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Numerical simulation of synthesis gas incineration

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Abstract. The authors have analysed the expediency of the suggested low-grade fuels application method. Thermal processing of solid raw materials in the gaseous fuel, called synthesis gas, is investigated. The technical challenges concerning the applicability of the existing gas equipment developed and extensively tested exclusively for natural gas were considered. For this purpose computer simulation of three-dimensional syngas-incinerating flame dynamics was performed by means of the ANSYS Multiphysics engineering software. The subjects of studying were: a three-dimensional aerodynamic flame structure, heat-release and temperature fields, a set of combustion properties: a flare range and the concentration distribution of burnout reagents. The obtained results were presented in the form of a time-averaged pathlines with color indexing. The obtained results can be used for qualitative and quantitative evaluation of complex multicomponent gas incineration singularities.

1. Introduction

One of the main problems of the global energy industry is the problem of low-grade fuels application. Low-grade fuels are characterized by a high moisture values. High fuel humidity causes high costs for its burning associated with the evaporation necessity. It is worth noting that the presence of such moisture amounts significantly facilitates fuel sticking and restricts its production and transportation in winter season. The mentioned disadvantages can be eliminated by heat processing of low-grade fuels into energy products of high quality gaseous fuel, called synthesis gas [1-5]. The aim of this work is the examination of low-grade raw fuel processing to gaseous fuel (synthesis gas) in order to assess the feasibility of this energy application method. The well-known advantages of the gaseous fuels energy use [6–8] (possibility of combustion process automating, ecological compatibility, low abrasive deterioration of heating surfaces and intensive heat transfer due to higher flow velocities available) expand the range of low-grade fuels useful applications.

Despite the fact, that nowadays synthesis gas has a high variety of applications in Power Engineering and Industrial services, there is still no commercially available equipment designed for its utilization. Therefore, the technical challenges concerning applicability of the existing gas equipment, developed and extensively tested exclusively for natural gas, often arise while designing synthesis gas burning power plants.

In this article the turbulent diffusive synthesis gas incineration was investigated using a computeraided simulation with ANSYS Multiphysics engineering software. The subjects of study were: a threedimensional aerodynamic flame structure, heat-release and temperature fields, a set of combustion properties: a flare range and the concentration distribution of burnout reagents. IOP Conf. Series: Materials Science and Engineering 124 (2016) 012110 doi:10.1088/1757-899X/124/1/012110

2. Initial data for investigation

The initial data for mathematical modeling are the following: the investigated gaseous fuel composition was simplified to H_2 - CH_4 -CO- CO_2 compound (Table 1); the oxidant is atmospheric oxygen (the air content is simplified to 0.23 and 0.77 mass fractions of the oxygen and nitrogen respectively); the air excess ratio is 1.02; the fuel-air mixture is supplied with the temperature of 20 $^{\circ}$ C; the coolant temperature is 368 K.

T, K	H ₂ , %	CH ₄ , %	CO, %	CO ₂ , %	Q, kJ/m ³
 500	30,32	15,9	10,98	42,8	10364,32
600	48,57	27,97	13,65	9,82	17001,7
700	50,1	27,59	7,59	14,72	16264,46
750	50,02	31,57	6,82	11,58	17586,52
800	48,09	37,1	8,17	6,63	19533,08
850	34 52	34 41	30.6	0.47	19938 86

Table 1. Content (mole fractions) of synthesis gas obtained by thermal decomposition of peat using different processing temperature (T) [9, 10]

For fuel-air mixing a simplified model of the prevalent automatic gas burner Weishaupt WKGL70 in the embodiment 3LN was analyzed. The investigated burner has 11 MW of thermal power and involves one primary fuel inlet orifice, four secondary fuel inlet orifices, primary and secondary air channels (Figure 1). The virtual cylindrical flame tube with the diameter of 2 m and the length of 10 m was considered as a combustion chamber. The temperature of the screening walls surface was assumed to be equal to the coolant temperature.

A simplified computational geometric model of the investigated burner with the partition into tetragonal finite elements was implemented. The mesh for simulation (Figure 2) was designed by means of the ANSYS Workbench. It consists of 1531011 tetrahedral cells with 196310 nodes. The integral volume of computational cells for combustion is 20 m³. The boundary zones are:

- 21333 triangular wall faces,
- 5133 triangular pressure-outlet faces,
- 7740 triangular mass-flow-inlet faces.

