NUMERICAL STUDY OF ELECTRODYNAMIC CONTROL
OF STRAW CO-FIRING WITH PROPANE

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Abstract. The mathematical modelling of straw co-firing with propane is performed with account of variations of combustible volatiles by increasing the supply of gas into the experimental device.In accordance with the experimental data the average values of molar density of combustible volatiles H_2 and CO at the inlet of the combustor depending on the electric field in the mathematical model are usedas the mass fraction of concentration in thetwo second-order exothermic chemical reactions.The mathematical model is developed using MATLAB for solving a system of parabolic type partial differential equations to describe the formation of the 2D compressible reacting swirling flow in a coaxial cylindrical pipe, the formation of the electric field, the variation of the mass fraction of volatiles, the flame species and the flame temperature. The electric field was applied to the flame base using an axially inserted electrode and the surface of the pipe. The charge and electron distribution are given at the surface.The maximal value for the temperature, velocities and the mass fraction of the product CO_2 are obtained for the value of the electric field.

Keywords: mathematical model, electric field, 2D reacting flow, flame.

Introduction

The main goal of the current research refers to the EU 2030 targets to reduce overall greenhouse gas (GHG) emissions by 40 %, to increase the energy production efficiency and the utilization of the renewable energy sources by 27 %, thus minimizing the effect of heat producers on GHG emissions and global warming. In this context, the use of differentagriculture and harvestingresidues (wood, wheat straw, rape straw)for energy production is severe [1]. Although, the use of biofuels for energy production nowadays reaches already 15 % of the world's total energy consumption and has already provided a significant reduction of greenhouse gas emissions, more efficient use of biofuels, such as straw [2].

This study combines the experimental research and mathematical modelling of the processes developing during co-firing of straw pellets with propane. The experimental and numerical study of the electric field effects on the combustion dynamics at co-firing of straw pellets with gas (propane) was carried out with the aim to provide control of the thermal decomposition and to minimize the negative effects using straw as fuel for energy production.The mathematical model is developed for formation of 2D compressible reacting swirling flow with the chemical reactions in the coaxial cylindrical pipe with the radius $r_0 = 0.05$ m and length $z_0 = 0.1$ m. The following two dominant second-order exothermic chemical reactions with 3 reactants CO, H_2, OH and 3 products CO_2, H, H_2O are considered:

$$H_2 + OH \rightarrow H_2O + H, \quad CO + OH \rightarrow CO_2 + H . \tag{1}$$

Mathematical modelling of the chemical reactions

To describe the chemical reactions the following parameters of Arrhenius kinetics are used [3;4]:

- $R = 8.314$ J·(mol·K)$^{-1}$ is the universal gas constant;
- $m_1 = 2$, $m_2 = 17$, $m_3 = 18$, $m_4 = 1$, $m_5 = 28$, $m_6 = 44$ g·m^{-3} are the molecular weights of 6 species $C_1(H_2)$, $C_2(OH)$, $C_3(H_2O)$, $C_4(H)$, $C_5(CO)$, $C_6(CO_2)$;
- $h_1 = 0$, $h_2 = 39.46$, $h_3 = -242$, $h_4 = 218$, $h_5 = -111$, $h_6 = -394$ kJ·mol^{-1} are the constant enthalpies of the species;
- $c_p = 1,000$ J·(kg·K)$^{-1}$ is the specific heat at a constant pressure;
- $E_1 = 14965.2$, $E_2 = 29930.4$ J·mol^{-1} are the activation energies;
- $\delta_k = E_k/(R \cdot T_0)$, ($T_0 = 300$ K, $\delta_1 = 6.0$, $\delta_2 = 12.0$) are the scaled activation energies;
- $A'_1 = 22$, $A'_2 = 15000$ m^3·(mol·s)$^{-1}$ are the reaction-rate pre-exponential factors;
- $A_1 = A'_1 \cdot \rho_0 \cdot r_0/(U_0 \cdot m_2) = 647.1$, $A_2 = A'_2 \cdot \rho_0 \cdot r_0/(U_0 \cdot m_5) = 2.7 \cdot 10^5$ ($\rho_0 = 1$ kg·m^{-3}, $U_0 = 0.1$ m·s^{-1}) are the scaled reaction-rate pre-exponential factors;

