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Steam Gasification of Wood Biomass in a Fluidized Biocatalytic System Bed Gasifier: A Model Development and Validation Using Experiment and Boubaker Polynomials Expansion Scheme (BPES)

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Abstract: One of the most important issues in biomass biocatalytic gasification is the correct prediction of gasification products, with particular attention to the Topping Atmosphere Residues (TARs). In this work, performedwithin the European 7FP UNIfHY project, we develops and validate experimentally a model which is able of predicting the outputs,including TARs, of a steam-fluidized bed biomass gasifier. Pine wood was chosen as biomass feedstock: the products obtained in pyrolysis tests are the relevant model input. Hydrodynamics and chemical properties of the reacting system are considered: the hydrodynamic approach is based on the two phase theory of fluidization, meanwhile the chemical model is based on the kinetic equations for the heterogeneous and homogenous reactions. The derived differentials equations for the gasifier at steady state were implemented MATLAB. Solution was consecutively carried out using the Boubaker Polynomials Expansion Scheme by varying steam/biomass ratio (0.5-1) and operating temperature (750-850°C).The comparison between models and experimental results showed that the model is able of predicting gas mole fractions and production rate including most of the representative TARs compounds.

Keywords: Biomass; Gasification; TAR; Hydrodynamic and kinetic model; BPES; Biocatalytic systems; Experimental test.

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1. Introduction

The current trend in the development of new-generation energy systems aims to integrate renewable energy sources feeding ‘community-scale’ energy systems integrated in the national grid. Biomass represents a suitable choice for such an approach: it is available locally in sufficient quantity, it can be easily stored, it has a quasi-zeroCO_2production/emission balance. Biomass absorbs CO_2 from the atmosphere during photosynthesis, and the CO_2 is then returned to the environment after thermal utilization. Because of this cycle, biomass is CO_2 neutral, making it an advantageous fuel source and a dominant choice for replacement of fossil fuels as the concern of global warming increases. Biomass materials known as potential sources of energy are agricultural residues such as straw, bagasse, and husk and residues from forest-related industries such as wood chips, sawdust, and bark (Werther et al., 2000; Strehler & Stutzle, 1987).

However, to foster the use of biomass in power generation, highly efficient and clean energy conversion devices must be developed and assessed, especially in the low-medium power range due to the low energy

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density of this fuel (Demirbaş, 2001; Rapagna *et al.* 2000).The gasifier used in this work, is based on the UNIQUE concept (UNIQUE Cooperative Research Project, 2013), consisting in a compact gasifier integrating into a single reactor vessel both the fluidized bed steam gasification of biomass and the hot gas cleaning system, by means of a bundle of ceramic filter candles operating at high temperature in the gasifier freeboard. Such a configuration produces a syngas free of TARs and Sulphur compounds and allows a remarkable plant simplification and reduction of costs (UNIQUE Cooperative Research Project, 2013; Foscolo & K. Gallucci, 2008; Heidenreich *et al*., 2008).

Fluidized bed gasifiers are advantageous for converting biomass, particularly agricultural residues, into energy: good contact between gas and solid, along with a high degree of turbulence, improves heat and mass transfer characteristics, enhances the ability to control temperature, and increases heat storage and volumetric capacity (Sadaka *et al*., 2002).

The activities described here are part of the simulations carried out in the European 7FP UNIfHY project. In particular the aim of this work is to develop and validate experimentally a model capable of predicting the performance of a steam blown fluidized bed biomass gasifier during steady state operation. This model will be utilized in future works for the simulations of a pilot scale dual fluidized bed gasifier (100 kWth) (Di Carlo *et al*., 2013) fed with different biomass feedstock. In this gasifier concept, the fuel is fed into the gasification zone and gasified with steam. The bed material, together with some charcoal, circulates to the combustion zone. This zone is fluidized with air and the charcoal is burned, heating the bed material that is circulated back to the gasifier supplying the thermal power needed for the gasification reactions. With this concept, the two reaction chambers (air combustion and steam gasification) are physically separated and it is possible to get a high-quality gas, with a reduced N_2 content even if air (instead of pure oxygen) is used for the combustion. The model described here will be utilized to simulate the steam gasification zone of the dual fluidized bed gasifier. The input variables of the numerical program included steam flow rate and steam to biomass ratio.P ine wood was chosen as biomass feedstock in the process. Many studies were done on TAR conversion to obtain a product gas with lower content of these compounds, increasing the efficiency of biomass utilization, and power generation (Han & Kim, 2008; Anis & Zainal, 2011).Most of the gasification models were reported for coal gasification and those dealing with biomass gasification did not include the hydrodynamic parameters which affect both the mass and heat interchange coefficients between the bubble and emulsion phases (Buekens & Schoeters, 1985). This model instead includes the hydrodynamic, transport and thermodynamic properties in the fluidized bed, composed of olivine sand. The hydrodynamic model is based on the two phase theory of fluidization where the fluidized bed consists of two regions, bubbles and emulsion, interacting with each other through interchange and diffusion of gas species simulated by a mass transfer coefficient. The properties of the fluidized bed, like bubble gas ascending velocity and bubble diameter along the reactor axis were calculated using typical correlations of the two phase theory of fluidization. The chemical model is based on the kinetic equations for the heterogeneous and homogenous reactions introduced in mass and heat balance equation. The gasifier model utilizes as input the results of the pyrolysis experimental tests carried out at the same temperature; biomass thermal decomposition (pyrolysis) is the first step of the thermochemical conversion process, and it influences strongly the final gas composition as well as TARs production resulting from the following gasification reactions. This model is based on a previous work of Di Carlo *et al.* (2013). In that work an enriched air gasifier was simulated and thus also the combustion reactions with oxygen were considered, differently to the model developed here that is used to simulate gasification only with steam.

Devi *et al.*(2005) used naphthalene component as the tar model and the catalytic activity of olivine is there investigated via steam-reforming. During dry reforming reaction with CO_2, naphthalene conversion of about 80% is observed. Jess (1996) uses naphthalene, toluene and benzene as aromatic hydrocarbons. The kinetics of the thermal conversion in the presence of hydrogen and steam were studied. The experiments were performed in a tubular flow reactor at a total pressure of 160 kPa, temperatures of 700–1400 °C, residence times of 0.3–2 s and different gas-phase concentrations of hydrogen, steam and the aromatics. Swierczynski *et al.* (2001,2008)use toluene as model component of tar. A model study in laboratory scale fixed bed reactor of toluene steam-reforming is performed, the toluene conversion obtained with Ni/olivine at 560 °C is the same as with olivine at 850 °C.

