Applied Chemical Engineering (2024) Volume 7 Issue 2
doi: 10.59429/ace.v7i2.2063

ORIGINAL RESEARCH ARTICLE

Numerical simulation of different types of CO_2 and O_2 gas mixers

S. Osipov, I. Komarov, P. Golosova, M. Oparin, M.M Shaikh*

Department of Innovative Technologies for High-Tech Industries, National Research University "Moscow Power Engineering Institute", Moscow 111250, Russia

*** Corresponding author:** M.M Shaikh. sheykhm@mpei.ru

ABSTRACT

The operating thermal power plants emit greenhouse gases which cause an undesirable greenhouse effect. One of the ways to reduce emissions of such gases is to create oxyfuel-energy units and use of carbon dioxide as diluent. However, for effective combustion efficient CO_2/O_2 mixing is required which is possible only by employing external gas mixer.

This paper presents the results of the gas mixer study design. Based on the results of numerical modeling of the flow of combustion components in the gas mixer it is established that the location of deflectors and diffusors plays important role in mixing of components in the mixing chamber.

Keywords: carbon dioxide CO_2; gas mixer; mixing in the burner; numerical modeling; supercritical parameters

ARTICLE INFO

Received: 2 January 2024
Accepted: 25 January 2024
Available online: 3 April 2024

1. Introduction

Currently, electricity is generated by burning fossil fuels in thermal power plants (TPPs). The process of TPP operation involves emission of combustion products into environment, which mainly consist of gases that provoke the greenhouse effect. In addition to using plants to capture harmful emissions, there is a potential to minimize them through the use of oxyfuel technologies[1,2]. Unlike conventional plants, oxyfuel power units (OFPUs) do not pollute the atmosphere with emissions, thanks to the closed-loop Brayton cycle, the use of oxyfuel for a combustion and the prevention of carbon dioxide by removing from the cycle. The Allam cycle power plant is one of the most efficient examples of the oxyfuel technologies, and its critical part is the use of carbon dioxide as diluent in combustion chamber (CC)[3–5].

A distinctive feature of this CC from conventional GTP CC is the use of pure oxygen as an oxidizer and use of carbon dioxide not only for cooling, but also as a diluent. The **Figure 1** shows the design of a CC with a vortex device[6].

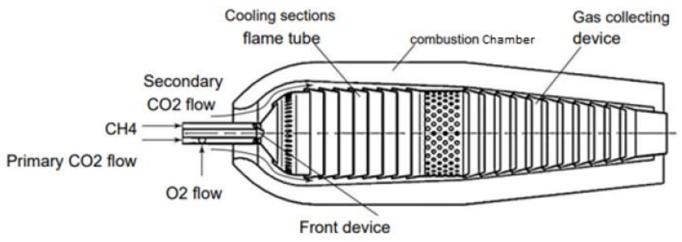


Figure 1. Flow distribution and CO_2 combustion chamber design[6].

Vortex burners are used to ensure high-quality mixing of gases. In the study of Osipov et al.[7], it was found that vortex burner devices do not provide high-quality mixing of oxidizer and diluent. For the combustion of oxyfuel in the environment of CO_2, high level of CO_2/O_2 mixing is required which create the foundation of employing external gas mixing device.

2. Overview of existing gas mixer designs

A mixer is a type of process equipment designed to prepare mixes from initial components in the same or different aggregate state. There are two main groups of mixers - dynamic and static, the classification is shown in **Figure 2**.

In a dynamic mixer, the main mixing function is provided by a moving rotating structural element: auger, blade, rotor, roller. It is fixed in the mixer body and is driven by an actuator. Two-blade mixers with Z-shaped blades, planetary mixers with one T-shaped or U-shaped blade, batch or continuous mixing rollers are used for mixing viscous materials. In terms of design, dynamic mixers are often designed as vertical mixers. The axis of rotation of the movable element coincides with the machine axis.

a) Static mixer.

