1	DEVELOPMENT OF A NEW STEADY STATE ZERO-DIMENSIONAL SIMULATION MODEL FOR
2	WOODY BIOMASS GASIFICATION IN A FULL SCALE PLANT
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13	Abstract
14	A new steady state zero-dimensional simulation model for a full-scale woody biomass
15	gasification plant with fixed-bed downdraft gasifier has been developed using Aspen Plus [®] .

16 The model includes the technical characteristics of all the components (gasifier, cyclone, 17 exchangers, piping, etc.) of the plant and works in accordance with its actual main control 18 logics. Simulation results accord with those obtained during an extensive experimental 19 activity. After the model validation, the influence of operating parameters such as the 20 equivalent ratio, the biomass moisture content and the gasifying air temperature on syngas 21 composition have been analyzed in order to assess the operative behavior and the energy 22 performance of the experimental plant. By recovering the sensible heat of the syngas at the 23 outlet of the gasifier, it is possible to obtain higher values of the gasifying air temperature and 24 an improvement of the overall gasification performances.

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Z	5

26 Keywords

- 27 Downdraft gasifier, Biomass gasification, Steady state simulation, Aspen Plus[®], Experimental
- 28 activity
- 29

30 **Nomenclature**

- 31 CGE [-]: cold gas efficiency
- 32 Cp_a [J/kg K]: specific heat of the wind air outside of the gasifier
- 33 Cp_i [J/kg K]: specific heat of the air/syngas within chipped biomass bed
- 34 D_{e_insulation} [m]: external diameter of the ceramic fiber insulation
- 35 D_{e_refractory} [m]: external diameter of the protective refractory layer
- 36 De_shell [m]: external diameter of the reactor shell
- 37 D_i [m]: internal diameter of the protective refractory layer
- 38 d_p [m]: mean equivalent diameter of the chipped biomass that is supposed as sphere
- 39 E_m [-]: the emissivity of the cover surface of the external thermal insulation of the gasifier
- 40 ER [-]: equivalent ratio
- 41 k_a [W/m K]: conductivity of the wind air outside the gasifier
- 42 k_i [W/m K]: conductivity of the air/syngas within chipped biomass bed
- 43 k_{insulation} [W/m K]: conductivity of the ceramic fiber insulation
- 44 k_{refractory} [W/m K]: conductivity of the refractory layer
- 45 k_{shell} [W/m K]: conductivity of the shell
- 46 L [m]: length of the reactor
- 47 I [m]: height of the chipped biomass bed within the gasifier
- 48 LHV [kJ/kg]: lower heating value

- 49 LHV_b [kJ/kg]: lower heating value of biomass
- 50 LHV_s [kJ/kg]: lower heating value of the syngas

51 MC [-]: moisture content

- 52 \dot{m}_{h} [kg/s]: biomass mass flow
- 53 m, [kg/s]: syngas mass flow
- ⁵⁴ m_{a_a} [kg/s]: actual gasifying air mass flow
- m_{a_s} [kg/s]: stoichiometric gasifying air mass flow
- 56 Nu_a [-]: Nusselt number for the convective heat exchange between the wind air and the cover
- 57 surface of the external thermal insulation of the gasifier
- 58 Nu_i [-]: Nusselt number for the convective heat exchange between the air/syngas and the
- 59 internal surface of the refractory layer of the gasifier
- 60 Pr_a [-]: Prandtl number of the wind air outside of the gasifier
- 61 Pr_i [-]: Prandtl number of the air/syngas within chipped biomass bed
- 62 Q [W]: thermal power that is dispersed by the gasifier into the environment
- 63 R_{c1} [K/W]: conductive thermal resistance of the internal refractory layer
- 64 R_{c2} [K/W]: conductive thermal resistance of the gasifier shell
- 65 R_{c3} [K/W]: conductive thermal resistance of the external thermal insulation of the gasifier
- 66 shell
- 67 R_e [K/W]: thermal resistance of the convective heat exchange between the wind air and the
- 68 cover surface of the external thermal insulation of the gasifier shell
- 69 Re_a [-]: Reynolds number of the wind air outside of the gasifier
- 70 Re_i [-]: Reynolds number of the air/syngas within chipped biomass bed
- 71 R_i [K/W]: thermal resistance of the convective heat exchange between the air/syngas and
- the internal surface of the refractory layer of the gasifier

- 73 R_r [K/W]: equivalent thermal resistance of the radiative heat exchange between the cover
- 54 surface of the external thermal insulation of the gasifier shell and the environment
- 75 R_{tot} [K/W]: total thermal resistance from the reactor core to the environment
- 76 T_e [K]: environment temperature
- 77 T_p [K]: the temperature of the cover surface of the external thermal insulation of the gasifier
- 78 T_r [K]: mean temperature of air/syngas within the reactor
- 79 u_a [m/s]: velocity of the wind air outside of the gasifier
- 80 u_i [m/s]: mean velocity of the air/syngas across the chipped biomass bed within the gasifier
- 81 Greek symbols
- 82 ΔP [Pa]: pressure drop of the air/syngas across the gasifier
- ϵ [-]:mean porosity of the chipped biomass bed within the gasifier
- μ_a [kg/m s]: dynamic viscosity of the wind air outside of the gasifier
- μ_i [kg/m s]: dynamic viscosity of the air/syngas across the chipped biomass bed within the

86 gasifier

- ρ_a [kg/m³]: density of the wind air outside of the gasifier
- ρ_i [kg/m³]: density of the air/syngas across the chipped biomass bed within the gasifier
- 89 σ [W/m² K⁴]: the Boltzmann constant
- 90

91 **1. INTRODUCTION**

92 Recently the growing awareness of the shortage of the traditional energy sources and the 93 concern for environmental protection have encouraged the wider use of renewable energy 94 sources. Among these, biomass is certainly one of the most important because of its 95 inexhaustibility and wide availability. In addition, more than wind and photovoltaic, energy 96 conversion of biomass can create concrete local economic opportunities.