- $Q_1 = (m_1 \cdot h_1 + m_2 \cdot h_2 - m_3 \cdot h_3 - m_4 \cdot h_4)/(m_1 \cdot m)$, $Q_2 = (m_2 \cdot h_2 - m_4 \cdot h_4 + m_5 \cdot h_5 - m_6 \cdot h_6)/(m_2 \cdot m)$ expressed in J·kg^{-1} are the heat effects of each reaction,
- $m = 18.3$ g·m^{-3} is the averaged value of the molecular weights of species,
- $q_1 = Q_1/(c \, p \cdot T_0) = 124.9$, $q_2 = Q_2/(c \, p \cdot T_0) = 9.42$ are the normed heat releases.

In a physical experiment during co-firing of wheat straw pellets with propane the average values of concentration of H_2 and CO for different propane flow series were obtained. In accordance to the results of the experimental measurements these values are used as the mass fraction for the exothermic chemical reactions (1) at the inlet of the combustor in the mathematical model, where OH is the third reactant. The 2D distribution of axial and radial components of velocity $w = u_z/U_0, u = u_r/U_0$, circulation $v = rv_\varphi/(r_0 V_0), V_0 = 0.3$ m·s^{-1} (azimuthal velocity v_φ), density ρ/ρ_0, temperature T/T_0, and mass fractions for 6 specie are calculated of the nonlinear 11parabolic type PDEs system,depending on the time $t/t_0,(t_0 = 1s)$ withthe normed axial and radial coordinates $x = z/r_0, r/r_0$.

In accordance with the experimental data the average values of molar density of combustible volatiles C_1 (H_2) and C_5 (CO) at the inlet of the combustor depending on the electric field are as follows:

- for 0.0 mA – $C_1 = 0.78$, $C_5 = 1.69$ mol·m^{-3};for 1.13 mA – $C_1 = 0.86$, $C_5 = 2.03$ mol·m^{-3};
- for 2.65 mA – $C_1 = 0.94$, $C_5 = 2.29$ mol·m^{-3};for 3.57 mA – $C_1 = 0.99$, $C_5 = 2.31$ mol·m^{-3};
- for 4.66 mA – $C_1 = 1.10$, $C_5 = 2.57$ mol·m^{-3} [5].

In the physical experiment the obtained values of molar density as the mass fraction of concentration C_k, $k = 1$ (1) 6 for initial conditions $C_1 + C_2 + C_5 = 1$(the mass fraction of the reactants), $C_3 = C_4 = C_6 = 0$ (the mass fraction of the products) in the mathematical model are used (decreasing the values of concentration 5 times).

Assuming negligible thermal diffusion and equal constant multi component diffusion coefficients, the diffusive ass flux vector of the species is decreased to $-\rho D \nabla C_k$, and the species equation for the mass fraction C_k reads as

$$\rho D/Dt \cdot C_k = \nabla(\rho D \cdot C_k) + m_k \Omega_k , \tag{2}$$

where D/Dt – substantial derivative;
$D = 5 \cdot 10^{-5}$ m^2·s^{-1} – constant molecular diffusivity of the species;
m_k – molecular weight of the k-th species;
ρ – density of the mixture,
Ω_k – production rate for k-th species [6].
The temperature equation is

$$\rho cp DT/Dt = \nabla \cdot (\lambda \nabla T) - \Sigma h_k \Omega_k m_k., \tag{3}$$

In the equation for the temperature, the source term is

$$1/(m\rho c_p) \sum_{k=1}^{K} h_k m_k \, \Omega_k, \text{K·s}^{-1},$$

where K – number of species,
$\lambda = 0.25$ W/(m·K)$^{-1}$ – thermal conductivity.

