NUMERICAL STUDY OF WASTE GASES PURIFYING USING A COMBINED SUPERSONIC SEPARATOR IN CHEMICAL INDUSTRY*

Viktor S.Vlasenko1**, Aleksandr A. Yudakov1,2, Vyacheslav V. Slesarenko1, Artur A. Karakozov1


Abstract

The article describes the principle of operation of the combined supersonic separator (CSS). The CSS proposed as an alternative to a three-flow vortex tube (TVT) in vortex installations for the chemical industry. On the example of the vortex installation M-100 Novomoskovsk stock company "Nitrogen" the process separation of methanol from the flue gas by the CSS. For these purposes computer systems Ansys CFX and UniSim Design R451 were used.

Keywords: waste gases, chemical industry, supersonic separation, clean technology, purification

1. Introduction

It is known that the wasted gases remaining after the main synthesis in the chemical production are burned in flares (Bellotti et al., 2017; Reddy et al., 2014; Sosna et al., 2018). Due to low-temperature separation with the three-flow vortex tube, valuable components

* Selection and peer-review under responsibility of the EIAETM
** Corresponding author: email: vkt_vl@mail.ru; vlasenko.vs@dvfu.ru
contained in these gases (Leonzio, 2018) can be extracted for further use (Devisilov et al., 2013, 2014). The efficiency and reliability of the tubes has been proved by long-term testing (Zhidkov et al., 2015), however, there are some factors that prevent effective separation in it (Vlasenko et al., 2018). Besides this, the less high-boiling components in the gas entering the pipe (so called «lean» gas), the weaker the separation. This happened when the wasted gas is used as a working fluid. In this regard, the combined supersonic separator (CSS), previously proved its higher separation degree, is offered instead of the three-flow vortex tube (Vlasenko et al., 2017, 2018).

The possibility of using the CSS in the wasted gas purification process has been studied. As the input data, the parameters of the vortex plant M-100 by Russian chemical company «Azot» were used.

This work is divided in three main parts:

- description of the device and the principle of operation of the combined supersonic separator;
- the formulation of the study, the selection of equations and programs for numerical research;
- analysis of the results, drawing a conclusion.

2. Combined supersonic separator

The basic principle of the combined supersonic separator is based on the combination of two designs of vortex devices (Fig.1). The twist of the gas-liquid flow is carried out both in the vortex tube (Gutak, 2015) by tangential twisting device and in the energy separation chamber includes the Laval nozzle design, which like the CSS accelerates the gas flow to supersonic speeds (Cao and Bian, 2019). Adjustment of the operating modes is carried out at the vortex tube, due to the throttle at the hot outlet. Operating fluid moves in the apparatus as inside a counterflow vortex tube. The condensate is removed through the separation gap in the energy separation chamber – similar to the 3S separator (Imaev et al., 2014).

![Fig. 1. The basic scheme of the combined supersonic separator:](image)

(1 - swirl zone, 2 - supersonic flow zone, 3 - separation zone, 4 - hot gas outlet zone, 5 - reverse vortex formation zone, 6 - dry cooled gas outlet zone)

Under certain modes, the CSS supports the supersonic flow regime in the energy separation chamber (Vlasenko et al., 2017). It promotes deep extraction of high-boiling components due to low static temperatures. At the same time, the energy separation
Numerical study of waste gases purifying using a combined supersonic separator in chemical industry

Inherent in the Ranka-Hilsch effect is maintained, however, with a decrease in temperature efficiency by 30-50% (depending on the mode) (Vlasenko et al., 2018).

3. Materials and methods

The possibility of using CSS in the chemical industry is considered. The data of a vortex unit for separation of methanol M-100 Novomoskovsk stock company "Azot" was taken (Devisilov et al., 2014). The vortex unit had the following characteristics for 2013:

- Average waste gas composition (% vol.): hydrogen - 52.87; nitrogen - 12.50; methane - 21.42; ethane - 1.26; carbon monoxide - 4.88; carbon dioxide - 5.55; methanol - 1.52;
- Consumption of 16000 Nm³/h;
- The pressure at the inlet to the vortex apparatus is 3.98 MPa, at the outlet of the apparatus through the cold flow 0.4 MPa;
- Temperature at the entrance to the heat exchanger is 326.25 K, at the entrance to the vortex apparatus 294.45 K;
- Mode of operation of the vortex apparatus μ = 0.7 (70% of the mass flow in the cold flow);
- The standard scheme of the vortex low-temperature unit is used to separate the components from the waste gas (Zhidkov et al., 2015).