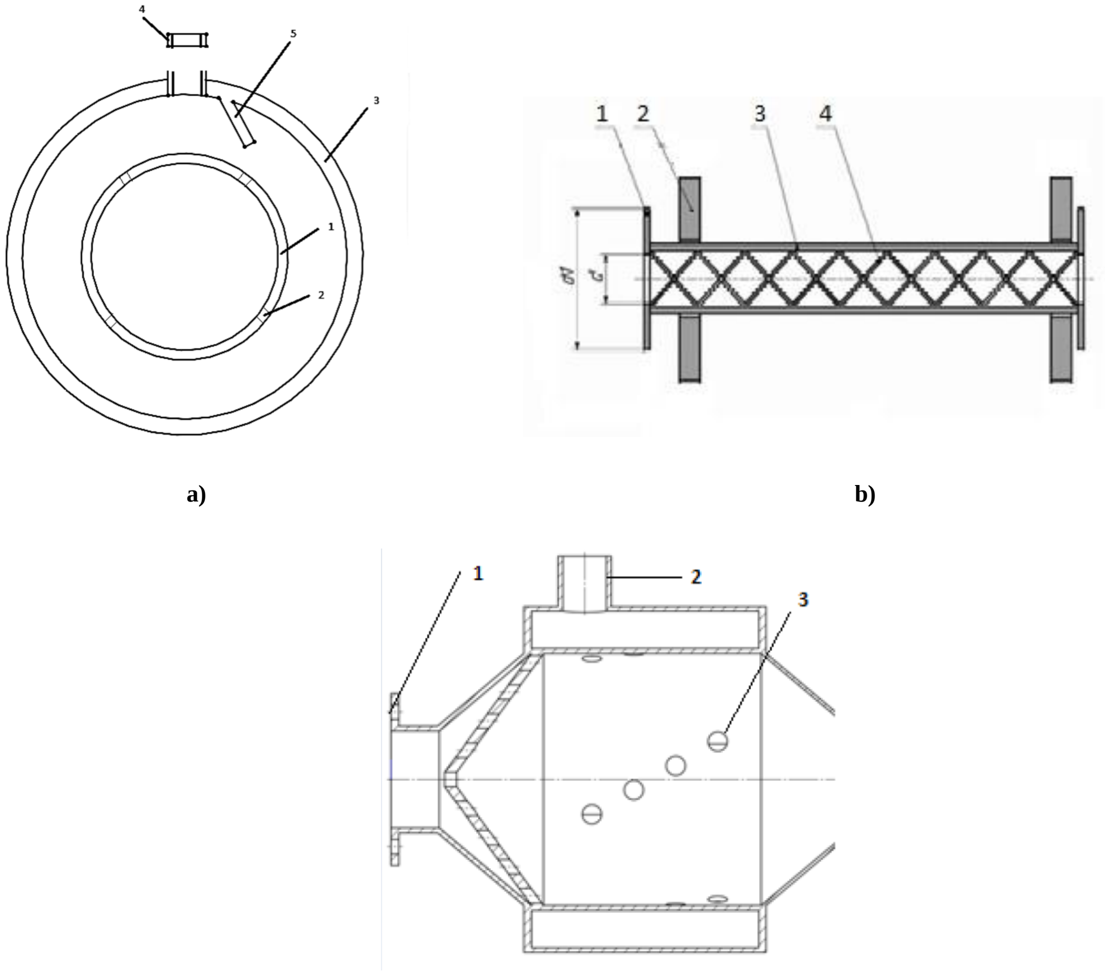
b) Dynamic mixer.

Figure 2. Classification of mixers.

In industrial applications, liquids and gases are most often mixed in pipelines. If it is necessary to mix the components directly in the pipe, static mixers are installed. A static mixer utilizes the energy of flow motion to mix components. This configuration requires no power consumption. This type of mixer has no moving parts. This maximizes the reliability of the mixing device and reduces the costs and simplifies the installation. With fixed mixers, regular maintenance of the equipment with inspection of the interior is practically eliminated, as the mixers are made of corrosion-resistant materials. The tubular mixer is a pipe section. It incorporates various kinds of fixed fillers: plate fillers, comb fillers or a row of equalizing grids. The fillers are placed in the pipe at various angles of inclination and 90° turns. The media to be mixed are fed to the inlet side.

At the transition points of the plate sections, the liquids are separated into individual flows, turned and fed again into a different pipe diameter. The required length of the mixing pipe in this case is about 2–5 diameters of this pipe. But in addition to the advantages listed above, this type of mixers has the following disadvantages: significant pressure loss compared to a hollow pipe, risk of clogging when the openings between the filler plates are occluded.

Let us review the designs of tubular mixers described in domestic patents[8,9]. shown in **Figure 3**.



a) **b)**

c)

Figure 3. Designs of jet mixers: **a)** - two-flow mixer **b)** - tubular mixer; **c)** jet gas mixer.

Figure 3a shows the design of the gas mixer from the research of Galitskaya et al.[8]. A cross-flow of one of the gas components is supplied through pipeline 1. The second flow enters manifold 3 through branch pipe 4, from where it is evenly distributed over orifices 2 joins the cross-flow in a pattern of transverse jets. The angle of jet efflux into the flow depends on the position of baffle plate 5. At the plate 5 maximum angle of deflection from the cut of branch pipe 4, the jets flow radially into the flow (with no tangential velocity component). As plate 5 approaches the cut of branch pipe 4, the jets flow chordally into the flow. This is due to the fact that the high-pressure flow hits baffle plate 5 and deviates from the radial direction, thus acquiring a tangential velocity component. The disadvantage of this design is the need for an automated plate position controller.

Figure 3b shows a tubular mixer. It includes a tubular body 3 having free cap flanges 2 on welded rings 1 at its ends. Inside the tubular body, mixing elements 4 designed for optimum mixing are located. The principle of operation of this mixer is that when a multi-component flow moves through a pipeline the flow is split by mixing elements into two parts which swap places. Each mixing element doubles the number of flow “layers”, which number reaches 2n after n mixing elements. By “splitting” the main flow the mixing efficiency is improved. The disadvantage of this type of mixer is high hydraulic losses.

Figure 3c schematically depicts a jet gas mixer[10]. It includes a body with inlet 1 and outlet branch pipes, nozzles 2 are arranged in rows and directed at an angle to the mixer axis connecting an annular manifold to the main pipe and an admixture supply branch pipe to the main flow. The main component flow, such as air-helium mix, is fed into the body through the inlet port and another admixture component, such as air or helium, is fed through a port on the annular manifold and nozzles to control the concentration of the mixt. Since all nozzles in adjacent rows have different directions and their projections on the plane perpendicular to the mixer axis are shifted relative to each other, all jets from these nozzles are exposed to the relatively unperturbed onrushing flow of the main component, i.e., they all intensively turbulize it.

