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Modeling and numerical simulation of basic thermodynamic processes of ideal gases

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ABSTRACT

Mathematical models of processes with ideal gases at open and closed thermodynamically systems, easy for numerical simulation by CFD software are developed. They include the main steps for computer simulations of laminar and turbulent flow, buoyancy, isobaric and isochoric heating, and adiabatic compression using simple geometrical models and changing the governing equations, boundary and initial conditions. Visualization and animations of stationary and transient thermal and fluid flow field are obtained as results. The models are easy for verification and validation on the base of the theory of thermodynamics, heat transfer and fluid dynamics. They can help to bachelor students to understand and learn the theory of transport phenomena at ideal gases.

Keywords: numerical simulation, CFD, ideal gases, thermodynamics, heat transfer, fluid flow.

INTRODUCTION

The gases that can be accepted as ideal are widely used in industry: air flows, gas fuels, flue gases, etc. Theoretical models, describing the ideal gas processes are well known, validated, verified and included in the bachelor engineering education. The development of hardware systems and software for finite volumes and elements analysis allows to simulate numerically and to visualize the temperature, pressure, velocity fields at different processes in 3D gas domains [1]. Such numerical analyses can help the students to understand the physical processes and to obtain additional knowledge about them. There are many tutorials at the common used CFD software as ANSYS/Flotran, Fluent or CFX, Open Foam, etc. [2]. They are oriented to simulation of more complicated and specific processes and require higher level of knowledge in mathematics and transport phenomena. That make them useful for engineers, researchers and PhD students. The aim of the present work is to compose and summarize conceptions for modeling and numerical simulations of widespread in industry ideal gas processes, suitable for easy solution by bachelor students using common CFD codes.

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Conceptions and algorithms for numerical simulations

Five processes at ideal gases are suggested for numerical simulation by bachelor students in the present paper. They can be done as exercises in computer laboratory with licensed or free CFD software. Before the simulations it is necessary for students to have studied mathematics, informatics, physics, thermodynamics, fluid dynamics, technical drawing and CAD and to have also a broad idea of the capabilities of the software. The main steps of the simulations are:

- Short discussion of the theory (thermodynamic, hydrodynamic and heat transfer aspects of the problems);
- Creation of the geometrical models and finite volume meshes;
- Duplications of the models according the number of processes;
- Setup the model options, boundary and initial conditions;
- Solution of the models;
- Post processing and discussion of the results.

Each simulation, preliminary calculations, discussion of the theory and the received results can be implemented in 2 or 3 teaching hours. Demonstrative solutions are implemented by ANSYS/ CFX software in the present work.

Isobaric processes at open systems

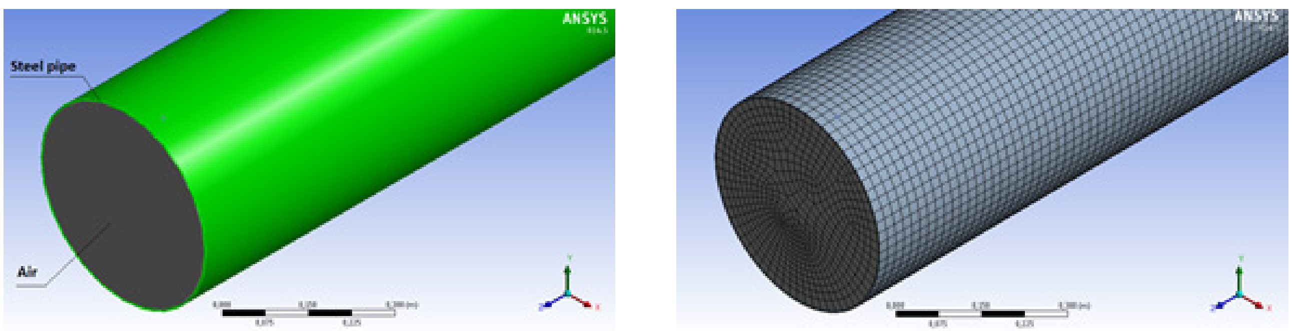
Gas flow in pipes at velocities less than 20 m s^{-1} can be accepted as isobaric due to relatively small pressure drop in comparison with the total pressure. In principle the length of the pipe must be higher than the entrance length to ensure modeling of the boundary layer and velocity profile at the entrance region and the fully developed flow. The entrance length can be predicted by well-known relations for laminar and turbulent flows on the base of internal diameter of the pipe and Reynolds number [3]. These conditions are approximately met at pipe sizes: internal diameter = 0.4 m, wall thickness = 0.003 m; length = 10 m.