Maxwell's equations and mathematical models of the electric field

The behaviour of an electrostatic field can be described by the Maxwell's equations [9]:

$$\text{div } E = q /\varepsilon \text{ ,div } B = 0, \text{ curl } E + \partial B /\partial t = 0, \text{ curl } H = J + \varepsilon \partial E/ \partial t , \varepsilon = \varepsilon_0. \varepsilon_r, \tag{4}$$

where q – the space charge density, Am^{-3};
H – the magnetic field Am^{-1};
E – the electric field, Vm^{-1};
J – the current density, Am^{-2};
B – the magnetic induction, N·(Am)$^{-1}$;
$\varepsilon_0 \approx 10^{-11}$ – the absolute dielectric constant, As·V^{-1};

$\varepsilon_r \approx 1$ the relative permittivity in the gas-air region.

Taking a divergence and the magnetic field B represented as $B = \text{curl } A$ (A the vector potential) gives:

$$\text{div } J + \partial q / \partial t = 0, E + \partial A / \partial t = -\text{grad } \Phi, \tag{5}$$

where Φ – scalar potential.

Make an assumption that it is possible to neglect $\partial A/\partial t$ (the quasi-stationary approximation), then the solution of the electric field can be based on the approximation $E = -\text{grad } \Phi$ and can be transformed to Poisson's equation $\Delta \Phi = -q / \varepsilon$. The Coulomb force $F = q E$. The current density in the air region is defined as [10] $J = K q E + q U - D \text{ grad } q$, where $K \approx 2.10^{-4} \text{ m}^2 \cdot (\text{Vs})^{-1}$ is the constant ion mobility, U the gas velocity vector, D the diffusion coefficient. Taking a divergence gives:

$$\partial q/\partial t = -\text{div } J = D\Delta q + K\text{grad } q \cdot \text{grad } \Phi - \text{grad } q \cdot U - q(\text{div } U + K q /\varepsilon_0). \tag{6}$$

We have the following two dimensionless equations for the charge density and scalar potential:

$$\partial q/\partial t = P_d\Delta q + P_k(\partial q/\partial r \cdot \partial\Phi/\partial r + \partial q/\partial x \cdot \partial\Phi \partial x) -$$
$$- P_u(q\text{div } U + u \partial q /\partial r + w \partial q/\partial x)-P_r q^2, \tag{7}$$

$$\partial\Phi/\partial t = \Delta\Phi + Q_e q, \tag{8}$$

where $\text{div } U = \partial w /\partial x + 1/ r \, \partial(r u/ \partial r)$;
$P_d = D t_0/ r_0{}^2 = 0.02$,
$P_k = K\Phi_0 t_0/ r_0{}^2$,
$P_u = U0 t_0/ r_0 = 2$,
$P_r = K q_0 t_0/\varepsilon_0 = 400$,
$Q_e = r_0{}^2 q_0/(\Phi_0\varepsilon_0)$.

The equation for scalar potential (8) for the numerical simulation is transformed to non-steady. The equations for the charge density and potential made dimensionless by scaling all the lengths to r_0, the time to t_0, the velocity vector to U_0, the potential to $\Phi_0 = 100$ [V], the charge density to $q_0 = 2 \cdot 10^{-5} \text{ C} \cdot \text{m}^{-3}$. For the Coulomb force $F = q E = -q \text{ grad } \Phi$ we have the electric parameter $P_{ar} = q_0 \Phi_0/(U_0{}^2 \rho_0)$. In accordance with the experimental data of the electric current I_0 and potential Φ_0 we use $\Phi_0 = 100$ V, $I_0 = 0.2$ to 1.0 mA. Then we have $P_{ar} = 0.2-1.0$, $P_k = 8$, $Q_e = 50$.

For the electric field the BCs at the walls of the combustor r = 1 we use following profile:

