The mathematical model structural-parametric synthesis of working processes in an oxygen-methane steam generator with flow swirl

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Abstract. While formulating a mathematical model of the flow and interaction between oxygen-methane fuel combustion products with tangentially swirled ballast water injected in the end of the combustion chamber in CAE product Fluent, which integrated into the ANSYS Workbench platform, the problem of structural-parametric synthesis is solved for structure optimization of the model. Equations are selected from the catalogue of Fluent physical models. Also optimization helps to find "regime" model parameters that determine the specific implementation of the model inside the synthesized structure. As a result, such solutions which were developed during creation of a numerical algorithm, as the choice of a turbulence model and the state equation, the methods for determining the thermodynamic thermophysical characteristics of combustion products, the choice of the radiation model, the choice of the resistance law for drops, the choice of the expression which allows to evaluate swirling flows lateral force, determination of the turbulent dispersion strength, choice of the mass exchange law, etc. Fields of temperature, pressure, velocity and volume fraction of phases were obtained at different ballast water mass flows. Dependence of wall temperature from mass flow of ballast water is constructed, that allows us to compare results of the experiment and mathematical modeling.

1. Introduction
Usage of standard schemes in the development of compact steam generators leads to a sharp decrease in their efficiency due to recuperative steam regeneration. Unstable condition of two phase flow and detritus of combustion products on heat transfer surfaces are appears and, as a result, burnout of working surfaces occurs. Solution of the problem which helps to improve efficiency of compact steam generators is possible supplying ballast water with tangential swirl directly into the combustion chamber. The scheme of compact steam generator provides combustion and vaporization in one chamber [1]. That allows to combine reduction of mass and dimensions of the unit with temperature regulation of gas at the output. Theoretical and experimental verification of such hypothesis will significantly increase the efficiency of steam generators, expand usage of hydrocarbon fuel - methane and improve reliability and durability of the steam generator, reduced burnout of combustion chamber walls [2].

Main goal of the work is a mathematical modeling methodology development of fluid dynamics and heat and mass transfer processes for a multiphase model in condition of phase transfer in compact oxygen-methane steam generators. This process conduct with interaction of a liquid film with high-
temperature flow of combustion products, in addition taking into account multicomponent nature of gas.

2. Geometry of the computational domain and boundary conditions
Sketch and photograph of steam generator experimental model are shown at Figures 1 and 2.

![Figure 1. Sketch of steam generator experimental model: 1 – mixing head, 2 – combustion chamber with flow swirl, 3 – evaporation chamber, 4 – nozzle, 5 – flange](image1)

![Figure 2. Experimental model: 1 – combustion chamber with flow swirl; 2 – mixing head; 3 – nozzle; 4 – electric-discharge spark](image2)

Computational experiment implementation requires the following boundary conditions set:
- the first phase - steam (CO₂ + water vapor), the second phase - water with droplet diameter at the inlet of 0.0015 m;
- tangential inflow. Water mass flow rate is 6-20 g/s with 290 K temperature;
- steam inflow. Steam mass flow rate is 10 g/s with ~ 3400 K temperature, the volume fraction is 1;
- outflow. The reference pressure is 2.57 MPa.

3. Structural-parametric synthesis of the mathematical model in the ANSYS Fluent
To perform mathematical modeling of work processes (heat and mass transfer and fluid dynamics) in a oxygen-methane steam generator under given conditions, it is necessary to develop a 3D adjoint mathematical model which describes processes of fluid dynamics and heat and mass transfer between moving liquid film and a high-speed steam flow under phase transition conditions [3, 4].

Generation of a mathematical model for description of multiphase turbulent flow in the ANSYS Fluent environment is a complex problem without precise guidelines (at the current level of CFD methods) for modeling of multidisciplinary adjoint tasks. The list of questions studied during development of a model, even without most important question about constructing a high quality design grid, includes several fundamental solutions of choice an internal physical model and its mathematical formalization. Therefore, process of mathematical model development in ANSYS environment is a task to structural-parametric synthesis, where some parameters are "structural" and can take a particular nominal value from a given set of possible ones. Specific set of these parameters determines a structure of the model and, correspondingly, a set of equations which formed physical models. Another part of parameters is "regime" parameters of a simulation. These parameters determine a specific implementation of a model inside a framework of synthesized structure.

There is no detailed discussion of a computational mesh development technique using manual generation algorithm supported with mandatory automatic control of mesh quality in specified ranges of boundary conditions parameters, because this is an independent problem of another scientific specialty. Formulation of structural-parametric synthesis of the developing CFD model is given further in the article. Results of synthesis are obtained for Eulerian multiphase model.
List of models "structural" parameters with their possible values includes the following variables:

- $c_1$ – gas state equation. This parameter can take the following values: ideal gas, Hall-Yarburg equation, Redlich-Kwong equation (and its modifications: Wilson modification and Soave modification), Peng-Robinson equation. Total number of values 6.

