

# Numerical simulation of biomass syngas combustion

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**Abstract.** The aim of this work was to comparatively assess the environmental characteristics of combustion products in the combustion of synthetic gas with air compared to the combustion of methane with air. Such characteristics have been so far studied for the use of methane as a fuel to a greater extent than for synthetic gases. Syngas was represented by products of a steam biomass gasification (agricultural residues). Numerical simulation of combustion processes was carried out using the kinetic model of a perfectly stirred reactor. The influence of the residence time of the chemically reacting mixture in the reaction volume on the completion of combustion processes and the emission of CO<sub>2</sub> and NO<sub>x</sub> was investigated. For the same thermal power of the energy device, CO<sub>2</sub> and NO<sub>x</sub> emissions from the syngas combustion exceed those from the methane combustion. Mass emission ratios were the following: CO<sub>2</sub>(syngas)/CO<sub>2</sub>(methane)≈1.55-1.57; NO<sub>x</sub>(syngas)/NO<sub>x</sub>(methane)≈2.56-3.4. The greatest impact on NO<sub>x</sub> emissions during syngas combustion is caused by higher combustion temperatures compared to the temperatures during methane combustion. To reduce NO<sub>x</sub> emissions when using syngas, it is necessary to develop and implement technical solutions that are more effective than those currently used for organizing the processes of mixture formation and combustion in energy setups.

## 1 Introduction

Use syngas produced from biomass gasification is a carbon neutral alternative fuel. Increasing the efficiency of using syngas to produce thermal energy in various setups that use combustion technologies is a challenging task [1-10]. It includes ensuring high quality mixing of syngas and air, stability and completeness of combustion processes, reducing emissions of nitrogen oxides and carbon monoxide, etc. To improve the safety of syngas storage and transportation, studying its explosive characteristics is required [1, 2]. One of potential syngas applications is using it as a fuel for an internal combustion engine in a vehicle [3].

For more complete understanding of the syngas combustion in a mixture with air, various models of chemical interaction that accurately reproduce experimental data, including the ignition delay time and flame speed, should be considered [4, 5].

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The energy value of syngas is largely determined by the processes of biomass gasification [6, 7].

The main characteristics of syngas are the concentrations of hydrogen, carbon monoxide, methane and other hydrocarbons. The amount of H<sub>2</sub> has a critical impact on the energy characteristics of syngas. Increasing the proportion of hydrogen in syngas causes an increase in lower heating value [8, 9]. The composition of the synthesis gas significantly influences the level of emissions. Hydrogen and carbon monoxide in syngases lead to an increased combustion temperature, which contributes to the thermal formation of NO and NO<sub>2</sub> [10].

The completion of syngas combustion processes and NO<sub>x</sub> emission depend on the temperature and the reagents' residence time in the reaction volume. Longer residence time promotes more complete combustion. However, with longer residence time at temperatures above 2000 K, the NO<sub>x</sub> concentration increases. One of the main trends in the production of thermal energy is the use of syngas instead of traditional gas fuel (natural gas, methane, a mixture of propane and butane, etc.) in already existing setups. For that, in most cases, only syngas supply devices are changed and the mixture formation system is slightly modified.

Here, we report the results of a numerical simulation of the effect of the residence time on the combustion completeness and NO<sub>x</sub> emissions when burning synthesis gas with air compared to burning methane with air. Based on the results obtained, a comparative assessment of NO<sub>x</sub> and CO<sub>2</sub> emissions for both types of fuel was carried out.

## 2 Materials and methods

The amounts of the main syngas components were taken in accordance with the results of modeling biomass gasification [11], vol. %: CO – 44.708; H<sub>2</sub> – 49.543; CH<sub>4</sub> – 1.371; H<sub>2</sub>S – 0.045; CO<sub>2</sub> – 3.904; N<sub>2</sub> – 0.428. Lower heating value of syngas  $LHV=16.511$  MJ/kg. Lower heating value of methane  $LHV=50$  MJ/kg.

Combustion processes were simulated using a kinetic model of a perfectly stirred reactor (PSR) [12]. The feed reagents (fuel and air) are supplied to the PSR. The transformation of initial reactants into final products occurs as a result of chemical interactions within the PSR volume. The end products of combustion are removed from the PSR. The residence time ( $\tau$ ) of the reacting mixture in the PSR was determined by the ratio of the PSR volume and the volumetric flow rate of combustion products. Heat losses to the external environment were not considered.