$$\Phi = q = \exp(-(x -0.025)^2)(2x -x^2)/0.6$$

with maximum value equal to 1; and at the axially inserted electrode for smooth round wire r = 1/80: $\Phi = q = 0$. These BCs are used also for initial conditions by $t = 0$. In [8] the electric field modelling is without the ion mobility and the charge distribution at the surface electrode. In Fig. 1 the levels of the dimensionless scalar potential are presented. In Fig. 2 we can see the profile of the dimensionless values of potential with the maximal value 1 for $r = 1$ increasing to 0 for $r = 0$.
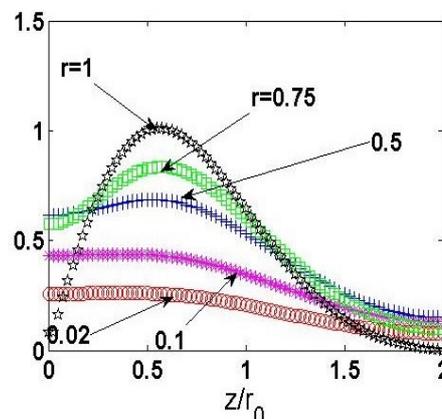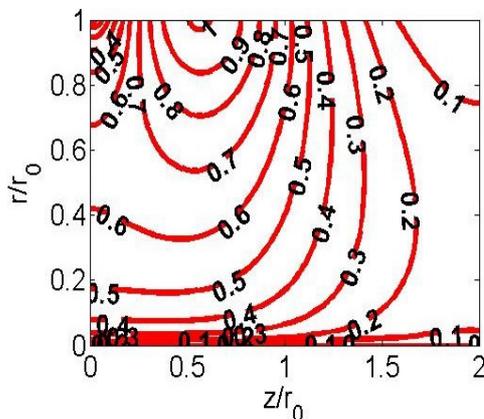
Fig. 1. **Levels of dimensionless scalar potential for $P_{ar} = 0.53$**

Fig. 2. **Dimensionless potential depending on x for fixed r and for $P_{ar} = 0.53$**

Mathematical models and equations

In the governing balance equations, some assumptions are made, i.e. constant physical properties, negligible soot and flame radiation, laminar flow, and validity of the ideal gas law. We focus on a configuration, in which a steady low-velocity laminar flame exists in a straight pipe in the base state. The 2D mathematical model is described by the 3 Navier–Stokes , temperature and 6 reaction-diffusion dimensionless equations in the cylindrical coordinates (r, x) and at the time . The equations for density, velocity, circulation and temperature are the following:

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + M(\rho) + \rho\left(\dfrac{1}{r}\dfrac{\partial(ru)}{\partial r} + \dfrac{\partial w}{\partial x}\right) = 0, \\[2mm] \dfrac{\partial u}{\partial t} + M(u) - S\dfrac{v^2}{r^3} = -\dfrac{1}{\rho}\dfrac{\partial p}{\partial r} + \mathrm{Re}^{-1}\left(\Delta u - \dfrac{u}{r^2}\right) + P_{ar}\dfrac{F_r}{\rho}, \\[2mm] \dfrac{\partial w}{\partial t} + M(w) = -\dfrac{1}{\rho}\dfrac{\partial p}{\partial x} + \mathrm{Re}^{-1}\Delta w + P_{ar}\dfrac{F_x}{\rho}, \\[2mm] \dfrac{\partial v}{\partial t} + M(v) = \mathrm{Re}^{-1}\Delta_* v, \\[2mm] \dfrac{\partial T}{\partial t} + M(T) = P_0\dfrac{1}{\rho}\Delta T + q_1\rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right) + q_2\rho A_2 C_2 C_5 \exp\left(-\dfrac{\delta_2}{T}\right) \end{cases} \qquad (9)$$

The equations for 6 chemical reactions are the following:

$$\begin{cases} \dfrac{\partial C_1}{\partial t} + M(C_1) = P_1\Delta C_1 - \rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right), \\[2mm] \dfrac{\partial C_2}{\partial t} + M(C_2) = P_2\Delta C_2 - \rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right)\dfrac{m_2}{m_1} - \rho A_2 C_2 C_5 \exp\left(-\dfrac{\delta_2}{T}\right), \\[2mm] \dfrac{\partial C_3}{\partial t} + M(C_3) = P_3\Delta C_3 - \rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right)\dfrac{m_3}{m_1}, \\[2mm] \dfrac{\partial C_4}{\partial t} + M(C_4) = P_4\Delta C_4 - \rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right)\dfrac{m_4}{m_1} + \rho A_2 C_2 C_5 \exp\left(-\dfrac{\delta_2}{T}\right)\dfrac{m_2}{m_1}, \\[2mm] \dfrac{\partial C_5}{\partial t} + M(C_5) = P_5\Delta C_5 - \rho A_2 C_2 C_5 \exp\left(-\dfrac{\delta_2}{T}\right)\dfrac{m_5}{m_2}, \\[2mm] \dfrac{\partial C_6}{\partial t} + M(C_6) = P_6\Delta C_6 - \rho A_2 C_2 C_5 \exp\left(-\dfrac{\delta_2}{T}\right), \end{cases} \qquad (10)$$