- $c_2$ – definition of isobaric heat capacity. Total number of values 4: constant, piecewise linear interpolation, piecewise-polynomial and kinetic theory formulation.

- $c_3$ – determination of thermal conductivity coefficient. Total number of values 4: constant, piecewise linear interpolation, piecewise-polynomial and kinetic theory formulation.

- $c_4$ – determination of viscosity coefficient. Total number of values 5: constant, piecewise linear interpolation, piecewise polynomial, Sutherland's law and kinetic theory formulation.

- $c_5$ – selection of turbulence model. Total number of values 5: k-ε model, k-ω, SST model, Reynolds stress model, LES model of large eddies [5 ÷ 8].

- $c_6$ – selection of radiation model. Total number of values 3: no radiation, Rosseland model, model S2S "surface to surface".

- $c_7$ – selection of method for specifying discrete phase particles. Total number of values 2: constant or model dimensions equilibrium distribution.

- $c_8$ – selection of resistance law for drops. Total number of values 3: Schiller and Naumann law, Morsi and Alexander and symmetric drag model.

- $c_9$ – selection of expression for calculating lateral force in swirled flows. Total number of values 3: Saffman Mei law, Moraga model, the Hibiki and Ishii model.

- $c_{10}$ – selection of law which determines strength of turbulent dispersion. Total number of values 3: Lopez de Bertodano law, Burns/Simonin law, diffusion in VOF law.

- $c_{11}$ – selection of mass exchange law. Total number of values 2: constant mass transfer rate and evaporation-condensation model.

- $c_{12}$ – determination of Nusselt number for interphase heat exchange. Total number of values 2: Ranz-Marshall and Hughmark.

- $c_{13}$ – selection of turbulent interaction model. Total number of values 3: Simonin model, Troshko-Hassan model and Sato model.

As the "regime" parameters of the model, it is necessary to identify following parameters values:

- $p_1$ – value of critical Weber number for drop. Lies in range 1 < We < 2.

- $p_2$ – value of lateral force Saffman coefficient. Lies in range 0.1 < $C_L$ < 1.

- $p_3$ – value of turbulent dispersion force coefficient $C_{TD} = 0.1 \ldots 0.5$.

- $p_4$ – value of frequency coefficient of individual events in evaporation-condensation model 0.05 < $c$ < 0.2.

Parameters $p_i, i = 1,4$ are independent, therefore number of different variants of mathematical model structure is more than one and a half million variants. In addition, for each variant of a structure 4 "regime" parameters are needed. That’s why genetic optimization algorithm was used for solution of structural-parametric synthesis problem. The results created during the synthesis of a mathematical model are valuable as a generation tool for mathematical modeling, as a mechanism for improving of understanding of the phenomenon. During the construction of mathematical model, physical laws, which uncover mechanism of processes progress, are identified. There are some of the most significant features of the synthesized steam generator flow model.

Optimal mathematical model structure definition was realized with response surface optimization technology. Design of experiment for 17 input variables (parameters) was compiled on the base of optimal space-filling design (OSF) algorithm. OSF plan assumes generation of the most distant points in a whole area of factor space. So the most uniform distribution of plan points in a factorial space hypercube under consideration is achieved.

Structural parameters at the first stage were encrypted and represented by real variables in accordance to usual rounding rules. For example, variable $c_1$ can take 6 values: 0 - ideal gas, 1 - Hall-Yarburg equation, 2 - Redlich-Kwong equation (its modifications: 3 - Wilson modification and 4 - Soave modification), 5 - Peng-Robinson equation. It means that, if the value of $c_1$ falls within the range from 1.5 to 2.5, so Redlich-Kwong equation was used in a model.

The OSF experiment plan has 291 plan points for 17 factors.
291 numerical calculations were carried out according to model of a corresponding structure generated in experiment plan. Total "clean" machine time was ~ 11190 hours, so multitasking regime was used for calculations. The root-mean-square error was determined as the discrepancy between the calculated and experimental values of the steam generator wall temperatures for each calculated model was derived. Also calculation time requires to reach convergence was obtained.

Response surface was formed according to two algorithms: polynomial regression and neural networks. Figures 3 to 5 shows some results are obtained during construction of response surface.

