

The concept of interfering with the homogeneity of air and CO₂ mixture by means of acoustic wave

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Abstract

The paper presents the results of numerical modelling of a rectangular tube filled with a mixture of air and carbon dioxide with an induced standing wave. Assumed frequency inducing the acoustic waves corresponds to the frequency of the thermoacoustic engine. In order to reduce the computational time the engine has been replaced by mechanical system consisting of a piston. This paper includes the results of model studies of an acoustic tube filled with a mixture of air and CO₂ in which a standing wave was induced.

Key words: CO₂ separation, thermoacoustic, CFD

INTRODUCTION

Carbon dioxide belongs, together with water vapour, methane, CFC's, ozone and nitrogen oxides, to a group called greenhouse gases. The gases are responsible for the accumulation of heat in the atmosphere of the Earth. It is estimated that CO₂ has a significant, 50% share (Kotowicz et al., 2007) in this effect. This results from its strong absorption of infrared radiation, as well as from the large quantities of CO₂ present in the atmosphere due to its emissions in conventional processes of heat and electricity generation. Therefore, the efforts of research circles are strongly focused on the methods to reduce CO₂ emissions into the atmosphere by means of an improvement in the efficiency of power engineering systems and of the introduction of CO₂ capture technologies.

The separation methods are divided into: pre-combustion and post-combustion techniques, fuel oxygen combustion, and the use of fuel cells to reduce CO₂ emissions (Kotowicz et al., 2007, Chmielniak et al., 2003). The carbon dioxide separation process itself can be divided into: absorption, adsorption, membrane separation, and cryogenic methods. Each of these processes can be used in all separation methods. Apart from the above-mentioned methods, which are already at a certain level of research advancement, other separation methods, based on different physical phenomena are being developed. One of them is separation which makes use of the acoustic or thermoacoustic wave. The thermoacoustic phenomenon was described for the first time by Lord Rayleigh in 1878. The original description comes down to the statement that if heat is added to gas when it is compressed the most, or extracted when the gas is expanded, an oscillatory wave will be formed. Naturally, the description does not specify the mechanism of the thermoacoustic wave formation; it merely presents a description of the concept of induction of such a wave. A scientific development of this phenomenon can be found in studies conducted in the 80's and 90's of the 20th century. In particular, they are the works of N. Rott from the 60's and 70's, and J. Weatley and G. Swift from the 80's and 90's, and others, such as (Geller et al., 2002, Swift et al., 1999, Swift et al., 2006, U.S. Patent, 2004). The simplest method to induce a thermoacoustic wave is the application of the Rijke

tube (Carrier et al., 1955, Rayleigh et al., 1945). From the thermodynamic point of view, the thermoacoustic phenomenon realises the Stirling cycle and, as such, it can be considered as a right- or left-running cycle, i.e. as the engine cycle or the cycle of the cooler. Both cases have already found application in prototype devices such as thermoacoustic engines and coolers, natural gas liquefaction facilities and many others. Studies of the thermoacoustic wave have also shown that, in certain conditions, the wave can be used in the gas separation process. The aim of this study is to investigate the possibility of using the thermoacoustic wave in CO₂ separation processes. It should be treated as preliminary research for further, more detailed, analyses. In particular, the aim of this study is to start a numerical model of the separation process, and its parametric analyses. The performer tentative calculations are original and are not based on the other calculations presented in literature.

THERMAL DIFFUSION

Thermal diffusion (thermodiffusion, the Soret effect) is a process of disturbance in the mixture homogeneity which is caused by the difference in temperatures in the medium, and which consists in the movement of particles in the mixture or solution resulting from a temperature gradient. The Soret effect is explained in Fig. 1. In subsequent time instances, the moving acoustic wave produces a temperature gradient, which in turn causes a momentary disturbance in the contents of individual components in the mixture. If the temperature gradient direction is properly correlated with the direction in which the mixture particles move, a lasting effect of separation can be obtained.

