The individual mass transfer coefficient on the gas phase [m/s] is: 7.295e+003

The individual mass transfer coefficient on the gas phase [kmol/(s·m²·bar)] is: 2.150e-003

The overall mass transfer coefficient on the liquid phase [m/s] is: 1.246e-004

The overall mass transfer coefficient on the gas phase [m/s] is: 8.302e-005

The volumetric mass transfer coefficient on the liquid phase [1/s] is: 6.268e-002

The volumetric mass transfer coefficient on the gas phase [kmol/(s·m³·bar)] is: 9.708e-003

The total mass transfer resistance [h/(m³·Pa·mol)] is: 3.53

The mass transfer resistance of the liquid phase [percentage] is: 18.86

The mass transfer resistance of the gas phase [percentage] is: 81.14

COLUMN MECHANICAL DESIGN



The height of one transfer unit [m] on the overall gas phase is: 3.71

The number of transfer units [-] on the overall gas phase is: 4.70

The nominal size of the filling [mm] is: 28.60

The specific surface area of the filling [m²/m³] is: 80.00

The void fraction of the filling [-] is: 0.955

The sphericity of the filling [-] is: 0.128

The packing factor of the filling [1/m] is: 37.00

K4 coefficient in operating conditions [-] is: 0.090

K4 coefficient when flooding occurs [-] is: 0.183

FLG parameter is [-] is: 2.15

The thickness of the column wall [mm] is: 10

The number of the liquid distributors needed is: 2

The weight [kg] of the empty column is: 15703.30

The weight [kg] of the fillings is: 106299.58

The total weight [kg] of the column is: 122002.87

The material of the column shell is stainless steel

COLUMN COST ESTIMATION

An approach of the direct costs [€] is: 1890140

An approach of the indirect costs [€] is: 756056

An approach of the total fixed capital costs [€] is: 2646196

An approach of the working capital [€] is: 132310

18.8. Complementary data of hypothetical neighbourhood study

18.8.1. Numerical data

BASIC STRIPPING COLUMN DESIGN DATA

The percentage removed is: 54.55

The height [m] of the column is: 5.55

The section [m²] of the column is: 0.20

The diameter [m] of the column is: 0.50

The best type of filling is: 'HIFLOW RING (Plastic - 3 1/2 in.)'

The flow of gas [L/min] required is: 7457.00

The gas operating velocity [m/s] is: 1.12



The liquid operating velocity [m/s] is: 0.11
The total pressure drop [mmH₂O/(column m)] is: 25.48
An approach of the total investment [€] required is: 216114
The total initial potential carcinogenic risk [-] is: 2.596e-005
The total final potential carcinogenic risk [-] is: 1.180e-005

DETAIL STRIPPING COLUMN DESIGN DATA

TRIHALOMETHANES POTENTIAL RISK

The initial oral potential carcinogenic risk [-] is: 1.716e-006
The initial dermal potential carcinogenic risk [-] is: 1.655e-007
The initial inhalation potential carcinogenic risk [-] is: 2.407e-005
The initial potential carcinogenic risk [-] of CHCl₃ is: 2.596e-005
The initial potential carcinogenic risk [-] of CHCl₂Br is: 0.000e+000
The initial potential carcinogenic risk [-] of CHClBr₂ is: 0.000e+000
The initial potential carcinogenic risk [-] of CHBr₃ is: 0.000e+000

STRIPPING SYSTEM

The constant temperature [K] of the whole system is: 293
The constant pressure [Pa] of the whole system is: 101325
The concentration [microg/L] of the gas at the top of the column is: 2.03
The partial pressure [Pa] at the top of the column is: 0.04
The concentration [microg/L] on the interphase is: 3.6036
The partial pressure [Pa] on the interphase is: 0.0113
The Henry constant [atm/(m³·mol)] on the whole system is: 0.0037
The liquid mass flow over the column section [kg/(m²·s)] is: 106.25
The gas mass flow over the column section [kg/(m²·s)] is: 1.12
The effective interfacial area of the filling [m²/m³] is: 1.029e+002
The individual mass transfer coefficient on the liquid phase [m/s] is: 1.077e-003
The individual mass transfer coefficient on the gas phase [m/s] is: 3.875e+003
The individual mass transfer coefficient on the gas phase [kmol/(s·m²·bar)] is: 5.141e-004
The overall mass transfer coefficient on the liquid phase [m/s] is: 3.531e-004
The overall mass transfer coefficient on the gas phase [m/s] is: 9.497e-005
The volumetric mass transfer coefficient on the liquid phase [1/s] is: 9.080e-002
The volumetric mass transfer coefficient on the gas phase [kmol/(s·m³·bar)] is: 1.630e-002
The total mass transfer resistance [h/(m³·Pa·mol)] is: 2.84