The geometrical model is consisted of gas domain and solid domain (pipe), shearing common interface (Fig. 1). They are meshed by finite volumes/elements with sizes, depending on the computer properties. As finer is the mesh, as higher is the time duration for meshing and solution.

Laminar and turbulent flow at horizontal pipe and chimney effect at vertical pipe are suggested for modeling at the geometry above. The governing equations, boundary conditions and processes features are given in Table 1. The air ideal gas relation and the thermal properties of the steel are available at the CFX library of material models.

Numerical simulation of horizontal laminar and turbulent flow

The preliminary discussions with the students include the explanation of ideal gas equation and processes, the nature of laminar and turbulent flow, the heat transfer with the environment, calculations of Re number at the conditions at



a) b)

Fig. 1. Geometrical model (a) and finite volumes mesh (b) including 337500 elements.

Table 1. Models and conceptions for numerical simulation of gas flow in pipes.

Process	Equations	Boundary conditions
1. Laminar non isothermal flow in a steel pipe • Steady state; • Conjugate heat transfer • Buoyancy is not taken into account • Fluid - air ideal gas • Pipe - steel	1. Continuity equation 2. Momentum equations at g_x=g_y=g_z=0 3. Energy equation (for solid and fluid domain) 4. Boundary layer model (wall functions) 5. Ideal gas law	Inlet: velocity, normal to the boundary V_n= 0.1 m s^{-1} and static temperature t = 0°C. Outlet: relative static pressure *p* = 0 Pa. External pipe walls: heat transfer at h_e=15 W m^{-2} K^{-1} and ambient temperature t = 30°C.
2. Turbulent non isothermal flow in a steal pipe • Steady state • Conjugate heat transfer • Buoyancy is not taken into account • Fluid - air ideal gas • Pipe - steel	1. Continuity equation 2. Momentum equations at g_x=g_y=g_z=0 3. Energy equation (for solid and fluid domain) 4. k-ε turbulence model 5. Boundary layer model (wall functions) 6. Ideal gas law	Inlet: velocity, normal to the boundary V_n=10 m s^{-1} and static temperature t = 0°C. Outlet: relative static pressure *p* = 0 Pa. External pipe walls: heat transfer at h_e=15 W m^{-2} K^{-1} and ambient temperature t = 30°C.
3. Turbulent flow in a steel chimney • Steady state • Conjugate heat transfer • Including buoyancy at reference (ambient) density of 1.2 kg/m^3 • Fluid- air ideal gas • Steel pipe	1. Continuity equation 2. Momentum equations at g_x=g_y=0; g_z= - 9.81 m s^{-2} 3. Energy equation (for solid and fluid domain) 4. k-ε turbulence model 5. Boundary layer model (wall functions) 6. Ideal gas law	Inlet: opening boundary, relative static pressure p = - 36 Pa and static temperature t = 150°C. Outlet: opening boundary, relative static (ambient) pressure p = - 118 Pa (corresponding to altitude 10 m) and static temperature t = 20°C. External pipe walls: heat transfer at h_e= 30 W m^{-2} K^{-1} and ambient temperature t = 20°C

the inlet in order to check the propriety of the inlet velocities.

A laminar flow is simulated first. After a view of the results the model is duplicated, the inlet velocity is changed and turbulence model is checked instead of the laminar one.

