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System Approach from Biomass Combustion in Packed Bed Reactor

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The combustion of bed fuel in a packed bed reactor can be assumed very complicated. Researchers have studied this problem for many years. Such studies have been performed by both empirical and computational methods. However, due to the sharp increase in the development of computer science-based packages, the Computational Fluid Dynamics (CFD) technique can be applied to simulate and analyze the performance of the combustion reaction. Consequently, this has saved on empirical expenditures and has provided more understanding about the research objective.

This paper models the computation of bed fuel combustion in a packed bed reactor using Fluent version 6.2. The User Defined Functions (UDFs) were created to define the system as well as the boundary conditions, initial conditions, and dynamic mesh deforming. Furthermore, the source terms, heat exchanges, and homogeneous reactions were also defined in UDFs. The species transport and volume reaction were used to model the gas phase, where the Eulerian model was employed to solve the problem using two-phase modelling. The k-ε submodel was employed for turbulence, together with an unsteady model, since the problem was regarded as unstable. The results obtained from the modelling work would give more understanding about bed fuel combustion in a packed bed reactor.

INTRODUCTION

The combustion in incinerator is considered as a very complicated process. Currently, the ways of the researchers studying the combustion process are the practical and modelling methods. The research in this field contributed more understanding to the combustion science (Yang et al. 2005a; Thunman and Leakner 2005; Khor et al. in press; and, Ryu et al. 2006). All the methods to study the combustion process are covered by the system approach methodology. However, there has not been any research performed to study the combustion process in the right way of the system approach methodology so far.

The Fluent modelling code is well known among computational fluid dynamics software users. Many applications in science and engineering employs Fluent modelling code to solve a problem. The combustion of solid fuel in packed bed reactor, however, has not been included in the Fluent code. Therefore, in order to solve the problem, the user defined functions (UDFs), which are, fortunately, supported by Fluent as an open source, were created to define the system.

This study presents the new method to study combustion in a packed bed reactor by using the system approach as a methodology, borrowing a proper solver, combining with the special definition for the system to solve the problem.

SYSTEM APPROACH METHODOLOGY

The System Approach (Le Xuan Hai 2007) is one of the most important methodology used for studying nature phenomena and social problems.

To study a technical object following the system approach method, the object could be partition into the sub-system, so that it could be understood clearly the process, properties of the substances in the sub-system. Then, the model will be built up and will be operated to predict the performance of the technical object. Figure 1 shows the logical procedure of the system approach.

APPLYING SYSTEM APPROACH TO STUDY COMBUSTION IN A PACKED BED REACTOR

Qualitative Analysis of the System Structure

Figure 2 shows the application of the system approach.