Fiaschi*et* & Michelini (2001) developed a mathematical model of biomass gasification kinetics in bubbling fluidized bed. It was one-dimensional, and considers two phases, a bubble and a dense phase. In addition to the reaction kinetics in the dense phase, mass transfer between the two phases and a quantitative estimation of local bubble and particle properties were included in the model.A comparison with experimental data from the literature was done, and showed a largely satisfactory agreement.

Nikooet & Mahinpey (2008) developed a model for biomass gasification in an atmospheric fluidized bed gasifier using the ASPEN PLUS simulator. This model addresses hydrodynamic and reaction kinetic parameters and different sets of operating conditions for a pine gasifier have been used to validate the model. Through this analysis they demonstrated that temperature increases the production of hydrogen and enhances carbon conversion efficiency, while carbon monoxide and methane show decreasing trends with increasing temperature; increasing steam-to-biomass ratio increases hydrogen and carbon monoxide production and decreases carbon dioxide and carbon conversion efficiency.

Sadaka *et al*. (2002) developed a two-phase biomass air-steam gasification model[8] that was then validated [20]using the experimental results obtained from a dual distributor fluidized bed reactor. The reactor was operated on wheat straw at various fluidization velocities, steam flow rates and biomass to steam ratios. They obtained a good agreement between the model predictions and experimental data under all operating conditions studied. The model predicted the temperatures of the bubble, emulsion and solid phases, the mole fractions of methane, hydrogen, carbon monoxide, carbon dioxide and nitrogen, and the HHV of the product gas with great accuracy (R2=0.88–0.98). The correlation coefficient (R2) for the gas yield was somewhat lower (0.75), which could be attributed to the assumption that the gases behaved ideally.

The analysis is based on a gasifier model that was developed by some of the authors in an earlier work [9] where only Naphthalene was chosen as TAR representative. In this work, TAR was divided in 4 main classes:Benzene, Toluene (1-ring), Phenol, Naphthalene (2-rings), aiming at improving the accuracy of the model.

2. Materials and Methods

2.1 gasification model

De-volatilization is a very complicated process and the distribution of products is particularly sensitive to the heat rate and the residence time in the reactor. The products of pyrolysis are composed of gas compounds CO_2, CO, H_2O, H_2, and CH_4, light and heavy hydrocarbons (TAR) and char. In fluidized bed gasifiers, the pyrolysis reactions can be considered as instantaneous (Nikoo & Mahinpey,2008). Then de-volatilization time was assumed negligible. In order to get realistic values for the input pyrolysis products and to validate the steam gasification model, experimental tests on a bench scale fluidized bed reactor were carried out.

The proposed gasification model was based on the following reactions, solved simultaneously:

$C+H_2O \rightarrow CO+H_2$ (R1)
$C+CO_2 \rightarrow 2CO$ (R2)
$C+2H_2 \rightarrow CH_4$ (R3)
$CH_4+H_2O \leftrightarrow CO+3H_2$ (R4)
$CO+H_2O \leftrightarrow CO_2+H_2$ (R5)
$C_6H_6+6H_2O \leftrightarrow 6CO+9H_2$ (R6)
$C_{10}H_8+10H_2O \leftrightarrow 10CO+14H_2$ (R7)
$C_7H_8+7H_2O \leftrightarrow 7CO+11H_2$ (R8)
$C_6H_5OH+5H_2O \leftrightarrow 6CO+8H_2$ (R9)

Kunii & Levenspiel (1990) proposed an improved fluidized bed reactor model for various fluidization conditions (Fig. 1).The hydrodynamic model is based on the two phase theory of fluidization where the fluidized bed consists of two regions, bubbles and emulsion, interacting with each other through one interchange mass transfer coefficient of gas, k_{be}.

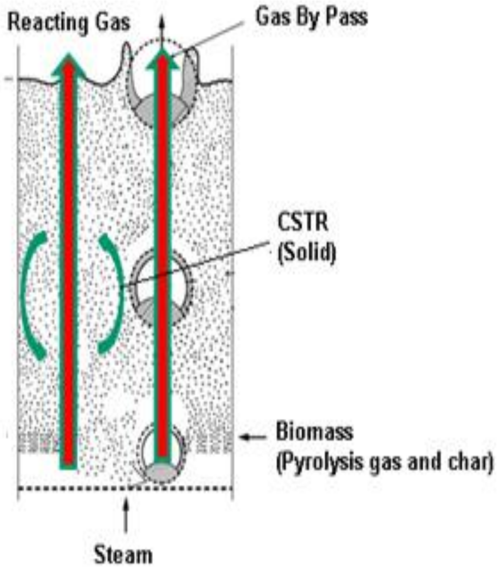

Figure 1: Kunii and Levenspiel fluidized bed reactor model

The model assumes plug flow for gas in emulsion and in bubble phase as well as complete mixing for solids in the emulsion phase. The combined hydrodynamic and chemical model was developed by Di Carlo *et al*.(2013) in earlier works.

Several assumptions are employed. The wake and cloud region is neglected. In the emulsion phase, gas ascends at the minimum fluidization velocity, u_{mf}.

$$u_{mf} = \left[\left(27.2^2 + 0.0408 \cdot Ar\right)^{0.5} - 27.2\right] \cdot \frac{\mu}{d_p \rho_{gas}}$$

In the bubble phase, bubble gas ascends at the velocity of u_b.

$$u_b(z) = 0.71\sqrt{g d_b} - \left(\frac{Q(z)}{A} - u_{mf}\right)$$

The bubble diameter is calculated by Davidson model at each bed height.

$$d_b(z) = 0.54\frac{\left(Q(z)/A - u_{mf}\right)^{0.4}}{g^{0.2}}\left[z + 4\sqrt{\frac{A}{N_{or}}}\right]^{0.8}$$

The volume fraction of bubble in the bed is δ and that of emulsion is (1- δ).

$$\delta(z) = \frac{Q(z)/A - u_{mf}}{u_b(z)}$$

For gas exchange between bubbles and emulsion the following transfer coefficient is considered:

$$k_{be}(z) = \frac{u_{mf}}{4} + \sqrt{\frac{4\varepsilon_{mf} D_r u_b(z)}{\pi d_b(z)}}$$