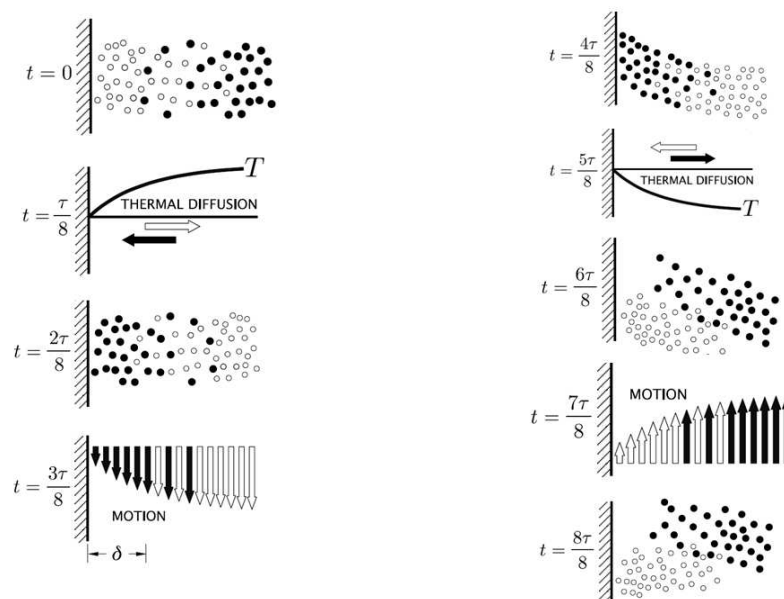


Fig.1 Thermal diffusion mechanism produced by the temperature gradient between the wave front and the tube wall (Spoor and Swift, 2002).

As it can be seen in Fig. 1, in subsequent time instances the moving front of the pressure wave produces a temperature gradient towards the tube walls, which entails a momentary separation of the mixture. It should be noted that, apart from this effect, there is also a purely mechanical impact of the wave on the mixture particles.

CFD MODEL

The numerical model of carbon dioxide separation was developed with the use of a computational fluid dynamics commercial code Ansys-CFX13. The scheme of the model is presented in Fig. 2. The following dimensions of the computational domain are adopted: $x=20$

mm, $y=50\text{mm}$, $z=1000\text{mm}$. Both for the lateral and the top as well as bottom areas, boundary conditions were assumed as symmetry (Fig. 4). Therefore, the model does not take account of the impact of the walls and the friction related to it on the behaviour of the acoustic wave.

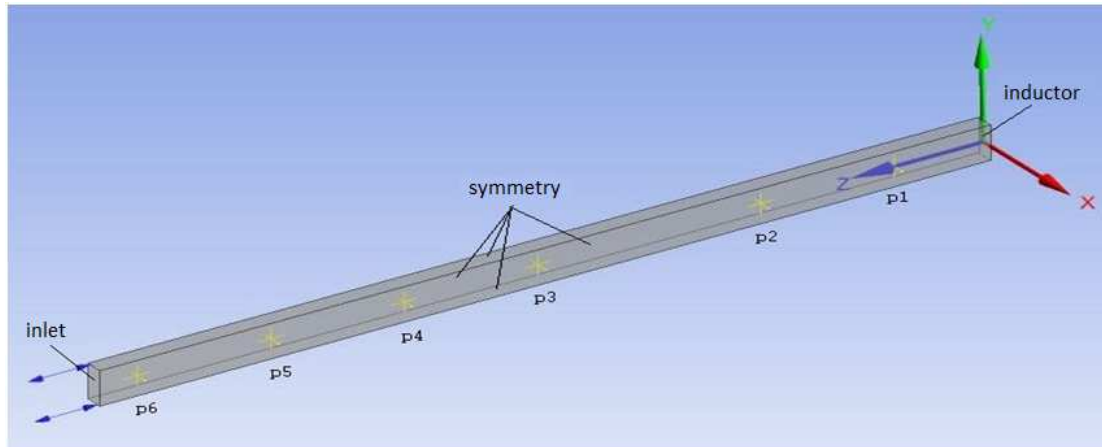


Fig. 2 View of the tube adopted for the calculations. Rectangular tube with dimensions: 20x50x1000mm.