97 The exploitation of energy from through biomass comes off bio-chemical and thermo-98 chemical processes [1]. Bio-chemical process involves biomethanization of biomass, 99 characterized by low cost effectiveness and efficiency. Actually, the three main thermo-100 chemical processes are combustion, pyrolysis and gasification. Combustion, apart from the 101 applications in small fireplaces and stoves, is used mainly to supply heat and power with by 102 means of large scale systems (typically above 500 kW_e), and the net efficiency for electricity 103 generation is usually very low and ranges from 15-20 % for the smallest plants (< 1 MW_e) [2]. Pyrolysis converts biomass to bio-fuels and bio-char in absence of oxygen (O2), but the 104 105 application of this technology is limited due to the thermal system complexity and the low 106 quality of the fuels that are produced. Gasification [3] converts biomass through a partial 107 oxidation into a gaseous mixture, called syngas, and represents, especially in the low power 108 range (< 500 kW_e), the process with the greatest development prospects mainly for its high 109 electric efficiency (20-25 %) [4-5]. Other advantages of gasification are the plant simplicity and 110 the lower capital cost for small scale applications with respect to other technologies. The main 111 drawback is represented by the syngas cleaning system complexity and efficiency.

112 The development of numerical simulation models is an important tool in order to provide 113 more accurate qualitative and quantitative information on biomass gasification. The possible 114 approaches for the modelling of the gasification process are: steady state models, transient 115 state models and models based on the computational fluid dynamics. The steady state 116 models, that do not consider the time derivatives, are further classified as kinetic rate models 117 and kinetics free equilibrium models [6-9]. For the evaluation of the syngas composition and 118 temperature as function of the process parameters, the kinetics free equilibrium models are 119 the most preferred models because they are very simple and reliable. They have the inherent 120 advantage of being generic but, at the same time, they have thermodynamic limitations, even though researchers have successfully demonstrated that this approach describes sufficiently
well the gasification process in downdraft gasifiers [10-13].

123 A commercial code, such as Aspen Plus[®], can be usefully and effectively adopted for the 124 construction of a reliable kinetic free equilibrium simulation model. This article aims at 125 presenting an innovative simulation approach, where the whole experimental gasification 126 plant, containing all the elements such as cyclone, heat exchangers, turbomachineries etc., 127 works following the main control logics of the real plant. Besides, it gives an experimental 128 contribution to the validation of a zero-dimensional steady state simulation model of a full-129 scale wood-fueled downdraft gasifier. Furthermore, it tries to demonstrate that it is possible 130 to define and tune a reliable equilibrium Aspen Plus® simulation model using detailed 131 experimental data of a real gasification plant (equipment and streams). This model makes it 132 possible to effectively predict the performance of the plant over a wide range of operative 133 conditions.

To the best of the authors' knowledge, simulative models for a whole gasification plant with fixed-bed downdraft gasifier have never presented in literature considering the actual performance characteristics and operative behavior of the plant equipments.

Hence, the work described in this paper is very innovative and can be an useful tool for thedevelopers and users of biomass gasification combined heat and power plants.

On the other hand, there are several papers that describe a steady-state biomass gasification model using Aspen Plus[®], mainly in the field of fluidised bed gasifiers. These are briefly summarized below. Ramzan et al. [14] reported an interesting comparative analysis between the simulation performances of a lab-scale up-draft biomass gasifier and the experimental data obtained in literature. Fu et al. [15] analyze without an experimental validation how the performances of an autothermal biomass gasifier are affected by the gasifying air flow and

temperature. Doherty et al. [16-18] using experimental data from literature proposed and
validated an Aspen Plus[®] model based on the Gibbs free energy minimisation for a circulating
fluidised bed gasifier and for a steam blown dual fluidised bed gasifier, in order to show the
dependence of the gasifier performance on the gasifying air temperature.

Several kinds of fluidized bed gasifiers have been simulated and validated using a kinetic
model in [19-23], while other authors [24-28] used an equilibrium approach.

A semi detailed kinetic model coupling Aspen Plus[®] and dedicated fortran subroutines is proposed in [29] for the simulation of an air-steam gasification of biomass in a bubbling fluidised bed. The results of the modelling are well aligned with experimental results available in literature.

Other authors focalized their studies on simulating and validating original two-stage biomass gasifiers [30-31], while in [32] the entrained flow gasification of wood waste is simulated in Aspen Plus[®] using a plug flow reactor with a kinetic approach. The model validation is executed with experimental results.