Among the main results presented in Figures 4, 5, the following features can be noted:
- determination coefficient for the calculation error function (criterion P18) did not reach 0.9, so this cell is marked with a "cross" in the table. In addition, recommended values (according to a theory of regression analysis) exceed the values of maximum and root-mean-square errors of the constructed regression function. Determination coefficient is 0.97253 for the calculation time function (criterion P19). Despite the fact that a determination coefficient for the calculation error function is 0.89, engineers engaged in practical calculations using computational fluid dynamics are sufficiently satisfied with this result;
- sensitivity analysis graph shows that a calculation error value is influenced by all factors except the factor p₄. At the same time, all regime parameters p₁ ÷ p₄ don’t noticeably influence to a value of calculation time.

Figure 3. Response surface as the dependence of the error function on the structural parameters c₁ and c₂

Figure 4. "Quality" coefficients of a response surface
Response surface optimization was realized with help of two algorithms. Optimization by one criterion (calculation error) was carried out using the NLPQL sequential quadratic programming method.

It can be noted that the minimum error was approximately 10.4%. This result was obtained with the following model structure:

\[ c_1 = 2 – \text{Redlich-Kwong gas state equation}; \]
\[ c_2 = 2 – \text{isobaric heat capacity definition according to a piecewise-polynomial interpolation}; \]
\[ c_3 = 0 – \text{constant coefficient of thermal conductivity}; \]
\[ c_4 = 0 – \text{constant coefficient of viscosity}; \]
\[ c_5 = 1 – k–\omega \text{ turbulence model}; \]
\[ c_6 = 1 – \text{Rosseland radiation model}; \]
\[ c_7 = 1 – \text{discrete phase particles specifying method according to the model of dimensions equilibrium distribution}; \]
\[ c_8 = 0 – \text{Schiller and Naumann resistance law for drops}; \]
\[ c_9 = 1 – \text{Moraga model for calculation of lateral force in swirled flows}; \]
\[ c_{10} = 2 – \text{diffusion in VOF model for determining the strength of turbulent dispersion}; \]
\[ c_{11} = 1 – \text{evaporation-condensation model}; \]
\[ c_{12} = 0 – \text{Ranz-Marshall model for determining the Nusselt number for interphase heat exchange}; \]
\[ c_{13} = 2 – \text{Sato model of turbulent interaction}. \]

"Regime" parameters have the following values:

\[ p_1 = 1 – \text{value of the critical Weber number for the drop}; \]
\[ p_2 = 0.4 – \text{value of the lateral force coefficient of Saffman}; \]
\[ p_3 = 0.5 – \text{value of the turbulent dispersion force coefficient } C_{TD}; \]
\[ p_4 = 0.125 – \text{value of frequency coefficient of individual events in the evaporation-condensation model}. \]

For multicriteria optimization (using two criteria - calculation errors and time costs), a multicriteria genetic optimization algorithm MOGA was used. Algorithm settings are shown in Figure 6.

Figure 7 shows candidate points, which provide both acceptable accuracy and time costs for the solution. In particular, the first point provides a solution error ~ 14.3% with a calculation time ~ 20.6 hours. In this case, the following structure of model can be used:

\[ c_1 = 0 – \text{ideal gas state equation}; \]
\[ c_2 = 1 – \text{piecewise linear interpolation of isobaric heat capacity}; \]
\[ c_3 = 0 – \text{constant coefficient of thermal conductivity}; \]
\[ c_4 = 0 – \text{constant coefficient of viscosity}; \]
\[ c_5 = 0 – k–\varepsilon \text{ turbulence model}; \]
\[ c_6 = 0 – \text{no radiation}; \]
\[ c_7 = 0 – \text{constant discrete phase particles specifying method}; \]
$c_8 = 0$ – Schiller and Naumann resistance law for drops;
$c_9 = 1$ – Moraga model for calculation of lateral force in swirled flows;
$c_{10} = 2$ – diffusion in VOF model for determining the strength of turbulent dispersion;
$c_{11} = 0$ – mass transfer constant rate;
$c_{12} = 0$ – Ranz-Marshall model for determining the Nusselt number for interphase heat exchange;
$c_{13} = 2$ – Sato model of turbulent interaction.

"Regime" parameters have the following values:
$p_1 = 1.0312$ – value of the critical Weber number for the drop;
$p_2 = 0.357$ – value of the lateral force coefficient of Saffman;
$p_3 = 0.471$ – value of the turbulent dispersion force coefficient $C_{TD}$;
$p_4 = 0.137$ – value of frequency coefficient of individual events in the evaporation-condensation model.

Figure 8 shows Pareto set of variants to the model structure and corresponding values of "regime" simulation parameters, obtained from results of multicriteria optimization.
4. Verification of Pareto-optimal mathematical model variants

Five candidate-points from the Pareto set of mathematical model different variants of working processes in the steam generator were tested. Below there are results of variant No.3 verification of the mathematical model. Main "structural" and "regime" parameters were shown in Figure 7.