Recent calculations for a thermoacoustic tube (Remiorz et al., 2010) with similar dimensions have been confirmed that there was no significant impact of this assumption on the calculation results. However, the assumed symmetry (Fig. 2) has a substantial impact on the computation time, which gets definitely shorter. As an enforcement, a sinusoidally changeable location of the closed end of the tube was assumed, while the other tube end remained open. The adopted computational model thus realises a computational scheme whose mechanical analogy is shown in Fig. 3. It is a long cylinder closed at one end with a movable piston. The piston location is described by the following equation:

$$x_t = s \cos(2\pi ft) \quad (0.1)$$

where:

- x_t – change in the location of the mesh enforcing (piston) oscillations
- s – maximum shift
- f – oscillation frequency
- t – simulation time.

The equation does not take account of the fluctuations of the connecting rod, and the changes in the piston location resulting from them. The change in location is caused only by the rotation of crank r . The maximum shift from the initial state was assumed at $s=2\text{mm}$. The tube was filled with a mixture of air and CO_2 with volume contents of 85% and 15%, respectively. At the outlet section, an open boundary condition was assumed with inlet pressure equal to 0 Pa (compared to reference pressure). The open boundary condition allows a two-way flow of gas, depending on the pressure distribution.

For the case under analysis, the mechanical enforcement of the acoustic wave was performed by the method of so-called movable meshes implemented within the code ANSYS-CFX. In our case, this allows a simplified modelling of the sound source, which most often is a properly selected loudspeaker, the target source being a thermoacoustic engine. It was assumed that one of the walls of the calculated area (the inductor) oscillated with a strictly defined frequency. This results in a local deformation of the numerical mesh. The oscillations are responsible for the formation of an acoustic wave in the device. At the same time, on the

inductor wall itself, the velocity value is assumed at zero (the velocity node), and the pressure at this point reaches its maximum value (the pressure antinode).

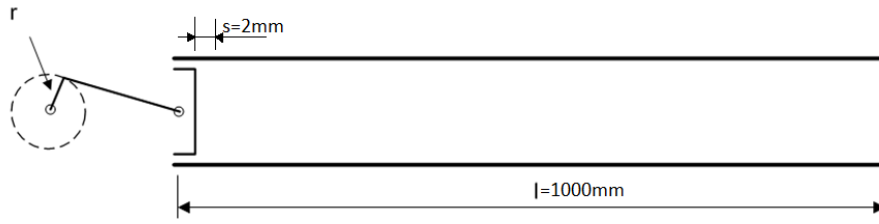


Fig. 3. Mechanical analogy of the computational model

The basic data of the numerical simulation are: frequency $f = 85.25$, temperature $T = 300\text{K}$, reference pressure $p = 0.1\text{MPa}$. Assumed physical model consists of two continuous phases, air and carbon dioxide, governed by Euler-Euler approach with the volume fraction 85% and 15%, respectively. The adopted basic time step of $3.91 \cdot 10^{-4}\text{ s}$ corresponds to 30 iterations per a single acoustic wave period. The impact of time discretisation will also be discussed in detail in one of the sections below. Additionally, in the case under consideration, the inductor oscillation frequency was adopted at 85.25 Hz – the value resulting from the frequency of the standing wave for this tube. The aim of the numerical analysis is to determine whether or not carbon dioxide, due to the effect of the acoustic wave, would be concentrated and whether or not the mixture homogeneity would be disturbed. For this purpose, the CO_2 content at individual locations was analysed. Fig. 4 presents the obtained results, which show that with passing time the CO_2 concentration at certain locations increases, while at other locations – it decreases. After 2.5s the carbon dioxide content increases near the inductor itself and reaches the value of approx. 0.28, whereas near the outlet area the CO_2 content is approx. 0.08. At the same time, all thermodynamic values and the CO_2 content at individual locations oscillate around their local average values. However, the oscillations are slight compared to the obtained differences in CO_2 contents. The control points were placed at a distance of 0.1m, 0.25m, 0.5m, 0.65m, 0.8m, 0.95m from the inductor.