As a result, the transport equations solved at steady state are:

$$\frac{\partial}{\partial z}\left[\left(Q(z) - u_{mf}A\right)C_{bi}\right] = k_{be}A\left(C_{bi} - C_{ei}\right)\frac{6}{d_b}\delta + \\ + \varepsilon_{mf}A\delta\sum_{j,b}\nu_{ij}R^g_{bj}$$

$$\frac{\partial}{\partial z}\left[\left(u_{mf}\cdot A\right)\cdot C_{ei}\right] = k_{be}A\cdot\left(C_{ei} - C_{bi}\right)\frac{6}{d_b}(1-\delta) + A(1-\delta)\cdot \\ \left[\begin{array}{l}(1-\varepsilon_{mf})\cdot\varepsilon_c\frac{\rho_c}{PM_c}\cdot\sum_{j,s}\nu_{ij}\cdot R^c_{ej} + \\ + \varepsilon_{mf}\cdot\sum_{j,e}\nu_{ij}\cdot R^g_{ej} + (1-\varepsilon_{mf})\cdot\varepsilon_{oliv}\cdot\nu_{ij}\cdot R^{oliv}_{ej}\end{array}\right]$$

$$\frac{dm_c}{dt} = \dot{m}^{in}_c + \int_{Vbed}(1-\delta)(1-\varepsilon_{mf})\varepsilon_c\left[\rho_c\sum_j\nu_{ij}R^c_{ej} + PM_cR_{10}\right]$$

$$\varepsilon_c = \frac{m_c}{\rho_c}\cdot\left(\frac{m_c}{\rho_c} + \frac{m_{oliv}}{\rho_{oliv}}\right)^{-1}$$

Where *j* indicates the reaction (1…13), *i* are the chemical species and ν_{ij} is the stoichiometric coefficient of species *i* in reaction *j*, negative for reagents and positive for products.

Finally ideal gas law was used to calculate the gas concentration:

$$C_{tot} = \frac{p}{RT}\cdot$$

In order to complete the model, the kinetic expressions for the reaction rates are required. Owing to the small char particles diameter, extra and intra particle diffusion resistances were neglected.

For reaction R1 and R2 (gasification of char with steam and CO2) the expressions deducted by Barrio *et al.* (2001) and Barrio & Husted (2001) were used.

$$R_1 = \frac{k_{w1}p_{H2O}}{1 + \left(k_{w1}/k_{w3}\right)p_{H2O} + \left(k_{w2}/k_{w3}\right)p_{H2}}\left(1/s\right)$$

$$R_2 = \frac{k_{c1}p_{CO2}}{1 + \left(k_{c1}/k_{c3}\right)p_{CO2} + \left(k_{c2}/k_{c3}\right)p_{CO}}\left(1/s\right)$$

The kinetic data, shown in Table 1, were deduced from the work of Konttinen *et al.*(2003).

Table 1:
Pre-exponential and activation energy values

	$k0_1$ ($s^{-1}bar^{-1}$)	$k0_2$ ($s^{-1}bar^{-1}$)	$k0_3$ ($s^{-1}bar^{-1}$)	EA_1 (J/mol)	EA_2 (J/mol)	EA_3 (J/mol)
R_1	6.49E+07	95.3	1.64E+09	204000	54315	243000
R_2	1.64E+07	4.59E+02	8.83E+07	1.88E+05	8.83E+04	2.25E+05

Reaction R3 was neglected because of its very slow rate at low operating pressure.

Gas phase reactions (R4, R5) were simulated using the expressions adopted by Wang & Kinoshita (1993) (R4 and R5 are expressed in mol/m^{3}s)

$$R_4 = 2.79e^{-12579/RT}\left(C_{CO}C_{H2O} - \frac{C_{CO2}C_{H2}}{K^{WGS}_{eq}}\right)$$

$$R_5 = 1.2863e^{-36150/RT}\left(C_{CH4}C_{H2O} - \frac{C^3_{H2}C_{CO}}{K^{REF}_{eq}}\right)$$

For the heterogeneous catalytic reactions taking place on olivine particles, the kinetic expression obtained by Simell et al. (1999) was used for benzene (R6), while for the reactions R7-R9 the results in (Devi, 2005) were used to extrapolate first order kinetic expressions (reactions are expressed in (mol/kgcat.h)).

$$R_6 = \frac{1.72\cdot10^{11}e^{-197000/RT}C_{C6H6}}{\left(1 + 4.24\cdot10^{-7}e^{-105000/RT}C_{H2} + 6.99\cdot10^{-7}e^{-54200/RT}C_{H2O}\right)}$$

$$R_7 = 498.15e^{-42262/RT}C_{C10H8}$$

$$R_8 = 56239e^{-83386/RT}C_{C7H8}$$

$$R_9 = 9 \cdot 10^{11} e^{-200000/RT} C_{C6H5OH}$$

2.2 Gasification model

High-temperature biomass pyrolysis is the first step of the thermo-chemical process taking place in a fluidized bed gasifier; it influences strongly the final produced gas composition as well as TAR (heavy organics) production. In the model, biomass de-volatilization time was considered negligible, and in order to get realistic values for the pyrolysis products, experimental tests on a bench scale fluidized bed reactor were carried out at temperature close to those adopted for the simulations (750-800 °C). The results of the pyrolysis tests were integrated in the model as input data. In order to consider TAR evolution in the gaseous stream during the gasification process different representative compounds were chosen: Benzene, Toluene (1-ring), Phenol, Naphthalene (2-rings).The bench scale rig used in this work is schematized in Fig.2.