![Fig. 2. The principal process flow diagram of a vortex unit with a CSS for the separation of components from the waste gas:](image)

As a basis for the temperature effects implemented in the CSS, previously obtained data by the authors were used (Vlasenko et al., 2018). As far as the temperature effects were obtained in air, it was necessary to recalculate the temperature effects on this gas mix of waste gas. According to research (Piralishvili et al., 2000) temperature efficiency ηₜ does not depend on the temperature in the region of 300 K ≤ Tᵢn ≤ 1500 K, at observance of optimum parameters of a design and degree of expansion of gas in a vortex tube π (Eq. 1):

\[ ηₜ = ΔTᵢ/Tᵢ = \text{const} \] (1)
where: $\Delta T_c$ - the absolute effect of reducing the temperature of the cooled flow; $T_s$ - the absolute effect of reducing the temperature with isentropic expansion of gas from the inlet pressure $P_{in}$ to the pressure of the medium into which the gas flows $P_{med}$.

Thus, for the transition from the air to the system with another gas as a working substance, knowing that the designs of vortex tubes are similar and have the same pressure ratio of the gas $\pi$, the following approximate dependence of determining the temperature of the cold flow was used (Eq. 2):

$$\eta_{t(j)} = \frac{((\Delta T_{c(j)} - \Delta T_{th(j)})/ \Delta T_{s(j)})}{\frac{((\Delta T_{c(i)} - \Delta T_{th(i)})/ \Delta T_{s(i)})}{\eta_{t(i)}}}$$

where: the indexes $j$ and $i$ relate to the air and gases mix respectively; $\Delta T_{th}$ it is the throttling effect reducing temperature.

The final formula for the definition of the fall of temperature for the mix of gases is given by Eq. (3):

$$\Delta T_{c(i)} = \frac{((\Delta T_{c(j)} - \Delta T_{th(j)})/ \Delta T_{s(j)})}{\Delta T_{s(i)} - \Delta T_{th(i)}}$$

By this means recalculation for the fall of temperature of hot flow can be done, taking fall of temperature of throttling by tested in air with the opposite sign (Eq. 4):

$$\Delta T_{h(i)} = \frac{(\Delta T_{h(j)} - \Delta T_{th(j)}/T_s(j))}{\Delta T_{s(i)} - \Delta T_{th(i)}}$$

Fig. 3. Technological scheme of CSS in supersonic separator mode for cold flow ratio $\mu = 0$ and hot flow ratio $\mu_h = 1$:
(1 - gas at the entrance to the vortex tube, 2 - gas-liquid flow after heat exchanger, 3 - condensate after regular separator, 4 - gas at the entrance to the CSS, 5 - gas-liquid flow after the Laval nozzle, 6 - condensate drainage from CSS, 7 - gas flow after the Laval nozzle, 8 and 9 - heated gas flow, 10 - gas to flaring, A - heat exchanger, B – regular separator, C - imitation of the swirling device of CSS, D - imitation of the separation unit of CSS, E - imitation of orifice CSS)

For determining the Mach number and static temperature in the Laval nozzle, the complex of mathematical simulation of Ansys CFX was used. The unstructured net contained 2645157 elements. Near-wall layer had 5 layers with the gross thickness 0.5 mm. Boundary conditions: total pressure at the input 4.02 MPa, total temperature at the input 294.45 K, the static pressure at the cold end 0.4 MPa, the mass flow at the hot end depending on the mode. As a working substance given composition of waste gas M-100 Novomoskovsk stock company "Azot" was used (Devisilov, 2014). Calculation was
Numerical study of waste gases purifying using a combined supersonic separator in chemical industry

produced in the steady-state with application of the turbulence model SST. The convergence of the problem by the moment and mass compiled $10^{-4}$, by energy $10^{-3}$.

To simulate the technological scheme of M-100 Novomoskovsk stock company "Azot" with CSS the software package UniSim Design R451 was used. The processes were set in the available devices, using the recalculation data and the results of mathematical modeling in Ansys CFX. Two principal diagrams have been applied. First (Fig. 3) for CSS in supersonic separator mode ($\mu = 0; \mu_h = 1$), the second (Fig. 4) for all other modes, where the proportion of cold flow is not equal to 0.

