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# Optimum design of a welded pressure vessel using different heat resistant steels

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## Abstract

In this article, analysis and optimization of a welded pressure vessel are presented for an ammonia synthesis converter, which could be made from different types of heat and corrosion resistant steels. As we know, there are three different types of these steels such as the ferritic steels, austenitic steels and the combination of the two before the duplex steels. These steels are widely used primarily in the chemical industry. Each type has advantages and disadvantages. In which case is it appropriate to use it depends on a consistency that's in contact with the steel, especially the corrosive property of it and it also depends on the mechanical stress.

Keywords: welded pressure vessel, heat and corrosion resistant steels, optimum design

### 1. Ferritic steels

The ferritic steels have the lowest toughness, but these are the only ones which could resist to sulphur-containing consists, and because of that, these types of steels most important use is the vehicle exhaust system. Their most important alloying element is the chromium, but some types can contain silicon and aluminium to improve their corrosion resistance, and they have an essential role in the genesis of the ferrite. This type has the worst weldability, because of the toughness and the impact strength also decrease during the welding procedure. To avoid this, heat treatment should be used after welding. For this reason, an annealing heat treatment should be applied. In general, this is the only heat treating procedure which is used in the case of these heavily alloyed steels. The main goal of this treatment to decrease the remaining stress of the welded workpiece after the wedding or the cold forming. The temperature of the hold is different for each type of ferritic steels, that is shown in Table 1 [1].

As filler material matching (or overmatching) welding electrodes are available for welding this type of steel, but this electrode is specified only those joints where the corrosion resistance is essential. But if the main requisitioning is dynamic, fatigue or any other type of non-static load is anticipated. In these cases, the selection of austenitic filler material can be a solution. This can lead a mismatch between the properties of the ferritic and austenitic steel [2].

The good thing is the austenitic weld is tough, and it can improve the toughness of the welded area by absorbing most of the impact that the joint may be exposed during the usage. The other problem with the austenitic filler material is which is the next if the cooling rate after the welding the austenitic filler material and the austenite which created through the dual-phase zone  $(\delta - \gamma)$  transform into martensite below the M<sub>s</sub> temperature [2].

| Type of steel         | Temperature [°C] |
|-----------------------|------------------|
| 405 (X6 CrAl 13)      | 650-815          |
| 430 (X8 Cr17)         | 595-900          |
| 430F (X14 CrMoS 17)   | 705-785          |
| 442(X16 CrNiSi 20-12) | 760-830          |
| 446 (X18 CrN 28)      | 760-830          |

1. Table: The range of the temperature of the hold of annealing heat treatment of different

ferritic steels [1]

The other purpose of this treatment is to cease the areas with precipitates and the modified regions because of the 475  $^{\circ}$ C embrittlement, and in this way, the homogeneity of the steel is increased, and with it, the resistance to the corrosion also increased. The normal temperature of this treatment is around 950  $^{\circ}$ C, and the cooling is usually happening in water or some other

strong coolant. This is necessary because in case of slow cooling, the chromium has more time to move to the edge of the grains and there they with carbon form  $Cr_{23}C_6$  complex carbide or sometimes nitrides. If the cooling is fast enough, one could avoid the formation of this carbide (or nitride) than the appearance of the martensite can be a problem. The problem with the martensite is the increasing the number of the grain borders, and with it, the corrosion resistant properties will decrease. Furthermore, the martensite is rigid, and because of that, the impact strength and the toughness will also decrease. To avoid this another, secondary heat treatment should be used [1].

With this heat treatment, the effect on the impact strength at room temperature and the hardness are shown in Table 2 in case of an X8 Cr17 (AISI 430) steel with different levels of temperatures.

| Hold temperature of the<br>annealing | Impact strength [J] | Vickers hardness (HV30) |
|--------------------------------------|---------------------|-------------------------|
| without heat treatment               | 3 <u>±</u> 0,5      | 251 <u>±</u> 4          |
| 600 °C                               | 18 <u>+</u> 0,5     | <i>231<u>+</u>3</i>     |
| 700 °C                               | 19 <u>±</u> 0,5     | <i>195<u>+</u>4</i>     |
| 800 °C                               | 22±0,5              | 177 <u>±</u> 5          |

Table 2: The range of the temperature of the hold of annealing heat treatment of different ferritic steels [1]

With this in mind, it can be stated that after welding annealing at 600  $^{\circ}$ C is definitely worth doing on the welded joint, since the impact strength, becoming six times better, but the hardness reducing to a lesser extent. Figure 1 shows the macrostructure of the welded metal, the heat affected zone and the base material, and in this picture, the grain growth is also can be observed [1].

The microstructure of the heat affected zone shows coarse grains in the welded condition without any heat treatment. After the welding procedure, the martensite appears in the welded joint. In very coarse grains, carbides and nitrides are also showable. The martensite contains less chromium than the ferritic matrix, and because of this, this area with martensite is particularly sensitive to electrochemical corrosion [2].



Figure 1: Macrostructure of the welded joint [1]

In Figure 2, the microstructure of the heat affected zone and the base material can be seen. On the left, there is a heat affected zone's microstructure after tempering at 700  $^{\circ}$ C and the base material on the right quenched from 950  $^{\circ}$ C.