The mass transfer resistance of the liquid phase [percentage] is: 40.04

The mass transfer resistance of the gas phase [percentage] is: 59.96

COLUMN MECHANICAL DESIGN

The height of one transfer unit [m] on the overall gas phase is: 3.91

The number of transfer units [-] on the overall gas phase is: 1.42

The nominal size of the filling [mm] is: 88.90

The specific surface area of the filling [m²/m³] is: 66.00

The void fraction of the filling [-] is: 0.958

The sphericity of the filling [-] is: 0.086

The packing factor of the filling [1/m] is: 30.00

K₄ coefficient in operating conditions [-] is: 0.125

K₄ coefficient when flooding occurs [-] is: 0.254

FLG parameter is [-] is: 3.00

The thickness of the column wall [mm] is: 5

The number of the liquid distributors needed is: 0

The weight [kg] of the empty column is: 406.35

The weight [kg] of the fillings is: 996.72

The total weight [kg] of the column is: 1403.07

The material of the column shell is stainless steel

COLUMN COST ESTIMATION

An approach of the direct costs [€] is: 147016

An approach of the indirect costs [€] is: 58807

An approach of the total fixed capital costs [€] is: 205823

An approach of the working capital [€] is: 10291

18.8.2. Graphical representations

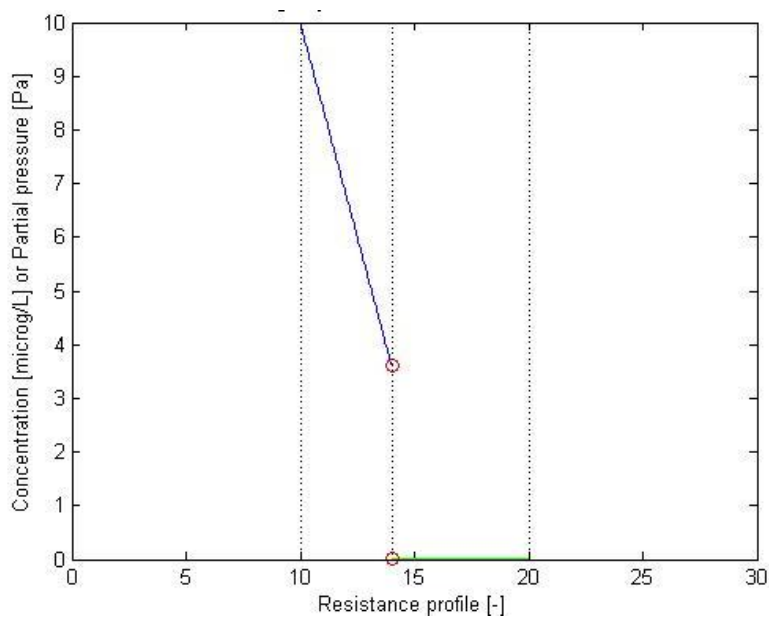


Figure 18.9. Double film theory representation at the bottom of the column.

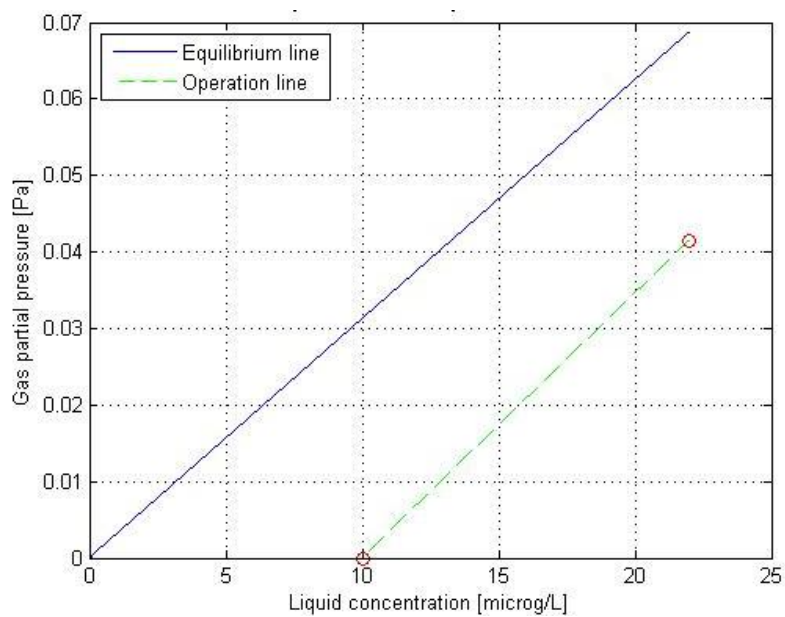


Figure 18.10. Equilibrium and operation lines of the stripping system.