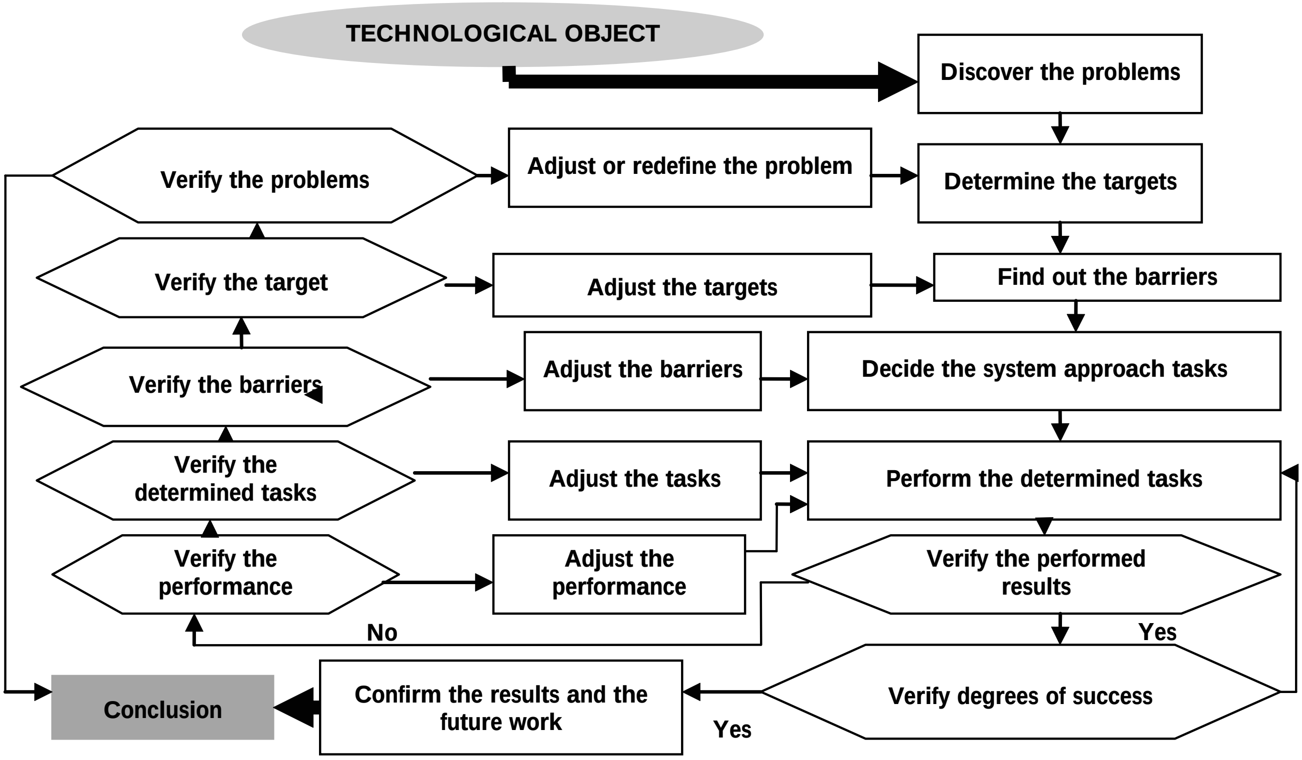


Figure 1. Logical Procedure of the System Approach

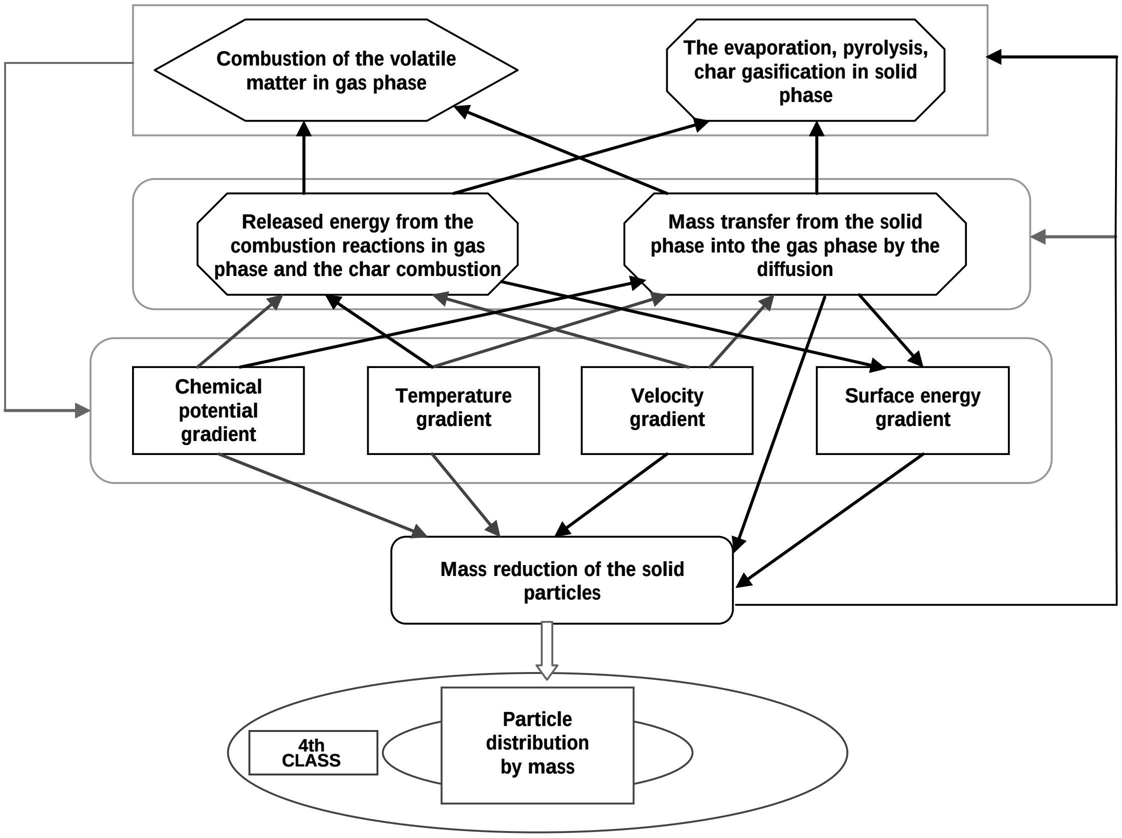


Figure 2. Qualitative Analysis of System Structure

MATHEMATICAL DESCRIPTION

Continuity equations.

Gas phase:

$$\frac{\partial(1-\varepsilon_s)\rho_f}{\partial t}+\nabla.((1-\varepsilon_s)\rho_f\upsilon_f)=S_m \qquad (1)$$

Solid phase:

$$\frac{\partial\left(\varepsilon_s\rho_s\right)}{\partial t}=-S_m \qquad (2)$$

t is the time, s

1-ε_s is the porosity of the fuel bed,

ρ_f is the density of gas phase in the system, kg/m^3 $\rho_f=\dfrac{p_{op}}{\frac{R}{M}T}$; and,

υ_f is the superficial velocity of the gas phase, *m/s*.

The source term S_m is the mass conversion rate from solid phase to gas phase due to moisture evaporation, devolatilization, and char combustion.

Energy conservation equations.

Gas phase:

$$\frac{\partial\left[(1-\varepsilon_S)\rho_f h_f\right]}{\partial t}+\nabla[(1-\varepsilon_S)\rho_f\upsilon_f h_f]=\nabla(k_f\nabla T_f)+S_{g,Q} \qquad (3)$$

Solid phase:

$$\varepsilon_s\rho_s C_{p,s}\frac{dT_{solid}}{dt}=\nabla(k_s\nabla T)+S_{s,Q} \qquad (4)$$

where, h_f is the gas phase enthalpy, *kJ/kg*.

$$h_{s,(f)} = \overline{C}_p \Delta T_{s,(f)} = \int C_{ps,(f)} dT_{s,(f)} \qquad (5)$$

The heat $S_{g,Q}$ represents the heat gain of the gas phase due to combustion in gas phase within the control volume.

Species conservation equations in gas phase.

$$\frac{\partial\left[(1-\varepsilon_S)\rho_f Y_i\right]}{\partial t} + \nabla[(1-\varepsilon_S)\rho_f \upsilon_f Y_i] = \nabla(D_{a,cff}(1-\varepsilon_S)\rho_f \nabla Y_i) + S_i \qquad (6)$$

where

i represents individual species: *i*=CO, CO_2, H_2, CH_4, C_xH_y, H_2O, O_2, and tar (gas); and,

$D_{a,eff}$ is the effective axial dispersion coefficient,

$$D_{a,eff} = D_i + 0.5\upsilon_f d_p \qquad (7)$$

D_i is the molecular diffusion coefficient.

The source term S_i represents the rate of individual species production during moisture evaporation, devolatilization, and the combustion of volatiles and char.

SOLVING THE PROBLEM

To solve the problem, the Fluent code was employed as a solver. Since the combustion of solid fuel in packed bed is considered very complicated and has not been included in the Fluent code, the user defined functions were created to solve the problem.

Main assumptions.

1. The gas is in plug-flow. The gas is described as an ideal gas.
2. No fragmentation, attrition, or agglomeration of solids takes place.
3. The effects of volume reduction during the drying, pyrolysis, and combustion are neglected. The packed bed is stationary when the air-flow rate is less than 0.27 kg/(m^2 s).
4. The fuel is composed of C, H, and O. The gas-phase species included in the model are CO, CO_2, H_2O, O_2, H_2, CH_4, tar (described by C_xH_y and CH_mO_n, respectively), and inert gas N_2.

Define source term. The source term can be expressed, in general, as:

$$S_\phi = S_u + S_p\phi_p \qquad (8)$$

where, ϕ is the dependent variable, S_u is the explicit part of the source term, and $S_p\phi_p$ is the implicit part.

Define heat transfer.

$$Nu = \frac{\alpha_1 1_s}{K_g} = 2.0 + 1.1\,\mathrm{Re}^{0.6}\,\mathrm{Pr}^{1/3} \qquad (9)$$

$$\mathrm{Pr} = C_{pf} \cdot \mu_f / K_g \qquad (10)$$

$$\mathrm{Re} = \rho_f \upsilon_f 1_s / \nu_f, \qquad (11)$$

Where C_p is the specific heat capacity, *J/kg·K*; ρ_f is the gas density, *kg/m³*; 1_s is a specific dimension of solid material, it can be calculated as the equivalent diameter of material, *m*; and, ν_f is the gas kinematics viscosity, *m²/s*.