The design shown in **Figure 3c** was chosen as a prototype for the development of a CO_2/O_2 gas mixing chamber due to the lack of moving parts and design simplicity. To simplify the modeling process, the perforated cone was removed to reduce the pressure loss of gas that is channeled through the main pipeline. Another simplification is a less complex design of the nozzles-they are replaced by holes 3 connecting the annular manifold and the mixing chamber. The diameters of the main pipeline and the feed branch pipes were determined from the known media flow rates ($G_{CO_2} = 6.505 kg/s$; $G_{O_2} = 1.428 kg/s$) and the required velocity at the pipeline outlet ($\omega = 20 m/s$). The drawing and 3D model are shown in **Figures 4** and **5**, respectively.

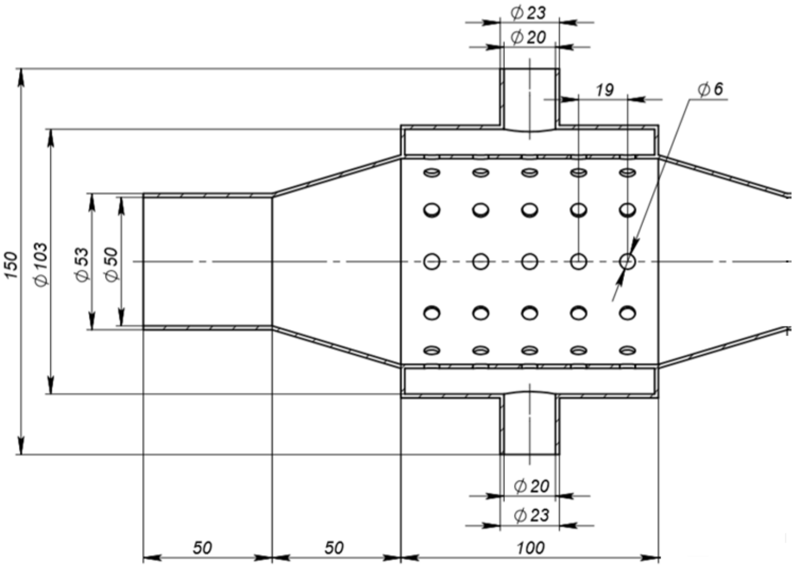


Figure 4. Drawing of the mixer with equalizing grid.

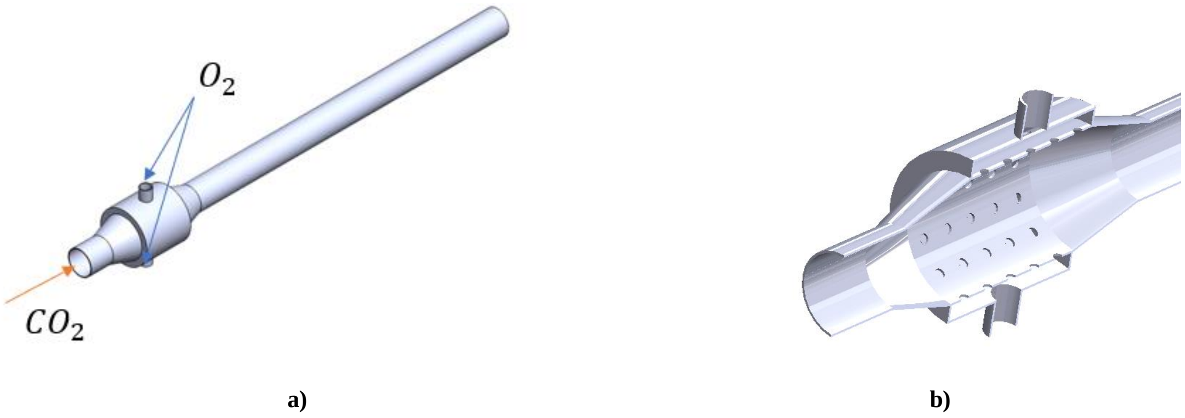


Figure 5. Prototype 3D model: **a)** - model of a mixer with channel in isometry; **b)** - mixing chamber in cross-section.

3. Methodology of mixer numerical modeling

After developing a 3D model of the mixer in the ANSYS software package, numerical modeling of gas flow in the mixer was carried out. The purpose of the modeling is to obtain the mixing results of the gas components and to estimate the hydraulic losses of the gas mixer.

The computational mesh was plotted in the Mesh module with mesh refinement in the equalizing grid area. The mesh parameters are specified in **Table 1**. For the selected turbulence model, the recommended range of values for the dimensionless distance from the first mesh node to the channel wall is $30 \leq y^{+} \leq 300$. The value of $y^{+} = 150$ was taken. The number of mesh elements was more than 3 million. The section of the computational mesh of the mixer flow section is shown in **Figure 6**.

Table 1. Mesh parameters.

Parameters	Values
Minimum element size	0.5 mm
Maximum element size	2 mm
Number of elements	3,076,474

The calculation was carried out in the ANSYS Fluid Flow (Fluent) software. The Reynolds averaging method of the Navier-Stokes equation system (RANS), a k-ε Realizable turbulence model was chosen as the modeling method.