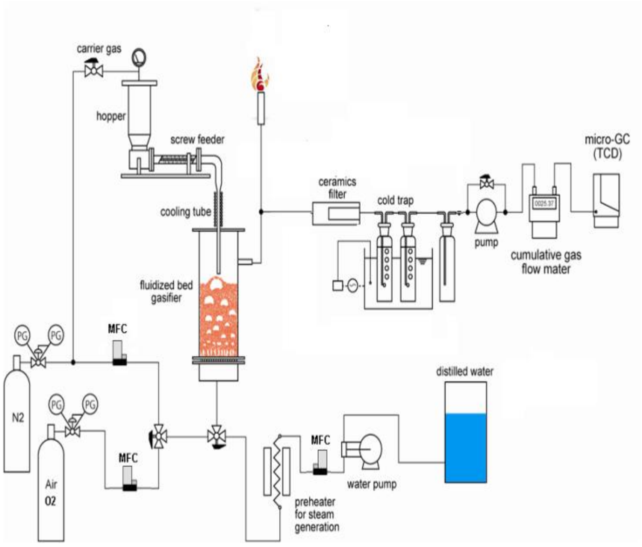

Figure 2. Experimental rig for pyrolysis and gasification tests

As shown in Fig. 2, the test rig consists of the following parts:

- ✓ Feeding systems for nitrogen, water (including steam generation), and air/oxygen.
- ✓ A fluidized bed reactor (80 mm ID) enclosed in a cylindrical electric furnace to maintain it at the desired temperature level. The bed consists of 350 μm olivine particles.
- ✓ A biomass feeding system at the top of the reactor that enables wood particles to be instantaneously dropped into the hot bed.
- ✓ A heated ceramic filter installed at the exit of the reactor for particulate removal.
- ✓ Gas cooling baths at ambient temperature and at −20 °C, respectively, to sample TARs in 2-propanol filled impingement bottles. TAR is then analysed by Agilent GC-MS 5975C.
- ✓ A gas cumulative flow meter.
- ✓ A gas chromatography analysers Varian micro GC to analyse the gas composition.
- ✓ Mass Flow Controller (MFC) allow to adjust the input flow-rates at the desired value

As mentioned above, pine wood was chosen as biomass feedstock, the elemental analysis is reported in Table 2, together with average particle size and density.

Table 2
Biomass Analysis

Type	Black Pine wood
Status	Raw
Moisture (wt %)	11
Ash (wt %)	0.5
Carbon (wt %)	49,1
Hydrogen (wt %)	6.36
Oxygen (wt %)	44.3
Particle size (mm)	1-2
Particle Density (kg/m^3)	510

Nitrogen was used as the fluidizing medium during pyrolysis tests. The composition of the produced gas was continuously monitored in terms of H_2, CO, CO_2 and CH_4. The mass flow of biomass was set equal to 170 g/h. Tests were carried out at 750 °C. The time-averaged results are reported in Table 3:

Table 3
Average gas composition obtained from pyrolysis tests

Gas yield (Nm^3/kg$_{bio(as\ received)}$)	0.81
Composition (%vol)	
H_2	32
CO	34
CH_4	19
CO_2	14

After pyrolysis, the feeding gas was switched to air to burn the residual char, allowing to evaluate CO and CO_2 produced in this process, measuring exit gas composition and flow. It was so possible to estimate that the carbon (char) produced during pyrolysis tests was equal to 0.18 (gchar/gbio(ar)).

Table 4 shows the produced TARs and their mass fractions, divided in 4 subgroups (Benzene, 1-ring, 2-rings, Oxygenated).

Table 4
Analysis of tar obtained from pyrolysis tests

TAR yield	108 g/Nm^3
Tar /bio(dry ash free)	0.09 (g/g)
Composition (weight fractions)	
Benzene	0.44
Toluene+Styrene+Xylene (1-ring)	0.20
Naphthalene+Indene (2-rings)	0.21
Phenol (oxygenated)	0.07

3. Model validation

3.1 Validation via ordinary differential equations (ODE) analysis and MATLAB calculation

The derived ordinary differential equations(ODE) for the gasifier model at steady state were implemented and solved with MATLAB. Simulations of thegasifier were carried out varying steam to biomass ratio (τ) and operative temperature from 0.5 to 1 and from 750 to 850 °C, respectively. In order to validate the model, experimental gasification tests were carried out at identical operative conditions, with the same test rig utilized for pyrolysis tests (Fig. 2), using steam instead of nitrogen as fluidization gas.

Fig. 3 shows, the gas composition and the gas product yields at different steam to biomass ratios, with a gasification temperature of 850 °C obtained by the model and compared with experimental results.

The comparison between the model and experimental results shows that model is fairly capable of predicting gas composition and production rate: in particular, the numerical and experimental results showed slight discrepancies lower than 2 % for the gas composition and lower than 4 % for gas product yields.

Figure 4 shows the gas composition and the total TAR concentration varying the gasification temperature in between 750 and 850°C maintaining the steam to biomass ratio equal to 0.7.

Also in this case, simulation and experimental results are in good agreement. The discrepancies is always lower than 2 % for CO_2, CH_4. H_2. CO shows a bigger discrepancy at 750 °C, but the difference is always lower than 5%. Figure 4 b) shows the comparison of simulated and experimental total TAR concentrations. Also for the TAR, the mayor difference between simulated and experimental data is always at low temperature, but, in this case, it is bigger. Indeed, at 750 °C the model shows a significant overestimation of 25 %.

Figure 5 below shows the comparison between simulated and experimental single TAR concentrations (Benzene, Toluene (1-ring), Naphthalene (2-rings), Phenol), obtained varying the temperature from 750 to 850°C, with steam to biomass ratio at 0.7.

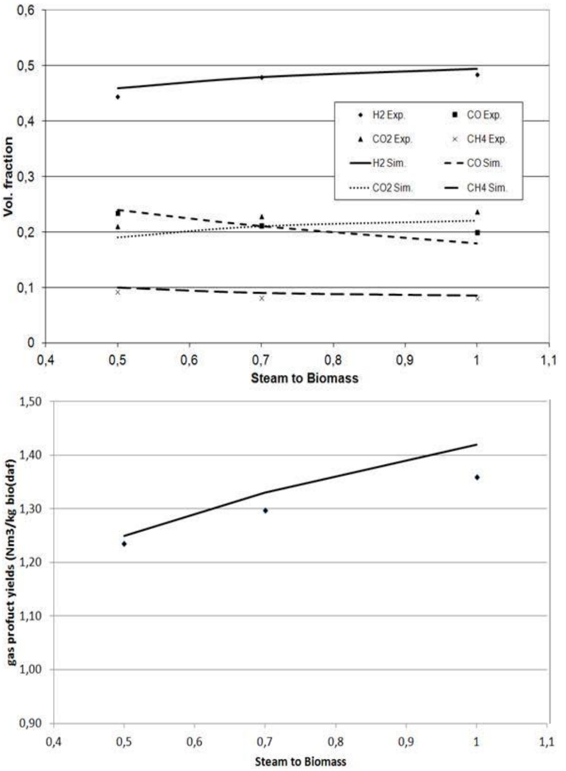

Figure 3. Gas composition (a) and gas product yield (b) at different S/B with T= 850 °C, obtained by simulation (line), and compared with experimental results (dots).

