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DEVELOPMENT OF A DIGITAL TWIN FOR GAS MIXING IN A GENERATOR

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The subject of this research is the development of a digital twin for the process of mixing the components of a gas mixture in the mixer of a mixture generator. The problem is motivated by the concept of digitalizing modern production and is considered in relation to the technology in question for generating a gas mixture of a given composition and homogeneity. A gas-dynamic model of an unsteady flow has been constructed and a numerical study carried out using the Ansys Fluent software. The Reduced Order Model was developed and used in the Ansys Twin Builder platform to build the digital twin.

Keywords: digital twin, reduced order model, numerical simulation, gas mixer

1. Introduction

The incentive for developing digital twins (DT) in the process of generating gas mixtures is the digitalization of modern technologies. A DT is a virtual copy of a real system characterized by continuous and automatic synchronization as well as feedback between the real and digital domains.

Many authors have diversified the typical development process of DTs [1]-[8]. All of the aforementioned referenced studies added their own values to define their DT. In almost all of these works, given the large number and variety of systems for which DTs can be created, the authors paid special attention to structuring the process of creating a DT. Therefore, the authors of [1] presented a five-dimensional model of a DT in which all stages for creating, implementing and monitoring the operation of equipment as well as recording data are accounted for. A more simplified scheme for creating a DT is provided by the authors of [2]-[4] in which the importance of individual aspects of the DT are emphasized. In [2], the authors insist on the importance of the digital component in the creation and implementation of a DT, which depends on the speed of process control and data exchange between elements of the system. In [3], the importance of communication as well as information exchange between a DT and a real system, in addition to monitoring the operation of a system in real time, is considered. A more unusual concept was proposed in [4], in which the evolution of the state of the object when creating a DT is considered. Furthermore, the peculiarities and relevance of creating duplicates of multiphysics models, which should process large arrays of heterogeneous data, are addressed in [4]. Currently, many studies provide a comprehensive theoretical justification for the concept of creating a DT as well as the importance of the stages necessary to create and implement a DT of a real system or process amongst other research objectives. Such works are analysed in a review article [5], moreover, a group of practically oriented studies [6]-[9] is provided. In [6], the authors proved the importance of creating a DT when designing a large complex system. They came to the conclusion that a preliminary analysis of the system in a digital format will help to avoid many expensive problems when constructing and adjusting real equipment. In light of this, a new wind turbine controller was created in [7] in which the Functional Mock-up Interface (FMI) was used to combine the CFX and Maxwell 3D models as well as the capabilities of the Ansys Twin Builder platform applied to create a DT. Lastly, an exemplary example of combining a real braking device with its DT into one system is given in which data exchange took place in real time [8]. Within the framework of this work, a DT to form a fuel mixture in the system in which it is generated is developed, which should automatically provide the required composition of components in the mixture and the degree of its homogeneity.

2. Problem statement

International standards [9]-[12] have been developed on the basis of state-of-the-art research into the digitalization of production, which regulate the construction of automation systems, integration of technical processes or operation of industrial equipment using digital technologies. These standards define two types of twins, namely digital and physical ones.

A DT consists of three parts:

1. A data collection and device management facility in which signatures are also combined. The collected data is pre-processed by the data collection facility.
2. The core, which is responsible for its general operation and management as well as consists of computing environments.
3. The user object, with the help of which various human-system interactions take place, can be provided both in the cloud and in the local network.

A physical twin consists of an experimental setup, sensors that facilitate data collection and a device control system to regulate executive functions. In the case of extremely complex non-stationary workflows or when it is not possible to install sensors, numerical modelling can provide an alternative source of data acquisition.

To ensure the specific heat consumption remains stable during cyclic thermal processing, simultaneous control of the mass of the fuel mixture and the pressure applied on the charge in the combustion chamber is necessary to form the mixture, fill the chamber and make subsequent corrections. In accordance with the specified requirements, a system for forming the fuel mixture in the thermal pulsation system was developed, which is described in detail in [13].