At the first step, a geometric 3D model of the investigated object, a calculated area, a mesh were constructed. Assumptions and boundary conditions were defined. Figure 9 shows the constructed flow area. Calculation is carried out in the flow area of steam generator without taking into account heat exchange between steam, walls and environment.

An irregular tetragonal mesh was used for creation of mesh model. Inflation on walls and refinement at areas of tangential water supply were added. An automatic mesh generator ANSYS Meshing was used.

Parameters of constructed with patch conforming method mesh model (Figures 10 and 11) are given below.

The total number of elements - 950038, surfaces - 2050070, nodes - 281114. This grid model provided the following values of Yplus: maximum – 133; average – 13.2. Independence of obtained solutions from the mesh was investigated during modeling.

Boundary conditions for solving problem:
1) Tangential inflow. Water mass flow rate is 6-20 g/s with a temperature 290 K, the volume concentration is 1;
2) Steam inflow. Steam mass flow rate is 10 g/s with a temperature 3400 K, volumetric concentration is 1;

3) Outflow. Outlet pressure is 0 MPa, the reference pressure is 2.57 MPa.

At the second step of modeling, model is transferred to the solver, where calculation settings are selected and the boundary value problem is solved.

An implicit algorithm of a solver was selected. It allows to solve transport equations separately. Separate resolving of momentum equations in projections to the axis of solution coordinate system was made at the beginning. Then pressure and velocity were corrected. Solution of the transport equations for scalar quantities were the final stage. As a result, the convergence criteria was checked.

At the third step (post-processing), analysis of results was performed and decision about completion or continuation of a problem investigation was taken.

Thus, a complete pattern of interaction of multiphase multicomponent flows inside the combustion chamber with a flow swirl was obtained for different values of cooling liquid (water) mass flow rate.

5. Analysis of the results

As a result of numerical simulation, temperature, pressure, velocity and volume concentration of phases fields were obtained at liquid film curtain water mass flow rate diapason from 6 to 20 g/s (Figure 12).

Figure 12. Temperature distribution of the first phase (steam) in the meridional section of the steam generator

Figure 13 shows evolution of the second phase (liquid curtain film) volume concentration along the length of steam generator.

Figure 13. Evolution of the second phase (water curtain film) volume concentration along the length of steam generator:
- water mass flow 20 g/s;
- water mass flow 15 g/s;
- water mass flow 10 g/s;
- water mass flow 6 g/s

Dependence of steam generator wall temperature from the axial coordinate is constructed (Figure 14) on the base of this distribution. The graph clearly shows a horizontal section with a wall temperature equal to 505 K what corresponds a water saturation temperature at pressure 2.75 MPa.
Then, at a distance from the fire bottom equal to \( \sim 130 \div 150 \) mm up to outflow from the steam generator, a monotonous increase in temperature is observed. This fact indicates the absence of a water film in this section. This conclusion agrees with averaged integral values of the second phase volume concentration, which are shown in Figure 13.

To compare the results of a numerical experiment and a natural one, a representative rated dependence of the steam generator wall temperature from the ballast water mass flow is constructed. This dependence is shown in Figure 15, where the results of full-scale experiment are also plotted. The root-mean-square error of simulation results and physical experiment is \( \sim 15 \% \). In our case this can be considered as a satisfactory coincidence with predicted parameters.

Figure 14. Dependence of steam generator wall temperature from the axial coordinate

![Figure 14](image)

Figure 15. Temperature dependence of the steam generator wall (265 mm from the fire bottom) from the water mass flow: ■ – experimental value; —— – calculated value

![Figure 15](image)

6. Conclusion
Formulating a mathematical model of the flow and interaction between oxygen-methane fuel combustion products with tangentially swirled ballast water injected in the end of the combustion chamber was made in CAE product Fluent, which integrated into the ANSYS Workbench platform. The problem of structural-parametric synthesis was solved for structure optimization of the model, i.e. equations were selected from the catalogue of Fluent physical models. Also optimization helped to find "regime" model parameters and determine the specific implementation of the model inside the synthesized structure. The model synthesizing procedure in this formulation is implemented using the toolkit of ANSYS DesignXplorer module, including the response surface optimization methodology and possibilities of evolutionary modeling methods, such as the genetic optimization algorithm and artificial neural networks. As a result, the choice of a specific turbulence model and state equations is...
substantiated. Methods for determining thermodynamic thermophysical characteristics of combustion products, choice of a radiation model, choice of a resistance law for drops, choice of an expression for calculating the lateral force for swirling flows, the choice of the law for determining the strength of turbulent dispersion, etc. are substantiated too.

Analysis and comparison of numerical and full-scale experiments results shows good convergence, and also confirms correctness of equations and modeling parameters selection.

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