Fig. 4. Technological scheme of CSS in vortex tube mode for cold flow ratio $\mu > 0$ and for hot flow ratio $\mu_h < 1$

(1 - gas at the entrance to the vortex tube, 2 - gas-liquid flow after heat exchanger, 3 - condensate after regular separator, 4 - gas at the entrance to the CSS, 5 - gas-liquid flow after the twisting device, 6 - condensate after the twisting device, 7 - gas flow after the twisting device, 8 - peripheral gas after in the Laval nozzle, 9 - gas-liquid flow after the Laval nozzle, 10 - condensate after the Laval nozzle, 11 - condensate drainage from CSS, 12 - gas flow after the Laval nozzle, 13 - heated gas flow, 14 - axial gas flow, 15 - cooled gas flow, 16 and 17 - compound gas flow, 18 - gas to flaring, A - heat exchanger, B – regular separator, C - imitation of the swirling device of CSS, D - imitation of condensate drainage from the swirling device to the inner wall of CSS, E - imitation of vortex flow separation in CSS, F - imitation of cooling in a Laval nozzle, G - imitation of the separation unit of CSS, H - imitation of condensate fusion, I - imitation of peripheral flow heating, J - imitation of orifice CSS, K - imitation of flows compound)

For the second scheme, it was decided to use the compounding of two flow (heated and cooled), due to the low refrigerating power of the cooled flow (Fig. 6) calculated by the known formula (Eq. 5) (Piralishvili, et al., 2000):

$$Q_c = G_c \cdot \mu \cdot c_p \cdot \Delta T_c$$ (5)

where: $Q_c$ - refrigeration capacity of the cooled flow, $G_c$ - mass flow of the cooled flow, $\mu$ –cold flow ratio, $c_p$ – heat capacity gas at constant pressure.

For the compound flow, Eq. (6) was applied.

$$Q_{co} = G_{co} \cdot c_p \cdot \Delta T_{co}$$ (6)

where: $Q_{co}$ - refrigeration capacity of the compound flow, $G_{co}$ - mass flow of the compound flow, $\Delta T_{co}$ - the absolute effect of reducing the temperature of the compound flow.
4. Results and discussion

The experimental and recalculation data are presented in Table 1. Figure 5 shows the Mach number, which was determined as a result of numerical simulation in Ansys CFX. According to the results, supersonic mode in the Laval nozzle exists at $\mu < 0.2$ and when $\mu > 0.2$ changes into subsonic. According to the obtained values, the optimal refrigerating capacity of the gas mix flow after CSS will be at the mode $\mu \approx 0.55$.

Let’s estimate the effect $\lambda_Q$ (Eq. 7):

$$\lambda_Q = \frac{(Q_{co} - Q_{th})}{Q_{th}}$$  \hspace{1cm} (7)

where: $Q_{th}$ is the refrigerating capacity of the throttle effect.

<table>
<thead>
<tr>
<th>Cold flow ratio</th>
<th>Hot flow ratio</th>
<th>Absolute effect of reducing the temperature of the cooled flow for air [K]</th>
<th>Calculated absolute effect of reducing the temperature of the cooled flow for gas mix [K]</th>
<th>Absolute pressure ratio for cold flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>0.15</td>
<td>0.85</td>
<td>3.67</td>
<td>11.83</td>
<td></td>
</tr>
<tr>
<td>0.18</td>
<td>0.82</td>
<td>7.39</td>
<td>14.86</td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>0.80</td>
<td>9.95</td>
<td>16.93</td>
<td></td>
</tr>
<tr>
<td>0.24</td>
<td>0.76</td>
<td>13.3</td>
<td>19.68</td>
<td></td>
</tr>
<tr>
<td>0.28</td>
<td>0.72</td>
<td>18.1</td>
<td>20.88</td>
<td></td>
</tr>
<tr>
<td>0.32</td>
<td>0.68</td>
<td>16.42</td>
<td>22.19</td>
<td>8.04</td>
</tr>
<tr>
<td>0.39</td>
<td>0.61</td>
<td>16.95</td>
<td>22.62</td>
<td></td>
</tr>
<tr>
<td>0.46</td>
<td>0.54</td>
<td>17.05</td>
<td>22.70</td>
<td></td>
</tr>
<tr>
<td>0.56</td>
<td>0.44</td>
<td>15.52</td>
<td>21.45</td>
<td></td>
</tr>
<tr>
<td>0.62</td>
<td>0.38</td>
<td>14.01</td>
<td>20.23</td>
<td></td>
</tr>
<tr>
<td>0.77</td>
<td>0.23</td>
<td>9.88</td>
<td>16.88</td>
<td></td>
</tr>
</tbody>
</table>