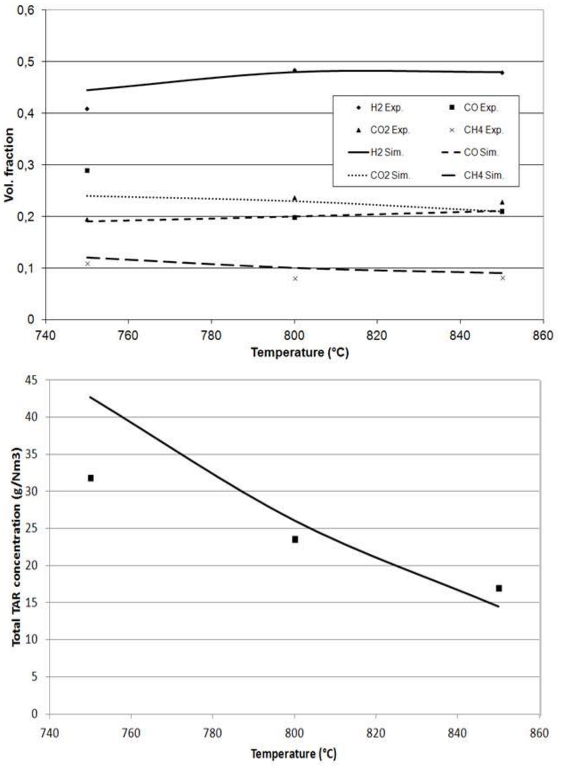

Figure 4. Gas composition (a) and total TAR concentration (b) at different T with S/B=0.7,obtained by simulation (line), and compared with experimental results (dots)

It was found also that Benzene, the lowest molecular weight TAR, is always the mayor TAR compound. It accounts for about 57% of all TAR compounds in all the conditions. 1-ring TAR accounts for about 25%, meanwhile 2-ring for about 17%, and Phenol for about 1%. Moreover it confirms that the mayor weight TARs are the ones that more decrease their concentrations at higher temperatures. Moreover the differences between simulated and experimental data are always below 20%, except for Benzene at 750°C, where the model overestimates the value of about 40% and at 850°C, where the model underestimates with discrepancies of about 30%.

3.2 Validation via the Boubaker Polynomials expansion Scheme BPES

3.2.a Fundamentals to the Boubaker Polynomials Expansion Scheme (BPES)

The Boubaker Polynomials Expansion Scheme BPES (Ghanouchi *et al*., 2008; Awojoyogbe & Boubaker, 2009; Labiadh & Boubaker, 2007; Slama *et al*., 2008, 2009; Tabatabaei *et al*., 2009; Fridjine & Amlouk, 2009; Belhadj *et al*., 2009a; 2009b, Barry & Hennessy, 2010; Yildirim *et al*., 2010; Kumar, 2010; Milgram, 2011; Rahmanov, 2011; Benhaliliba *et al*.,2011) is a resolution protocol which has been successfully carried out no several applied-physics and mathematics problems. The BPES protocol ensures the validity of the related boundary conditions regardless main equation features. The BPES is mainly based on Boubaker polynomials first derivatives properties:

$$\begin{cases} \left.\sum_{q=1}^{N} B_{4q}(x)\right|_{x=0} = -2N \neq 0; \\ \left.\sum_{q=1}^{N} B_{4q}(x)\right|_{x=r_q} = 0; \end{cases}$$

and:

$$\begin{cases} \left.\sum_{q=1}^{N} \frac{dB_{4q}(x)}{dx}\right|_{x=0} = 0 \\ \left.\sum_{q=1}^{N} \frac{dB_{4q}(x)}{dx}\right|_{x=r_q} = \sum_{q=1}^{N} H_q \\ \text{with} : H_n = B'_{4n}(r_n) = \left(\frac{4r_n[2-r_n^2] \times \sum_{q=1}^{n} B_{4q}^2(r_n)}{B_{4(n+1)}(r_n)} + 4r_n^3 \right) \end{cases}$$

Several solution have been proposed through the BPES in many fields such as numerical analysis, theoretical physics, mathematical algorithms, heat transfer, homodynamic, material characterization, fuzzy systems modeling and biology.

3.2.b Application of the Boubaker Polynomials Expansion Scheme (BPES)

In order to assess the validity of the actual model along with experimental results, simulations of the gasifier were carried out using the Boubaker Polynomials Expansion Scheme and by varying steam to biomass ratio and operative temperature from 0.5 to 1 and from 750 to 850 °C, respectively. The following assumptions are introduced to develop its mathematical model:

- ✓ Steam to biomass τ S/B lie between $\tau_{\min}$ =0.5 and $\tau_{\max}$ =1.0
- ✓ Compounds are accurately defined through molecular mass.
- ✓ Heat losses are neglected (adiabatic process).
- ✓ Ambient air is composed of 78.2% N_2, 20.7% O_2, 0.03% CO_2, and 1.0% H_2O in mole.
- ✓ Steam to biomass T lie between $T_{\min}$ =750° and $T_{\max}$ =850°

For normalization purposes, each experimental value of the variable M_i (here *H* values of τ_i or T_i)which varies inside the range $[M_{\min}, M_{\max}]$, is normalized as following.

$$\tilde{M}_i = \left[\frac{M_i - M_{\min}}{M_{\max} - M_{\min}} \right]$$

Consecutively, for each component, indexed as j, concentration in the gas $\left.\eta_j\right|_{j=0..4}$ is defined as a function of τ and T .

$$\left.\eta_j(\tilde{\tau}_i, \tilde{T}_i)\right|_{i=1..H,\, j=1..4} = \frac{1}{2N_0} \sum_{k=1}^{N_0} \lambda_{k,i,j} \times B_{4k}(r_k \tilde{\tau}_i) B_{4k}(r_k \tilde{T}_i)$$

where B_{4k} are the *4k*-order Boubaker polynomials, r_k are B_{4k} minimal positive roots, N_0 is a prefixed integer and $\left.\lambda_{k,i,j}\right|_{\substack{k=1..N_0 \\ i=1..H,\, j=1..4}}$ are unknown pondering real coefficients.