Figure 2: Microstructure of the heat affected zone and the base material [1]

#### 2. Austenitic steels

In the industry, the most widely used stainless steels are the austenitic steels. The weldability of this type is relatively good. They can be welded by most of the welding processes without any problem, and there is a wide selection of different kinds of filler materials. This type of steel has two groups: one is containing delta-ferrite the others don't this is pure austenitic steel. So the austenitic stainless steel's properties and performance are strongly related to their microstructure, especially the amount and distribution of delta ferrite and this mainly depends on the chemical composition and the cooling rate of the steel during the solidification. The amount of the delta-ferrite can be decided with the help of the DeLong diagram, which can be seen in Figure 3 [3].



Figure 3: The Delong-diagram [4]

On this Figure the x-axis is the chrome equivalent:

$$Cr_e = Cr + 1,5 \cdot Si + Mo + 0,5 \cdot Nb \tag{1}$$

And the y-axis is the nickel equivalent:

$$Ni_e = Ni + 30 \cdot C + 0.5 \cdot Mn \tag{2}$$

The main problem with these steels in term of the welding is the intergranular corrosion. Is, therefore responsible for the  $Cr_{23}C_6$  complex carbide, which can be seen in Figure 4 [5].



Figure 4:  $Cr_{23}C_6$  complex carbide at the border of an austenite grain [5]

To terminate these carbides, we have three options:

- 1. Choose steel with low carbon content (the ELC steels)
- 2. Use microalloys to create more stable carbides (Ti, Nb, Ta, Mo)
- 3. Use a solution heat treatment

The heat treatments which are used on austenitic steels can be seen in Figure 5 as a function of time and temperature.



Figure 5: The most used heat treatments on austenitic steels [5]

The solution annealing is the most widely used treatment to terminate these phases which precipitated during a previous thermomechanical process or welding. As the precipitations of M<sub>23</sub>C<sub>6</sub> types most forms between 450 to 900 °C, so the maximum temperature of the treatment should be higher than 900 °C. But not too high to avoid the harmful growth of the grains. This is usually between 1010 °C and 1120 °C, but it depends on the carbon content of the steel, steels that contain more carbon this temperature is a little bit higher with around 30 °C. The other thing is what influence the temperature is the microalloying. The austenitic steels that stabilized with Ti or Nb, in this case, the temperature of the heat treatment decreasing between 965 and 1065 °C. After the temperature holding a fast cooling should be used. The most common is water cooling. The most critical part of the cooling is when the temperature is between 650 and 870 °C especially when the steel is alloyed with molybdenum, because of the intermetallic precipitates like the Laves-phase (Fe<sub>2</sub>Mo). The probability of these precipitations increases if the steel contains  $\delta$  ferrite. In the case of austenitic steels with relatively high carbon content, the appearance of the martensite can also cause problems. In the case of austenitic steels the Ms temperature is below the room temperature, more person involved the calculation of it. For example, the calculation by Eichelmann and Hull [5,6]:

 $M_{s} = 1305 - [1667 \cdot (C\% + N\%) + 28 \cdot (Si\%) + 33 \cdot (Mn\%) + 42 \cdot (Cr\%) + 61 \quad (3) \cdot (Ni\%)].$ 

Because of the low formation temperature of the martensite so the amount of it will be small. But it can change with because of the precipitation of the chrome-carbide.

Because inside of the grain the quantity of the chromium and carbon is decreasing, and with it, the Ms temperature is increasing and can increase above the room temperature and because of that  $\alpha$ ' phase can appear. The martensite may also appear as a result of high mechanical stress; then the stress can be the 30-50% of the tensile strength. In this case, the Md temperature by Angel [6]:

$$M_{d} = 413 - [462 \cdot (C\% + N\%) + 9.2 \cdot (Si\%) + 8.1 \cdot (Mn\%) + 13.7 \cdot (Cr\%) + 9.5 \quad (4) \cdot (Ni\%) + 18.5 \cdot (Mo\%)].$$

Singh has determined that martensite, whether  $\alpha$  or  $\varepsilon$ , is stable to about 200 °C in cold-rolled austenitic stainless steel. According to Guy's experience, martensite can be reduced to zero at a temperature of 600 ° C for two minutes. According to Martins, the type of steel does not have a significant effect on the return temperature, which is more influenced by the stress and the amount of precipitation occurring during cold forming [6].

After the welding process, if the amount of the remaining is high, stress-reducing heat treatment should be used. As it is known, the decreasing of the remaining stress is happening in the heating period of the treatment. After it, the next step is a short holding at a chosen temperature, which could be around 925-1010 °C without the harmful growth of the grains if the austenitic steel contains stabilizing alloys such as titanium or niobium. But the cooling procedure can be problematic because if it is too fast, the level of stress won't be decreasing considerably after the treatment. If too slow, the harmful precipitation of the carbides will happen. To reduce the temperature of the treatment around 425 to 550 °C could be a solution, but at this lower temperature the decrease of the remaining stress will be less, but at the same time, the danger of the appearance of the stress corrosion cracks is also decreasing [5,7].

Part of the manufacturing of the austenitic steels is the austenitic quenching. It is used, for example, for annealing purposes between the steps of cold forming. In this case, the thickness of the plates is between 0,1-0,2 mm. This heat treatment also used to terminate the harmful carbides.