159 In the present work, simulation results have been analyzed and compared with the 160 experimental ones obtained from a commercial-scale gasification plant based on a downdraft 161 gasifier. The plant, with the potential of roughly 80 kW_e, allows to control and adjust many 162 parameters like air flow and temperature into the gasifier or biomass moisture content (MC) 163 and also to measure chemical composition, temperature and flow of syngas coming out from 164 the gasifier.

Using a full-scale experimental biomass gasification plant many operative results were available. This fact allowed both to make a detailed comparative analysis with simulation results and to set some parameters of the model so to achieve an accurate model validation. In this paper, after a brief introduction about the gasification principles, the technical and

operative characteristics of the full-scale experimental plant are described. Then, Aspen Plus[®] model of the gasifier and the whole gasification plant are presented. After that, the experimental and simulated data are compared and, successively, the performance assessment of the gasification plant is discussed.

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174 **2. GASIFICATION PRINCIPLES**

175 Gasification is a well-known thermochemical process that converts a solid fuel (usually 176 biomass or coal) into a combustible gaseous product (syngas) through partial oxidation, using 177 a gasifying agent in sub stoichiometric conditions [2-3]. When air is used as gasifying agent the 178 syngas consists mainly of carbon monoxide (CO), hydrogen (H_2), carbon dioxide (CO₂), steam 179 (H₂O), methane (CH₄) and nitrogen (N₂) with proportions that depend on air/biomass ratio 180 and MC. In addition there are trace amounts of higher hydrocarbons (such as acetylene, 181 ethene, ethane), and various contaminants such as small char particles, fly ash and tar [33-182 34].

183 It is well known that the entire gasification process can be divided into four successive stages:

184 drying, pyrolysis, combustion and gasification [5,9].

185 In a downdraft fixed bed gasifier, the required heat for the endothermic biomass drying and 186 pyrolysis is provided via heat conduction through the biomass bed by the exothermic 187 combustion zone at the gasifying air inlet. The main reactions in combustion and gasification 188 processes are summarized in Table 1.

189 The thermodynamic performances of the gasification process can be evaluated using the190 following parameters:

191 - the equivalent ratio (ER), defined as follows:

192

193
$$ER = \frac{m_{a_a}}{m_{a_s}}$$
(1)

197
$$CGE = \frac{\dot{m}_{s}*LHV_{s}}{\dot{m}_{b}*LHV_{b}}$$
(2)

Therefore CGE represents the ratio between the inlet biomass chemical energy and thecorresponding chemical value of the syngas.

Table 1 Main gasification reactions.

Heterogeneous reactions:		
$C_{(s)} + O_{2(v)} \rightarrow CO_{2(v)} + 394 \text{ kJ/mol}$	C complete combustion	(R1)
$C_{(s)} + 0.5 \ O_{2(v)} \rightarrow CO_{(v)} + 111 \ kJ/mol$	C partial combustion	(R2)
$C_{(s)} + CO_{2(v)} \rightarrow 2 CO_{(v)} - 172 kJ/mol$	Boudouard	(R3)
$C_{(s)} + H_2O_{(v)} \rightarrow CO_{(v)} + H_2 - 131 \text{ kJ/mol}$	Water-gas	(R4)
$C_{(s)} + 2 H_{2(v)} \rightarrow CH_{4(v)} + 75 \text{ kJ/mol}$	Methanation	(R5)
Homogeneous reactions:		
$CO_{(v)} + 0.5 O_{2(v)} \rightarrow CO_{2(v)} + 283 \text{ kJ/mol}$	CO partial combustion	(R6)
$H_{2(v)} + 0.5 O_{2(v)} \rightarrow H_2 O_{(v)} + 242 \text{ kJ/mol}$	H ₂ combustion	(R7)
$CO_{(v)} + H_2O_{(v)} \rightarrow CO_{2(v)} + H_2 + 41 \text{ kJ/mol}$	CO shift	(R8)
$CH_{4(v)} + H_2O_{(v)} \rightarrow CO_{(v)} + 3 H_2 - 206 \text{ kJ/mol}$	Steam-methane reforming	(R9)
H ₂ S and NH ₃ formation reactions:		

$H_{2(v)} + S_{(s)} \rightarrow H_2 S_{(v)}$	H ₂ S formation	(R10)
$N_{2(v)} + 3 H_{2(v)} \rightarrow 2 NH_{3(v)}$	NH ₃ formation	(R11)

3. THE EXPERIMENTAL GASIFICATION PLANT

205 **3.1 Layout**

The experimental gasification plant (Figure 1) is the result of a long research activity that has been performed at the "Dipartimento di Ingegneria Civile e Industriale" (DICI) and "Dipartimento di Ingegneria dell'Energia, dei Sistemi, del Territorio e delle Costruzioni" (DESTEC) of the University of Pisa (Italy).

The virgin chipped biomass is dried using a stand-alone concurrent rotating dryer that is equipped, to accomplish the drying process, with a LPG fired burner. In a future commercial configuration, the hot exhaust gas of the internal combustion engine fuelled by syngas will be used for drying. Periodically, a sample of dried chips is analysed to evaluate its MC and composition.