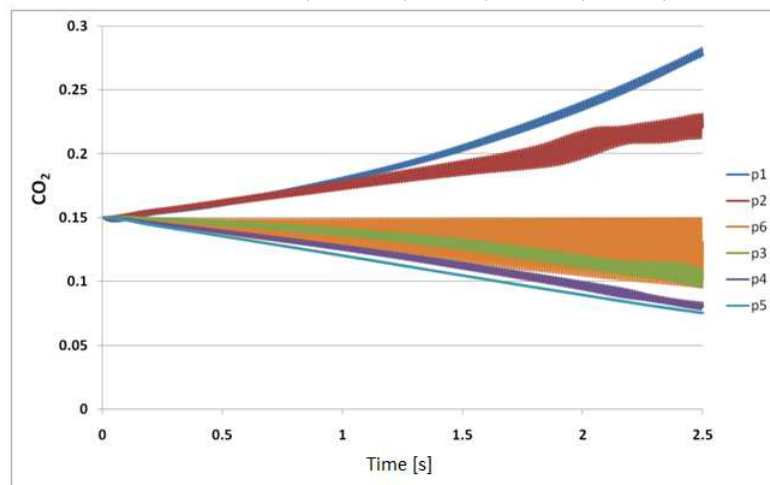


Fig. 4. Chart of CO_2 contents for Mesh I

CALCULATION RESULTS

The conducted numerical analysis shows that if in a rectangular tube filled with a mixture of air and CO_2 an acoustic wave with an appropriately selected frequency is generated, due to the effect of the wave a slow-changing process of the separation of the gases occurs. The

process has a lasting nature with respect to the running acoustic wave, i.e. subsequent wave cycles do not disturb the process, but they intensify it. This is shown in Fig. 10. At instant $t=0s$ the whole tube is filled with a homogenous mixture of air and CO_2 . After time $t=0.6s$, places appear with an increased concentration of CO_2 , and after time $t=1.2s$ the lasting inhomogeneity is already clearly visible.

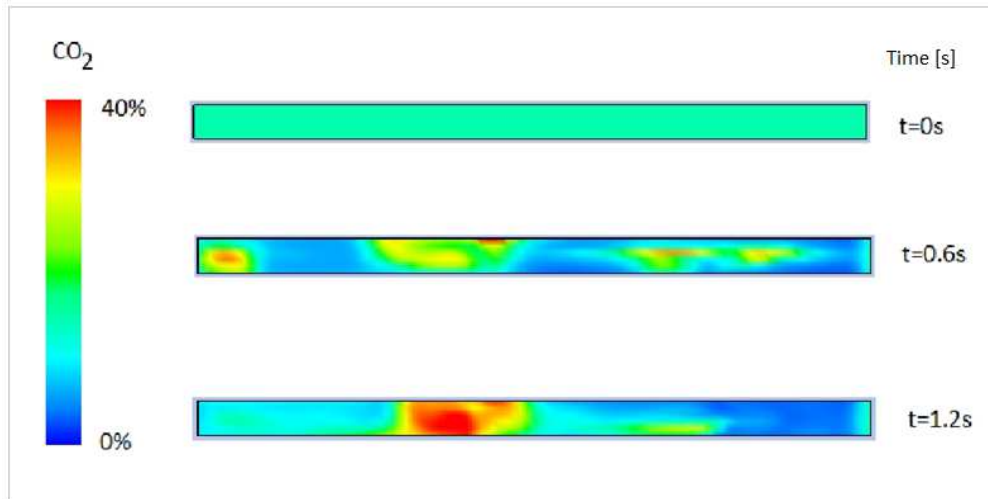


Fig. 10. CO_2 separation. Image of the modelled tube at subsequent time instances: $t=0s$, $t=0.6s$, $t=1.2s$. The red colour denotes places of CO_2 concentration.

In the numerical model the separation process did occur and it is intense. However, the obtained result has to be verified by laboratory tests.

CONCLUSIONS

The paper presents the results of numerical modelling of an acoustic tube filled with a mixture of air and CO_2 . A rectangular testing tube with dimensions: $20 \times 50 \times 1000mm$ was assumed. One end of the tube was left open, whereas an acoustic wave inductor was modelled at the other end. Due to the effect of an acoustic wave, a disturbance in the mixture homogeneity occurred in the modelled tube. The homogeneity disturbance had a lasting character with respect to the subsequent oscillation cycles in the tube. The observed phenomenon was not qualitatively affected by parameters such as the numerical mesh size, the adopted time step or the pressure in the tube. The separation could be observed regardless of the values of adopted parameters, within the set limits, of course. At the same time, the values adopted for the modelling had an impact on the level and time of separation, which was the case for space and time discretisation in particular. The presented results need experimental verification, which is the subject of further studies.

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