In these thin plates, the heat should be as fast as possible a there is no need to hold at temperature. The holding time should calculate with the following formula [8]:

$$t_h = 20 + \frac{a}{2}.$$
 (5)

Where the *a* is the maximum value of the wall thickness.

When designing a heat treatment, it should be taken into account that the thermal conductivity of these steels is about one third as high as that of conventional steels, while their thermal expansion coefficient is 50% higher. During the heat treatment, too rapid heating is the risk of cracking, so heating up to 400 °C should be done slowly. The usual temperature at which steel is heated is 1050 °C [8].

One of the most used austenitic stainless steel is the AISI 304 type (X5 CrNi 18-10, DIN: 1.4301). This steel is widely used in the ship manufacturing and as pipes in the oil industry. In these cases, usually we have to deal with thin plates, and one of the most economical ways of welding these plates is the submerged-arc-welding. The microstructure of the welded joint can be seen in Figure 6 [8].



Figure 6: Microstructure of (a) the base metal, (b) the heat-affected zone, (c) the welded metal [3]

After welding, if a heat treatment will be used, its temperature could be different. If its temperature is around 650 °C the size of the austenite grains doesn't change significantly compared to the welded state. The strips that already exist in the base material remain after the treatment. If the temperature of the heat treatment raising around 850 °C the volume of the strips will decrease that can be seen in Figure 7. The temperature of the treatment effects the thickness of the delta ferrite strips. And this also affects the hardness of the joint as can be seen in Figure 8 [3].



Figure 7: Microstructure of the base metal and the heat affected zone, on the top line the temperature of the treatment 650 °C and the lower 850 °C, at (a) and (d) the hold time is 0,5 h, at (b) and (e) the hold time is 1 h, at (c) and (c) the hold time is 4 h [3]



Figure 8: Hardness of the welded joint [3]

### 3. Duplex steels

Duplex steels combine the properties of ferritic and austenitic steels. These steels are often manufactured by hot forming because their formability is excellent around 1230 °C than a small load of force is enough. If the temperature of the hot forming is not high enough, then the deformation that indicated by the forming could lead to cracks, especially in the ferritic zones. Furthermore, at a lower temperature, the chance of the forming of the  $\sigma$  phase is higher the temperature of the hot forming can be seen in Table 3 in case of different duplex steels. The most critical part of the cooling is between 700 and 1000 °C because of the intermetallic precipitates [9].

| DIN number of steel | Heat temperature [°C] | Hold temperature [°C] |
|---------------------|-----------------------|-----------------------|
| 1.4162              | 900-1100              | 950                   |
| 1.4362              | 950-1150              | 980                   |
| 1.4462              | 950-1230              | 1040                  |
| 1.4410              | 1025-1230             | 1050                  |
| 1.4507              | 1000-1230             | 1080                  |
| 1.4501              | 1000-1230             | 1100                  |
| 1.4301              | 925-1205              | 1040                  |
| 1.4401              | 925-1205              | 1040                  |

Table 3: Temperatures of the hot forming [9]

Two types of heat treatment could use after the welding procedure: the solution annealing and the tempering. The temperature of the tempering treatment is around 900 °C. The holding time could be 30, 45 or 60 minutes. The cooling should be completed at dormant air. With the increase of the holding time, the impact strength is also increasing. However, the hardness is decreasing. This treatment is used to improve the mechanical properties of the welded joint. In this case, the temperature is usually 800 °C, and the holding time is around 10 minutes. The effect of the soaking time on the impact strength can be seen in case of different heat treatments on Figure 9 [9].



Figure 9: Effect of the soaking time on the impact strength [9]

The main goal of the solution annealing is similar to the purpose in case of austenitic steels. Its temperature is usually between 800 and 1100 °C. The holding time is around 10 minutes. For the cooling, an intensive refrigerant should use, such as water. If the temperature of the treatment is lower, the amount of the  $\sigma$  phase is increasing. The average microhardness after the treatment is around 274,1 to 281,4 HV0, 01 in the ferritic regions, meanwhile in the austenitic regions it's value is 221,3 to 236,2 HV0, 01. The effect of the solution annealing on duplex steel can be seen on a forged workpiece in cases of different temperatures on Figure 10 [9].



Figure 10: Duplex steel microstructures (a) forged condition without heat treatment, (b) treated at 800  $^{\circ}$ C (c) treated at 900  $^{\circ}$ C (d) treated at 1000  $^{\circ}$ C (e) treated at 1100  $^{\circ}$ C [9]

# 4. Wall thickness of the pressure vessel

As mentioned these steels widely used in the chemical industry as a commodity of a pressure vessel, for example, an ammonia synthesis converter. This is the central unit of ammonia production in this ammonia equilibrium reaction. This reaction always happens in elevated temperature the value of it's most often between 200 and 700 °C. At this temperature, the heat

and corrosion resistant steels similar to the structural steels their mechanical properties change with the rise of the temperature.