Some of the obtained results of the processes are visualized on Figs. 2 and 3.

The models can be validated by comparison of the mass flows, obtained by the software and computed by hand. Possible issues that can be disused by the students, based of the results at

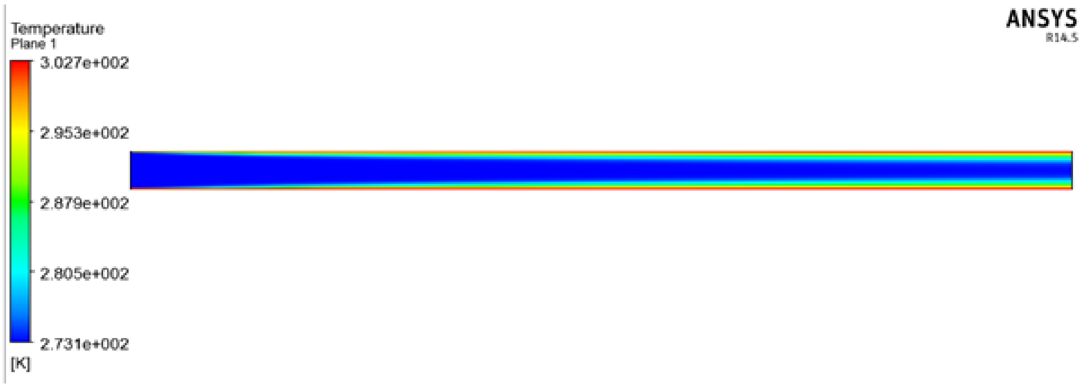


Fig. 2A. Temperature field in a longitudinal cross-section at laminar flow.

Fig. 2B. Velocity field in a longitudinal cross section at laminar flow.

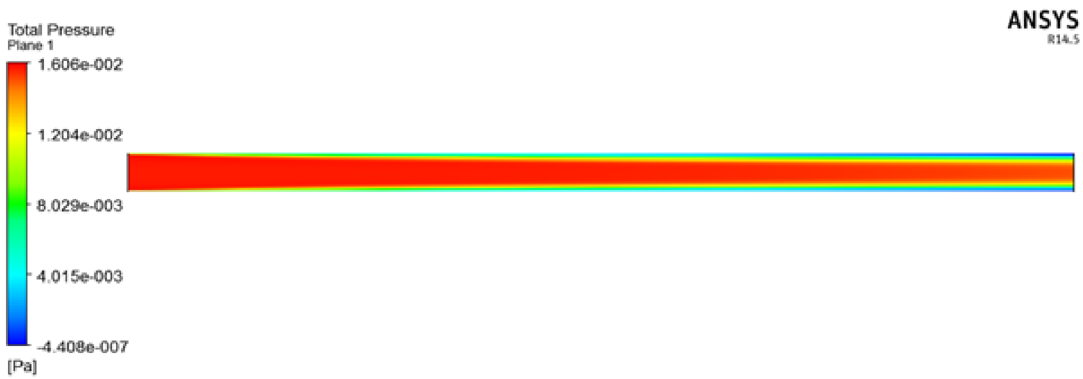


Fig. 2C. Total pressure (relative) in a longitudinal cross section at laminar flow.