where $M(q) = w{\cdot}\partial q/\partial x + u{\cdot}\partial q/\partial r$, $\Delta q = \partial^2 q/\partial z^2 + r^{-1}\partial/\partial r(r{\cdot}\partial q/\partial r)$ – the convective and diffusion terms;

$S_1 = \rho{\cdot}A_1{\cdot}C_1{\cdot}C_2{\cdot}\exp(-\delta_1/T)$, $S_2 = \rho{\cdot}A_2{\cdot}C_2{\cdot}C_5{\cdot}\exp(-\delta_2/T)$ are the chemical source terms;

$P_k = D/(U_0{\cdot}r_0) = 0.01$, $k = [1; 6]$, $P_0 = \lambda/(cp{\cdot}\rho_0{\cdot}U_0{\cdot}r_0) = 0.05$,

$\mathrm{Re} = U_0{\cdot}r_0{\cdot}\rho_0/\mu = 10000$ is the Reynolds number,

$\mu = 5{\cdot}10^{-7}$ kg${\cdot}$(m${\cdot}$s)$^{-1}$ – the kinematic viscosity,

$S = V_0/U_0 = 3$ – the swirl number.

The equations were made dimensionless by scaling all the lengths to r_0, the meridian velocity to U_0, the azimuthal velocity to V_0, the temperature to T_0, the density to ρ_0, the pressure to $\rho_0 U_0^2$, the time to t_0. The value of the finite Reynolds number Re = 10000 is the stabilization factor to approximate the velocity equations. For the dimensionless pressure p we use a model for perfect gas: $p = \rho T$.

The boundary of the combustor ($r = r_0$) is subjected to a heat loss modelled by the Newtonian cooling to the ambient surroundings at temperature T_0, and with heat transfer coefficient $h = 0.1$ J${\cdot}$(s${\cdot}$m$^2{\cdot}$K)$^{-1}$. The dimensionless boundary conditions are described in [8].

Results and discussion

In the physical experiment the effects of wheat straw co-gasification/co-combustion with propane were studied using a batch-size pilot device, which combines a biomass gasifier and the water-cooled sections of a combustor. The gasifier was filled with straw briquettes by varying the electric field from 0 up to 4.66 mA. The thermal decomposition of the mixture was initiated by an external heat source – by a propane flame flow with average heat input 1 kW and duration of the heat input up to 1000 s.

In the numerical experiment the additional heat supply for co-firing straw with propane is neglected. It should be noticed that increasing the propane and additional heat supply into the device, the inlet temperature of volatiles increases, determining the variations of the reaction rates and the temperature in the flame reaction zone. Hence, reviewing the obtained numerical results from the mathematical modeling, it is suggested, that more factors should be counted in the mathematical model to improve the numerical results and make them more applicable to the simulation of the experimentalwork.

The approximation is based on implicit finite difference vector-schemes.To solve the discrete problem, the ADI method of Douglas and Rachford (1956) was used in the vector form of 11 elements from unknown values. The discrete 2D problem with 40x80 uniform grid points and the time step 0.0008 s were solved. For the stationary solution with the maximum error 10^{-7} approximately 5000-7000 time steps were used (the final time $t_f = 5$ s).The numerical results depending on (x, r, t) are obtained for $0 < x < 2$; $0 < r < 1$; $0 < t < 5$.The maximal values of the temperature max$T$, of the axial and radial flow velocities Maxw, Maxu and mass fractions of species are obtained. The mass fraction of reactants OH decreases to zero by $t = t_f$. The numerical results depending on the electric current and parameter Par are obtained in Tab. 1