This means the decrease of the tensile strength and the yield strength. This change could be described as a polynomial function of the mechanical properties and the temperature with the help of the DIN EN 10028 standard and the software named "TableCurve 2D". Or linear interpolation also can be used instead of the polynomial function. This is necessary because during the calculations in case of a plant that operates at elevated temperature hen the mechanical characteristics of the given temperature should use instead of room temperature. The formula for the calculation of the yield strength of the X5 CrNi 18-10 austenitic steel and the linear interpolation in general [10]:

## X5CrNi18-10:

$$f_{y}^{-1} = 0,0039 + 1,296 \cdot 10^{-5} \cdot T - 1,013 \cdot 10^{-7} \cdot T^{2} + 3,913 \cdot 10^{-10} \cdot T^{3} - 6,23$$
  
 
$$\cdot 10^{-13} \cdot T^{4} + 3,43 \cdot 10^{-16} \cdot T^{5},$$
(6)

$$f_{y} = \frac{T - T_{1}}{T_{2} - T_{1}} \cdot \left(f_{y2} - f_{y1}\right) + f_{y1}.$$
(7)

The values can be seen in Table 4 for the X5 CrNi 18-10 steel (DIN 1.4301).

|                  | 1 1                              | 0 1                              | E _ J                         |
|------------------|----------------------------------|----------------------------------|-------------------------------|
| Tomporatura [°C] | Minimum 0,2 % proof              | Minimum 1,0 % proof              | Minimum tensile               |
|                  | strength R <sub>p0,2</sub> [MPa] | strength R <sub>p1,0</sub> [MPa] | strength R <sub>m</sub> [MPa] |
| 50               | 190                              | 228                              | 494                           |
| 100              | 157                              | 191                              | 450                           |
| 150              | 142                              | 172                              | 420                           |
| 200              | 127                              | 157                              | 400                           |
| 250              | 118                              | 145                              | 390                           |
| 300              | 110                              | 135                              | 380                           |
| 350              | 104                              | 129                              | 380                           |
| 400              | 98                               | 125                              | 380                           |
| 450              | 95                               | 122                              | 370                           |
| 500              | 92                               | 120                              | 360                           |
| 550              | 90                               | 120                              | 330                           |
| 600              | -                                | -                                | -                             |

| Table /l. Machanical proportion of aiven temperatured L   |    |   |
|---|----|---|
| <b>1</b> and $2$ is the matrix of the method. At the methods $1$ is the matrix of |    | Ł |
| 1 abie 4. Micenanical properties at given temperatures [1]  | 11 | Ł |

So the wall thickness of the pressure vessel can be calculated at the temperature which it operates. The MSZ EN 13445-3 gives the formula in case of cylindrical shell [12]:

$$s = \frac{D_e \cdot P}{2 \cdot f_d \cdot z + P} + c. \tag{8}$$

Where the members are the followings:

- $D_e$  is the outer diameter of the cylindrical shell
- *P* is the pressure inside the vessel
- $f_d$  is the design stress
- *z* is the welding factor
- *c* is the corrosion allowance.

The value of the welding factor is usually 1 or 0,85 depending on the testing group of the pressure vessel. The corrosion allowance depends on the corrosion, erosion properties of the material of the plant and the atmosphere inside of it. From the side of corrosion, the ammonia

is not dangerous. However, the temperature is relatively high inside of the converter, so the value of the corrosion allowance will be 1,6 mm, which applies to the hot gases.

The  $f_d$  contains the yield strength or the tensile strength of the steel divided by the security factor. Which mechanical property should be used and how much is the value of the safety factor that depends on the structure of the steel and the elongation of the steel. These are presented in the MSZ EN 13445-3 in tabular form, which can be seen in Table 5 [12].

|  | Normal load cases   | Test, exceptional load cases   |  |  |
|--|---|--|--|--|
| Steels other than<br>austenitic<br>A<30%   | $f_d = \min\left\{\frac{R_{p0,2/t}}{1,5}; \frac{R_{m/20}}{2,4}\right\}$   | $f_{test} = \left\{ \frac{R_{p0,2/t \ teszt}}{1,05} \right\}$                                |  |  |
| Austenitic steels<br>30% <a≤35%< td=""><td><math display="block">f_d = \left\{ \frac{R_{p1,0/t}}{1,5} \right\}</math></td><td><math display="block">f_{test} = \left\{ \frac{R_{p1,0/t \ teszt}}{1,05} \right\}</math></td></a≤35%<> | $f_d = \left\{ \frac{R_{p1,0/t}}{1,5} \right\}$   | $f_{test} = \left\{ \frac{R_{p1,0/t \ teszt}}{1,05} \right\}$                                |  |  |
| Austenitic steels<br>A>35%   | $ \int_{a}^{f_{d}} = max\left[\left\{\frac{R_{p1,0/t}}{1,5}\right\}; min\left\{\frac{R_{p1,0/t}}{1,2}; \frac{R_{m/t}}{3}\right\}\right] $ | $f_{test} = max \left\{ \frac{R_{p1,0/t \ teszt}}{1,05}; \frac{R_{m/t \ teszt}}{2} \right\}$ |  |  |
| Cast steels  | $f_d = \min\left\{\frac{R_{p0,2/t}}{1,9}; \frac{R_{m/20}}{3}\right\}$   | $f_{test} = \left\{ \frac{R_{p0,2/t \ teszt}}{1,33} \right\}$                                |  |  |

Table 5: The calculation of the design stress [12]

The pressure in the ammonia synthesis reaction is between 100 and 1000 at (9806650 and 98066500 Pa). Based on this, there are three different methods for ammonia production. The low pressure, also known as Uhde Mont Cenis procedure, the medium pressure the Haber-Bosch procedure and the high-pressure Claude-Casale procedure. The pressure values which chosen to the calculations are 100, 150, 200 bars ( $p_1$ ,  $p_2$  and  $p_3$ ). The temperature values are 200, 400 and 500 °C ( $T_1$ ,  $T_2$  and  $T_3$ ) [10].