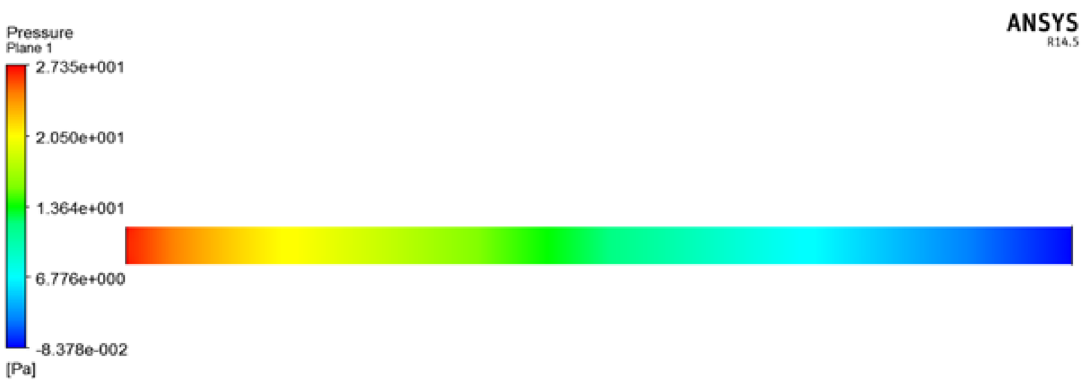


Fig. 2D. Static pressure (relative) in a longitudinal cross section at laminar flow.

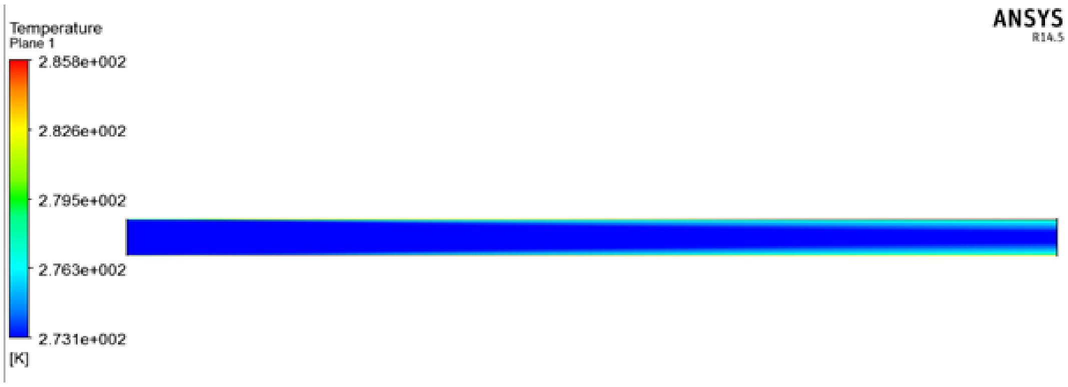


Fig. 3A. Temperature field in a longitudinal cross-section at turbulent flow.

Fig. 3B. Velocity field in a longitudinal cross section at turbulent flow.

Fig. 3C. Total pressure (relative) in a longitudinal cross section at turbulent flow.

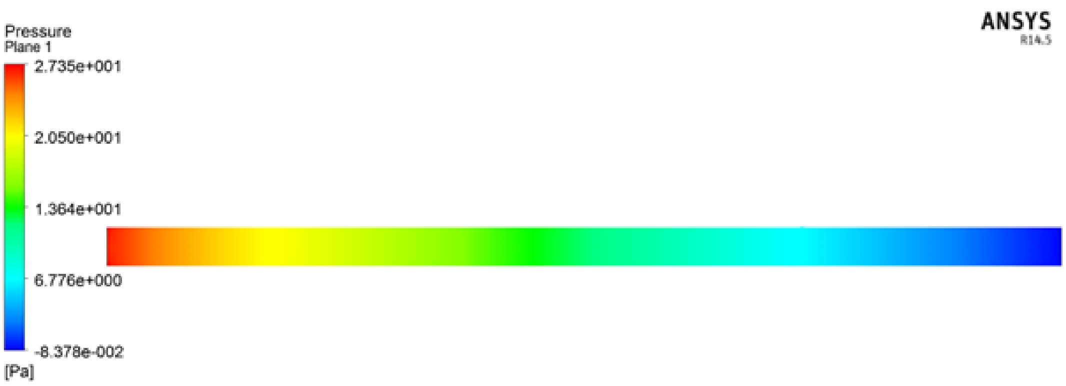


Fig. 3D. Static pressure (relative) in a longitudinal cross section at turbulent flow.