The main advantage of this formulation is the evidence of verifying the boundary conditions, in advance to problem resolution thanks to the properties of the Boubaker polynomials (Awojoyogbe & Boubaker, 2009; Labiadh & Boubaker, 2007; Barry & Hennessy, 2010; Yildirim et al., 2010; Kumar, 2010; Milgram, 2011; Rahmanov, 2011), besides proposing differentiable and piecewise continuous solutions (Ghanouchi *et al*., 2008; Awojoyogbe & Boubaker, 2009; Benhaliliba *et al*.,2011).

The Boubaker Polynomials Expansion Scheme BPES is a resolution protocol which has been successfully applied to several applied-physics and mathematics problems. Several solutions have been proposed through the BPES in many fields such as numerical analysis, theoretical physics, mathematical algorithms, heat transfer, homodynamic, material characterization, fuzzy systems modelling and biology . The BPES protocol ensures the validity of the related boundary conditions regardless of main equation features. In fact, thanks to Boubaker polynomials first derivatives properties boundary conditions are inherently verified.

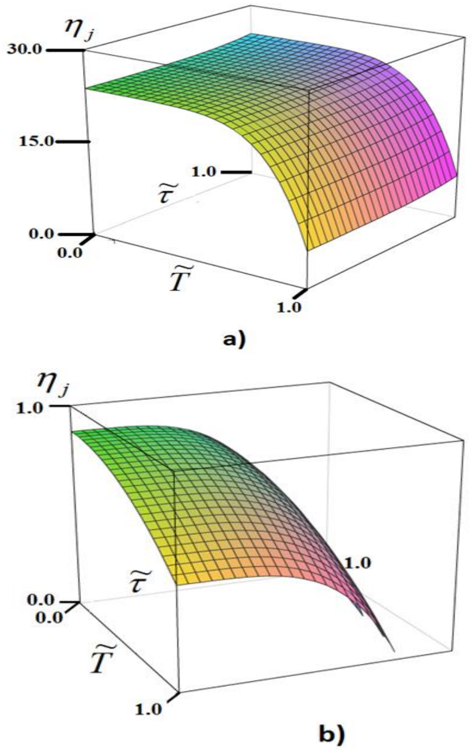

Figure 5. BPES solution plots in the $(\tilde{T},\tilde{\tau})$ plane < (a) Benzene (b) Phenol in g/Nm^3>

By taking into account the given expressions, boundary conditions become redundant since already verified by the proposed expansion and optimality of protocol-dependent efficiency . The BPES solution is obtained through six steps:

- Setting an arbitrary value of N_0.
- Calculation model values of the concentrations $\eta_j\Big|_{j=0..4}$ in the gas using experimental values $(\tilde{\tau}_i,\tilde{T}_i)\Big|_{i=1..H}$
- Computing the optimal set $\hat{\lambda}_{k,i,j}=\lambda_{k,i,j}\Big|_{k=1..N_0}$ which minimizes the quadratic error between the experimental values and those calculated through the formula:

$$\eta_j(\tilde{\tau}_i,\tilde{T}_i)\Big|_{i=1..H,j=1..4} = \frac{1}{2N_0}\sum_{k=1}^{N_0}\hat{\lambda}_{k,i,j}\times B_{4k}(r_k\tilde{\tau}_i)B_{4k}(r_k\tilde{T}_i)$$

- Incrementing the value of N_0.
- Testing convergence
- Setting final values of the unknown parameters $\hat{\lambda}_{k,i,j}=\lambda_{k,i,j}\Big|_{k=1..N_0}$

Figure 5 shows partial results for concentration in the gas of representative components: Benzene and Phenol. The obtained plots confirm the experimentally obtained efficiency range as well as recorded distribution (§2). They are also in good agreement with the records of Ruoppolo *et al*., (2012), Mastellone *et al*. (2012), Kobayashi *et al*., (2009) and Arena *et al*., (2011).

4. Conclusion

A hydrodynamic and kinetic model capable of predicting steady state product gas composition of a steam blown fluidized bed biomass gasifier, including four different representative TARs compounds has been developed and validated at different temperatures and steam to biomass ratios.

The comparison between the simulated and experimental data shows that the model predicts gas composition and product yields with a very good accuracy. In particular, the difference between simulated and experimental data is lower than 2 % for the gas composition and lowers than 5 % for gas product yields. Regarding the TAR concentrations, the results confirms that Benzene, the lowest molecular weight compound, is the greater TAR compound representative, showing that it amounts for about 60% of the total TAR compounds concentrations. The model and experimental results confirm that the heavier TARs are reformed at high temperature more than the lighter TARs. In detail, the experimental results show that Benzene concentration increases from about 50% at 750°C to about 70% at 850 °C; meanwhile the model, even if maintain a difference, in the total TARs concentration, with the experimental data below 20% at medium-high temperatures, great overestimates at 750°C and underestimates at 850°C the Benzene concentration.

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LIST OF NOTATION

Latin Letters

A	the cross-sectional surface area of the bed (m^2)
Ar	Archimedes number
C_{bi}	Concentr. of specie *i* in bubble phase ($mol \cdot m^{-3}$)
C_{ei}	Concentration of specie *i* in emulsion phase ($mol \cdot m^{-3}$)
d_b	bubble diameter (m)
d_p	particle diameter (m)
D_r	Reactor diameter (m)
g	gravity acceleration ($m \cdot s^{-2}$)
H	Height of expanded bed(m)
k	Arrhenius of reactions
k_{be}	gas interchange coefficient between bubble and emulsion phases ($m \cdot s^{-1}$)
LHV	Low Heating Value of the incoming biomass dry and ash free (see Table 2) ($kJ \cdot kg^{-1}$)
m_c	mass of char in the bed (kg)
$\dot{m}_c^{in}$	inlet mass flow rate of char(from pyrol.) ($kg \cdot s^{-1}$)
m_{oliv}	mass of olivine in the bed (kg)
N_{or}	Number of orifices per unit area of distributor plate (m^{-2})
p	pressure ($N \cdot m^{-2}$)
PM_c	Molecular weight of char
Q	Volumetric flowrate of gas ($m^3 \cdot s^{-1}$)
R_{bj}	Rate of reaction *j* in bubble phase *b* (R4,R5 R11,R12,R13)($mol \cdot m^{-3} \cdot s^{-1}$)
R_{ej}^{g}	Rate of reaction *j* in emulsion phase *e* for the gas phase *g* (R4,R5 R11,R12,R13) ($mol \cdot m^{-3} \cdot s^{-1}$)
R_{ej}^{c}	Rate of char gasification (R1-R2*)* in emulsion phase *e* with char *c* (s^{-1})
R_{ej}^{oliv}	Rate of tar reaction (R6..R9) in emulsion phase *e* catalyzed by olivine *oliv*($mol \cdot kg^{-1}_{cat} \cdot h^{-1}$)
T	Temperature (K)
V_{bed}	Volume of reactor bed (m^3)
u_b	velocity of bubble ($m\ s^{-1}$)
u_{mf}	minimum fluidization velocity ($m\ s^{-1}$)

