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## Literature Review

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## CFD Modelling of heat exchanger equipment

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A report presented to Imperial College London in partial fulfillment of the requirements for the degree of Master of Sience in CHEMICAL ENGINEERINGFebruary 2013Table of contentsIntroductionMany experimental and modeling attempts have been carried out to analyze the effects of fouling on heat exchanger efficiency. So far, the research has been focused on the deposition of fouling elements on the tube inner side and its corresponding thermal-hydraulic effects. This project aims at investigating these aspects inside the tube but also on the shell side of a shell and tube heat exchanger by CFD simulations. First, we will examine whether the deposition models established for the tube side can be applied to the heat exchanger shell side. Then we search in the literature for the existing shell side models. The next step starts with modeling of fouling in the inside and outside of a single tube, and then we refine and extend the model to more real cases by relaxing the limiting hypotheses. Finally, the numerical results for a shell and tube heat exchanger with a single tube will be compared with experimental data.

## Chapter 1

## Fouling in heat exchangers

This chapter describes the basics and science of fouling process. Different types of fouling and mechanisms that generate fouling are explained in this part.

## Different types of fouling

The fouling refers to the deposits that appear in the heat exchangers surfaces. It can be found in different shapes: crystallization, sediments, biological residues, chemical reaction products, etc. These deposits have a thermal conductivity between 0. 2 and 1 W. m-1. K-1 [4] that reduces the heat exchanger‘ s performances and lead to an early ageing of the facilities. The fouling process rolls out in five stages: Initiation: the first stage is connected to the time before the first appearance of deposits in the facilitiesThe deposits transport until the wallThe deposit attachment: every particle does not necessary settle in the wallParticle removal: some particles can be extracted from the deposit layerDeposit ageing: the chemical layout or crystalline of deposit can change over time which reduces the particle bond and weaken the deposit.

## Particulate fouling

DescriptionThe heat exchangers are in contact with fluid that may contain airborne particles. These particles can settle in the heat exchanger’s walls and accumulate creating a deposit.

## Particle deposit mechanisms in the walls

Many processes are involved in the transfer of the particles to the wall. Transfer due to Brownian diffusion: the airborne particles are subjected to random motions. Transfer due to gravity: particles are subjected to the gravitation field (P= mparticle. g). The gravity effect is significant in case of horizontal installations, with a slow fluid flow and regarding large particles (particles with a size superior to 1µm). Transfer due to centrifugal force: the bond attraction is high -under the centrifugal force- in areas where the fluid flow re-circulates as shown in Figure 1. recircualtion. pngFigure 1: Flow profile in a right angle bend [5]Transfer due to thermal precipitationWhen the fluid is subjected to a temperature gradient, particles move to the areas where the fluid is the coldest. In a heat exchanger, particles move to the areas with hot/cold interface. Consequently, when there is a considerable temperature difference between the two fluids of a heat exchanger, the bond to walls due to thermal precipitation is high. Transfer due to electrical precipitationRegarding small particles (size under 1µm), the electrical interaction is stronger than the gravity force and so affects the motion of these particles. Transfer due to turbulenceThe turbulence projects particles against the wall creating the deposit. The Figure 2 summarizes these mechanisms that generate the deposit: mecanisms deposit. pngFigure 2: Mechanisms creating deposit [5]To conclude, the deposit is more likely to be generated from the gravitational and centrifugal forces in a heat exchanger that is horizontal and contains many bends. Besides, a high thermal gradient increases considerably the deposit. However, the deposit can be partly prevented by maintaining a high flow velocity.

## Scaling [7]

DescriptionScaling is a kind of fouling that appears in the presence of calcium (Ca2+), magnesium (Mg2+) and bicarbonate (HCO3) ions in water. This is exemplified by a limestone deposit (calcium carbonate CaCO3) on the walls, according to the following reaction: Ca2+ + CO32- ↔ CaCO3. Risk factorsWater hardness, characterized by the presence of magnesium and calcium ions, is a significant scaling risk factor. Another factor to bear in mind is the water temperature. Indeed, the increase of water temperature leads to the release of carbon gas which accelerates the previous reaction. That is why scaling is low on cold water pipes while it is common on hot water pipes such as water heaters. A third risk factor is the presence of other ions in water such as iron Fe2+ ion that favors deposit. Conversely, when copper or zinc ions are present, the limestone does not attach the walls but stays airborne in water. The amount of these elements needed is very low such as 10-5 g. L-1 respectively. Therefore, copper pipes must be favored. Scaling is a type of fouling that is most commonly found within aqueous environment. It is often combined to other fouling mechanism such as corrosion fouling.