To simulate the combustion of syngas and methane, the same mechanism of chemical reactions was used. This mechanism involved 182 reversible chemical reactions typical of the combustion of methane with air. Since H<sub>2</sub>S is present in the syngas, reactions involving S, S<sub>2</sub>, H<sub>2</sub>S, HS, SO, and SO<sub>2</sub> were included in the mechanism.

The calculations were performed with equivalent ratio values  $ER=1.0$  and  $ER=1.2$ .

The degree of combustion processes completion was assessed using the indicator  $\eta=T_{kin}/T_{eq}$ , where  $T_{kin}$  is the temperature of combustion products determined using the kinetic model depending on the residence time,  $T_{eq}$  is the temperature of combustion products determined under the condition of chemical equilibrium (equilibrium model) regardless of the residence time.

### 3 Results and discussion

Tables 1-4 show the calculations obtained when burning syngas with air (Tables 1 and 2) and methane with air (Tables 3 and 4) at different values of the equivalent ratio  $ER$ .

**Table 1.** Composition and temperature of syngas combustion products at  $ER=1.0$ .

Composition and temperature	Kinetic model				Equilibrium model
	$\tau=12$ ms	$\tau=24$ ms	$\tau=48$ ms	$\tau=96$ ms	
CO, vol. %	0.27903E-01	0.24876E-01	0.23306E-01	0.22178E-01	0.21571E-01
CO <sub>2</sub> , vol. %	0.14027E+00	0.14300E+00	0.14517E+00	0.14621E+00	0.14765E+00
NO, vol. %	0.81940E-03	0.13048E-02	0.19741E-02	0.24899E-02	0.33878E-02
NO <sub>2</sub> , vol. %	0.16792E-06	0.29392E-06	0.47477E-06	0.61563E-06	0.86072E-06
SO <sub>2</sub> , vol. %	0.15046E-03	0.14962E-03	0.15056E-03	0.14888E-03	0.14854E-03
O <sub>2</sub> , vol. %	0.14566E-01	0.12663E-01	0.11485E-01	0.10614E-01	0.98500E-02
H <sub>2</sub> , vol. %	0.58514E-02	0.51085E-02	0.47156E-02	0.44576E-02	0.43008E-02
H <sub>2</sub> O, vol. %	0.16607E+00	0.16705E+00	0.16835E+00	0.16876E+00	0.16992E+00
N <sub>2</sub> , vol. %	0.62746E+00	0.63033E+00	0.63003E+00	0.63084E+00	0.62918E+00
$T$ , K	2272.4	2294.0	2314.1	2321.5	2335.6
$\eta$	0.97294	0.98219	0.99079	0.9939	-

**Table 2.** Composition and temperature of syngas combustion products at  $ER=1.2$ .

Composition and temperature	Kinetic model				Equilibrium model
	$\tau=12$ ms	$\tau=24$ ms	$\tau=48$ ms	$\tau=96$ ms	
CO, vol. %	0.12740E-01	0.10126E-01	0.82012E-02	0.69431E-02	0.54481E-02
CO <sub>2</sub> , vol. %	0.13319E+00	0.13615E+00	0.13825E+00	0.13957E+00	0.14152E+00
NO, vol. %	0.42607E-03	0.74536E-03	0.12460E-02	0.19484E-02	0.45896E-02
NO <sub>2</sub> , vol. %	0.14344E-06	0.29161E-06	0.54730E-06	0.92143E-06	0.23329E-05
SO <sub>2</sub> , vol. %	0.13124E-03	0.13145E-03	0.13147E-03	0.13155E-03	0.13148E-03
O <sub>2</sub> , vol. %	0.34570E-01	0.33159E-01	0.31996E-01	0.31063E-01	0.29135E-01
H <sub>2</sub> , vol. %	0.26418E-02	0.20556E-02	0.16427E-02	0.13816E-02	0.10791E-02
H <sub>2</sub> O, vol. %	0.14657E+00	0.14800E+00	0.14899E+00	0.14962E+00	0.15069E+00
N <sub>2</sub> , vol. %	0.65343E+00	0.65467E+00	0.65556E+00	0.65601E+00	0.65492E+00
$T$ , K	2141.9	2169.8	2188.4	2199.2	2212.6
$\eta$	0.96805	0.98066	0.98906	0.99394	-