Figure 11: Geometry of the ammonia synthesis converter

#### 5. Optimization of the pressure vessel

The height of the shell is 16700 mm, and the outer diameter of it is 1400 mm while the inner is 1200 mm. The calculated values of the wall thickness have to be equal to the difference between the outer and the inner radius. The change of the volume of the converter could be maximally 10% of the original value. This is necessary because of the optimal temperature curve of the converter, which can be seen in Figure 12 [10,13].



Figure 12: Optimal temperature curve [10]

So the limits of the volumes and the radiuses could be calculated with the following equations. The original inner volume of the converter:

$$V = \pi \cdot r^2 \cdot h = \pi \cdot ((600mm)^2) \cdot 16700mm = 1,8887 \cdot 10^{10}mm^3.$$
(9)  
The original volume of the converter, including the shell:

$$V = \pi \cdot R^2 \cdot h = \pi \cdot ((700mm)^2) \cdot 16700mm = 2,5707 \cdot 10^{10}mm^3.$$
(10)

The limits of the internal volume:

$$1,6983 \cdot 10^{10} mm^3 \le V \le 2,0757 \cdot 10^{10} mm^3.$$
<sup>(11)</sup>

The limit of the volume with the outer radius:

$$2,3137 \cdot 10^{10} mm^3 \le V \le 2,8278 \cdot 10^{10} mm^3.$$
<sup>(12)</sup>

The limits of the radius:

$$r_{ilower} = \sqrt[2]{\frac{V_{ilower}}{\pi \cdot h}} = \sqrt[2]{\frac{1,6983 \cdot 10^{10} mm^3}{\pi \cdot 16700 mm}} = 568,9499 mm,$$
(13)

$$r_{iupper} = \sqrt[2]{\frac{V_{iupper}}{\pi \cdot h}} = \sqrt[2]{\frac{2,0757 \cdot 10^{10} mm^3}{\pi \cdot 16700 mm}} = 628,9978 mm,$$
(14)

$$R_{eupper} = \sqrt[2]{\frac{V_{eupper}}{\pi \cdot h}} = \sqrt[2]{\frac{2,8278 \cdot 10^{10} mm^3}{\pi \cdot 16700 mm}} = 734,1607 mm,$$
(15)

$$R_{elower} = \sqrt[2]{\frac{V_{elower}}{\pi \cdot h}} = \sqrt[2]{\frac{2,3137 \cdot 10^{10} mm^3}{\pi \cdot 16700 mm}} = 664,0799 mm.$$
(16)

With these conditions, an optimizing procedure could be completed. This optimization is the main goal is to find the optimal value of the wall thickness with the following conditions:

- The value of the wall thickness has to be higher than the one which calculated before (this is necessary because the wall thickness and the radiuses are the variables of the optimizing procedure),
- The difference of the radii has to be equal to the wall thickness produced by the optimization,
- The volume calculated with the optimized radiuses and wall thickness has to be between the limits.

The results of the optimization in case of the X5 CrNi 18-10 steel can be seen in Table 6. The optimization procedure was done using Microsoft Excel's Solver extension. With this, the mass of the vessel could be minimized. The cost could be another question, but it significantly depends on the steel which is used and its commercial price because the selection of steel grade determines the cost and the mechanical properties, which has a significant effect on the wall thickness and with it, the mass and with the cost of the converter.

|                                   | The volume<br>of the shell<br>[mm <sup>3</sup> ] | The mass<br>of the shell<br>[kg] | Inner<br>radius<br>[mm] | Outer<br>radius<br>[mm] | Wall<br>thickness<br>[mm] | The cost<br>of the<br>base<br>material<br>[EUR] |
|-----------------------------------|--|----------------------------------|-------------------------|-------------------------|---------------------------|---|
| $T_1$ and $p_1$                   | 3544215124                                       | 27822,09                         | 611,0756                | 664,0799                | 53,0043                   | 37702,28  |
| $T_1$ and $p_2$                   | 5022987851                                       | 39430,45                         | 587,5483                | 664,0799                | 76,5316                   | 53433,01  |
| T <sub>1</sub> and p <sub>3</sub> | 6484121682                                       | 50900,36                         | 568,9499                | 668,8475                | 99,8976                   | 68976,11  |
| T <sub>2</sub> and p <sub>1</sub> | 4507500918                                       | 35383,88                         | 595,8552                | 664,0799                | 68,2247                   | 47949,42  |
| T <sub>2</sub> and p <sub>2</sub> | 6418027451                                       | 50381,52                         | 568,9499                | 667,9046                | 98,9547                   | 68273,02  |
| T <sub>2</sub> and p <sub>3</sub> | 8976811861                                       | 70467,97                         | 568,9499                | 703,4863                | 134,5364                  | 95492,58  |
| T <sub>3</sub> and p <sub>1</sub> | 4868333555                                       | 38216,42                         | 590,0528                | 664,0799                | 74,0271                   | 51787,85  |
| T <sub>3</sub> and p <sub>2</sub> | 7113716819                                       | 55842,68                         | 568,9499                | 677,7636                | 108,8137                  | 75673,55  |
| T <sub>3</sub> and p <sub>3</sub> | 10016361729                                      | 78628,44                         | 568,9499                | 717,438                 | 148,4881                  | 106551  |

| I | able | 6: | Results | of | the | 0 | ptim | iza | itio | n |
|---|------|----|---------|----|-----|---|------|-----|------|---|
|   |      |    |         |    |     |   |      |     |      |   |