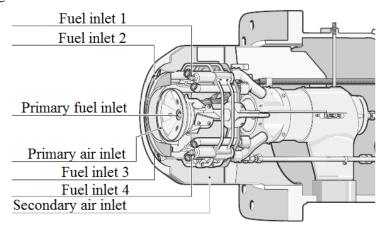


Figure 1. Layout of the investigated burner

Chemical oxidation of fuel components in a turbulent air flow was simulated by a finite-element method using a computer-aided engineering software ANSYS Multiphysics and a widely-used set of mathematical models [7, 11, 12]. Fuel oxidation was supposed to be proceeded by means of these

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reactions between combustible components and oxygen irreversibly: $CH_4+2O_2=CO_2+2H_2O$; $2CO+O_2=2CO_2$; $2H_2+O_2=2H_2O$. The chemical process in a turbulent flow was simulated with combined "Finite rate/Eddy-Dissipation" model.

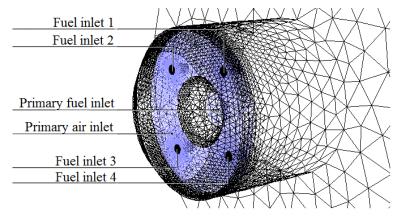


Figure 2. A simplified computational geometric model of the investigated burner with the partition into tetragonal finite elements.

For the mathematical description of the three-dimensional combustion dynamics in the concurrent flows of atmospheric air and synthesis gas the model of nonisothermal incompressible multicomponent gas was adopted. The flow process was considered to be steady, and, therefore, mathematical models of the continuity equation, mass-energy conservation were used in the steady-state formulation in the Euler's approximation.

Heat exchange by radiation was simulated with the spherical harmonics method in the first approximation (P1-model). A standard k- ϵ model was implemented for calculating pulsational (turbulent) flow characteristics.

The obtained results were presented in the form of a time-averaged pathlines with colored, according to heat release dissipation, temperature and the mass fraction of reactants in the gas mixture.

3. Calculation results

Table 2. Comparative analysis of natural gas and synthesis gas thermal characteristics

Type of fuel	Caloric value, MJ/m ³	The volumetric flow rate of air for the stoichiometric combustion related to 1 cubic meter of gaseous fuel, m ³ /m ³	The combustion products volume related to 1 cubic meter of gaseous fuel, m ³ /m ³
Natural gas	37,01	9,78	11,29
Synthesis gas	16,2	3,92	4,83

The less, in comparison with natural gas, syngas calorific value (Table 2) at same burner power leads to a higher fuel massflow rate through the nozzle, whereas the amount of air required for stoichiometric combustion is significantly lower because of high ballast content [9, 10], thereby the massflow rate through the air channels reduces. Mathematical modeling is an effective tool to assess the enumerated features impact of the tested fuel on the intensity of mixing processes, flame range and temperature. The approved EBU-model proposed by Spalding [13] was applied for the numerical simulation of chemical reactions behaviour in turbulent flow conditions.

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The numerical simulation results display the synthesis gas combustion via the mean pathlines colored according to different thermal characteristics. Despite the existence of massive vortices generated by local flow resistance in a burner slot, the process of combustion takes place in a short section of a straight continuous-flow without large scale eddies (Figure 3).

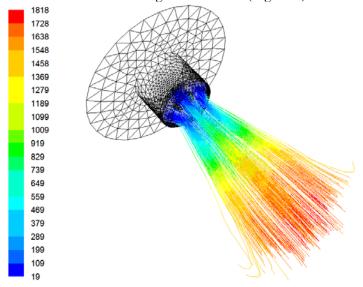


Figure 3. Synthesis gas burning flame pathlines colored according to temperature (°C).

According to the results of numerical experiments hydrogen burning (Figure 4) occurs in the close area from the burner orifice, due to the low activation energy for its oxidation. As the volume content of hydrogen in synthesis gas is about 50%, then there is a more intensive temperature rise in the region close to the burner slot rather than the combustion of natural gas, where the hydrogen content is much lower. The temperature of the gaseous flow reaches its maximum at the narrow boundaries of the flame wherein there is no intensive burning. The area beyond the boundaries of the flame is filled with combustion products: CO_2 and H_2O .

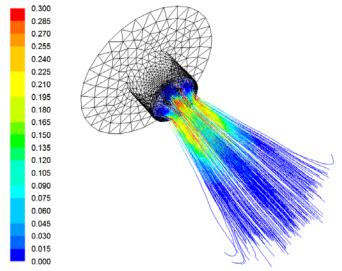


Figure 4. Synthesis gas burning flame pathlines colored according to the reaction rate of $2H_2 + O_2 = 2H_2O$ (kgmol·m⁻³·s⁻¹).

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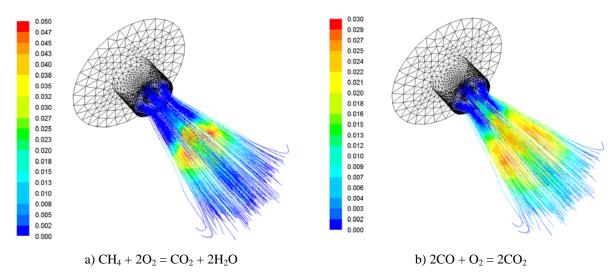


Figure 5. Synthesis gas burning flame pathlines colored according to the reaction rate (kgmol·m⁻³·s⁻¹).