In solid phase, during combustion, heat is transferred from the top to the bottom of the bed fuel by radiation. The radiative heat transfer can be assumed as following:

$$(-1)^{i-1}\frac{dI_j^i}{dx_j} = -k_a\left(I_j^i - \frac{1}{4}E_b\right) \qquad (12)$$

where, *i* denotes the radiation intensity for incident (*i* = 1) or reflex (*i* = 2) rays;

j is spatial variable, denoted by the x, y, or z or direction;

k_a denotes the absorption coefficient,

$$k_a = -[1n(1-\varepsilon_s)]/l_s \qquad (13)$$

and, E_b is the black body radiation.

Define mass transfer.

$$Sh = \frac{k_c l_s}{D} = 2.0 + 1.1\,\mathrm{Re}^{0.6}\, Sc^{1/3} \qquad (14)$$

$$\mathrm{Sc}=\mu_f/(\rho_f \mathrm{D}) \qquad (15)$$

k_c is the mass transfer rate coefficient, *m/s*;

D is the diffusion coefficient in the bulk, m^2/s; and,

K_g is the thermal conductivity of gas phase, *W/m.K.*

Define moisture evaporation and heterogeneous reaction rate.

Moisture evaporation

When the temperature is less than the evaporated temperature, the rate of evaporation can be calculated as following:

$$r_{H_2O} = k_c \cdot A_S \cdot (C_{w,s} - C_{w,g}) \qquad (16)$$

where, k_c is the mass transfer coefficient, *m/s*.

The concentration of vapor at the surface is evaluated by assuming that the partial pressure of vapor at the interface is equal to the saturated vapour pressure, p_{sat}, at the solid temperature, T_s.

$C_{w,s}$ is the vapor concentration at the surface, $C_{w,s} = p_{sat}/RT_s$, kgmol/m^3.

The concentration of vapor in the bulk gas is known from solution of the transport equation for species H_2O.

$C_{w,g}$ is the vapor concentration in the bulk gas, $C_{w,g} = X_i \cdot p_0/RT_g$, kgmol/m^3.

p_{sat} is the saturated vapor pressure, *Pa*.

R is the universal gas constant, $R = 8.314$, *L·kPa/mol·K*

X_i is the local bulk mole fraction of species i, here, the species *i* is the vapour.

p_0 is the operating pressure, *Pa*.

T_g is the local bulk temperature in the gas, K

In case of temperature in solid phase is higher than the boiling point of water, the rate of evaporation should be:

$$r_{H_2O} = \frac{1}{L_w}\left[k_1 A_s (T_g - T_s) + \mathrm{e}_s A_s \sigma (T_{rad}^4 - T_s^4)\right] \qquad (17)$$

where, L_w is the latent heat of water evaporation, *J/kg.*

The evaporation is assumed to stay at constant temperature while the boiling rate is applied. The energy required for vaporization appears as a (negative) source term in the energy equation for the gas phase.

De-volatilization

The volatiles are composed mainly of CO, CO_2, H_2, CH_4, C_xH_y, CH_mO_n, and other trace compounds. The pyrolysis may be described simply as a one-step global reaction:

$$\text{Material} \rightarrow \text{char} + \text{volatiles}$$

The single kinetic rate de-volatilization model assumes that the rate of de-volatilization is first-order dependent on the amount of volatiles remaining in the solid:

$$r_{vol} = K_{vol}\cdot[m_s - (1-f_{v,0})(1-f_{w,0})m_{s,0}] \qquad (18)$$

where, K_{vol} is the rate constant of de-volatilisation, s^{-1}.

$$K_{vol} = k_2 Exp(-E_V/RT_s) \qquad (19)$$

r_{vol} is the de-volatilization rate, *kg/s.*

m_s is the mass of solid fuel at time *t, kg.*

$m_{s,0}$ is the initial mass of solid fuel, kg.

$f_{v,0}$ is the mass fraction of volatiles initially present in the solid.

$f_{w,0}$ is the mass fraction of water in evaporating and boiling process.

k_2 is the constant in the Arrhenius equation, s^{-1}.

The yields and evolution patterns of the volatile products are a function of temperature and, to a minor extent of heating rate and particle size, among others. The volatiles composition mass fraction used in the model is obtained from literature data. For simplification, hydrocarbons such as acetaldehyde (CH_3CHO), acetic acid (CH_3COOH), and other very minor compounds are treated as tar.

Combustion of volatiles

Combustion of volatiles, particularly tar, is an important process in fixed-bed combustion. *Tar* is a complex mixture of condensable hydrocarbons. The amount and composition of tar that forms from pyrolysis depend on the type and properties of the material (moisture, particle size) and pyrolysis conditions (e.g. temperature, heating rate). For simplification, tar is modeled as hydrocarbon $CH_{1.84}O_{0.96}$, with a molecular weight equal to 95. The tar is oxidized to produce CO and H_2O:

$$CH_{1.84}O_{0.96} + 0.48O_2 \rightarrow CO + 0.92H_2O$$

The kinetic rate for tar oxidation is obtained from Bryden and Ragland:

$$r_{tar} = 2.9x10^5 T_e \, Exp\left(-\frac{9650}{T_e}\right) C^{0.5}_{CH_{1.84}O_{0.96}} C_{O_2} \qquad (20)$$

where,

$$\begin{cases} T_e = \alpha T_f + (1-\alpha)T_s, & T_f \le T_s \\ T_e = T_f, & T_f > T_s \end{cases} \qquad (21)$$

α is a weighting factor.

r_{tar} is the reaction rate per unit volume.

T_e is the mean temperature at which the rate should be calculated.

T_f is the temperature of the gas.

$C_{CH1.84O0.96}$ and C_{O2} are the species concentration.

Char oxidation

The char forms as volatiles escape from the materials. The reactivity of char, which is important for the development and optimization of the combustion system, not only depends on the properties of the materials and the pyrolysis conditions but also on the mineral content, such as potassium.

The primary products of char combustion are CO and CO_2. The char oxidation reaction is:

$$C + \gamma O_2 \rightarrow 2(1-\gamma)CO + (2\gamma - 1)CO_2$$

where, γ is the stoichiometric ratio for char combustion,

$$\gamma = (1/2 + 1/r_{CO/CO2})/(1 + 1/\, r_{CO/CO2}), \qquad (22)$$

$r_{CO/CO2}$ is the ratio of CO–CO_2 formation rate, which can be estimated by:

$$r_{CO/CO2} = CO/CO_2 = 12Exp(-3300/T_s) \quad (23)$$

Following the researches of Wu et al. (2002) and Yu et al. (1997), the rate of char combustion under chemical reaction control can be derived from thermal gravimetric analyzer (TGA) measurements at 973K and 10% O_2, and fitted to a first-order rate in the oxygen concentration:

$$r_{char} = K_{char} \cdot m_{char} \cdot p_{s,0} \quad (24)$$

$$K_{char} = k_3 Exp(-E_c/RT_s) \quad (25)$$

where,

r_{char} is the chemical reaction rate, s^{-1}.