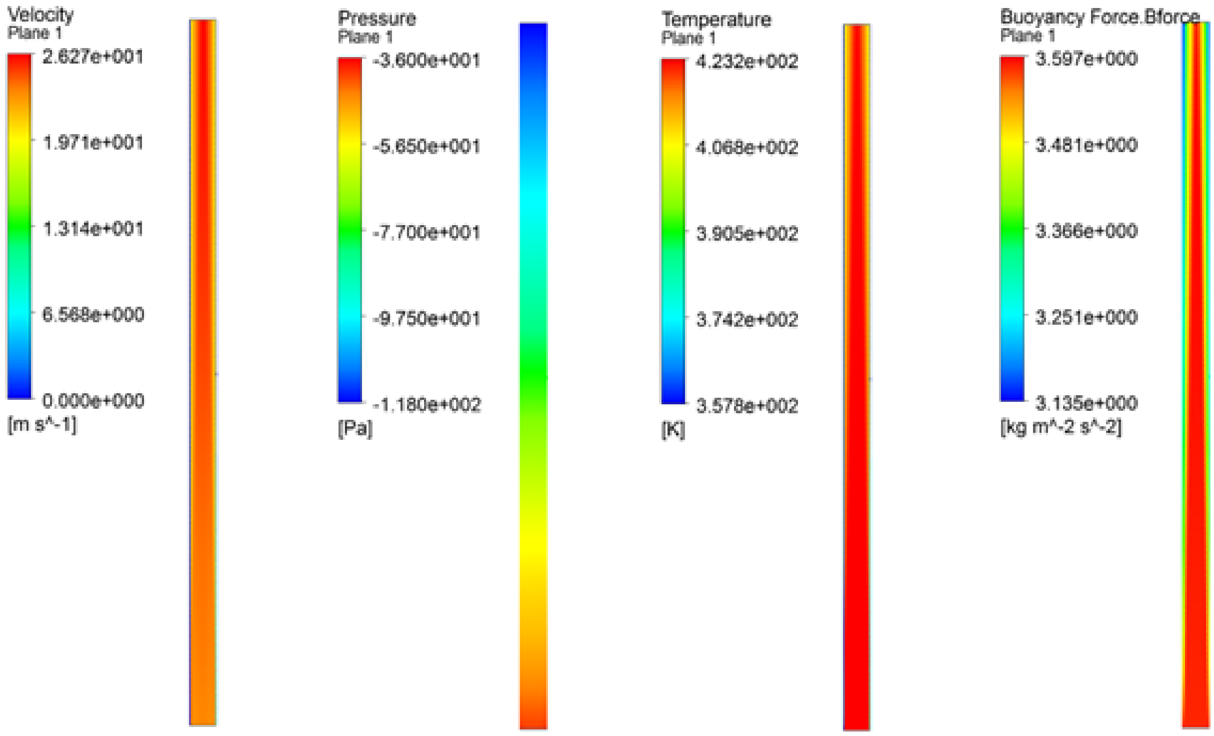


Fig. 4. Velocity, static pressure, temperature, and buoyancy force at Process #3 (chimney effect).

the two processes, are:

- differences between local and average velocities;
- differences between the total and the static pressures;
- difference between the pressure drops at the turbulent flow and the laminar flow;
- difference between the temperatures fields at the turbulent flow and the laminar flow;
- reasons to accept the processes as isobaric.

Numerical simulation of chimney effect

It is enough to include buoyancy model and to activate the gravity in direction, pointing the expected inlet to simulate chimney effect by the same geometrical model. A gas temperature, higher than the ambient one, has to be applied on the pipe inlet. The relative pressure on the outlet is the ambient pressure at a height of the pipe (10 m), computed according the ambient pressure of the bottom of the chimney that usually is accepted as zero. The relative pressure at the bottom is the static pressure, computed by Bernoulli equation and the density of the hot air at the inlet temperature. The hot air density, ambient pressure at the top of the pipe and static pressure at the bottom are computed by the students before numerical simulations of the process.