The high gas mixture temperature (Figure 3) initiates methane (Figure 5, a) and carbon monoxide (Figure 5, b) ignition in the immediate vicinity of the burner, but the values of the oxidation reaction rate in the combustion chamber is generally lower than those values for the natural gas combustion, due to the burner jet ballasting. A consequence of the described factors is a uniform heat release distribution (Figure 7) for the entire length of the flame, which favorably affects the reliability of the combustion chamber.

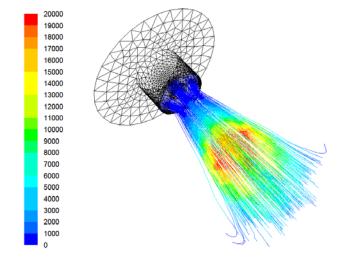


Figure 7. Synthesis gas burning flame pathlines colored according to heat release of three simultaneous reactions in the gas mixture (W).

4. Conclusion

Using the ANSYS Multiphysics engineering software a detailed description of the synthesis gas turbulent combustion is given. The obtained results can be used for qualitative and quantitative evaluation of complex multicomponent gas incineration singularities.

The synthesis gas caloric value is 2.3 times lesser than the natural gas caloric value. For this reason, the volumetric flow rate of synthesis gas through the burner of the same capacity is 130% higher. This increases the velocities in the fuel injectors and reduces its life because of the higher abrasive solids contained in synthesis gas. However, the combustion of synthesis gas requires less air (3.92 m³/m³).

For this reason aerodynamic flow resistance and power consumption of burners using VFD fans (with frequency adjustment) is reduced while incinerating synthesis gas.

The amount and composition of the combustion products resulting from the synthesis gas combustion do not significantly change compared to natural gas, so it allows using exhaust fans of the same capacity. In other words, for the synthesis gas incineration in the rarefied gas furnaces (developed for the natural gas combustion with the aerodynamic rarefaction) there is no modernization of draft equipment required.

As a result of the conducted research it is possible to conclude that the low-temperature catalytic conversion, allowing receiving synthesis gas, enriched with hydrogen, from the solid initial raw is a promising way of low-grade fuel recycling. The resulting synthesis gas can be effectively used in Power Engineering to produce heat and electricity without expensive upgrades of gas equipment.

Acknowledgments

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References

- [1] Sarker M, Mohammed A S M D, Rashid M M, Schiralli N, Zaman A, Kabir A, Rahman S, Islam K, Molla M 2009 New alternative energy from solid waste plastics. ICDRET: Proc. of 1st Intern. Conf. on the Developments in Renewable Energy Technology, Bangladesh: Dhaka, (5454177) 100–103
- [2] Lorincz J, Bule I 2013 Renewable *International Journal of Business Data Communications and Networking* **9(3)** 53–74
- [3] Aysu T 2015 *Bioresource Technology* **191** 253–262
- [4] Sircar I, Sane A, Wang W, Gore J P 2014 Fuel **119** 38–46
- [5] Kazakov A V., Tabakaev R B, Novoseltsev P Y and Astafev A V 2014 Low-temperature conversion of low-grade organic raw, part 1 (technical aspects) ed P A Strizhak, A A Kozyreva and R Z Reshetova MATEC Web Conf. 19 01014
- [6] Liu G, Chen Z, Li Z, Li G and Zong Q 2015 Appl. Therm. Eng. 75 1034–45
- [7] Zavorin A S, Khaustov S A and Zaharushkin R N A 2014 *IOP Conf. Ser. Mater. Sci. Eng.* **66** 012029
- [8] Gergelizhiu P S, Khaustov S A, Tabakaev R B, Novoseltsev P U, Kazakov A V and Zavorin A S 2014 International Conference on Mechanical Engineering, Automation and Control Systems (MEACS) (IEEE) 1–4
- [9] Tabakaev R B, Gergelizhiu P S, Kazakov A V and Zavorin A S 2014 *IOP Conf. Ser. Mater. Sci. Eng.* **66** 012052
- [10] Tabakaev R B, Kazakov A V. and Zavorin A S 2015 Solid Fuel Chem. 49 267-73
- [11] Zavorin A S, Khaustov S A and Sheikin V A 2014 International Conference on Mechanical Engineering, Automation and Control Systems (MEACS) (IEEE) 1–4
- [12] Khaustov S A, Zavorin A S, Buvakov K V, Kudryashova L D and Tshelkunova A V 2015 Computer simulation of vortex combustion processes in fire-tube boilers ed G V. Kuznetsov, P A Strizhak, A O Zhdanova and E E Bulba EPJ Web Conf. 82 01041
- [13] Spalding D B 1971 Proc. Combust. Inst. 13 649-657