So the mass of the shell is given and with the knowledge of the price per kilogram of the steel the cost of the base material can also calculate, and it could be a benchmark for steels that can help to make a choice between them. 23 different steels were compared in the calculations, and which are the following:

• The austenitic grades: X1 CrNiMoCuN 25-20-7, X1 CrNiMoCuN 25-25-5, X2 CrNiMo 17-12-2, X2 CrNiMoN 17-11-2, X2 CrNiMoN 17-13-3, X2CrNi 18-9,

X2CrNiMo 18-14-3, X2CrNiMo 18-15-4, X5 CrNiN 19-9, X5CrNi18-10, X6 CrNiMoTi 17-12-2, X6 CrNiTi 18-10,

- The ferritic grades: X2 CrMoTi 17-1, X2 CrMoTi 18-2, X2 CrNiN 23-4, X2CrTi 12, X2CrTiNb18, X3CrTi 17, X6 CrMoNb 17-1,
- The duplex grades: X2 CrNiMoN 22-5-3, X2 CrNiMoN 25-7-4, X2 CrNiN 18-7.

The result of the calculation of the cost and the mass the steel with the best result at given pressure and temperature are shown in Table 7.

| Tuble 7. The best steels by weight and east |                   |                   |  |  |
|---|-------------------|-------------------|--|--|
|   | By weight         | By cost           |  |  |
| T <sub>1</sub> and p <sub>1</sub>           | X2 CrNiMoN 25-7-4 | X2 CrNiMoN 25-7-4 |  |  |
| T <sub>1</sub> and p <sub>2</sub>           | X2 CrNiMoN 25-7-4 | X3 CrTi 17        |  |  |
| T <sub>1</sub> and p <sub>3</sub>           | X2 CrNiMoN 25-7-4 | X2 CrNiMo 17-12-2 |  |  |
| T <sub>2</sub> and p <sub>1</sub>           | X2 CrNiMoN 25-7-4 | X2 CrNiMo 17-12-2 |  |  |
| T <sub>2</sub> and p <sub>2</sub>           | X2 CrNiMoN 25-7-4 | X2 CrNiMo 17-12-2 |  |  |
| T <sub>2</sub> and p <sub>3</sub>           | X2 CrNiMoN 25-7-4 | X2 CrNiN 18-7     |  |  |
| T <sub>3</sub> and p <sub>1</sub>           | X6 CrMoNb 17-1    | X2 CrNiMo 17-12-2 |  |  |
| T <sub>3</sub> and p <sub>2</sub>           | X6 CrMoNb 17-1    | X2 CrNiMo 17-12-2 |  |  |
| T <sub>3</sub> and p <sub>3</sub>           | X6 CrMoNb 17-1    | X2 CrNiMo 17-12-2 |  |  |

Table 7: The best steels by weight and cost

#### 6. Calculation of the welding costs and the welding time

The other side of the cost of manufacturing is the cost of the welding procedure. For this, the length of the joint and the cross section of the joint have to be known. Furthermore, there is a question about the filler material and the welding technology. The selection of the filler material is relatively simple. Because these steels are heavily alloyed, the main point of the filler material selection is the corrosion resistant properties of the welded joint and also the base material. And for that, most of the filler material production company recommends the selection, and it is based on the chemical composition of the steel. In this study, four welding procedures were compared, which are the following: SMAW (111), SAW (121), MIG (131) and TIG (141) [12]. The calculations showed that the wall thickness of the vessel is relatively high, and during the manufacturing, the plates have to be bent. And because of the significant value of the wall thickness, the maximum width which could be bent is 2000 mm. So the complete 16700 mm should be built from these 2000 mm sections. That means for the manufacturing 9 sections are needed. And to complete the joint 10 circumferential welded joint and the total height of the converter have to be welded. This welded length is changing for each, and each temperature and pressure value, because the optimization produces the optimal inner and outer diameter of the pressure vessel and the welding length depends on them [14].

The next is the cross section area of the welding seam. For this some geometric formula available on the internet, there is also a possibility such as on the Böehler-Voestalpine site the Welding-Calculator. On the website, a few incoming parameters are needed.

For example, the welding procedure, shape of the seam preparation, angulation angle, root gap, chamfering, plate thickness, etc. The cross section for the geometric calculation can be seen in Figure 13.