The model of the turbulent flow, described above, is duplicated and model options and boundary conditions are changed according Table 1. The explanation of the chimney effect and the preliminary calculations can be implemented in one teaching hour. The simulation and the discussion of the results can be done in maximum 2 teaching hours.

Results, received by the numerical simulation of the chimney effect, are visualized on Fig. 4. The geometry of the pipe on the figure is oriented vertically just to visualize better the results according the expectance. It is obvious the existing of the non-zero velocity due to buoyance.

The models are validated by the students by comparison of the expected and computed buoyancy force. Parameters, influencing on that force can be an object of discussion.

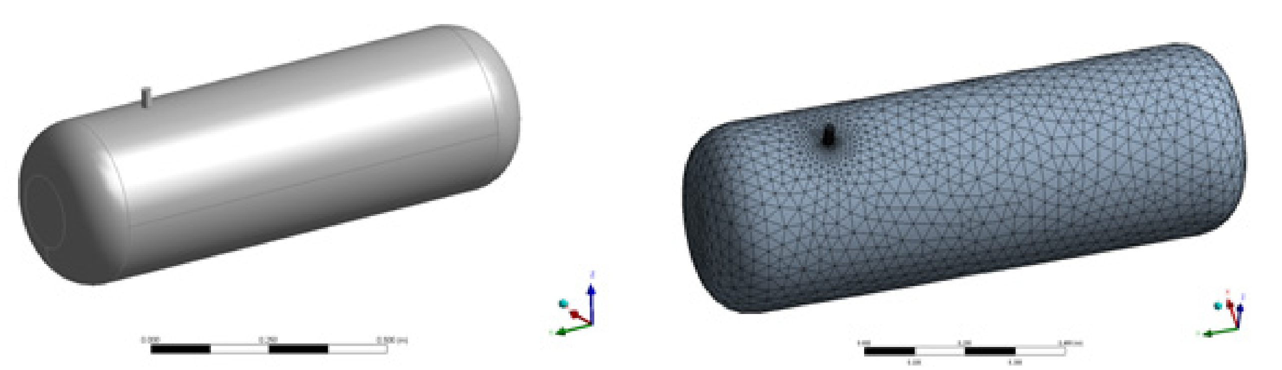
Table 2. Mathematical models and conceptions for numerical simulations of processes with compressed gases.

Process	Equations	Boundary conditions
1. Adiabatic compression in a steel air receiver • Transient process: time; duration - 60 s; adaptive time step; • Buoyancy is not taken into account; • Initial conditions: relative pressure p_{in}= 6 bar; initial temperature t = 20°C; $V_x=V_y=V_z=0$ • Fluid domain only - air ideal gas	1. Continuity equation 2. Momentum equations at $g_x=g_y=g_z=0$ 3. Energy equation for fluid domain 4. k-ε turbulence model 5. Boundary layer model (wall functions) 6. Ideal gas law	Inlet: relative static pressure p = 8 bar and temperature t = 70°C (measured at the real receiver). Adiabatic walls (zero heat flux)
2. Isochoric heating of compressed air in a steel receiver • Transient process: time duration - 35 s; adaptive time step • Including buoyancy • Initial conditions: relative pressure p_{in}= 7 bar; temperature t = 0°C; $V_x=V_y=V_z= 0$ • Fluid domain - air ideal gas. • The existing of metal walls is modeled by the boundary conditions.	1. Continuity equation 2. Momentum equations at $g_x=g_y=0;$ $g_z= - 9.81$ m s^{-2} 3. Energy equation for fluid domain 4. k-ε turbulence model 5. Boundary layer model (wall functions) 6. Ideal gas law	All boundaries: walls, heat transferring with the environment at temperature t = 30°C. Effective heat transfer coefficient: $h_{ef} = \dfrac{1}{\dfrac{\delta_{steel}}{K_{steal}} + \dfrac{1}{h_e}}$ h_{ef} = 15 W m^{-2} K^{-1}; δ_{steal} - wall thickness (4 mm); K_{steal} - thermal conductivity (70 W m^{-1}K^{-1}); h_e - heat transfer at the external walls: h_e = 15 W m^{-2} K^{-1}