The object of this study is to develop a mixer for mixing gaseous components, which is part of the fuel generator of an automated thermal pulse processing unit, described in detail in [14]. Mixing is frequently one of the most important processes in various industries. All starting materials and products, for example, in the chemical industry, must be homogeneous. In a paper where mixing in reservoirs was studied, a relationship was established between the flow structure in a tank and its geometry [15]. The aforementioned study considered a DT of the process of mixture formation in a mixing chamber by determining the composition of components and degree of homogeneity of the gas mixture obtained.

The physical twin of our research objective is a two-component mixer (*Figure 1*), which partly consists of a steel body (1), lid (2) and technological plugs (corks) (3). The components of the gas mixture enter through special jets (nozzles) (4) which are further mixed by counter currents in the chamber (5). Differences in the cross-sectional areas of the through hole in the jets through which the fuel and oxidizer enter control the stoichiometric ratio of the components of the mixture being a supercritical flow at a constant pressure [16].

An aPriori physical twin consists of an experimental setup, components that collect data (sensors) and a device
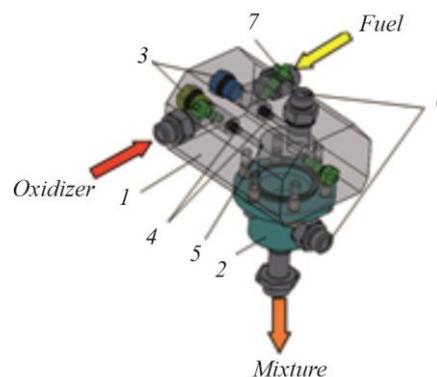

Figure 1. Mixer model
1 – body; 2 – lid; 3 – corks; 4 – nozzles;
5 – chamber; 6 – fittings; 7 – sensors

control system (executive function). The latest approach to the creation of DTs suggests the possibility of representing a physical twin by mathematically modelling it, which is necessary due to the complexity and sometimes even the impossibility of installing sensors as well as measuring the control parameters of processes in real time. For example, this applies to hermetic objects of a small or limited volume and fast-acting processes that occur in them. The mixer in question required to mix the components of a gas mixture also falls into this category, that is, where the control parameters are the total mass of the components and the degree of homogeneity of the mixture. By studying the simulation of this process, special and extremely expensive equipment is not required to experimentally determine these parameters in the mixer.
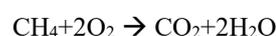
3. Modelling of gas mixing in a mixer

The calculation area is the internal cavity of the gas mixer (*Figure 2a*). The calculation grid (*Figure 2b*), consisting of 152042 polyhedral elements, was built in the Ansys Fluent Meshing module to make further calculations in the Ansys Fluent system [17]. In order to model the wall flow of gases accurately, 5 prismatic layers with a growth factor of elements equal to 1.2 were built.

To solve the defining equations of the model, the Finite Volume Method (FVM) was used, according to which the values of physical variables were calculated only at the center of the elements, while the mass flows, momentum and energy were calculated at the edges of these elements.

3.1. Boundary and initial conditions

Mixing of the methane-oxygen mixture in the expected stoichiometric ratio according to the reaction

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

was investigated. The directions of the supersonic flow of the gaseous components were normal at the inlets. The calculations were made while the system was stationary. At the tip of the jet, the speed of the gas flow was equal to the speed of sound. The computational model consisted of two domains with a common interface. While a force was applied, the average molar concentrations of oxygen and methane at the outlet of the mixer were monitored.

The pressures of methane and oxygen gas at the inlet to the mixer were set at 4.340 and 4.104 atm, respectively. The initial temperature of both gases at the inlets was 20 °C.

A single-phase multicomponent flow model was used to describe the mixing. The equations used to calculate the composition of the mixture were as follows [18]:

$$\frac{\partial \rho}{\partial t} + div(\rho \vec{u}) = 0 \qquad (1)$$

$$\rho \frac{d\vec{u}}{dt} = divP + \vec{f} \qquad (2)$$

$$\rho \frac{de}{dt} = div(\lambda gradT) + P \cdot grad\vec{u} \qquad (3)$$

where ρ denotes the density of the mixture; $\vec{u}$ represents the velocity vector; P stands for the stress tensor; T refers to the gas temperature; λ is the thermal conductivity coefficient of the gas; and e denotes the internal energy of the gas.