Greek Letters

δ	Volume fraction of bubble in the bed
ε_c	volume fraction of char *c* in the solid phase of the bed (char+olivine)
ε_{mf}	volume fraction of gas at minumum fluidization
ε_{oliv}	volume fraction of olivine *oliv* in the solid phase of the bed (char+olivine)
ρ_c	density of char ($kg \cdot m^{-3}$)
ρ_g	density of gas phase ($kg \cdot m^{-3}$)
ρ_{oliv}	density of olivine ($kg \cdot m^{-3}$)
μ_g	viscosity of gas phase ($kg \cdot m^{-1} \cdot s^{-1}$)
ν_{ij}	stochiometric coefficient of species *i* in reaction *j*

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References

Anis S. , Z. A. Zainal, "Tar reduction in biomass producer gas via mechanical, catalytic and thermal methods: A review," Renewable and Sustainable Energy Reviews, vol. 15, no. 5, pp. 2355–2377, Jun. 2011.

Arena, U., F. Di Gregorio, C. Amorese, M.L. Mastellone, A techno-economic comparison of fluidized bed gasification of two mixed plastic wastes, Waste Management, 31(7) 2011, 1494-1504

Awojoyogbe, O.B. and K. Boubaker, 2009. A solution to Bloch NMR flow equations for the analysis of homodynamic functions of blood flow system using m-Boubaker polynomials. Curr. App. Phys., 9: 278-288.

Barrio M. , J. E. Hustad, "CO2 gasification of birch char and the effect of CO inhibition on the calculation of chemical kinetics," Progress in Thermochemical Biomass Conversion, vol. 1, pp. 47–60, 2001.

Barrio, M., B. Gøbel, H. Risnes, U. B. Henriksen, J. E. Hustad, and L. H. Sørensen, "Steam gasification of wood char and the effect of hydrogen inhibition on the chemical kinetics," 2001.

Barry, P. and A. Hennessy, 0000. Meixner-type results for riordan arrays and associated integer sequences, section 6: The Boubaker polynomials. J. Integer Sequences, 13: 1-34.

Belhadj, A., J. Bessrour, M. Bouhafs and L. Barrallier, 2009a. Experimental and theoretical cooling velocity profile inside laser welded metals using keyhole approximation and Boubaker polynomials expansion. J. Thermal Analysis Calorimetry, 97: 911-920.

Belhadj, A., O. Onyango and N. Rozibaeva, 2009b. Boubaker polynomials expansion scheme-related heat transfer investigation inside keyhole model. J. Thermophys Heat Transf., 23: 639-642.

Benhaliliba, M., Benouis, C.E., Boubaker, K., Amlouk M., Amlouk, A., A New Guide To Thermally Optimized Doped Oxides Monolayer Spray-grown Solar Cells: The Amlouk-boubaker Optothermal Expansivity ψab in the book : Solar Cells - New Aspects and Solutions, Edited by: Leonid A. Kosyachenko, [ISBN 978-953-307-761-1, by InTech], 2011, 27-41.

Buekens A. G., J. G. Schoeters, "Modelling of Biomass Gasification," in Fundamentals of Thermochemical Biomass Conversion, R. P. Overend, T. A. Milne, and L. K. Mudge, Eds. Springer Netherlands, 1985, pp. 619–689.

Davidson J. F. , D. Harrison, Fluidised particles, vol. 3. Cambridge University Press New York, 1963.

Demirbaş, A., "Biomass resource facilities and biomass conversion processing for fuels and chemicals," Energy Conversion and Management, vol. 42, no. 11, pp. 1357–1378, Jul. 2001.

Devi, L. , K. J. Ptasinski, and F. J. Janssen, "Pretreated olivine as tar removal catalyst for biomass gasifiers: investigation using naphthalene as model biomass tar," Fuel Processing Technology, vol. 86, no. 6, pp. 707–730, 2005.

Devi, L., K. J. Ptasinski, F. J. J. G. Janssen, S. V. B. van Paasen, P. C. A. Bergman, and J. H. A. Kiel, "Catalytic decomposition of biomass tars: use of dolomite and untreated olivine," Renewable Energy, vol. 30, no. 4, pp. 565–587, Apr. 2005.

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Di Carlo, A., D. Borello, and E. Bocci, “Process simulation of a hybrid SOFC/mGT and enriched air/steam fluidized bed gasifier power plant,” International Journal of Hydrogen Energy, 2013.

Di Carlo A., E. Bocci, and V. Naso, “Process simulation of a SOFC and double bubbling fluidized bed gasifier power plant,” International Journal of Hydrogen Energy, vol. 38, no. 1, pp. 532–542, Jan. 2013.

Fiaschi D. , M. Michelini, “A two-phase one-dimensional biomass gasification kinetics model,” Biomass and Bioenergy, vol. 21, no. 2, pp. 121–132, Aug. 2001.

Foscolo, P. U. , K. Gallucci, “Integration of particulate abatement, removal of trace elements and tar reforming in one biomass steam gasification reactor yielding high purity syngas for efficient CHP and power plants,” in 16th european biomass conference and exhibition, 2008.

Fridjine, S. and M. Amlouk, 2009. A new parameter: An ABACUS for optimizig functional materials using the Boubaker polynomials expansion scheme. Modern Phys. Lett. B 23: 2179-2182.

Ghanouchi, J., H. Labiadh and K. Boubaker, 2008. An attempt to solve the heat transfert equation in a model of pyrolysis spray using 4q-order m-Boubaker polynomials. Int. J. Heat Technol., 26: 49-53.