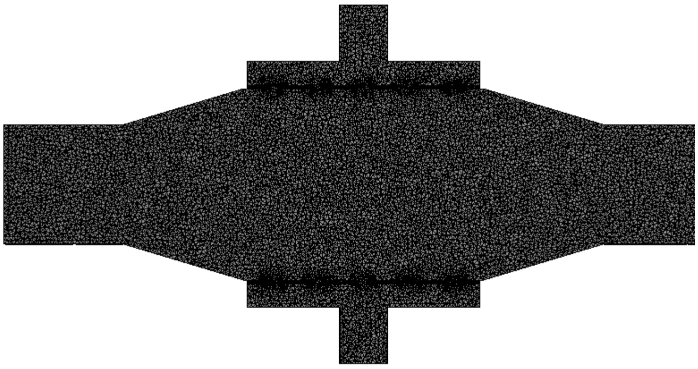


Figure 6. Section of the computational mesh of the mixer flow part.

The mass flow rates of the components at the inlets ($G_{CO_2} = 6.505 kg/s$;$G_{O_2} = 1.428 kg/s$) into the corresponding branch pipes, the inlet temperatures of the components ($T_{CO_2} = 939K$;$T_{O_2} = 503K$) and the outlet pressure ($P_{out} = 30MPa$) were set as boundary conditions. The specified boundary conditions are shown in **Figure 7**.

Figure 8 shows the velocity distribution profile in the longitudinal section of the channel, and **Figures 9a** and **9b** show the profile of component concentration distribution in the longitudinal section of the channel.

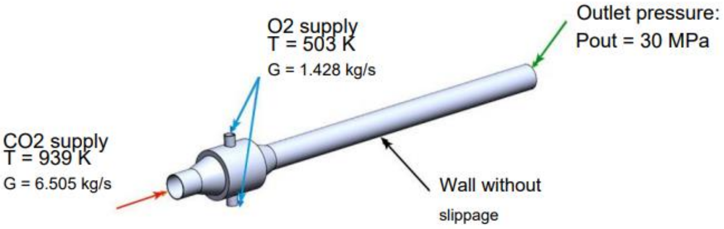


Figure 7. Calculation boundary conditions for CO_2 and O_2 mixer modeling.

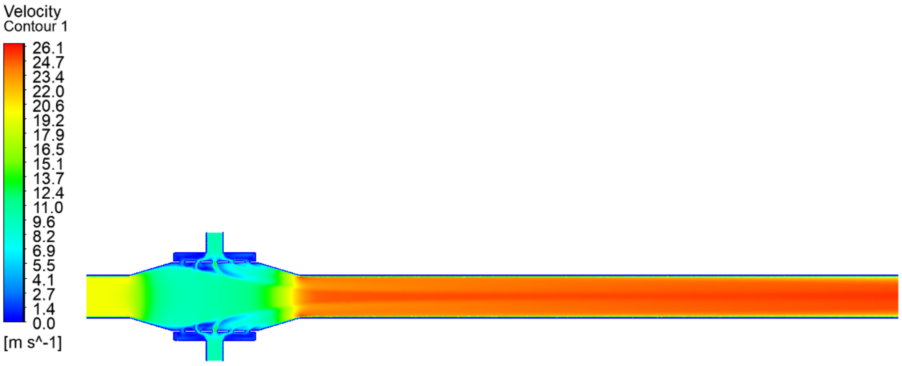
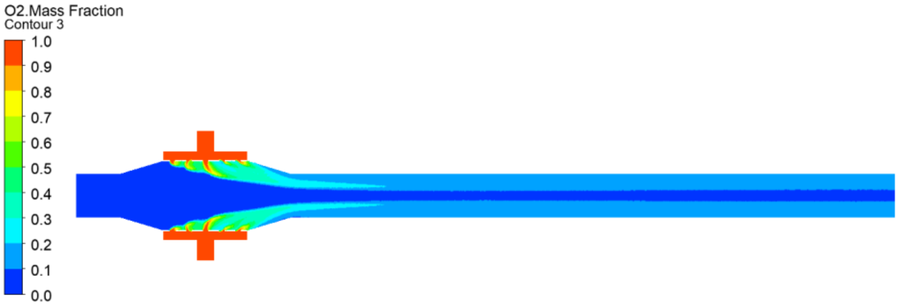


Figure 8. Velocity distribution profile in the cross section.

These profiles show that in this embodiment of the mixer the CO_2 stream forms the core of the flow while O_2 fed through the annular manifold is not mixed with the main carbon dioxide flow but is distributed in the near-wall zone. To assess the quality of mixing, a concentration non-uniformity factor is introduced which will be defined as the ratio of the maximum cross-sectional concentration to the average cross-sectional concentration in the pipeline.

The results of the concentration non-uniformity factor calculation are presented in **Table 2**.

a)



b)

Figure 9. Concentration distribution profiles in the longitudinal section: **a)** - distribution profile CO_2; **b)** - distribution profile O_2.

Oxygen concentration profiles in cross-sections along the length of the pipeline are shown in **Figure 10**. These profiles show that the highest oxygen concentration even downstream outlet of the mixing pipeline is observed at the periphery of the pipe in the area of its supply branch pipes. Local hydraulic losses in the mixing chamber were 0.27 MPa.