To ensure that the fuel mixture is stratified from components of different densities, the effect of volume forces, namely gravity, was taken into account $(\vec{f})$. When calculating the density and gas constant of the mixture, standard mixing rules were used:

$$\frac{1}{\rho} = \sum_{i=1}^{N} \frac{c_i}{\rho_i}, \quad R = \sum_{i=1}^{N} c_i R \qquad (4)$$

where (ρ_i) denotes the density of the components i of the mixture; R is the universal gas constant, c_i, represents the molar concentration of the components i.

To determine the degree of homogeneity of the mixture (ϑ), the following expression was used:

$$\vartheta = \frac{\sigma C_f}{[C_f]} \qquad (5)$$

where $[C_f]$ denotes a given value of the molar concentration of the fuel, which corresponds to the stoichiometric ratio and σC_f stands for the best estimate of the root-mean-square deviation of the molar concentration of the fuel as defined as:
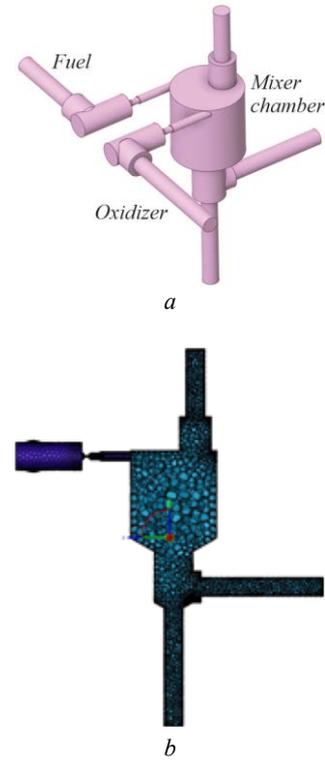

a

b

Figure 2. Cross-section of the calculated model of the mixer (a) and finite element grid (b)

$$\sigma C_f = \sqrt{\frac{\int_s (C_f - MC_f)^2 \, ds}{S_{outlet}}} \qquad (6)$$

where S_{outlet} denotes an area of an outlet from the mixer; C_f stands for the molar concentration of the fuel, MC_f denotes the following mathematical expression of the molar concentration of the fuel:

$$MC_f = \frac{\int_s C_f \, ds}{S_{outlet}} \qquad (7)$$

The mixture was considered to meet the requirements in accordance with the conditions below:

$$[C_f] - \delta \cdot [C_f] \leq MC_f - \sigma C_f \cup \qquad (8)$$
$$\cup \; MC_f + \sigma C_f \leq [C_f] + \delta \cdot [C_f]$$

where δ denotes the given permissible deviation in the mass concentration of the fuel.

An automatic time step was used for the calculation. The pressure-velocity coupling scheme was selected as the Pressure-Implicit with Splitting of Operator (PISO). For the discretization of parameters, Second Order Upwind Scheme was used.

3.2. The obtained results

The velocity fields of gas flows, the mass flow of the components of the gas mixture through the mixer as well as the pressure and temperature fields were obtained by applying Computational Fluid Dynamics (CFD) modelling. The temperature and pressure distribution across the cross-section of the mixer and in the nozzles is presented in *Figures 3 and 4*.

After travelling through the jet, a significant local decrease in temperature and pressure was observed due to the acceleration of the gas flow and the supercritical flow regime (*Figure 5*).

Undoubtedly, such heterogeneous flow conditions affect how accurately the components of the fuel mixture are dosed and must be taken into account when performing calculations. The distribution of the molar concentration of methane across the cross-sections of the mixer and at its outlet is shown in *Figure 6*.

CFD simulation results show that the mixer ensured that the fuel mixture was highly homogenous. According to the normalized estimate of the root-mean-square deviation of the molar concentration of methane, the deviation of the methane content from the stoichiometric value did not exceed 3 %.