Table 1

Values of Maxw ,Maxu, MaxT, Ckend, k = 1;3;4;6, tf = 5

I mA; P_{ar}	0;0	1.13; 0.23	2.65;0.53	3.57; 0.71	4.66; 0.93
C10 (H_2)	0.16	0.17	0.19	0.20	0.22
C50 (CO)	0.34	0.41	0.45	0.46	0.51
C20 (OH)	0.50	0.42	0.36	0.34	0.27
C1 end (H_2)	0.123	0.143	0.164	0.174	0.193
C3 end (H_2O)	0.311	0.183	0.110	0.096	0.064
C4 end (H)	0.029	0.025	0.021	0.020	0.016
C6 end (CO_2)	0.634	0.641	0.684	0.658	0.633
max w, m·s^{-1}	0.431	0.464	0.473	0.420	0.382
max u, m·s^{-1}	0.254	0.265	0.272	0.259	0.255
max T, K	1014	1290	1450	963	850

In the table we can see that for the fixed electric field 2.65 mA, ($P_{ar} = 0.53$) the maximal value for the temperature, velocities and mass fraction of the product CO_2 are obtained. This is in accordance with the data of the experimental study [11]. The mass fraction of reactants CO in the reactions decreases for all way of the electric field.

In the following Fig. 3-8 for the fixed value Par are represented the development, temperature, axial velocity, vectors of current density, electric field and concentrations in the time and space. The concentrations of products (CO_2,H,H_2 O) are increasing, but the concentrations of reactants (CO,H_2,OH) are decreasing. In figures the following results are represented:

Fig. 3 – maximum of the dimensionless temperature in a short time interval [0,0.1] is increasing from 1 (300 K) to 5.5 (1650 K) and then decreased in the time to asymptotic value 4.3 (1290 K).

Fig. 4 – minimal value of the mass fraction of reactant OH in a short time interval [0,0.05] is decreasing from 0.27 to zero.

Fig. 5 – maximal value of the mass fraction of the product H_2O in a short time interval [0,0.1] is increasing from 0 to asymptotic value 0.311.

Fig. 6 – profile of dimensionless density with the maximal value 1 for $x = 0$ (at the inlet) is decreasing in x and r to asymptotic value 0.1 for $x = 2$ (at the outlet).

Fig. 7 – profile of dimensionless axial velocity with the maximal value $w = 4.73$ ($u_z = 0.473$ m·s^{-1}) for $x = 2$ (at the outlet) is increasing in x from 1 ($u_z = 0.1$m/s) for $x = 0$ (at the inlet).