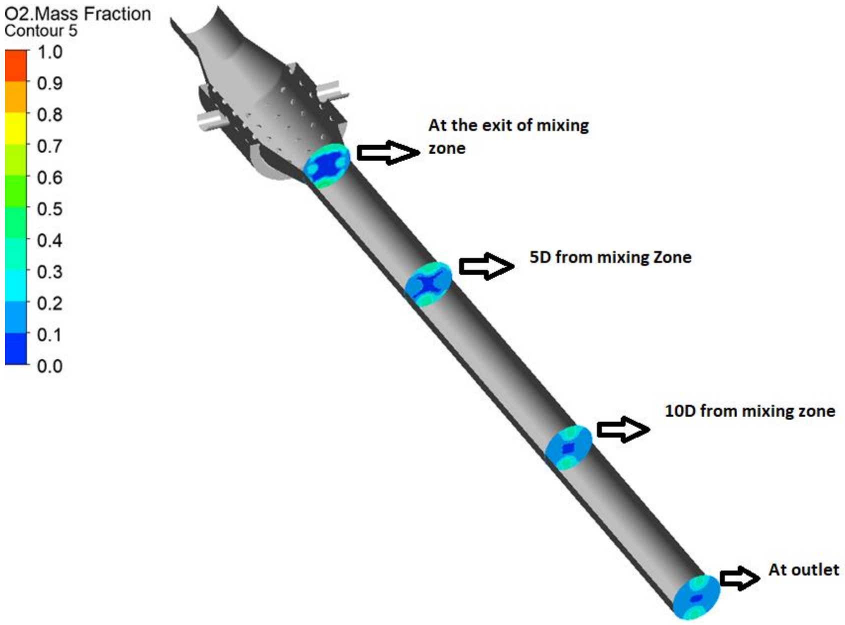


Figure 10. Oxygen concentration profiles in cross-sections along the length of the pipeline.

Table 2. Concentration non-uniformity factor in the mixer with equalizing grid.

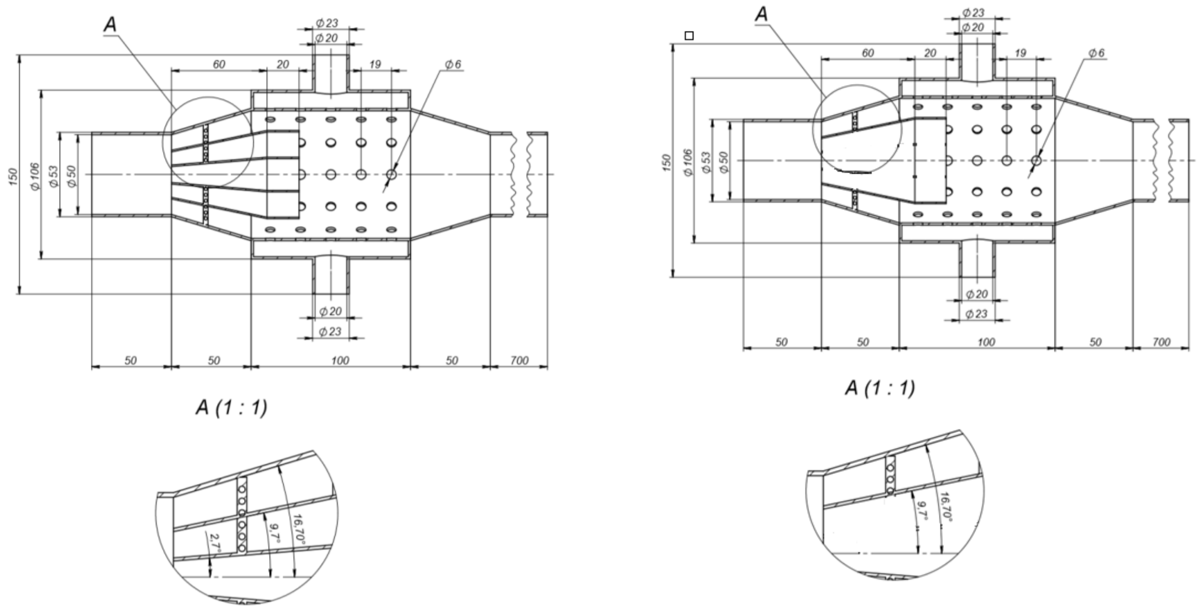
Section	Concentration non-uniformity factor calculation
At mixing chamber outlet	$K_{CO_2}=\frac{1}{0.822004}=1.2165$ $K_{O_2}=\frac{0.460394}{0.177996}=2.586$
At 14D from the outlet of the mixing chamber	$K_{CO_2}=\frac{0.820031}{0.818339}=1.0020$ $K_{O_2}=\frac{0.179969}{0.181661}=0.9906$

4. Development of solutions to reduce pressure losses through a gas mixer

A hypothesis was made that reducing the flow rate in the mixing chamber and directing the flow of CO_2 toward the oxygen outflow ports would allow the components to mix better within the chamber. It was decided to reduce the flow rate of carbon dioxide by installing coaxial diffuser channels (baffle plates) at the beginning of the mixing chamber. A new mixer design has been developed to reduce hydraulic losses and improve the mixing quality. The peculiarity of the new design is the absence of the equalizing grid as the main hydraulic resistance of the channel and the presence of elongated coaxial diffuser channels at the inlet to the mixing chamber. The drawing and 3D model of the upgraded version are shown in **Figures 11** and **12**, respectively.

Numerical modeling of the flow of CO_2 and O_2 the new mixer design in the ANSYS software was carried out. The numerical modeling parameters were assumed to be the same as those used for modeling the basic mixer design (**Table 2**). The section of the finite element computational mesh is shown in **Figure 13**. The grid parameters were assumed to be the same as in the case of analog mixer modeling.