4. Development of a DT of the mixer connected to the system generating the fuel mixture

The concept of a DT using Ansys Twin Builder numerical modelling technologies was proposed by ANSYS, Inc. [19]. The results of simulations using DTs can be calibrated based on the operating parameters of the physical process. The direct connection between the finite element method in its usual sense and the control scheme slows down the calculation speed when predicting the output parameters. Therefore, when developing a DT, Reduced Order Models (ROM) were used. Creating a ROM is possible by studying the physics of the process and extracting its global behaviour from the offline simulation. This can be obtained directly on the basis of the preliminary results from finite-element modelling by only taking into account the main features of the system and process. Since the calculation of the result in a separate object subjected to digital Reduced Order Modelling requires only simple algebraic operations, e.g. the addition of vectors and evaluation of response surfaces, the calculation process only requires technical resources for a short period of time and the result can be obtained in almost real time.
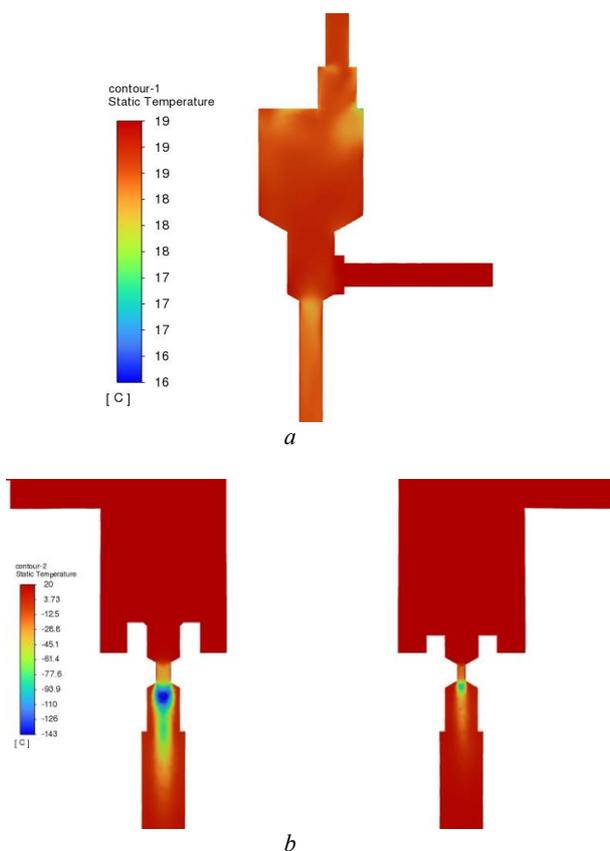

Figure 3. Temperature fields in the central section (a) of the mixer and its nozzles (b)
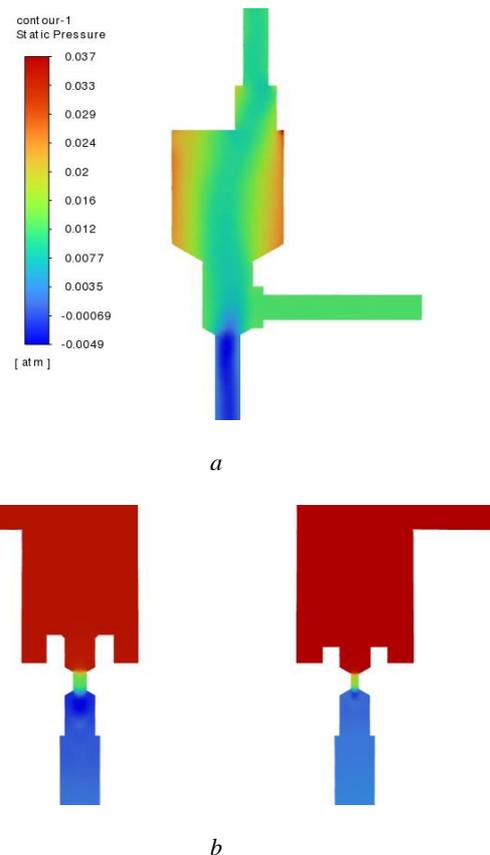