$m_{char} = m_s -(1-f_{c,o})(1-f_{v,o})(1-f_{w,o})m_{s,o}$ the mass of char remaining, *kg.*

$p_{s,O2}$ is the oxygen partial pressure at the solid surface.

RESULTS AND DISCUSSIONS

The material used was is pinewood with a dimension of 1cm cube. The amount of pinewood was 1kg. The moisture content, volatile matter, fixed carbon, ash, and calorific value were obtained from the proximate analysis. The air supplied was 400L/min, which is equivalent to 0.212m/s superficial velocity or 0.27kg/(m^2·s). The air entered the computing domain at the bottom.

The UDFs were created to define the properties of solid fuel, sources of mass, energy, momentum, and species in both primary and secondary phases. The heat transfer, mass transfer, and heterogeneous reactions were also defined in UDFs to model the system.

In this study, the Fluent modelling code was employed to solve the conservation equations, that have been presented in the preceding section. Furthermore, to solve the multiphase problem, the Eulerian model was used. The unsteady model, together with the segregated solver, was used to conduct the solution.

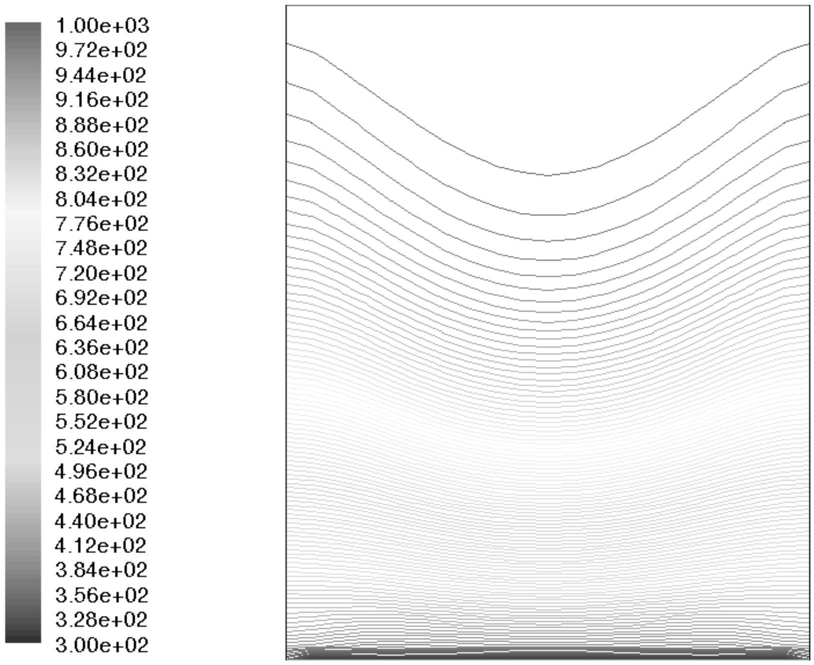
The calculated results are shown in Figure 3.

Within the first three hundred seconds, the flame moved down from the top to the bottom of the bed fuel. The temperature gradient of the bed fuel while the combustion occurs is very clear in the figures. There were three main regions within the bed fuel: the burning, pyrolyzing/gasifying, and drying areas. There have been two transition regions between the three main areas in the bed fuel. Furthermore, there was a phenomenon of the temperatures at bed wall were lower than temperatures at the middle of the bed fuel in the same section. These results reflected the genuine comprehensive combustion in the packed bed reactor.

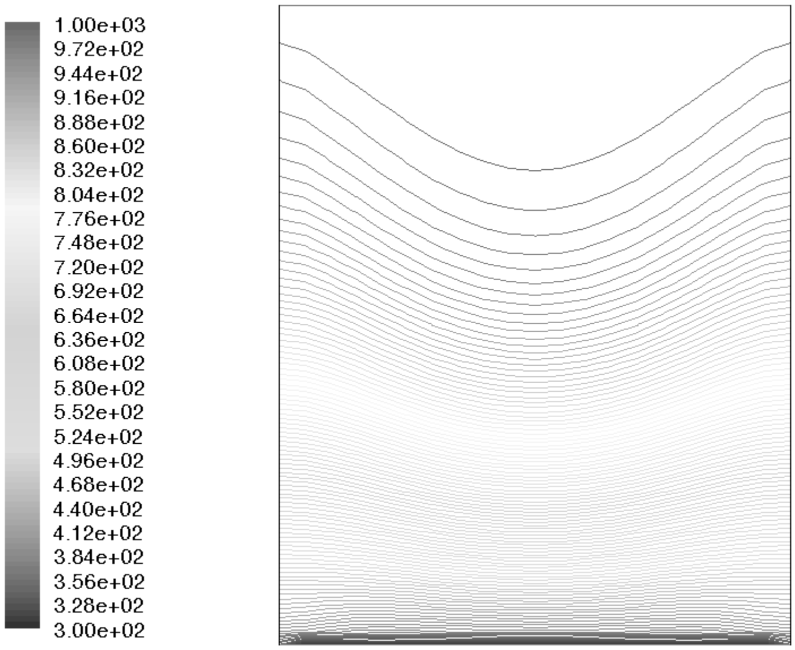
The maximum temperatures in solid phase and gas phase have been changed while the combustion was happening. For the first hundred seconds, the solid fuel absorbed energy from gas burning to increase the internal temperature. This caused the temperature in solid phase to lower than in gas phase as it increased while the combustion took place. When the temperature in solid phase was high enough, the heterogeneous reactions occurred and discharged energy. This caused the maximum temperatures to be similar in both solid and gas phases in this stage.

While the combustion was taking place within three hundred seconds and eight hundred seconds, the ignition was moving down slowly. This was because the stage of char combustion was occurring. This stage also released a huge amount of energy which caused the temperature of the entire computing domain to be high. These obtained computing results have played the similar rule with the real combustion phenomenon.

From the 700th to the 850th second, the computing results have shown that the combustion was going to finish. The temperature started going down quickly within 150 seconds to reduce 600°C. This may be because the combustible material has been finished while the air was still supplying to the computing domain.