Processes at air receivers

The receivers for compressed gases are open systems during the charging and discharging processes and closed systems if these processes are stopped. Conception for modeling of charging of air receiver (open system) and fluctuations of gas pressure and temperature at variation of the environmental temperature at closed system are presented in Table 2. A laboratory compressed receiver complied whit 1.5 kW piston compressor is an object of modeling. The volume and the surface of the receiver are 0.10923 m^3 and 1.3581 m^2, respectively. The geometrical model (Fig. 5a) can be drown in advance and imported at the start of simulation. It can be simplified to cylinder with the same volume and surface in order to facilitate the modeling process.

Two processes - at open and closed system (receiver), are suggested for modeling at the same geometrical model and mesh in the present paper. The main points of the conceptions for numerical simulations are summarized in Table 2.



a) b)

Fig. 5. Geometrical model (a) and finite volumes mesh including 35498 elements (b).

Adiabatic compression in the receiver (open system)

The compression of the gases in the receivers actually is not adiabatic process. The reason to be accepted as adiabatic is to explain to the students in which cases such assumption can be made and when the heat transfer with the environment has to be taken into account. The preliminary discussion includes an explanation of processes of compression in the receivers, gas inflows that can be with critical and subsonic velocity depending on the pressure in the tank, heat transfer with the environment, buoyancy effects and driving force.

The velocity of the gas, inflowing in the receiver is critical during the filing of the receiver if the process starts from zero gage pressure until achieving the critical pressure. The numerical simulation of that process is possible but has to be implemented at very small time step in order to obtain stable solution. The solution of such task needs a long computational time if it is done with non-powerful computers in students laboratory. If the process starts from pressure, higher than the critical, the velocity of the inflowing gas in the receiver is subsonic and the process is possible for the simulation within 3 teaching hours.

A process of filing of the receiver from start gage pressure of 6 bars to end pressure gage pressure of 8 bars is suggested for simulation in the present paper. An increasing of the air temperature from initial value of 293 K to the end value of 323 K is established during that process. The air streamlines at the start of the charging of the receiver are visualized on Fig. 6.

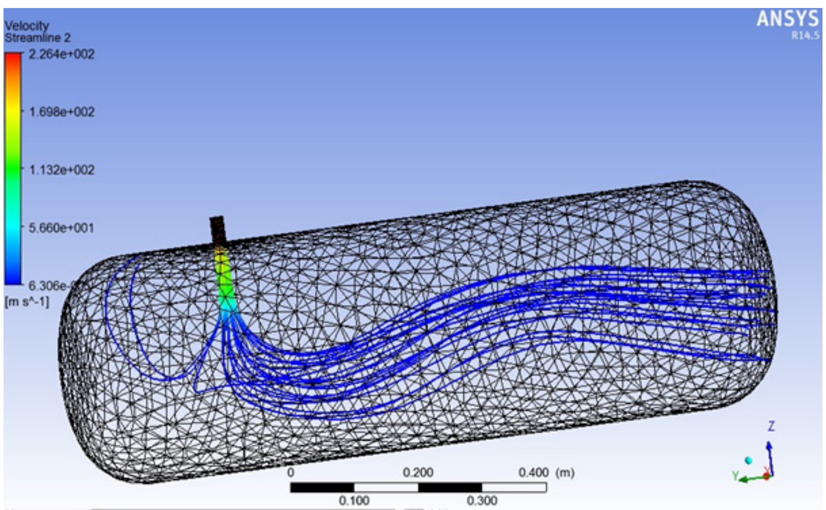


Fig. 6. Streamlines of the air at the start of the process.