Figure 4. Pressure fields in the central section of the mixer (a) and its nozzles (b)
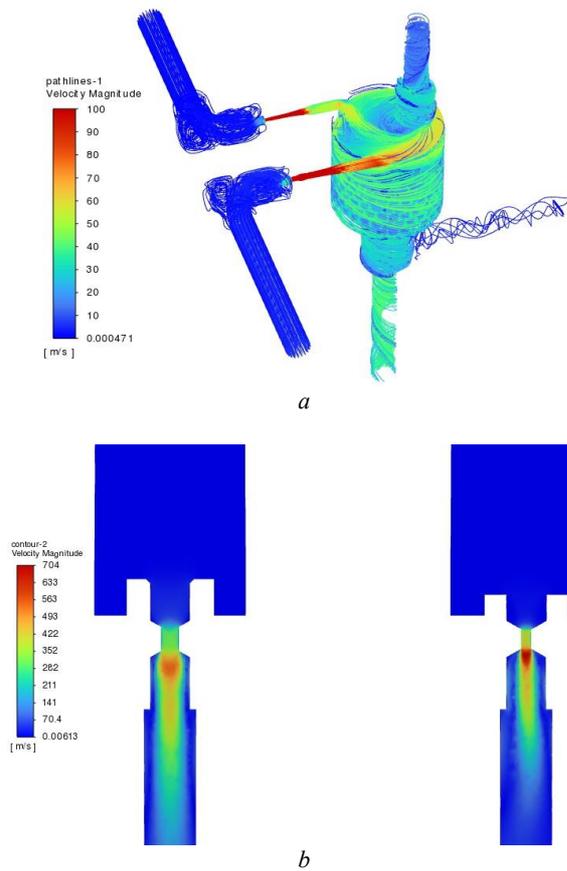
a

b

Figure 5. Velocity field throughout the volume of the mixer (a) and in the jets (b)

a

b

Figure 6. Molar concentration of the fuel injected into the mixing chamber (a) and at the outlet from the mixer (b)

With parametric ROM, the model can be evaluated and variations in the results quickly investigated depending on the values of the input parameters, thereby emphasizing the importance of suitable ROMs when simulating the operation of a complex multifunctional system.

Of course, the results of a DT will be as reliable as the input data used to describe the object or process being modelled as comprehensively as possible. Typically, an enormous number of data points were recorded from the full-scale model. Several of the most likely characteristic modes were selected from the set of all the generated data, from which a simplified numerical calculation was subsequently made. Therefore, it is possible to thoroughly understand how the equipment is operated in different modes. To implement this approach in Ansys Twin Builder, a special hierarchy of input data was drawn up. Having such a hierarchy of data files is undoubtedly advantageous because from this it is possible to immediately match the data coming from analog sensors with a DT, that is, a calculation program.

The DT of the mixer in the current study was created using the Ansys Fluent and Ansys Twin Builder programs.