18.9. Complementary data of San Diego study

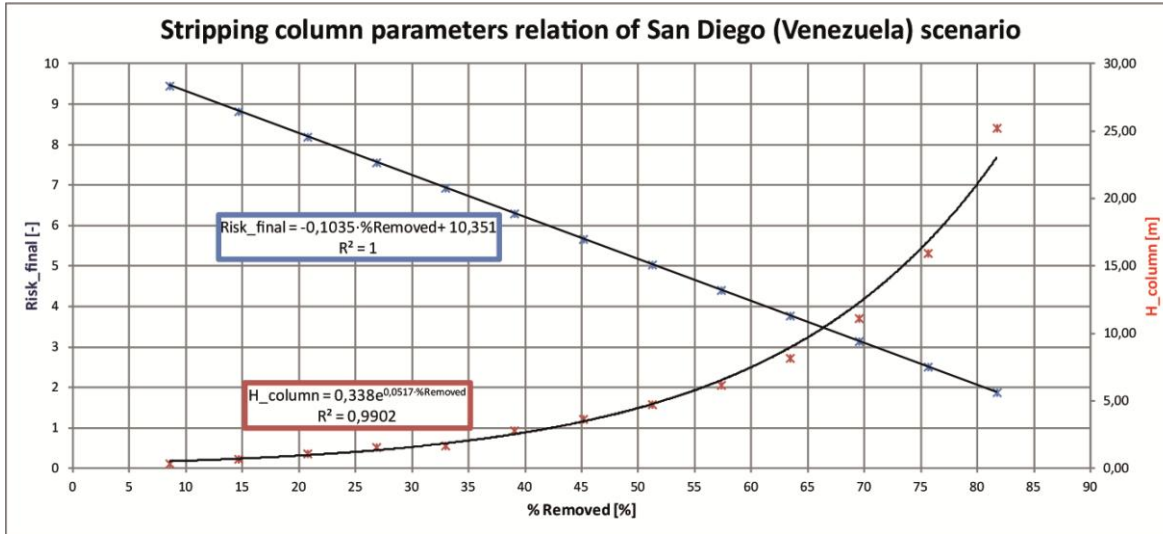


Figure 18.11. Stripping column parameters relation of San Diego (Venezuela) scenario.

18.9.1. Numerical data

BASIC STRIPPING COLUMN DESIGN DATA

The percentage removed is: 73.41

The height [m] of the column is: 13.95

The section [m²] of the column is: 2.35

The diameter [m] of the column is: 1.73

The best type of filling is: 'HIFLOW RING (Plastic - 3 1/2 in.)'

The flow of gas [L/min] required is: 93502.21

The gas operating velocity [m/s] is: 1.12

The liquid operating velocity [m/s] is: 0.11

The total pressure drop [mmH₂O/(column m)] is: 25.48

An approach of the total investment [€] required is: 2118552

The total initial potential carcinogenic risk [-] is: 1.035e-004

The total final potential carcinogenic risk [-] is: 2.752e-005

DETAIL STRIPPING COLUMN DESIGN DATA

TRICHALOMETHANES POTENTIAL RISK

The initial oral potential carcinogenic risk [-] is: 1.554e-005

The initial dermal potential carcinogenic risk [-] is: 6.584e-007

The initial inhalation potential carcinogenic risk [-] is: 8.731e-005

The initial potential carcinogenic risk [-] of CHCl_3 is: 8.259e-005

The initial potential carcinogenic risk [-] of CHCl_2Br is: 1.646e-005

The initial potential carcinogenic risk [-] of CHClBr_2 is: 4.462e-006

The initial potential carcinogenic risk [-] of CHBr_3 is: 0.000e+000

STRIPPING SYSTEM

The constant temperature [K] of the whole system is: 293

The constant pressure [Pa] of the whole system is: 101325

The concentration [microg/L] of the gas at the top of the column is: 9.66

The partial pressure [Pa] at the top of the column is: 0.19

The concentration [microg/L] on the interphase is: 8.2253

The partial pressure [Pa] on the interphase is: 0.0233

The Henry constant [atm/(m³·mol)] on the whole system is: 0.0035

The liquid mass flow over the column section [kg/(m²·s)] is: 106.25

The gas mass flow over the column section [kg/(m²·s)] is: 1.12

The effective interfacial area of the filling [m²/m³] is: 1.029e+002

The individual mass transfer coefficient on the liquid phase [m/s] is: 1.076e-003

The individual mass transfer coefficient on the gas phase [m/s] is: 1.222e+003

The individual mass transfer coefficient on the gas phase [kmol/(s·m²·bar)] is: 5.030e-004

The overall mass transfer coefficient on the liquid phase [m/s] is: 3.375e-004

The overall mass transfer coefficient on the gas phase [m/s] is: 9.559e-005

The volumetric mass transfer coefficient on the liquid phase [1/s] is: 9.070e-002