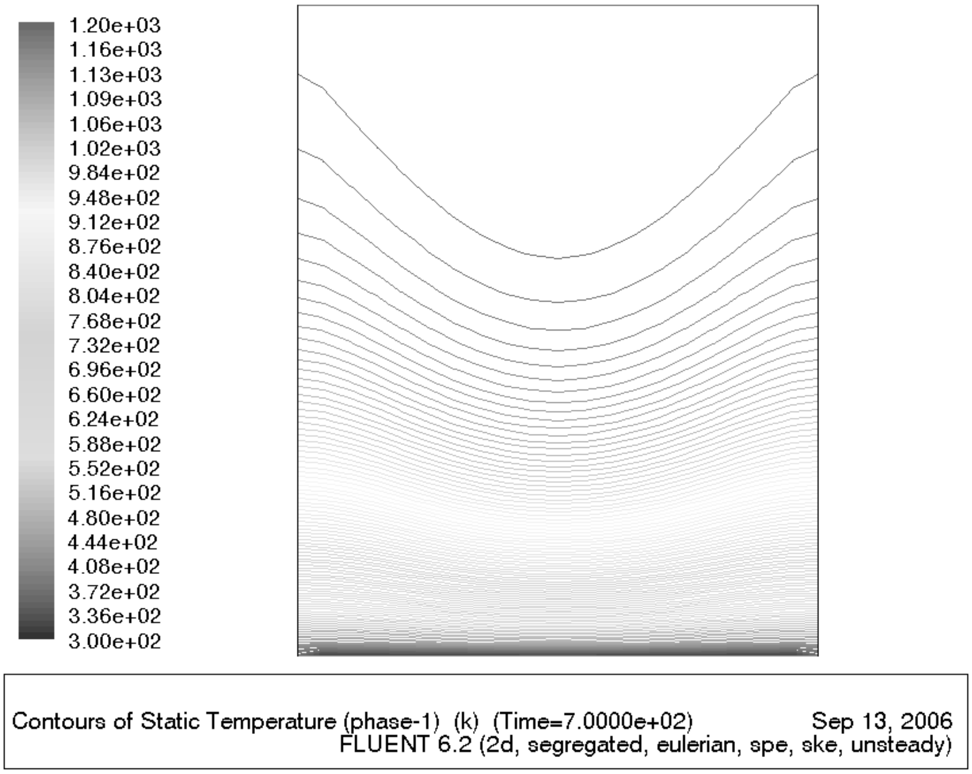


Contours of Static Temperature (phase-1) (k) (Time=3.0000e+02) Sep 13, 2006
FLUENT 6.2 (2d, segregated, eulerian, spe, ske, unsteady)



Contours of Static Temperature (phase-2) (k) (Time=3.0000e+02) Sep 13, 2006
FLUENT 6.2 (2d, segregated, eulerian, spe, ske, unsteady)

Figure 3. Temperature Profiles for the First 300



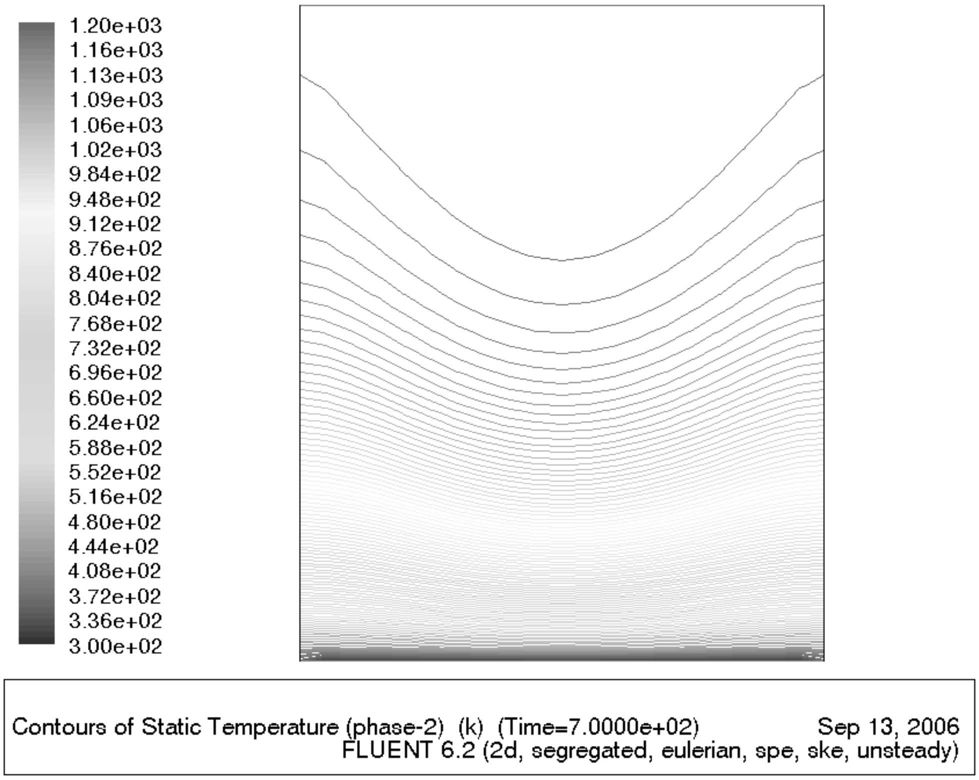
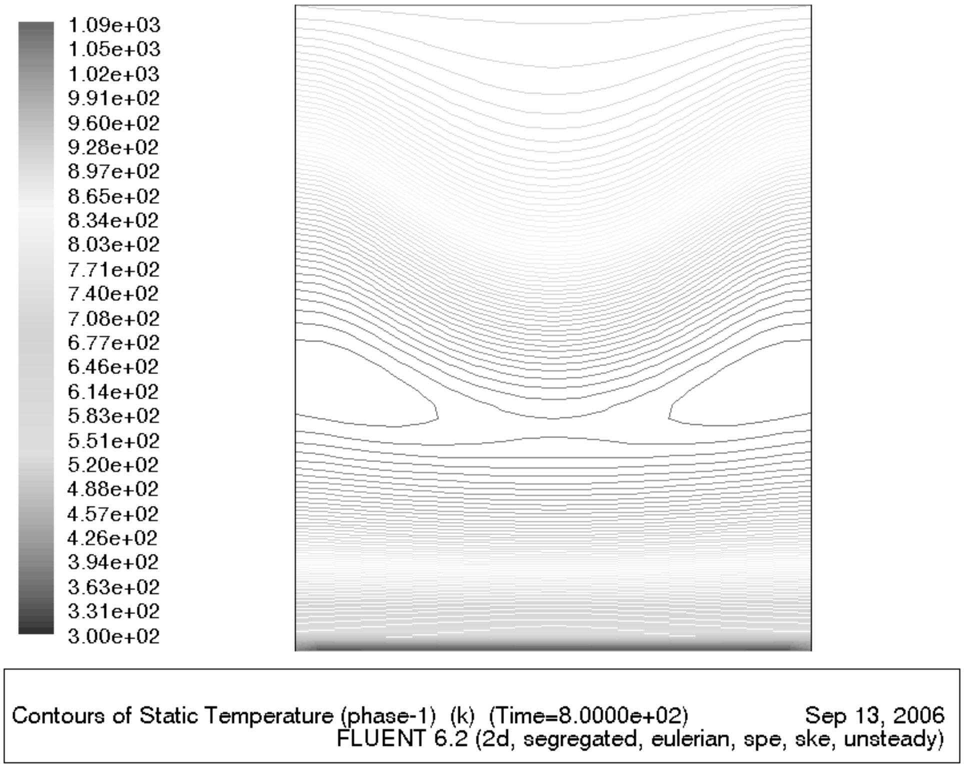