In the first stage, a complex model of the gas-dynamic process of mixture formation of different component compositions was carried out in Ansys Fluent in order to determine the parameters that were later transferred to the ROM block of the model necessary for
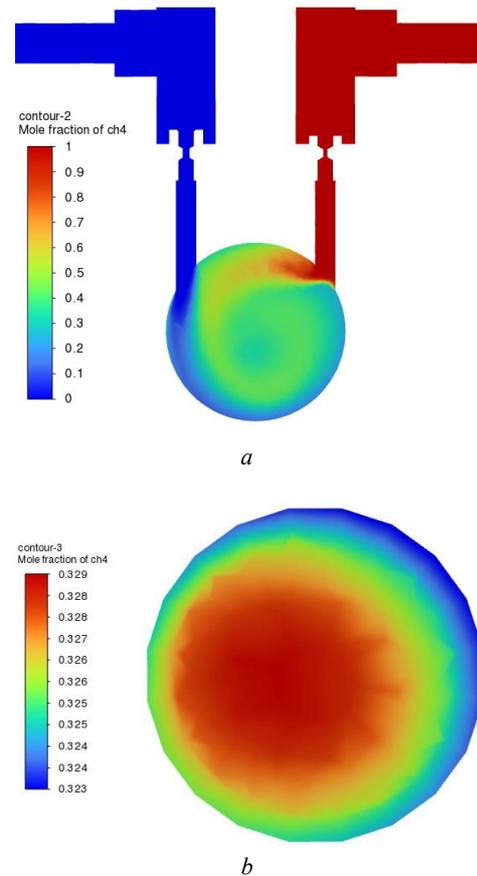
creating a DT in Ansys Twin Builder. The ROM of the model was transferred in Functional Mock-up Unit (FMU) format. A series of calculations was carried out to prepare the personnel unit required for the construction of the DT using the ROM model according to the established range of varied parameters.

To create a digital counterpart to this process, the pressures of the fuel and oxidizer at the inlets were selected as the initial parameters. As control (output) parameters, the molar concentration of the components of the gas mixture and its quality were selected. The parameter describing the quality of the gas mixture showed the non-compliance rate along with the stoichiometric value of the gas component in the following form:

$$\mathrm{sqrt}(\mathrm{areaAve}((\mathrm{areaAve}(\mathrm{CH4IdealGas.MolarFraction})\,@\,\mathrm{Outlet} -$$
$$-\mathrm{CH4IdealGas.MolarFraction})^{\wedge 2}\,@\,\mathrm{Outlet})\,/$$
$$/(\mathrm{areaAve}(\mathrm{CH4IdealGas.MolarFraction})\,@\,\mathrm{Outlet}).$$

According to the algorithm of the parametric calculation, the number of variations (the design points that were used to build the so-called learning points or snapshots of the ROM) required was determined. In the case under consideration, 16 of them were found. The scatter plot of variations in the initial data lies within 10 % of the deviations and is determined randomly. Therefore, in the framework of solving a parametric problem, after a series of gas-dynamic calculations on the
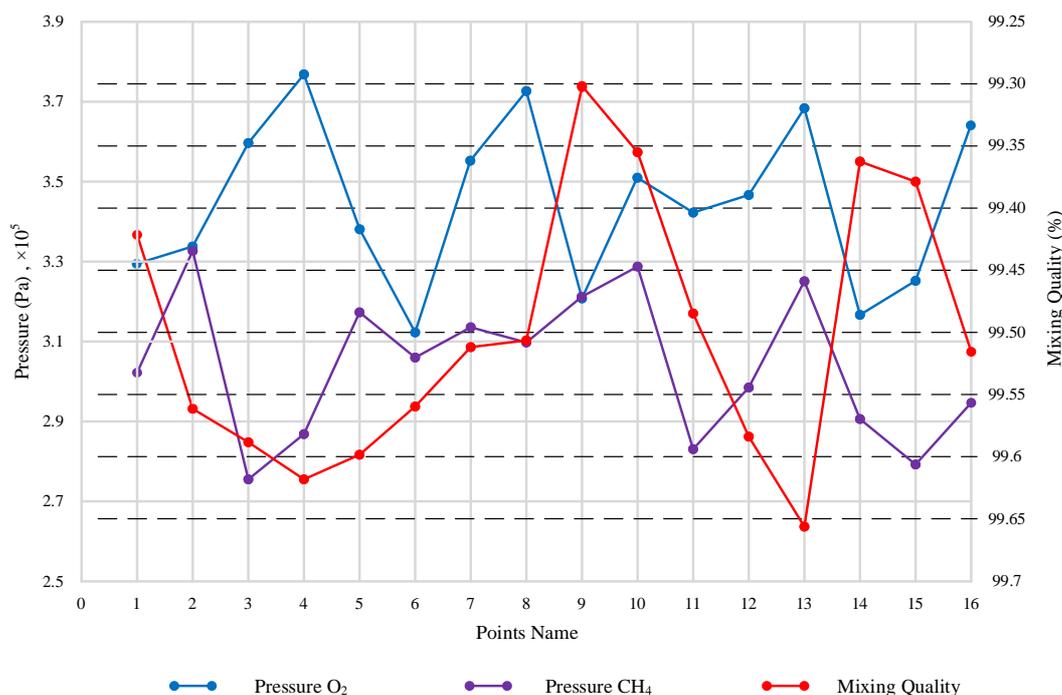
Figure 7. Design points vs. parameters