Fig. 7. Temperature field at the start of the heating process.

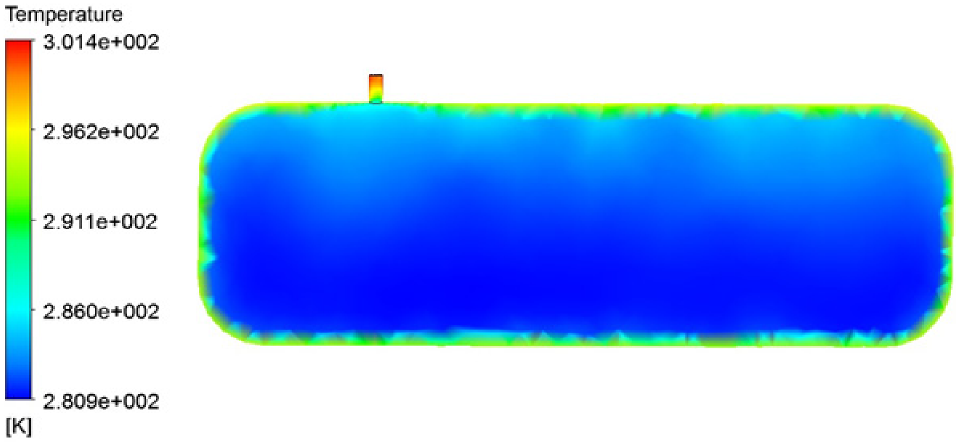


Fig. 8. Temperature field at the end of the heating process.

An interesting parameter for visualization is the density of the air. It is increasing at the process. It can be calculated by hand and compared to the obtained one during the numerical simulation in order to validate the model.

Issues that can de discussed by the students, based on the results above, are:

- if the simulated process is equilibrium or quasi-equilibrium.
- what differences are expected in the end parameters if the process is modeled as non-adiabatic.

A real process can be realized at the modeling condition with the laboratory receiver to demonstrate the difference between the adiabatic and non-adiabatic walls.

Isochoric heating of the compressed air in the receiver (closed system)

Isochoric heating or cooling of the compressed gas can occur if the ambient temperature is different according the temperature in the receiver (at receiver displacement from one room to another or ambient temperature change). The numerical simulation of that process can be implemented at duplication of the model, described above, and changing the boundary and initial conditions according to Table 2.

Results about the temperature, obtained by the numerical simulation of an isochoric heating of compressed air at closed system (receiver), are visualized on Figs. 7 and 8. The average temperature of the air is changed from 273 K to

285 K during the heat transfer. In the same time the gage pressure of the air is increased form 7 bars to 7.27 bars.

The pressure at the average end temperature in the receiver can be computed by hand and compared to the end simulated pressure in order to validate the models of the process.

The issues that can be discussed at the end of the lessons are:

- if the obtained end fields are equilibrium;
- which of the two-simulated processes (adiabatic compression or isochoric heating) is closer to an equilibrium (and why).

If possible, the process can be continued to equalizing the temperature of the gas in the receiver and the environment.

The numerical simulations of the processes are implemented for the first time by the second year students of specialty "Chemical Engineering" at the University of Chemical Technology and Metallurgy in Sofia. It was established that the students cope with the simulation in time. Better demonstration of the capabilities of the software and faster solution were established in cases at which the professor is doing and presenting the simulation in parallel with the students during the lessons.

CONCUSIONS

The developed conceptions for numerical simulation allow visualizations and animation of common processes with ideal gases. They can result in positive effects for students as:

- development of capacity to imagine scalar and vector fields;
- better understanding of theory;
- an idea for the development of the theory;
- awareness of the important role of the pure and applied mathematics in understanding and control of engineering processes;
- an idea for the possibility of the advanced hardware and software systems for solving of engineering problems;
- creation of interests in the science and research;
- development of skills for use of information technologies.

Acknowledgements

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