**Table 3.** Composition and temperature of methane combustion products at  $ER=1.0$ .

Composition and temperature	Kinetic model				Equilibrium model
	$\tau=12$ ms	$\tau=24$ ms	$\tau=48$ ms	$\tau=96$ ms	
CO, vol. %	0.13862E-01	0.11973E-01	0.10402E-01	0.95786E-02	0.89485E-02
CO <sub>2</sub> , vol. %	0.79927E-01	0.81453E-01	0.82450E-01	0.83568E-01	0.85278E-01
NO, vol. %	0.24292E-03	0.36832E-03	0.53020E-03	0.84296E-03	0.19236E-02
NO <sub>2</sub> , vol. %	0.36819E-07	0.61225E-07	0.93926E-07	0.15819E-06	0.38113E-06
O <sub>2</sub> , vol. %	0.86217E-02	0.73046E-02	0.62059E-02	0.55160E-02	0.45555E-02
H <sub>2</sub> , vol. %	0.57717E-02	0.49140E-02	0.42296E-02	0.38550E-02	0.35530E-02
H <sub>2</sub> O, vol. %	0.17902E+00	0.17959E+00	0.17944E+00	0.18061E+00	0.18326E+00
N <sub>2</sub> , vol. %	0.69799E+00	0.70093E+00	0.70417E+00	0.70386E+00	0.70065E+00
$T$ , K	2165.8	2179.1	2184.1	2198.0	2223.6
$\eta$	0.97401	0.97999	0.98224	0.98849	-

**Table 4.** Composition and temperature of methane combustion products at  $ER=1.2$ .

Composition and temperature	Kinetic model				Equilibrium model
	$\tau=12$ ms	$\tau=24$ ms	$\tau=48$ ms	$\tau=96$ ms	
CO, vol. %	0.42618E-02	0.31488E-02	0.23012E-02	0.17632E-02	0.85569E-03
CO <sub>2</sub> , vol. %	0.75667E-01	0.76900E-01	0.77559E-01	0.78489E-01	0.79423E-01
NO, vol. %	0.11839E-03	0.17527E-03	0.24008E-03	0.39061E-03	0.32656E-02
NO <sub>2</sub> , vol. %	0.46742E-07	0.80039E-07	0.12465E-06	0.22365E-06	0.21627E-05
O <sub>2</sub> , vol. %	0.33646E-01	0.33049E-01	0.32510E-01	0.32327E-01	0.30513E-01
H <sub>2</sub> , vol. %	0.16911E-02	0.12563E-02	0.92502E-03	0.71179E-03	0.35835E-03
H <sub>2</sub> O, vol. %	0.15587E+00	0.15687E+00	0.15713E+00	0.15832E+00	0.15918E+00
N <sub>2</sub> , vol. %	0.71478E+00	0.71554E+00	0.71706E+00	0.71618E+00	0.71567E+00
$T$ , K	2000.7	2016.5	2023.1	2037.3	2043.0
$\eta$	0.9793	0.98703	0.99026	0.99721	-

The main end products of combustion of syngas and methane are CO<sub>2</sub> and H<sub>2</sub>O. At a short residence time (for example, at  $\tau=12$  ms), the concentrations of these substances differ slightly from the concentrations at a long residence time (for example, at  $\tau=96$  ms). The incompleteness of combustion, assessed by the index  $\eta$ , can be considered quite acceptable for practical purposes. However, the residence time determines the emission of nitrogen oxides. To adequately compare CO<sub>2</sub> and NO<sub>x</sub> emissions when burning syngas and methane, the following circumstance must be considered. To achieve the thermal power obtained by burning 1 kg of methane, it is necessary to burn 3.028 kg of syngas. At  $ER=1.0$ , the amount of combustion products for the methane combustion is 18.211 kg, while for syngas, it is 16.415 kg. At  $ER=1.2$ , the amount of combustion products for the methane combustion is 21.654, while for syngas, it is 19.092 kg. Under these conditions, CO<sub>2</sub> and NO<sub>x</sub> emissions from syngas combustion exceed CO<sub>2</sub> and NO<sub>x</sub> emissions from methane combustion, respectively. Mass emission ratios are the following: CO<sub>2</sub>(syngas)/CO<sub>2</sub>(methane) $\approx 1.55$ -1.57; NO<sub>x</sub>(syngas)/NO<sub>x</sub>(methane) $\approx 2.56$ -3.4. The greatest impact on NO<sub>x</sub> emissions during syngas combustion is caused by higher combustion temperatures compared to temperatures during methane combustion.

## 4 Conclusion

The presented results can be used in practical applications of syngas as a fuel. The identified effects of the temperature levels and residence time allow us to estimate the expected levels of CO<sub>2</sub> and NO<sub>x</sub> emissions. To reduce NO<sub>x</sub> emissions when using syngas, it is necessary to develop and implement technical solutions that are more effective than those currently used for organizing the processes of mixture formation and combustion in energy setups.

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