full Fluent model of the mixing process were made, basic data were obtained for the ROM of the DT (*Figure 7*), which clearly show the variations in the values of the inlet pressure parameters of the components of the mixture and the corresponding values at the outlet, that is, the parameter defining the quality of the gas mixtures.

To view the goodness of fit for the output parameters in a ROM, the absolute error (L-Infinity Norm Error) was calculated for each snapshot (*Figure 8*) according to the following expression:

$$Y_i = max_{j=1...N}\left|Y_{i,j} - \overrightarrow{Y_{i,J}}\right| \qquad (9)$$

where Y_i denotes the i-th snapshot; $Y_{i,j}$ refers to the j-th entity of the i-th snapshot; and $\overrightarrow{Y_{i,J}}$ represents the ROM approximation of the j-th entity of the i-th snapshot.

A simplified mixer model can be considered to be a complete DT. Meanwhile, considering the mixer as a separate structural component of some hydraulic system, the resulting FMU model of the mixer will act as a structural unit of a higher-order circuit, e.g. "cylinder -
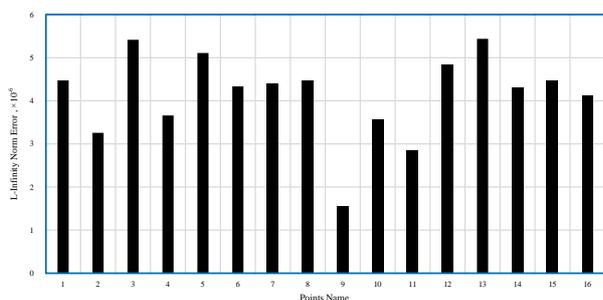

Figure 8. L-Infinity Norm Error for the points taken into account in the construction of the response surface

mixer - working tank". In terms of all these calculations, the resulting model should be loaded into the Ansys Twin Builder platform as a separate component.

When adding a model of an FMU mixer, attention must be paid to the model-carrying input and output parameters created when the ROM was built.

Therefore, when adding a mixer to the scheme of the digital double, all the parameters of the model of interest were noted before it was imported. The initial parameters here were the values of the Fluel_in_Press and Fluel_in_Oxi pressures specified in the Ansys Fluent parametric study at the outlets of the two cylinders of gases that were being mixed. Since the mass content of each component of the mixture at the outlet of the mixer was determined as initial and control parameters, the DT was successfully added to the DT project.

In Ansys Twin Builder, data can be assigned in many ways to describe how the equipment is operated or its individual link. The input parameters for this ROM of the mixer can be loaded from an external medium in tabular format, the data of "frames" - pre-saved measurements from analog devices (sensors) at a certain time interval - used or a continuous streaming of data recorded from when the equipment was used with the help of additional macros. When using this mixer as part of a DT of a higher order, the input parameters for the mixer were determined by the output parameters of the previously stationary element, e.g. the gas pressure at the outlet of each of the cylinders. In this work, given that the mixer itself was calibrated and verified, it is sufficient to use the standard "2D Lookup Table" scheme to determine the pressure of the two oxidizers at each inlet of the mixer. With the help of "2D Lookup Table" schemes, since the pressures at the inlets to the mixer are represented as tabular functions over time, it is important
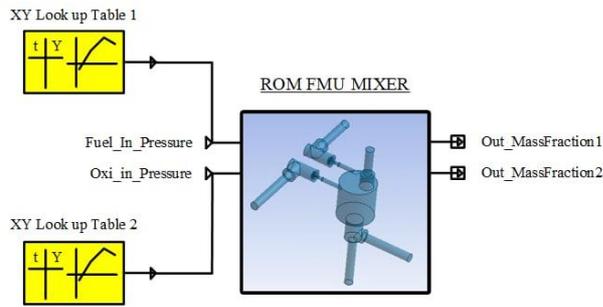
Figure 9. The scheme of the DT of the mixer

to match the time ranges of the input parameters with the time settings of the entire solution defined for the project (*Figure 9*).