215 The dry wood chips are then filled into the gasifier using a screw conveyor and a rotary valve, 216 while the air flow coming into the gasifier is preheated initially through an electric preheater 217 (during the starting of the gasification plant when the syngas temperature is not enough high). 218 Later, when the steady state regime is reached, the air is heated passing through a shell-and-219 tube heat recuperator, where the high-temperature syngas at the outlet of the gasifier is 220 cooled. In order to avoid the obstruction blockage of the syngas outlet section, and 221 consequently the stoppage of the reactor, the unburnt char is periodically extracted from the 222 gasifier.

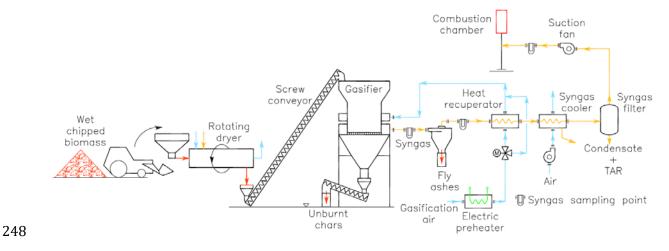
223 The syngas light carbonaceous residues The char residues and fly ash are removed from the 224 syngas in a cyclone. The syngas is further cooled in a second air-cooled shell-and-tube heat 225 exchanger. In the experimental facility this cooling air is dispersed into the atmosphere, but 226 in a commercial layout of the gasification plant the sensible heat of the syngas could be 227 effectively recovered for cogeneration application. At the outlet of the cooler, the contents of 228 pollutants in the syngas, such as fly ash and tar, are lowered using a custom-made filter. Then, 229 the syngas passes through the suction fan, which is responsible of the gasifying air-syngas 230 flow.

The syngas is finally oxidized in a custom combustion chamber equipped with a LPG burner. This special combustion chamber has been adopted in place of a conventional torch for safety reasons, since it ensures long residence time of CO at high temperatures and, consequently, its complete oxidation. In the commercial version of the plant an internal combustion engine in combination with a torch will replace the combustion chamber. The torch will be used to oxidize the syngas when the quality of the gas is not suitable for the engine (for example, during the plant starting) or when the engine does not work due to failures.

The operation of the experimental gasification plant is supervised by a programmable logic controller (PLC) that can be managed by the user with a user-friendly touch screen system. The temperature and pressure of each stream are measured and the measurement signals are connected to the PLC system. Moreover, air and syngas flows are continuously measured via two dedicated Honeywell flow transmitters (the syngas one includes the compensation of temperature) based on the orifice plate method.

244 Using some sampling points located in different places along the syngas stream line, it is 245 possible to extract the syngas in order to evaluate its macro-components with an off-line gas-

- 246 chromatograph and also tar and ash content via a sampling probe. This probe was designed
- and constructed in accordance with the tar Protocol [35-36].



249

Figure 1 Layout of the biomass gasification power plant.

- 250
- 251 The most important design data of the experimental plant are summarized below:
- 252 biomass mass flow feeding the gasifier with MC of 10 %: 90 kg/h
- 253 gasifying air temperature at the inlet of the gasifier: 450 °C
- syngas mass flow: 200 kg/h
- 255 syngas temperature at the inlet of the suction fan: 75 °C.
- 256

3.2 Main control logics for the operative management of the experimental gasification plant

- 258 The experimental gasification plant operates in accordance with some fundamental control
- logics that were implemented and managed by a governing PLC. These rules logics assure large
- 260 flexibility from the operative point of view and the possibility to test different configurations.
- 261 In particular the logics are:

automatic adjustment of the opening of the motorized three way valve located upstream
 of the heat recuperator (air-side) so that the air temperature just upstream the gasifier
 reaches a specified set-point value;

265 2. the cooling air mass flow in the syngas cooler is tuned by modifying the rotational speed of
266 the fan via electric motor inverter, in order to obtain a set-point value of the syngas
267 temperature at the outlet of the cooler;

268 3. gasification flow logic: the speed of the syngas suction fan is modified via electric motor

inverter in order to obtain a specified syngas mass flow upstream the combustion chamber.

270 Similarly the logic can be modified using a set-point of the gasifying air mass flow as control

271 objective;

- 4. the filling of the reactor starts periodically in accordance with a time log and stops when
 the level of the biomass chips inside the gasifier reaches the highest allowable level
 activating a blade sensor level;
- 5. the unburned char is periodically discharged in order to avoid the blockage of the reactor
 when the pressure drop across the reactor reaches the set-point level and then extracted
 with a dedicated screw conveyor.

278

279 **4. Aspen Plus® model**

Referring to the plant layout (Figure 1) the simulation flowsheet of the plant (Figure 2) hasbeen created.

282

283 **4.1 Gasifier**

A kinetic free equilibrium steady state model has been developed for the gasification process.

285 Initially the model simulates the biomass drying, reducing its MC up to a predetermined value.

Afterwards, biomass is decomposed into volatile components and char and then oxidation and gasification reactions are simulated by minimizing Gibbs free energy.