Figure 13: The cross section of the welding seam

The first step is to calculate the height of the right triangles, which is represented by the letter m:

$$m = t \cdot \tan(\alpha). \tag{17}$$

With this the area of one triangle:

$$A_{triangle1} = t \cdot (\tan(\alpha) \cdot t) \cdot \frac{1}{2}.$$
 (18)

There are two triangles, so their total area is:

$$A_{triangle} = t \cdot (\tan(\alpha) \cdot t). \tag{19}$$

The width of the crown:

$$b = 2 \cdot (\tan(\alpha) \cdot t) + i.$$
<sup>(20)</sup>

To calculate the area of the crown section before the radius of the crown must be known:

$$r = \frac{\frac{b^2}{4} + h^2}{2 \cdot h}.$$
 (21)

r is radius of the arch of the welding seam, the angle  $\beta$  of the corner point of the circle and the vertical radius of the circle:

$$\sin(\beta) = \frac{b}{2 \cdot r}.$$
(22)

The circular slice area:

$$A_{slice} = \frac{r^2}{2} \cdot \left(\beta - \sin(\beta)\right) \tag{23}$$

In this formula, the first  $\boldsymbol{\beta}$  which is not in the trigonometric function should be replaced by radian.

The area of the rectangle in the middle:

$$A_{rectangle} = i \cdot t. \tag{24}$$

The whole cross-section area of the welding seam:

$$A_{seam} = A_{triangle} + A_{slice} + A_{rectangle}.$$
(25)

The next step is the calculation of the mass of the welded seam. The length of it is known, also the cross-section area. The last thing that's needed is the density of the welded metal, for the calculations, the general density of the steel (7850 kg/m<sup>3</sup>) has been used.

The formula for the mass of the welded seam:

$$m_{seam} = A_{seam} \cdot L_{weld} \cdot \rho_{steel}.$$
 (26)

With it, and with the cost of one kilogramme filler material, the total cost of it can be calculated. But this value rarely matches the actual value, because of the welding losses, such as a damaged electrode, not properly stored electrode, that part of the wire electrode which the machine cannot pull out. This effect could be taken into account as a multiplying factor, which value is different for each welding procedure. The value of the factor assumes the manufacturing happens in pure bondage without any further loss. About the value, some manufacturer may give information about it in their catalogues, and its change with the diameter of the electrode and the type of the wire. The value of the factor can be seen in Table 8. The chosen filler materials for X5 CrNi 18-10 steels can be seen in Table 9, and the welding cost can be seen in table 10.

Table 8: Value of the factor1 [15]

| Welding procedure | Multiplying factor |
|-------------------|--------------------|
| SMAW (111)        | 1,5                |
| <i>TIG</i> (141)  | 1,1                |
| MIG (131)         | 1,05               |
| SAW(121)          | 1,02               |

Table 9: The filler materials for X5 CrNi 18-10 steel with different welding procedures

| Steel         | <b>SMAW (111)</b> | MIG (131)      | SAW (121) Flux | TIG (141)        |
|---------------|-------------------|----------------|----------------|------------------|
| X5 CrNi 18-10 | OK 61.34          | OK Autrod 308L | OK Flux 10.92  | OK Tigrod 308LSi |

|                                   | <b>SMAW (111)</b> | MIG (131) | SAW (121) | <b>TIG</b> (141) |
|-----------------------------------|-------------------|-----------|-----------|------------------|
| $T_1$ and $p_1$                   | 24053,957         | 4863,431  | 7365,252  | 6409,043         |
| T <sub>1</sub> and p <sub>2</sub> | 50324,149         | 10174,96  | 15409,11  | 13408,59         |
| T <sub>1</sub> and p <sub>3</sub> | 86373,344         | 17463,69  | 26447,27  | 23013,7          |
| T <sub>2</sub> and p <sub>1</sub> | 39930,403         | 8073,465  | 12226,57  | 10639,23         |
| T <sub>2</sub> and p <sub>2</sub> | 84662,98          | 17117,87  | 25923,56  | 22557,98         |
| T <sub>2</sub> and p <sub>3</sub> | 162813,42         | 32918,99  | 49853     | 43380,73         |
| T <sub>3</sub> and p <sub>1</sub> | 47067,881         | 9516,58   | 14412,05  | 12540,98         |
| T <sub>3</sub> and p <sub>2</sub> | 103509,87         | 20928,5   | 31694,42  | 27579,63         |
| T <sub>3</sub> and p <sub>3</sub> | 201329,49         | 40706,49  | 61646,51  | 53643,12         |

Table 10: The cost of the filler material for X5 CrNi 18-10 steel

The welding time can also be a question if manufacturing has an urgent deadline. Parallel to the formula of the velocity, the welding time also can be calculated with the welded length and the melting power of the welding procedure. The melting power can be seen in Table 11. But another method can also be used to determine the melting power. For this, a piece of the steel which want to be welded is needed, and before welding, the mass of it should be measured. Complete a welded seam on the workpiece, and during it, the time should be measured after it measures the mass of the workpiece with the welded seam, and divided the measured mass by the time the melting power definable. But the welding time similar to the cost of the filler material needed a little correction because the arc is not burning the whole time while the joints are preparing. This correction is the operating factor. This shows the burning time of the arc relative to the time of the completion of the full joint. The value of the factor can be seen in Table 11 [15,16].