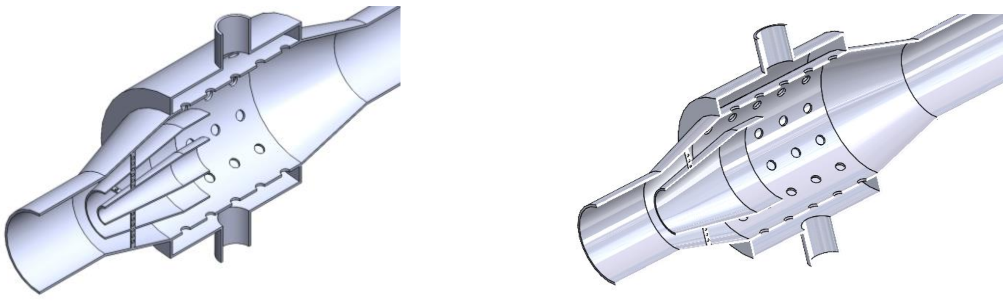
Similar conditions for numerical modeling of the flow in the basic mixer were adopted (see **Figure 7**). The results of numerical modeling of carbon dioxide and oxygen flow in the redesigned mixer are shown in **Figures 14** and **15**.



a) With two diffusers.

b) With one diffuser.

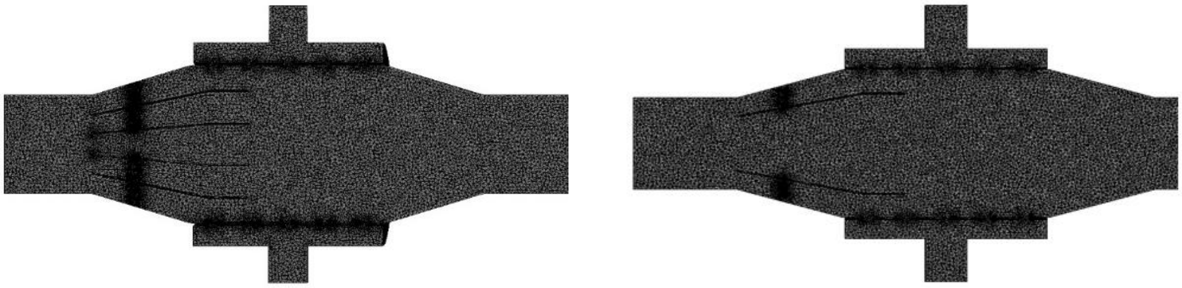
Figure 11. Drawing of the upgraded mixing chamber.



a) With two diffusers.

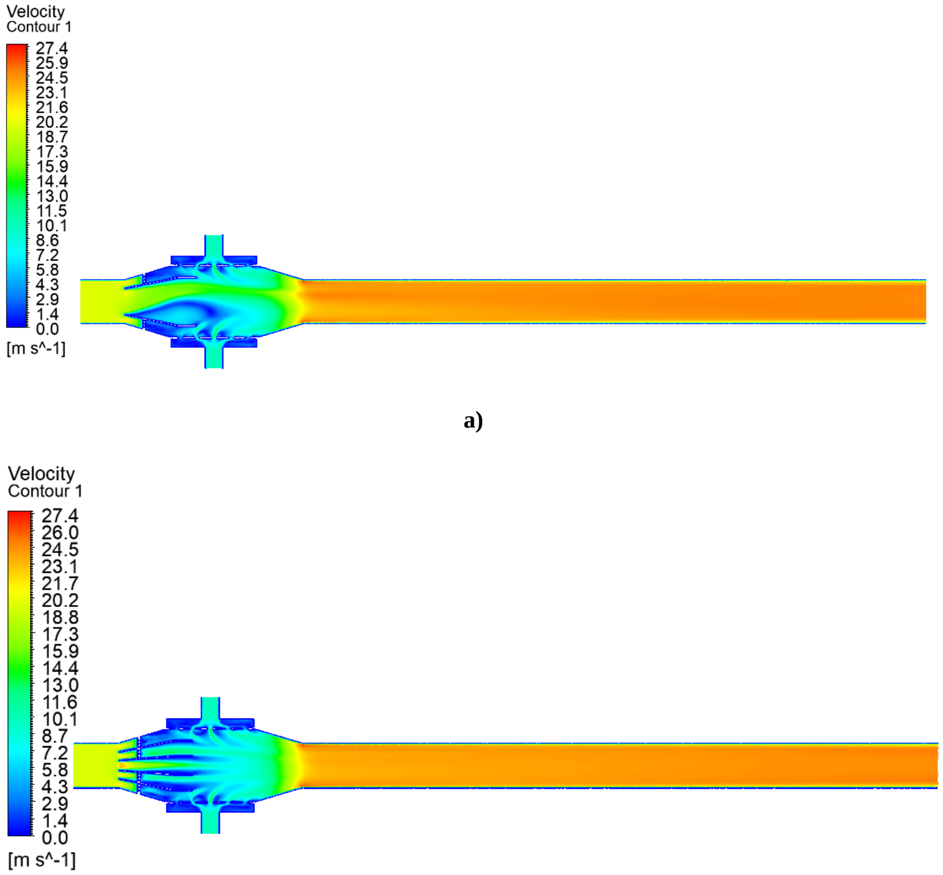
b) With one diffuser.

Figure 12. Section of the 3D-model of upgraded mixer.



a) With two diffusers. **b)** With one diffuser.