288 The block DRIER1 has been used to reduce the MC of moist biomass, simulating biomass drying controlled by a Fortran statement routine. Excess water is separated in the block DRYER2 (Sep 289 290 type), while dry biomass with the right MC at the inlet of the gasification reactor is then 291 decomposed into its conventional elements (C, H, O, N, S etc.) in the block DECO (Ryield type), 292 that uses calculations based on the component yield specification, controlled by a Fortran 293 statement. Ash and specified percentage of carbon of the dry biomass are separated in the 294 block CHAR-SEP (Sep type) in order to simulate the unburnt char that is extracted from the 295 bottom of the gasifier. The remaining elements are carried with the heat of reaction 296 associated with the decomposition of the biomass into the block GASIFIER (RGibbs type), 297 where the preheated gasifying air enters and the combustion and gasification reactions occur. 298 The gasification products are calculated by minimizing the Gibbs free energy and assuming 299 complete chemical equilibrium. Finally, taking into account the reactor geometry and thermal 300 insulation, pressure drop across the gasifier and heat losses to the ambient are calculated with 301 a user routine (see Appendix A).

Biomass is specified as a non-conventional component, with a chemical composition defined by the ultimate and proximate analysis in accordance with the results of the laboratory analysis, as shown in Table 2.

305

306

Table 2 Ultimate and proximate analyses of chestnut wood.

Proximate Analysis		Ultimate Analysis	
Moisture	10 %	Carbon	50.96 %

50 %	Hydrogen	5.978 %
48 %	Nitrogen	0.49 %
2 %	Chlorine	0.0098 %
	Sulphur	0.0392 %
	Oxygen	40.523 %
	Ash	2 %
	48 %	48 % Nitrogen2 % ChlorineSulphurOxygen

308 **4.2 Other equipment**

309 In order to reproduce the thermodynamic plant operation accurately and, after an 310 experimental validation, to predict the behavior of the system in general operating conditions, 311 the geometrical and operative characteristics of the equipment that are actually installed at 312 the experimental facility have been inserted within the simulation model. In particular:

313 - pressure drop ratio factor, the pressure recovery factor and the valve flow coefficient of the 314 valves (VA01, 3W-VALVE, VG01, VG02 in Figure 2) have been specified in accordance with 315 the real data from the equipment datasheets. In this way it is possible to predict the 316 pressure drop of the valve as a function of its geometrical dimensions and percent opening; 317 - geometrical data, such as internal diameter, length and material have been inserted for the 318 piping (PIPE-1, PIPE-2, PIPE-3 in Figure 2). Further, with the addition of the calculator tool 319 of Aspen Plus[®], the heat losses to the ambient have been calculated in function of the 320 actual insulation characteristics, the ambient air temperature and wind speed during the 321 experimental tests;

the geometry of the heat exchangers (HEATER and E02 in Figure 2) has been designed using
 the specific code of Aspen Plus[®] for the shell and tube heat exchangers and their simulation
 model has been linked within that of the gasification plant implemented into the main one.

In this way it is possible to assess the real thermodynamic off-design performance of the heater when the operating conditions change with respect to the design point. The electric heater (E-HEATER in Figure 2) has been simulated using a particular user routine in order to assess its actual thermal performance in function of the thermal load and air mass flow. The heat losses of the heaters to the environment have been calculated in function of their specific geometry and the insulation characteristics;

- geometrical data of the cyclone (CYCLONE in Figure 2) have been inserted considered in order
 to assess its fly ash separation performance. A specific routine has been added in order to
 evaluate the heat loss to the environment, adopting the approach described above for the
 piping and inserting a heater block (D01-Q-P in Figure 2) downstream the cyclone;

- the simulation of the air and syngas fans (AIR-FAN and S-FAN in Figure 2) has been executed
 inserting their characteristic curves in terms of head and efficiency as a function of flow at
 different shaft rotational speeds in accordance with the manufacturer datasheets. The
 actual operating speed of the fans is calculated once the flow and the head have been
 evaluated in agreement with the control logics described in the previous section and
 assuring the gas flow with the calculated pressure drop, respectively;

the final complete oxidation of the syngas within the combustion chamber (CC in Figure 2)
has been simulated using a RGibbs type block. The pressure loss through the combustion
chamber has been inserted as an input of the model using the experimental data. The
overall chemical power that is associated with the syngas flow is calculated via the cooling
of the combustion products with a heater block (QSYNGAS in Figure 2);

- the simulation of the syngas filter (COOLER in Figure 2) that is positioned upstream the fan
is executed using a separation block (Sep type) with a pressure loss that has been
experimentally evaluated in function of the actual syngas flow;

349 - the air and syngas flowmeters (F01 and F02 in Figure 2), which are based on the orifice plate 350 technology, have been simulated with valves whose pressure losses are in accordance with 351 formulation reported in [37] as function of the volume flow.

352 The control logics of the experimental plant have been implemented in the simulation model 353 using the Design Specs tool of Aspen Plus[®]. In this way it is possible to find the value of one or more control variables, such as, for example, the motor speed of the syngas fan, in order to 354 355 iteratively reach a specified goal, such as the syngas mass flow.