Figure 4. Temperature Profiles for the First 700



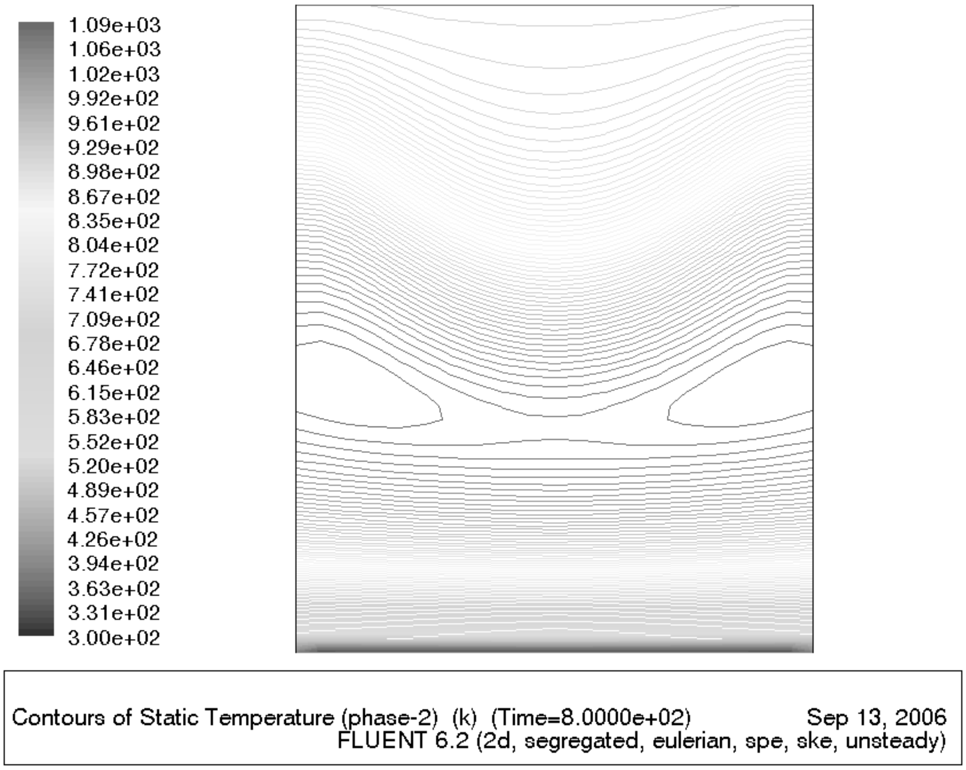
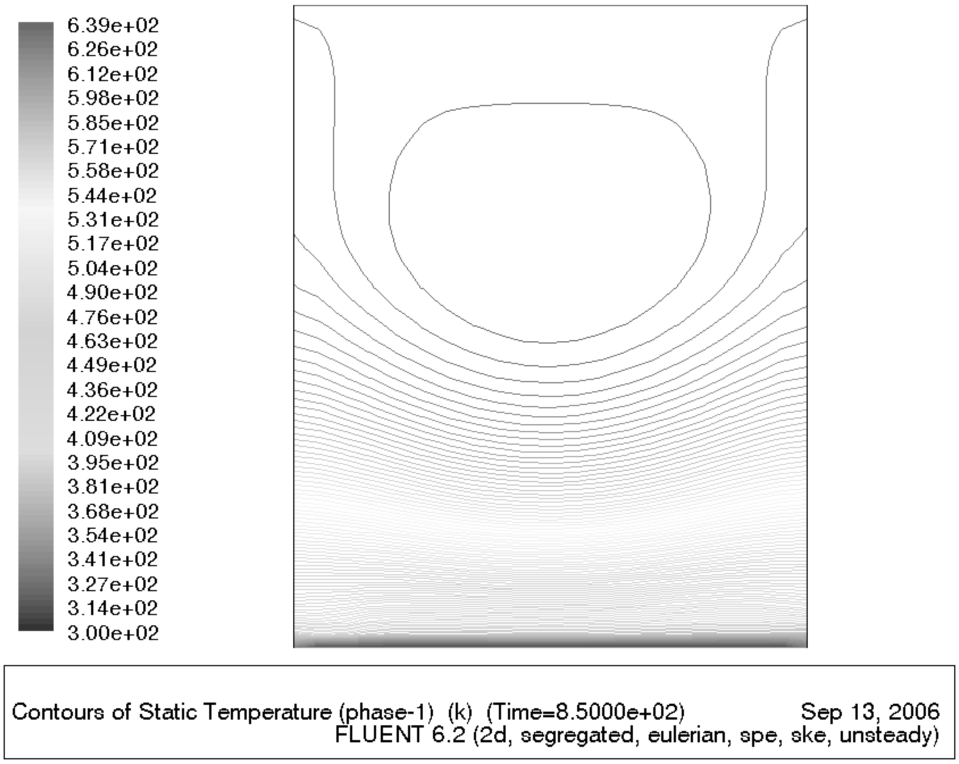