**Fig 5.** Mach number depending on the mode of operation of the CSS certain by numerical simulation in Ansys CFX
As can be seen from the formula (7), the parameter $\lambda Q$ shows how many times the refrigerating capacity of the waste gas flow exceeds the refrigerating capacity during throttling (a positive number is the flow supercooling, a negative number is the flow overheating). For CSS under given conditions, most modes have refrigerating capacity in excess of the effect of throttling (Fig. 6). In this case, the most advantageous position is also taken by the mode $\mu \approx 0.55$. A similar picture of the peak displacement of the refrigerating capacity of the CSS, which for traditional vortex tubes is in the modes $\mu \approx 0.6 ... 0.7$, is down to the reduction of the length of the CSS energetic separation chamber between the swirling device and the critical section of the Laval nozzle (Vlasenko et al., 2018).

Fig. 6. Refrigerating capacity of the CSS and throttle, parameter $\lambda Q$ depending on the mode for cooled and compound flows

The calculated quantity of condensate $f$ is presented in the form of graphs in Fig. 7, as the sum of the fluid from the heat-transfer device and the vortex apparatus.

Fig. 7. Condensate extraction depending on the CSS mode for compound flow: ($f_e$ - approximation of experimental data with moist air, $f_n$ - numerical calculation)
As we can see, there are two trends on the chart. Initially, values for \( f_n \) (the index \( n \) denoted numerical calculation) were obtained. In this case were used Ansys CFX and UniSim Design R451. The results showed a downward trend with a peak for the extraction of fluid in the mode of supersonic separator (\( \mu_h = 1 \)). This is directly related to the decrease in the efficiency of the Laval nozzle, with numerical simulation, expressed as a decrease in the Mach number, and as consequence, an increase in the static temperature with an increase in back pressure at the heating end. However, this picture does not correspond to the previously obtained results in humid air (Vlasenko et al., 2018), where it can be seen that CSS has a more difficult trend with a peak of condensate entering the mode (\( \mu \approx 0.4 \)).

In this connection, an approximation of the experimental data with humid air for these conditions was performed and a trend \( f_e \) (the index \( e \) denoted approximation from experimental data with moist air) was constructed. At the same time, it was found that in the mode range \( \mu = 0.3 \ldots 0.6 \), the methanol vapor is completely released from the waste gas.

![Fig. 8. The extraction of methanol, depending on the mode of operation of the CSS for the compound flow in the numerical simulation](image)

It is also important to note the potential level of methanol extraction for the \( f_n \) trend (Fig. 8). Even in this situation, the CSS will ensure the release of 75-100% of methanol vapors at modes \( \mu < 0.2 \), which in itself will increase the efficiency of the M-100 vortex plants of Novomoskovsk stock company "Azot" (Devisilov et al., 2014). A comparison of the graphs in Fig. 7-8 shows the presence of an additional 50 kg/h of condensate in the \( \mu_h = 1 \) mode. This additive consists of 99% of liquefied carbon dioxide, which, when the condensate stabilizes, can be easily separated from methanol.

5. Conclusions

As a result of calculation, the thermodynamic characteristics of CSS when working with the waste gas of the M-100 vortex unit of Novomoskovsk stock company "Azot" were determined. It was determined that in the recuperative scheme, under the given conditions and design, it is necessary to mix cooled and heated flows after CSS.

Numerical simulation in the Ansys CFX software package showed the presence of a supersonic mode for CSS on modes \( \mu < 0.2 \) during exploitation on a given composition of the waste gas.
Numerical study of waste gases purifying using a combined supersonic separator in chemical industry

Calculations of phase equilibria in UniSim Design R451 with recalculation parameters from experiments in air for heated and cooled flows, as well as parameters within the CSS defined by ANSYS CFX, showed the condensation of 75-100% methanol vapor at modes \( \mu < 0.2 \). Approximation of the experimental data, when CSS is working in humid air, showed the release of 100% methanol vapor in the \( \mu_h = 1 \) and \( \mu = 0.3 \ldots 0.6 \) modes.

As a result of the simulation of vortex processes, a number of features of the CSS operation in the separation of the liquid phase were revealed in comparison with earlier experiments in humid air. It was found that the design of a vortex-type apparatus CSS can be successfully applied in the chemical industry after passing pilot development tests.

Acknowledgements
The work was performed [partially] as part of the state assignment of the Federal State Budgetary Institution of Science Institute of Chemistry, Far Eastern Branch of the Russian Academy of Sciences, subject № 265-2019-0002.

References