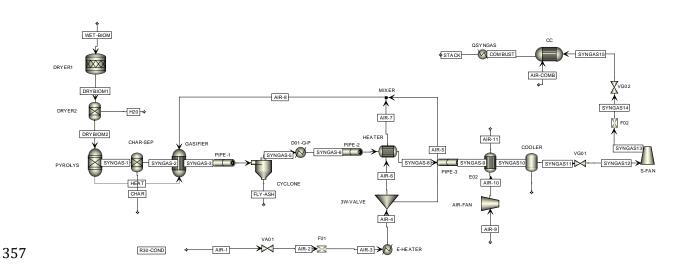




Figure 2 Aspen Plus[®] simulation model of the experimental gasification plant. 358

359

4.3 Physical property method 360

361 The equation of state that is used to estimate all physical properties of the conventional 362 components is the Peng-Robinson equation with Boston-Mathias alpha function (PR-BM), 363 which is appropriate for gasification processes where temperature is quite high.

365 **4.4 Simplifying assumptions**

366 Within the model some simplifying assumptions that do not markedly affect the goodness of 367 the simulation results are:

steady state conditions: as demonstrated by the experimental data, after roughly two
 hours from the starting of the gasification reactions, the temperature profile within each
 equipment, such as the gasifier and the heat exchangers, fluctuates slightly. This assures
 that the operating conditions do not practically change in time.

kinetic free model: as stated in the Introduction, the estimation of reliable kinetic data for
 the specific gasification configuration can be an hard task without assuring the goodness
 of the results. The adoption of the equilibrium approach in combination with a detailed
 geometrical simulation of the plant equipment can assure in any case to obtain a good
 representation of the experimental data;

• the sulphur reacts forming H₂S, as demonstrated by the experimental analysis;

no nitrogen oxides are considered and N₂ forms only NH₃: the study of the formation of
 the micro-pollutant is not an objective of the paper. They do not affect the overall energy
 balance of the gasifier and the macro-composition of the syngas;

the formation of the tars and other heavy products at equilibrium conditions are not
 simulated. It is important to note that their influence on the overall energy balance of the
 gasifier is marginal.

384

385 **5. Results and Discussion**

386

387 **5.1 Experimental activity vs simulation results**

Several different operative conditions have been considered during the experimental activity, varying the ER (modifying the suction fan rotational speed and consequently the air mass flows) and the gasifying air temperature at the inlet of the reactor (changing the opening of the bypass valve of the air preheater). As stated above, the thermodynamic data of each stream of the plant, the biomass characteristics and the syngas composition have been measured during the tests. Some experimental data have been used as inputs of the Aspen Plus[®] simulation model. In particular:

- the ambient gasifying air: temperature, pressure, relative humidity and mass flow,
 temperature at the inlet of the gasifier;
- biomass: chemical composition, MC, mass flow;
- 398 syngas: temperature at the outlet of the cooler;
- unburnt char that is extracted from the bottom of the gasifier: mass flow, chemicalcomposition;
- 401 fly ashes from the gasifier: size distribution, concentration.

Using these inputs, the simulation model calculates the syngas composition, temperature and
mass flow at each point of the plant (and consequently the rotational speed of each fan), the
thermal power of each heat exchanger, the aperture of the control valve of the air preheater.
The comparison of the experimental data and the results of the simulations, that have been
executed using data of about twenty experimental tests (Appendix B), are reported in Figures
3, 4, 5, 6 and 7. The trend and the values of the mass composition of the syngas are well

408 simulated by Aspen Plus[®] and the percentage error is marginal, also considering the intrinsic

409 error of the experimental measurements, which can be summarized in the following:

410 (i) the measurements of the temperature that are executed using thermocouples of type K

411 have a standard intrinsic tolerance of \pm 6 %;

412 (ii) the mass flow of the biomass has not been continuously monitored, but it is evaluated
413 measuring in average the biomass that is consumed;

(iii) the MC of biomass, that is not an homogeneous fuel, is not evidently measured in
continuous way, but some representative samples have been analysed. Some MC
differences between the measurement instant and the moment of gasification are
inevitable due to the fact that the material is not homogeneous and some moisture is
slightly absorbed from the environment;

(iv) as the experimental experience of the authors, the syngas composition is not perfectly
stable and fluctuates due to the fact that the biomass within the gasification bed is
evidently heterogeneous and the air and syngas fluid-dynamic through the biomass is
affected by inevitable variations;

423 (v) the volume flow measurement of air and syngas is affected by an error by about \pm 1 %;

424 (vi) there are inevitable errors of the laboratory measurements that can be estimate equal to 425 about \pm 0.5 %.

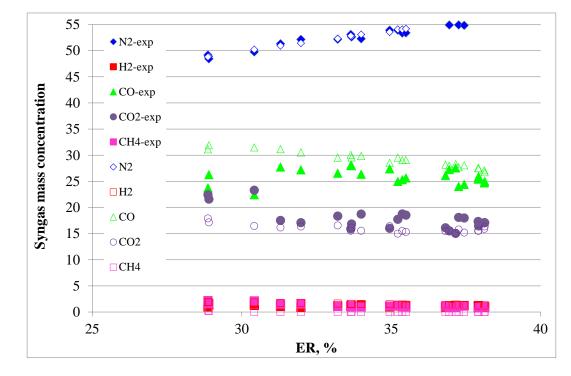
The average value and the standard deviation of the percentage difference between the experimental and simulated results are summarized in Table 3. The parity plot of the molar composition between the simulated values and the experimental ones, reported in Figure 8, allows to assess the prediction accuracy of the simulation model. The average differences between the measured LHV of the syngas and the simulated values and between the experimental CGE and the simulated ones as well are about 7 % and 5 %, respectively.