Figure 5. Temperature Profiles for the First 800



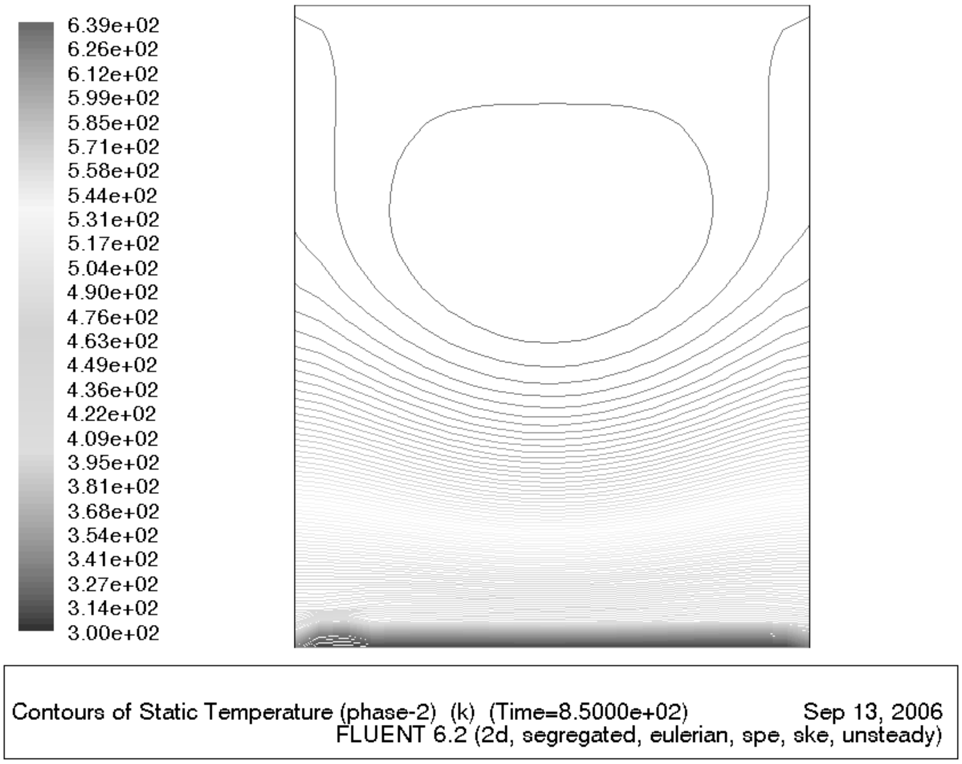
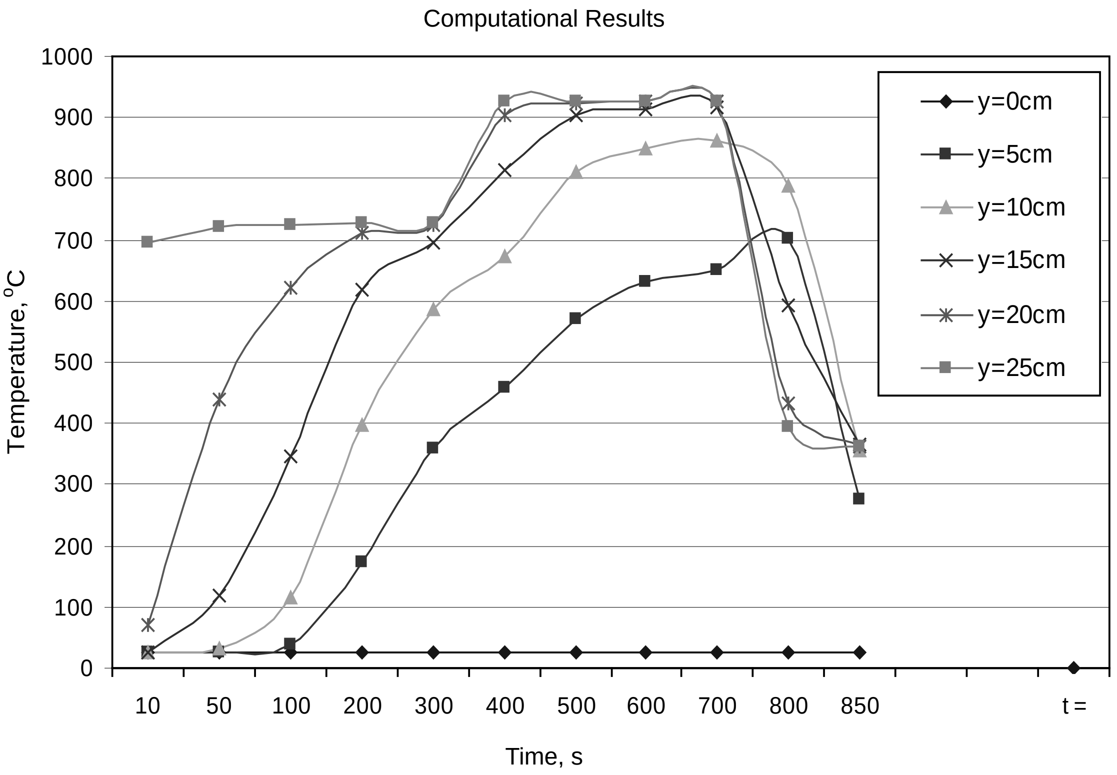


Figure 6. Temperature Profiles for the First 850



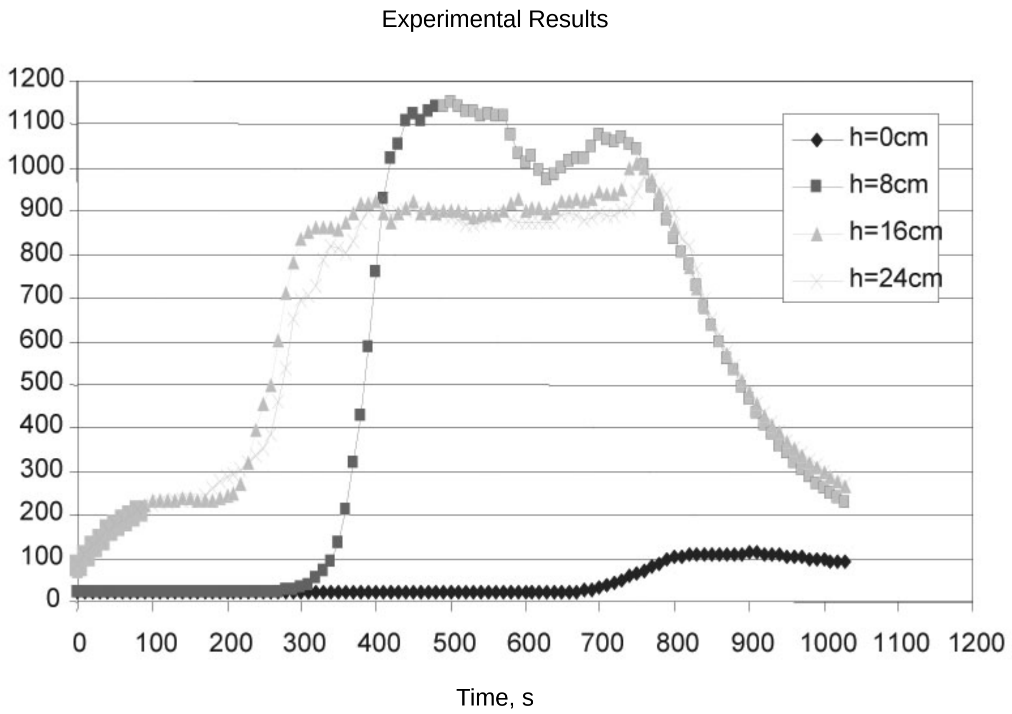
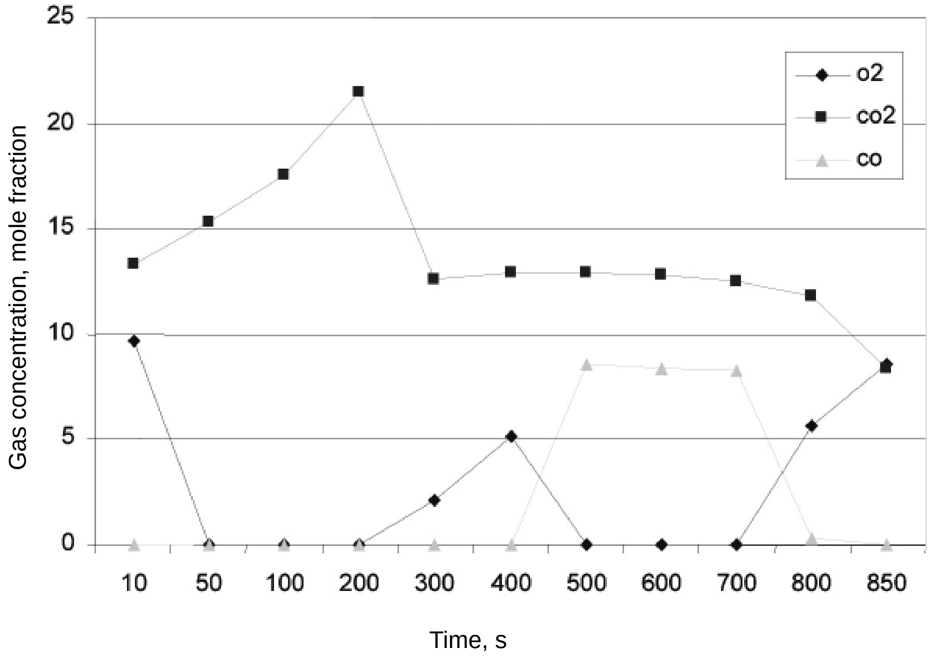