Han J. , H. Kim, “The reduction and control technology of tar during biomass gasification/pyrolysis: an overview,” Renewable and Sustainable Energy Reviews, vol. 12, no. 2, pp. 397–416, 2008.

Heidenreich, S., M. Nacken, P. U. Foscolo, and S. Rapagna, “Gasification apparatus and method for generating syngas from gasifiable feedstock material,” App. 12/598,508Apr-2008.

Jess, A., “Mechanisms and kinetics of thermal reactions of aromatic hydrocarbons from pyrolysis of solid fuels,” Fuel, vol. 75, no. 12, pp. 1441–1448, 1996.

Kobayashi, N., M. Tanaka, G. Piao, J. Kobayashi, S. Hatano, Y. Itaya, S. Mori, High temperature air-blown woody biomass gasification model for the estimation of an entrained down-flow gasifier, Waste Management, 29(1) 2009, 245-251

Konttinen, J., A. Moilanen, J. Vepsäläinen, S. Kallio, M. Hupa, and E. Kurkela, “Modelling and experimental testing of gasification of biomass char particles,” in Proceedings of the European Combustion Meeting, 2003, pp. 26–29.

Kumar, A.S., 2010. An analytical solution to applied mathematics-related Love’s equation using the Boubaker polynomials expansion scheme. J. Franklin Institute., 347: 1755-1761.

Kunii D. , O. Levenspiel, “Fluidized reactor models. 1. For bubbling beds of fine, intermediate, and large particles. 2. For the lean phase: freeboard and fast fluidization,” Ind. Eng. Chem. Res., vol. 29, no. 7, pp. 1226–1234, Jul. 1990.

Labiadh, H. and K. Boubaker, 2007. A Sturm-Liouville shaped characteristic differential equation as a guide to establish a quasi-polynomial expression to the Boubaker polynomials. Diff. Eq. and Cont. Proc., 2: 117-133.

Mastellone, M. L., L. Zaccariello, D. Santoro, U. Arena, The O2-enriched air gasification of coal, plastics and wood in a fluidized bed reactor, Waste Management, 32(4), 2012, 733-742

Milgram, A., 2011. The stability of the Boubaker polynomials expansion scheme (BPES)-based solution to Lotka-Volterra problem. J. Theoretical Biolog., 271: 157-158.

Nikoo M. B., N. Mahinpey, “Simulation of biomass gasification in fluidized bed reactor using ASPEN PLUS,” Biomass and Bioenergy, vol. 32, no. 12, pp. 1245–1254, Dec. 2008.

Rahmanov, H., A Solution to the non Linear Korteweg-De-Vries Equation in the Particular Case Dispersion-Adsorption Problem in Porous Media Using the Spectral Boubaker Polynomials Expansion Scheme (BPES), Studies in Nonlinear Sciences, 2011, 2 (1) 46-49.

Rapagna, S., N. Jand, A. Kiennemann, and P. U. Foscolo, “Steam-gasification of biomass in a fluidised-bed of olivine particles,” Biomass and Bioenergy, vol. 19, no. 3, pp. 187–197, 2000.

Ruoppolo, G. , P. Ammendola, R. Chirone, F. Miccio, H2-rich syngas production by fluidized bed gasification of biomass and plastic fuel, Waste Management, 32(4), 2012, 724-732

S. Sadaka, S., A. E. Ghaly, and M. A. Sabbah, “Two phase biomass air-steam gasification model for fluidized bed reactors: Part I—model development,” Biomass and Bioenergy, vol. 22, no. 6, pp. 439–462, Jun. 2002.

Sadaka, S. S., A. . Ghaly, and M. . Sabbah, “Two-phase biomass air-steam gasification model for fluidized bed reactors: Part III—model validation,” Biomass and Bioenergy, vol. 22, no. 6, pp. 479–487, Jun. 2002.

Simell, P. A., E. K. Hirvensalo, V. T. Smolander, and A. O. I. Krause, “Steam Reforming of Gasification Gas Tar over Dolomite with Benzene as a Model Compound,” Ind. Eng. Chem. Res., vol. 38, no. 4, pp. 1250–1257, Apr. 1999.

Slama, S., J. Bessrour, M. Bouhafs, K.B. Ben and M. Num et al., 2009. Heat Transf. Part A. 55: 401-404.

Slama, S., M. Bouhafs, K.B. Ben and A. Mahmouda, 2008. boubaker polynomials solution to heat equation for monitoring a3 point evolution during resistance spot welding. Int. J. Technol., 26: 141-146.

Strehler A., W. Stutzle, “Biomass residues,” Biomass: regenerable energy, pp. 75–102, 1987.

Swierczynski, D. , C. Courson, and A. Kiennemann, “Study of steam reforming of toluene used as model compound of tar produced by biomass gasification,” Chemical Engineering and Processing: Process Intensification, vol. 47, no. 3, pp. 508–513, Mar. 2008.

Świerczyński, D., S. Libs, C. Courson, and A. Kiennemann, “Steam reforming of tar from a biomass gasification process over Ni/olivine catalyst using toluene as a model compound,” Applied Catalysis B: Environmental, vol. 74, no. 3, pp. 211–222, 2007.

Tabatabaei, S., T. Zhao, O. Awojoyogbe and F. Moses 2009. Cut-off cooling velocity profiling inside a keyhole model using the Boubaker polynomials expansion scheme. Int. J. Heat Mass Transfer. 45: 1247-1255.

UNIQUE Cooperative Research Project, Contract N.211517 7FP.” [Online]. Available: www.uniqueproject.eu. [Accessed: 02-May-2013].

Wang Y. , C. M. Kinoshita, “Kinetic model of biomass gasification,” Solar Energy, vol. 51, no. 1, pp. 19–25, Jul. 1993.

Werther, J., M. Saenger, E.-U. Hartge, T. Ogada, and Z. Siagi, “Combustion of agricultural residues,” Progress in Energy and Combustion Science, vol. 26, no. 1, pp. 1–27, Feb. 2000.

Yildirim, A., S.T. Mohyud-Di and D.H. Zhang, 2010. Analytical solutions to the pulsed klein-gordon equation using Modified Variational Iteration Method (MVIM) and Boubaker Polynomials Expansion Scheme (BPES).Computers Math. Appl., 12: 026. DOI:10.1016/j.camwa.