432 Moreover, the average difference between the simulated values of the syngas temperature 433 at the outlet of the gasifier and the experimental values is lower than 7 %. On the basis of 434 these negligible differences, the Aspen simulation model can be considered particularly accurate for the estimation of the most important energy performance indicators and 435 436 operative data of the experimental facility. The most relevant difference between the 437 experimental and simulated results concern the mass and molar concentration of H₂, that is 438 overestimated, and CH₄, that is underestimated. Using the equilibrium hypothesis in the 439 simulation model, the conversion of the methane into hydrogen, which depends on the actual 440 crossing time of the gasification bed, is overestimated. Indeed, the methane that is produced 441 during the pyrolysis is progressively converted along the gasifying bed into H₂ and CO in 442 accordance with the steam reforming reaction. Using the hypothesis of equilibrium, the steam 443 reforming reaction is completed shifted toward the products, as reported also by other 444 authors [38-39]. This condition is hardly confirmed in real situations. However, it is important 445 to note that the differences are lower with higher values of ER, when the hypothesis of 446 equilibrium is more respected. Moreover, considering the overall amount of hydrogen moles and mass the differences reduce largely (Table 3). 447

However, as a whole, the dependence of the syngas composition on the ER is in good
agreement with the values of literature [7, 40-41]. Notwithstanding this difference for the H₂
estimation, the results concerning the plant operation and its energy balance are well
simulated by the Aspen Plus[®] model.

In general, the increasing ER implies a larger extension of the combustion process within the reactor (hence the temperature inside the reactor increases, as shown in Figure 5), with a lower content of the combustible components in favor of the nitrogen content that increases.
When the gasifying air increases, the LHV of the syngas consequently decreases (Figure 7) due

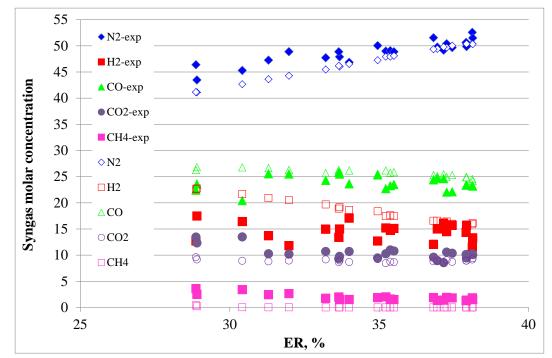
to the oxidation of the hydrogen and CO and the dilution due to the nitrogen. Consequently,



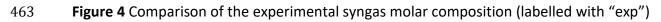
457 CGE decreases with ER (see Figure 7), too.

458

Figure 3 Comparison of the experimental syngas mass composition (labelled with "exp")
 with the results of the Aspen Plus[®] simulation model (dry basis).



462



464

with the results of the Aspen Plus® simulation model (dry basis).

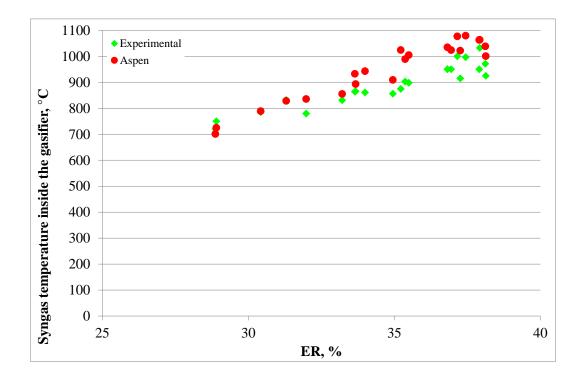




Figure 5 Comparison of the experimental syngas temperature inside the gasifier with the

results of the Aspen Plus[®] simulation model.

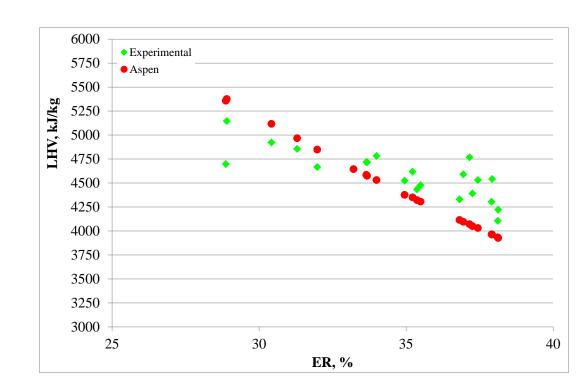
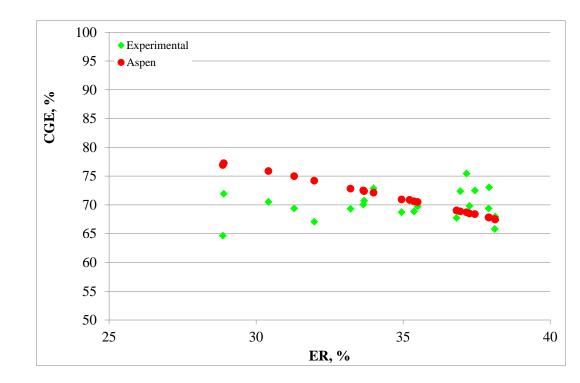




Figure 6 Comparison of the experimental syngas lower heating value with the results of the

Aspen Plus[®] simulation model.