Figure 7. Temperature Profile of Computational and Practical Results

Computational Results



Experimental Results

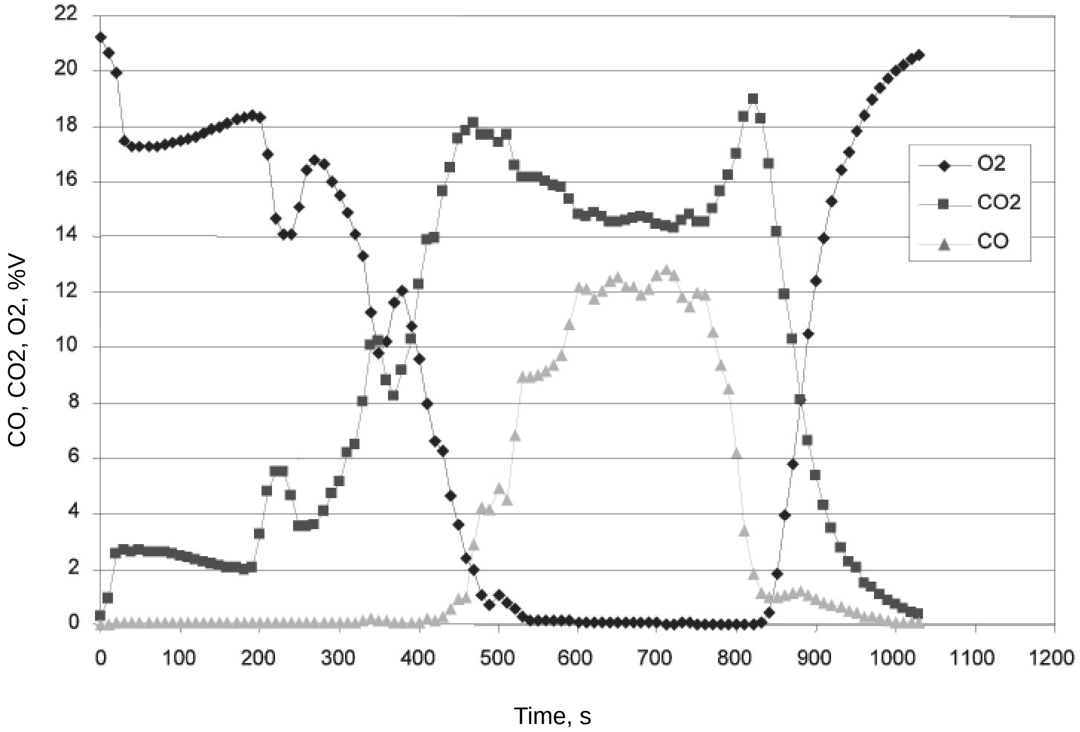


Figure 8. Gas Compositions of Computational and Practical Results

The comparison between practical and computational results, which are shown in Figure 7, gives more understanding of the predicted accuracy.

Within the first 700 seconds, computing results showed the temperatures at the bed heights of 10 and 5 cm were lower than temperatures at at bed heights 15, 20, and 25 cm of bed height while the practical results played the same rule only within the first 400 seconds. Furthermore, the maximum temperature in case of experiment was higher than the maximum temperature of prediction at around 10cm of bed height. This was because in the simulation assumptions, the collapse and shrinkage of the bed fuel were neglected while the combustion was taking place. The prediction was conducted as the material burned gradually from the top to the bottom of the bed fuel while the real burning played the different rule.

The moving flame, however, in case of the experiment was faster than in the prediction. The prediction burning temperature started at the beginning and at the 210th in case of experiment. In the experimental results, the ignition took 170 to get through 16cm while it was 20cm per 250. The ignition speed variation of experiment and simulation was 15%. This was able to accept with the current prediction.

Gas compositions in predicted results were collected in whole computing domain using Mass–Weighted Average panel. The results in both cases played the analogous rule. This reason could be explained in the above section.

CONCLUSION

In this study, the temperature profile and gas composition during the combustion progress were monitored. This method can model the effects of particle size and optimal air supply to the combustion results. This method can also predict the combustion of different types and properties of material.

This method opens a new window for the researcher to understand properly the combustion of solid fuel in packed bed reactor. By employing the proper solver and new techniques of Fluent modelling code, the researcher saves much energy and time to concentrate on technical problems.

This study still has some gaps that need to be filled in future work. The main gaps are located in the main assumption, the user-defined function to obtain the mass loss data, and the database of kinetic reaction rates, which are available in literature.

This paper would introduce the system approach logical diagram which is considered an effective and strong methodology to study the complicated combustion of the set of solid waste elements in the packed bed reactor, one of the typical poly-disperse processes, in particular and to study the technological system in general.

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