The calculation is performed by applying standard solver settings using the Adaptive Step Trapezoid Rule method to integrate time. Temporary settings cover all the calculation frames.

After preparing and adjusting the model of the DT of the two-component mixer, a calculation was made, the result of which was presented in the form of two-dimensional dependence graphs (*Figure 10*) showing changes in the mass fractions of the components of the mixture against the number of snapshots (time). The horizontal axis indicates the number of the calculated snapshot and the vertical axis indicates the mass fraction of the component of the gas mixture.

Given that the mass fraction of the components of the gas mixture controlled at each calculation point was one, the law of conservation of mass was not violated. The graphs obtained from the built DT with regard to the process of generating the fuel mixture provide visual representations of the percent composition of the mass

fractions of each gas mixture depending on the pressure at the outlet of each cylinder. Furthermore, how the composition of the mixture changes when the pressure of each component of the fuel mixture at the inlet to the mixer deviated from its optimal value was determined.

5. Conclusion

The construction of a DT of the system generating the fuel mixture based on the results of a numerical simulation was considered. A combined approach was used to build a DT. An element of the generation system with a complex flow pattern was modelled by a numerical experiment, the results of which were used to build its ROM. This model was used as the structural unit of the higher-order contour.

The graphs obtained from the built DT of the process used to generate the fuel mixture provide a visual representation of the percent composition of mass fractions of each gas mixture depending on the pressure at the outlet of the cylinders. Furthermore, how the composition of the mixture changed when the pressure of each component of the fuel mixture at the inlet to the mixer deviated from the optimal value could be determined.
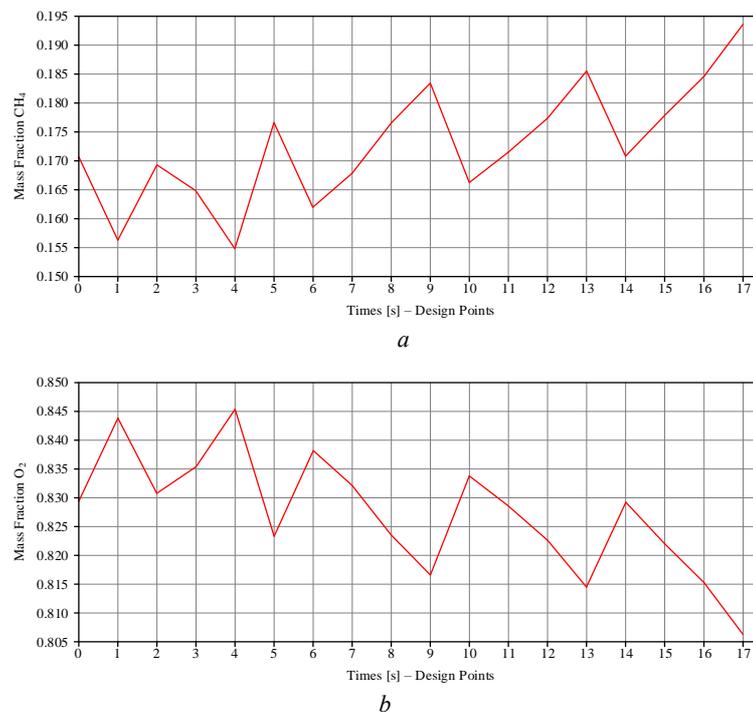
Acknowledgements

a

b

Figure 10. Mass fractions in the form of particles of the components of the gas mixture (a – CH_4; b – O_2)

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