Figure 13. Section of the mesh model of upgraded mixer.



a)

b)

Figure 3. Velocity distribution profile in the cross section of upgraded mixer **a)** one diffuser **b)** 2 diffusers.

(With one diffuser)

(With two diffusers)

a)

(With one diffuser)

(With two diffusers)

b)

Figure 15. Concentration distribution profiles in the longitudinal section of the redesigned mixer: **a)** Distribution profile CO_2; **b)** Distribution profile O_2.

These profiles show that in the upgraded version of the mixer, the flow is slowed down by CO_2 diffuser channels and directed to the oxygen outflow orifices. In this case, the main flow will stop "pushing" oxygen to the periphery, and the process of mixing the two components in the mixing chamber will begin. This can be observed in the flow lines presented in **Table 3**.

Figures 16 and **17** show the profiles of oxygen concentration distribution in cross sections of the mixing chamber and along the length of the pipeline. It can be seen that in the upgraded version already there is a uniform distribution of oxygen concentrations along the pipeline cross-section, which is not true for the design with equalizing grid, in it the non-uniform distribution of oxygen concentration is preserved along the entire length.

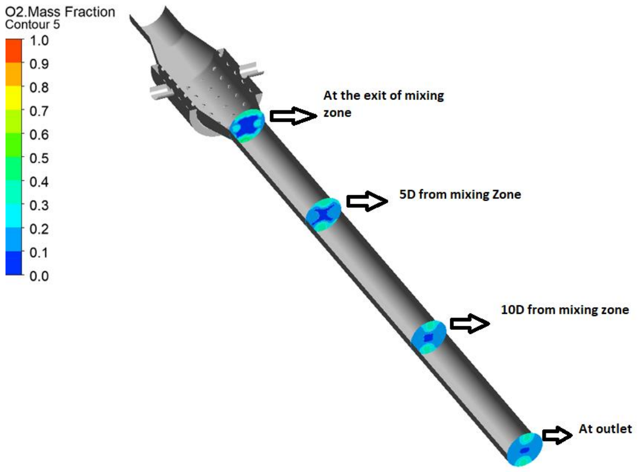
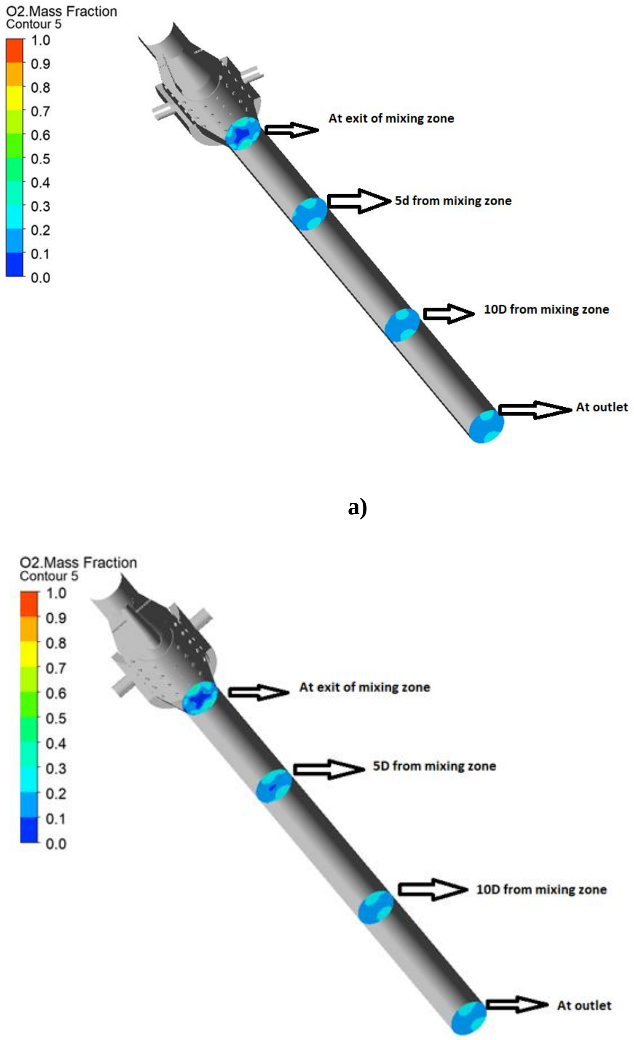


Figure 16. Oxygen concentration profiles in cross-sections along the length of the pipeline with equalizing grid.

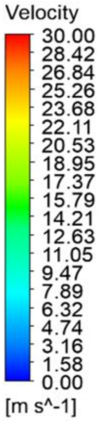
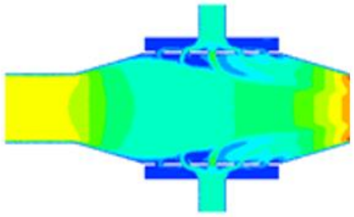
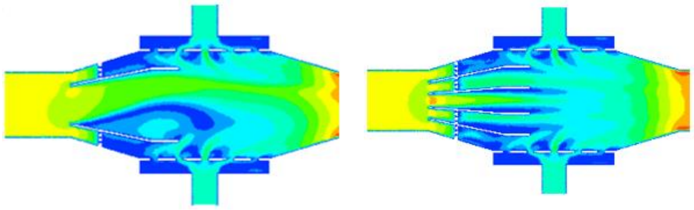


a)

b)

Figure 17. Oxygen concentration profiles in cross-sections along the length of the pipeline: **a)** with one diffuser; **b)** with two diffusers.