## Corrosion fouling

DescriptionLike scaling, corrosion fouling results from a chemical reaction. This reaction is an oxidation- reduction equation: metal + n. H+ → metal ions + n/2 (H2)Figure 3: Corrosion fouling mechanism [5]Figure 3 presents the corrosion mechanism: it results from redox reactions that correspond to material migration and create cavities.

## Biological fouling

Biological fouling is the result of the growth of micro- organisms that attach heat exchanger surfaces. Three types of micro- organisms are involved in this phenomenon: bacteria, algae and fungi. Bacteria: the bacteria growth is due to nutrient such as hydrocarbons, ammonia, etc. The bacterial cell is a living cell capable of feeding, growing and multiplying in the environment in which it operates. Algae: they are living organisms that grow in the presence of solar energy with photosynthesis. Green and brown algae are those commonly found in cooling system. It is of high importance to identify the presence of algae because it causes silica deposit which can create blockages. Fungi: these plants have neither root nor stem or leaf. They grow thanks to nutrients, but mainly thanks to changes in their physical conditions such as pH, humidity and ambient temperature.

## Chemical reaction fouling

This type of fouling occurs when a chemical reaction takes place next to a heat exchange surface and the solid products of the reaction attach the surface. Most of the time, it consists in a polymerization by auto- oxidation that spreads like a chain reaction with free radicals. Molecular oxygen plays a controlling role. The reaction scheme is the following: Initiation: RH + Z- → R- + HZPropagation: R¨ + O2 → ROO¨ROO¨ + RH → ROOH + R¨Stop: R¨ + R¨ → RRROO¨ + R¨ → ROORRH is a hydrocarbon molecule and Z¨ is a free radical originates from metal ions and nitrogen or sulfur compounds. Chemical reaction rates depend on temperature, pressure, concentration and the presence of catalysts. This type of fouling is mainly found in petrochemical and food industries, and heating circuits using an organic fluid.

## Solidification fouling

This type fouling results from a pure liquid solidification in contact with an exchange surface sub cooled. This means that an ice layer is formatted inside the pipes. It can also refer to the deposit of an element in his high melting point within a liquid that is in contact with a cold surface exchange. Vapor may attach as well as a solid, without passing through the liquid state which corresponds to the frost formation.

## Conclusions

Five major fouling categories exist: particulate fouling, crystallization fouling, corrosion fouling, chemical reaction fouling and biological fouling. Besides, installations can be subjected, at the same time, to several of these mechanisms that create a deposit. The parameters that affect the fouling rate of exchange walls are various: temperature, pressure, the fluid nature and velocity, materials used… Consequently, fouling does not affect all exchangers in the same way because their configurations are dissimilar.

## Impact

## Chapter 2

## Description, fouling and caution of shell and tube heat exchangers

A great number of heat exchangers exist to meet the needs of the different industry sectors. The aim of this chapter is to present these different heat exchangers by specifying the fouling risks according to their design.

## 2. 1 Shell and tube heat exchanger’s description

This is one of the most common heat exchanger. It is composed of a bundle of tubes in a shell. One of the fluids circulates inside the tubes while the other circulates outside the tubes, through the shell side. Baffles are often added inside the shell and guide the fluid that circulates outside the tubes. They generate turbulence, possibly increase the fluid velocity and improve the heat transfer coefficient. However, they can create at the same time a resistance to the flow and damaging vibrations. There are also void regions at the corners that favor fouling and limit the heat exchange area. Consequently many studies on baffle types have been carried out involving CFD modeling [17]. For instance, we can find in the literature the following baffles that have been designed for shell and tube heat exchangers: rod [18- 19], orifice [20] and helical baffles [21- 22]. More recently, a numerical modeling of the shell side of a shell- and- tube heat exchanger with flower baffles [23] have been developed and validated by experimental data. The computation results with the flower baffles shows a better overall thermal hydraulic performance than the heat exchanger with the helical baffles. These latter were so far considered to have outstanding thermal hydraulic performance, low vibrations and less subject to fouling. Figure ?: Shell and Tube heat exchanger [8]The tubes are supported at their ends by tube sheets. These are the sensitive parts of the heat exchangers as they are easily subjected to corrosion fouling. Two tubes configurations can be found: in square and triangular pitch. The square pitch gives access to all of the external part of the tubes while the triangular pitch is more compact as shown in Figure ?. Figure ?: Square pitch (on the left), triangular pitch (on the right) [5]