The results of the welding time calculation in case of X5 CrNi 18-10 steel can be seen in Table 12. In Table 13, the result of the ranking can be seen by the welding time and also the filler material.

| Welding procedure     | Operating factor<br>[%] | Melting power<br>[kg/h] |     |
|-----------------------|-------------------------|-------------------------|-----|
|                       |                         | min                     | max |
| SMAW (111)            | 15-30                   | 0,4                     | 5,5 |
| TIG (141)             | 25-40                   | 0,1                     | 7   |
| Automatized TIG (141) | 80-90                   |                         |     |
| MIG (131)             | 30-45                   | 0,6                     | 12  |
| Automatized MIG (131) | 80-90                   |                         |     |
| SAW (121)             | 80-95                   | 3                       | 16  |

Table 11: Value of the operating factor [15]

Table 12: Welding time in case of X5 CrNi 18-10

|                                      | Welding time [h] |              |              |              | Adjusted welding time [h] |                        |                           |              |              |                        |
|--------------------------------------|------------------|--------------|--------------|--------------|---------------------------|------------------------|---------------------------|--------------|--------------|------------------------|
|                                      | SMAW<br>(111)    | MIG<br>(131) | SAW<br>(121) | TIG<br>(141) | SMAW<br>(111)             | Manual<br>MIG<br>(131) | Automated<br>MIG<br>(131) | SAW<br>(121) | TIG<br>(141) | Automated<br>TIG (141) |
| T <sub>1</sub> and<br>p <sub>1</sub> | 243,77           | 146,26<br>2  | 81,256       | 731,31       | 1059,87                   | 384,9                  | 172,0729                  | 92,337       | 2216,091     | 860,365                |
| T <sub>1</sub> and p <sub>2</sub>    | 510              | 306          | 170          | 1530         | 2217,391                  | 805,2632               | 360                       | 193,182      | 4636,364     | 1800                   |
| T <sub>1</sub> and<br>p <sub>3</sub> | 875,333          | 525,2        | 291,778      | 2626         | 3805,797                  | 1382,105               | 617,8824                  | 331,566      | 7957,576     | 3089,412               |
| T <sub>2</sub> and<br>p <sub>1</sub> | 404,667          | 242,8        | 134,889      | 1214         | 1759,42                   | 638,9474               | 285,6471                  | 153,283      | 3678,788     | 1428,235               |
| T <sub>2</sub> and<br>p <sub>2</sub> | 858              | 514,8        | 286          | 2574         | 3730,435                  | 1354,737               | 605,6471                  | 325          | 7800         | 3028,235               |
| T <sub>2</sub> and<br>p <sub>3</sub> | 1650             | 990          | 550          | 4950         | 7173,913                  | 2605,263               | 1164,706                  | 625          | 15000        | 5823,529               |
| T <sub>3</sub> and<br>p <sub>1</sub> | 477              | 286,2        | 159          | 1431         | 2073,913                  | 753,1579               | 336,706                   | 180,682      | 4336,364     | 1683,529               |
| T3 and<br>p2                         | 1049             | 629,4        | 349,667      | 3147         | 4560,87                   | 1656,316               | 740,471                   | 397,349      | 9536,364     | 3702,353               |
| T <sub>3</sub> and p <sub>3</sub>    | 2040,333         | 1224,2       | 680,111      | 6121         | 8871,014                  | 3221,579               | 1440,235                  | 772,854      | 18548,48     | 7201,176               |

|                                   | By the cost of the | By the adjusted   |
|-----------------------------------|--------------------|-------------------|
|                                   | iller material     | weiding time      |
| T <sub>1</sub> and p <sub>1</sub> | X2 CrNiMoN 25-7-4  | X2 CrNiMoN 25-7-4 |
| T <sub>1</sub> and p <sub>2</sub> | X2 CrNiMoN 25-7-4  | X2 CrNiMoN 25-7-4 |
| T <sub>1</sub> and p <sub>3</sub> | X2 CrNiMoN 25-7-4  | X2 CrNiMoN 25-7-4 |
| T <sub>2</sub> and p <sub>1</sub> | X2 CrNiMoN 25-7-4  | X2 CrNiMoN 25-7-4 |
| T <sub>2</sub> and p <sub>2</sub> | X2 CrNiMoN 25-7-4  | X2 CrNiMoN 25-7-4 |
| T <sub>2</sub> and p <sub>3</sub> | X2 CrTiNb 18       | X2 CrNiMoN 25-7-4 |
| T <sub>3</sub> and p <sub>1</sub> | X2 CrTiNb 18       | X6 CrMoNb 17-1    |
| T <sub>3</sub> and p <sub>2</sub> | X2 CrTiNb 18       | X6 CrMoNb 17-1    |
| T <sub>3</sub> and p <sub>3</sub> | X6 CrMoNb 17-1     | X6 CrMoNb 17-1    |

Table 13: The best steels by the cost of the filler material and the welding time

# 7. Summary

During the tests, 23 different heat or corrosion resistant steel grades, which were compared with the ammonia synthesis converter could be made. The heat treatments of some properties of these steels that relate to their welding have been promoted. The particular subject of the study was ammonia, which can make of these high alloy steels. During the tests, these steels were compared by different reasons which are the followings: mechanical properties, the mass of the shell, the base material cost of the shell, filler material cost of the welding and the welding time. These calculations were performed at different inner pressure and temperature values, all of which are characteristic of ammonia production. Thus, at the end of the process, the optimum steel grade was determined by several aspects.

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