Table 3. Flow lines in the longitudinal section of the mixing chamber.

Design	Legend	Flow lines
Mixer with equalizing grid		
Mixer with 1 and 2 deflectors		

The calculation of the concentration non-uniformity factor which quantifies a more uniform mixing, is summarized in **Table 4**. The calculation results show that already at the outlet of the mixing chamber in the both new mixer the values of the concentration non-uniformity factor for both components reach lower values than at the outlet of the mixing chamber of the prototype.

Table 4. Concentration non-uniformity factor in the redesigned mixer with deflectors plates.

Section	Concentration non-uniformity factor calculation for one diffuser	Concentration non-uniformity factor calculation with two diffusers
At mixing chamber outlet	$K_{CO_2} = \frac{0.966905}{0.821757} = 1.176$ $K_{O_2} = \frac{0.395743}{0.178243} = 2.22$	$K_{CO_2} = \frac{0.989452}{0.822949} = 1.202$ $K_{O_2} = \frac{0.394834}{0.177051} = 2.23$
At the distance of 14D main pipeline diameters from the outlet of the mixing chamber.	$K_{CO_2} = \frac{0.862042}{0.819375} = 1.052$ $K_{O_2} = \frac{0.249841}{0.180625} = 1.383$	$K_{CO_2} = \frac{0.822949}{0.819629} = 1.004$ $K_{O_2} = \frac{0.254831}{0.180371} = 1.412$

5. Conclusions

Three simplifies design of gas mixers is been numerically simulated using Ansys fluent. These three designs of gas mixers are following: without any diffusors, with one diffusor and with two diffusors. During simulation following results are observed,

- Gas mixer device having no diffusors has a minimum pressure loss of 0.27. However, the concertation ratio of O_2 at outlet is also minimum 0.99.
- Gas mixer device with one diffusor has a maximum pressure loss of 0.48. Concentration of O_2 is 1.38 which is comparatively better than previous design.

- Gas mixer with two diffusors has a nominal pressure loss of 0.45. However, concentration of O_2 at outlet is 1.41 which is the most among all previous design of gas mixer.

Therefore, after careful consideration and analyzing results, it is found that gas mixer with 2 diffusor is more efficient and effective in O_2/CO_2 mixing.

Author Contributions:

Conceptualization, SO and IK; methodology, SO; software, MMS; validation, MMS, PG; formal analysis, SO; investigation, MMS, MO; resources, SO; IK, writing—original draft preparation, MMS; writing—review and editing, SO; visualization, PG; supervision, IK; project administration, SO; funding acquisition, SO. All authors have read and agreed to the published version of the manuscript.

Acknowledgments

This study conducted by National Research University "Moscow Power Engineering Institute" was supported by the Russian Science Foundation under Agreement No. 23-79-10291, https://rscf.ru/project/23-79-10291/.

Conflict of interest

The authors declare that they have no conflict of interest.

References

1. E. M. Lisin, V. O. Kindra Technical and economic aspects of forming the market for environmentally friendly power generation based on the use of oxyfuel technologies // New in the Russian electric power industry. - 2020. - No. 9.-P. 31-44.
2. Krieger, G. C., Campos, A. P. V., Takehara, M. D. B., Da Cunha, F. A., & Veras, C. G. (2015). Numerical simulation of oxy-fuel combustion for gas turbine applications. Applied Thermal Engineering, 78, 471-481.
3. Allam R. et al. Demonstration of the Allam Cycle: an update on the development status of a high efficiency supercritical carbon dioxide power process employing full carbon capture //Energy Procedia.-2017.-T. 114.-C. 5948-5966.
4. Rogalev, A., Rogalev, N., Kindra, V., Komarov, I., & Zlyvko, O. (2021). Research and Development of the Oxy-Fuel Combustion Power Cycles with CO_2 Recirculation. Energies, 14(10), 2927.
5. Kindra, V., Rogalev, A., Lisin, E., Osipov, S., & Zlyvko, O. (2021). Techno-economic analysis of the oxy-fuel combustion power cycles with near-zero emissions. Energies, 14(17), 5358.
6. I.I. Komarov, A.N Rogalev, D.M. Kharlamova, P.N. Nesterov, V.P. Sokolov Development and study of high-pressure oxygen-fuel combustion chamber // Bulleting of Moscow Aviation Institute. - 2022. - T.29. - No. 4. – P. 196-207.
7. Osipov S. K. T.P. Karev, A.I. Gubanova, P.V. Golosova, M.V. Oparin Investigation of the process of mixing of combustible mixture components in vortex burner devices // New in the Russian electric power industry. - 2023. - No. 9. – P. 39-51.
8. Pat. SU 1 693 320 A1. Two flow mixer/ V.A. Galitskaya, V.P. Stelmakov, R.A. Zakirov, Yu.Ya. Gelitskiy 1991.
9. Static mixers "IKhL SS" [Electronic resource] //Engineering and Chemical Laboratory. URL: https://labudgup.ru/ss.html. (Access date 19.10.2023).
10. Pat. SU 633574 A1. Gas mixer/ R.V. Bizyaev, A.I. Dukhov, O.M. Lvovskiy, V.L. Ronin,A.I. Usmanov, A.Ya. Cherniakhovskiy 1978.