Fig. 8 – maximal value of the mass fraction of the product CO_2 in a short time interval [0,0.1] is increasing from 0 to asymptotic value 0.684.
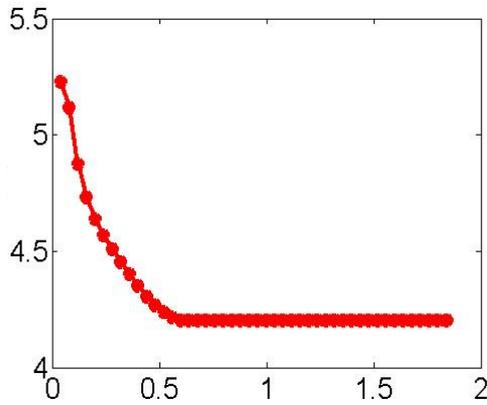
Fig. 3. **Maximal temperature T/T_0 depending on $P_{ar} = 0.23$**
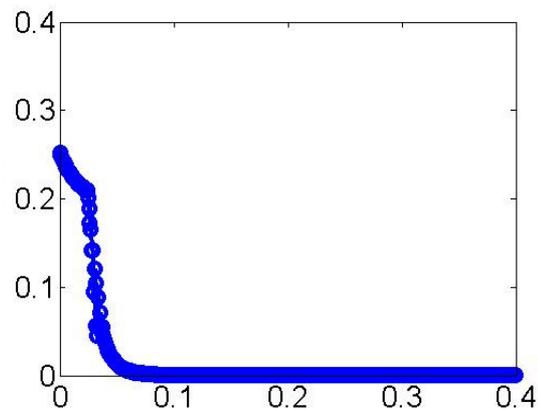
Fig. 4. **Minimal value OH depending on t for $Par = 0.93$**
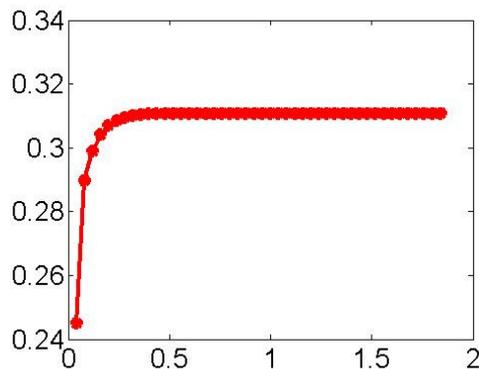
Fig. 5. **Maximal value of H_2O depending on $P_{ar} = 0$ for fixed r**
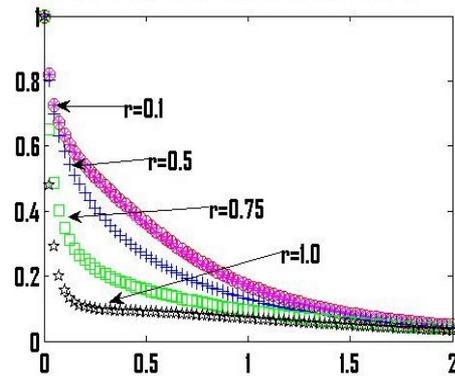
Fig. 6. **Profile of density ρ/ρ_0 depending on x on t for $P_{ar} = 0$**
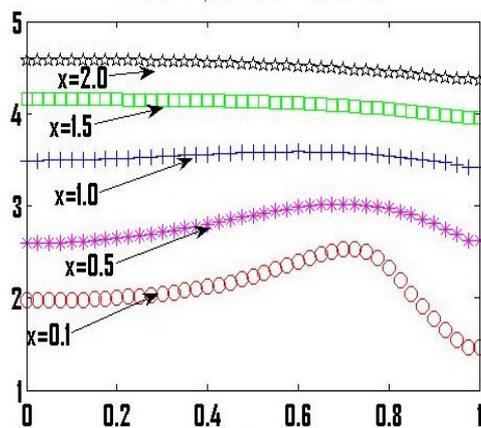
Fig. 7. **Axial velocity w depending on r for $P_{ar} = 0.53$ with maximum 0.473**
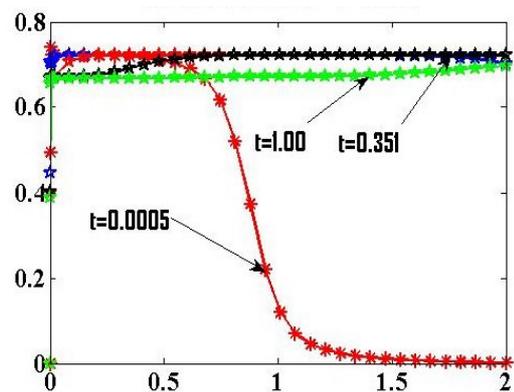
Fig. 8. **Concentration of CO_2 (max = 0.684) depending on x for fixed t, $P_{ar} = 0.53$**

Conclusions

1. Two dominant second-order exothermic chemical reactions with reactants CO, H_2 , OH and products CO_2 , H, H_2O are analysed.

2. The electric field is modelled with the charge and electron distribution at the surface of the cylindrical pipe by using constant ion mobility.

3. The results of the numerical simulation have revealed that at thermo-chemical conversion of biomass pellets and their mixtures the maximal values of the temperature, flow velocity and mass fractions of the product CO_2 are obtained during co-firing straw with propane for fixed value of the electric field 2.65 mA ($P_{ar} = 0.53$).

4. The comparison of the experimental and modelling results is rather qualitative in some cases due to complexity; reviewing the obtained numerical results from the mathematical modelling it is suggested that more factors should be counted in the mathematical model to improve the numerical results.

Acknowledgements

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