The volumetric mass transfer coefficient on the gas phase [kmol/(s·m³·bar)] is: 1.595e-002

The total mass transfer resistance [h/(m³·Pa·mol)] is: 2.82

The mass transfer resistance of the liquid phase [percentage] is: 38.30

The mass transfer resistance of the gas phase [percentage] is: 61.70

COLUMN MECHANICAL DESIGN

The height of one transfer unit [m] on the overall gas phase is: 3.88

The number of transfer units [-] on the overall gas phase is: 3.59

The nominal size of the filling [mm] is: 88.90

The specific surface area of the filling [m²/m³] is: 66.00

The void fraction of the filling [-] is: 0.958

The sphericity of the filling [-] is: 0.086

The packing factor of the filling [1/m] is: 30.00



K4 coefficient in operating conditions [-] is: 0.125

K4 coefficient when flooding occurs [-] is: 0.254

FLG parameter is [-] is: 3.00

The thickness of the column wall [mm] is: 7

The number of the liquid distributors needed is: 2

The weight [kg] of the empty column is: 5038.30

The weight [kg] of the fillings is: 29801.72

The total weight [kg] of the column is: 34840.02

The material of the column shell is stainless steel

COLUMN COST ESTIMATION

An approach of the direct costs [€] is: 1441192

An approach of the indirect costs [€] is: 576477

An approach of the total fixed capital costs [€] is: 2017669

An approach of the working capital [€] is: 100883

18.9.2. Graphical representations

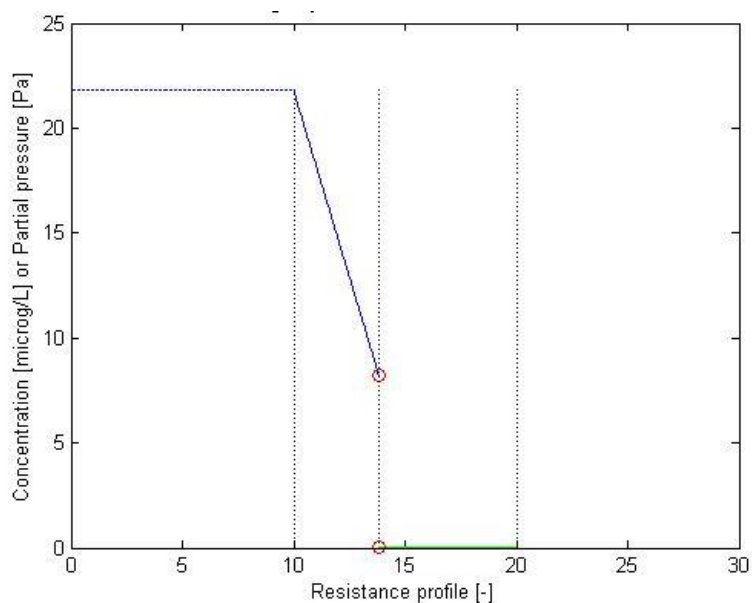


Figure 18.12. Double film theory representation at the bottom of the column.

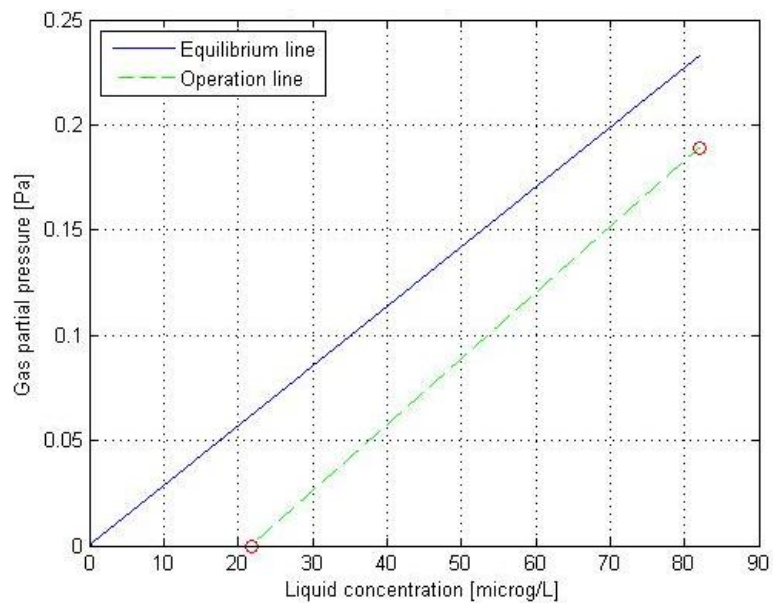


Figure 18.13. Equilibrium and operation lines of the stripping system.