## 2. 2 Fouling risks and caution

If a very fouling fluid is being used, exchangers- type U should be avoided because they do not allow mechanical cleaning of the tubes inside. Besides, it is essential to circulate the more fouling fluid inside the tubes since tube side is easier to clean than the shell side. As explained previously, the square pitch is a better configuration for cleaning matters. The baffle’s configuration should be considered regarding the flow in the shell. In order to have a uniform velocity and to avoid re-circulating flows that lead to deposit, it is essential to consider the following configuration: To define a limited clearance between the baffles and the shellTo set a distance between the baffles slightly smaller than the shell diameterClearance between the baffles and the shellShellBaffles should define an opening of approximately 20% of the shell diameterDistance between bafflesBaffles openingFigure ?: Baffle’s configurations [5]By implementing vents in the installation, the corrosive vapors can be released out of the exchanger. To avoid further fouling, preexisting micro cracks in the material should be minimized.

## Chapter 3

## CFD Modeling of heat exchangers undergoing chemical reaction fouling

Numerical modeling methods are sought increasingly to study the performance of heat exchangers. One of the main advantages of this method compared to the experimental method is economical. In addition, it allows visibility of the phenomena that are not necessarily possible experimentally and often saves time compared to experimental method. However, the modeling of loaded configurations is complex and often requires a simplification of the studied element and validation of computation results by comparison with experimental data.

## 3. 1 Fouling models

This research project focuses in the chemical reaction type of fouling. Many correlations have been developed over the years for this fouling model trying to take into account the variables affecting it (composition, temperature, pressure, velocity, shear stress and surface conditions) [3]. The common method to assess the fouling dynamics is to calculate the fouling resistance that would be added to the mass transfer equations.

## 3. 1. 1 Fouling resistance

We can find in literature two main methodologies to design heat exchanger that take into account fouling: the LMTD (log mean temperature difference) method [9] and the ε- NTU approach [10] [11]. The following figure shows the fouling phenomenon for a single tube heat exchanger and describes the nomenclature used in the mass transfer equations detailed below: tFigure ?: Fouling layer within the tube and the shell side [3]LMTD methodologyFirst, the heat duty Q (W) is calculated for both (shell and tube) sides of the tube wall:(3. 1)Where and (kg. s-1) are the mass flow rate of the hot and cold fluids, and (J. kg-1. K-1) the specific heat capacity, , and , (K) the inlet and outlet temperature of the two fluids. The total heat transfer Q (W) in the exchanger can also been expressed by the Hausbrand formula: Where U (W. m-2. K-1) is the overall heat transfer coefficient; S (m²) is the surface area of the exchanger, ΔTlm is the appropriate mean temperature difference between the hot and cold fluids. According to the configuration of the heat exchanger, the mean temperature is adjusted with a dimensionless coefficient ε departing from the counter- current flow so that: ΔTlm = ε ΔT°lm (3. 3)where ΔT°lm is the mean temperature for a counter- current flow. [2]The formula of the mean temperature is defined by:(3. 4)The overall heat transfer coefficient U (W. m-2. K-1) is equal to the sum of the resistances including the tube- side and shell- side fouling resistances, Rf, t and Rf, s:(3. 5)Where So (m²) and Si (m²) are the outer and inner heat transfer areas, , ht and hs are the tube- side and shell- side convective heat transfer coefficients, δw is the wall thickness, λw is the thermal conductivity  (W·m-1·K-1), Sm is the logarithmic mean area [3]:(3. 6)Models inside the tubeRésumé de la theseModels for shell sideWhile there are a considerable number of numerical modeling studies to improve the performance of the tube side [12-16], there is little research on the shell side in the literature and even fewer studies considering fouling. This is due to the complexity of the velocity and temperature fields increased by the complicated geometry (baffles) of this side.