475 Figure 7 Comparison of the experimental cold gas efficiency with the results of the Aspen
476 Plus[®] simulation model.

- **Table 3** Average value and standard deviation of the percentage difference between

the experimental and simulated results.

	Syngas mass concentration				
	N ₂	H ₂	СО	CO ₂	CH₄
Average	0.7	35.2	12.2	10.2	95.9
Standard deviation	0.4	27.4	9.1	7.7	14.9
	Syngas molar concentration				
	N ₂	H_2	СО	CO ₂	CH₄
Average	4.0	29.0	8.4	13.1	95.5
Standard deviation	3.1	22.2	7.0	8.8	17.1
	CGE	LHV	Syngas temperature	H_2 mass	H ₂ mole
Average	5.5	6.6	6.3	13.2	4.6
Standard deviation	5.2	4.5	5.1	12.6	3.4



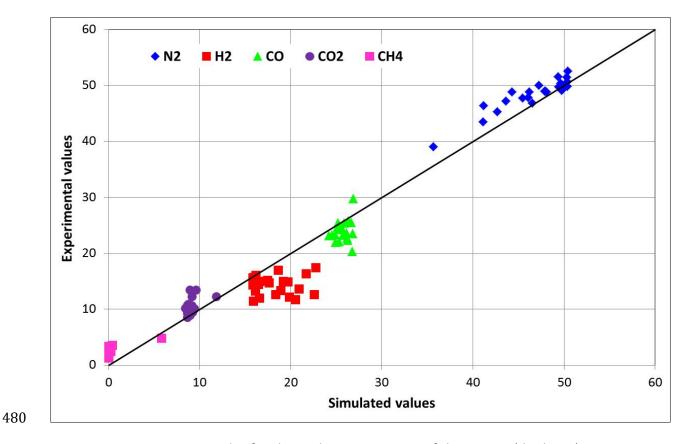
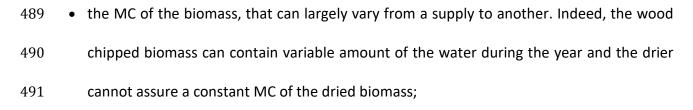


Figure 8 Parity plot for the molar composition of the syngas (dry basis).

482

483 **5.2** Performance assessment of the experimental gasification plant with Aspen Plus®

Once the reliability of the simulation model has been demonstrated using the comparison with the experimental data, it is possible to use it to predict and assess the thermodynamic and energy performance of the experimental gasification plant in various operative conditions without the necessity to execute further experimental tests. The most important controllable parameters for the gasification plant user are:



• the ER that largely affects the gasification efficiency and the syngas composition. It is the

493 most simple controllable plant parameter that the user can easily modify, operating the494 suction fan;

the gasifying air temperature, that can be simply modified with the control valve and
 affects the overall thermal performance of the gasification plant.

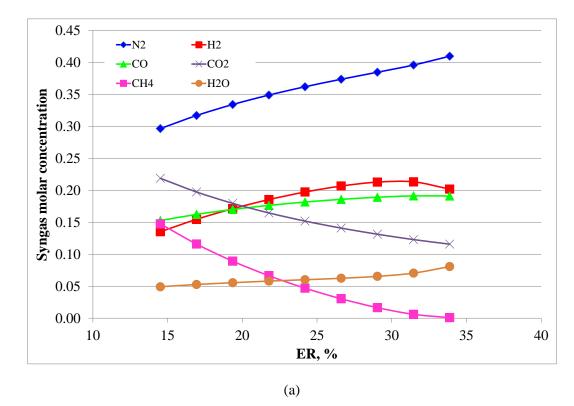
497 Hence, the simulations have been executed at different values of biomass MC and gasifying 498 air temperature vs. ER. In particular, two extreme values have been adopted for the biomass 499 MC (6 % and 14 %) and for the gasifying air temperature (20 °C and 300 °C). When the MC of 500 biomass has been increased, we assumed to maintain constant its dry matter mass flow equal 501 to 72 kg/h. The lowest value of the biomass MC can be considered the lower bound that can 502 be practically obtained using commercial industrial driers. The highest value is generally 503 considered the maximum allowable value in order to avoid an excessive production of tar in 504 the syngas. The maximum value of the gasifying air temperature can be easily obtained using 505 the air preheating with suitable gas-gas heat exchangers. The lowest value, that corresponds 506 to the atmospheric temperature, represents the absence of the air preheating and the heat 507 exchanger is completely bypassed by the air. So, ambient air is directly used as gasifying agent. 508 In this case the sensible heat of the syngas can be recovered during the successive cooling 509 with the atmospheric air.

The reduction of the biomass MC (Figures 9 and 10) ensures a higher production of CO, with an increase in LHV_s (Figure 11) and CGE (Figure 12). Indeed, the absorption of latent heat (required for the water vaporization) reduces the useful heat for the gasification reaction and the presence of steam tends to dilute the syngas. The value of ER with the highest H₂ and CO content in the syngas is slightly lower with high gasifying air temperature (Figures 9 and 10). Figures 11 and 12 show that the reduction of ER increases syngas LHV and CGE, so the

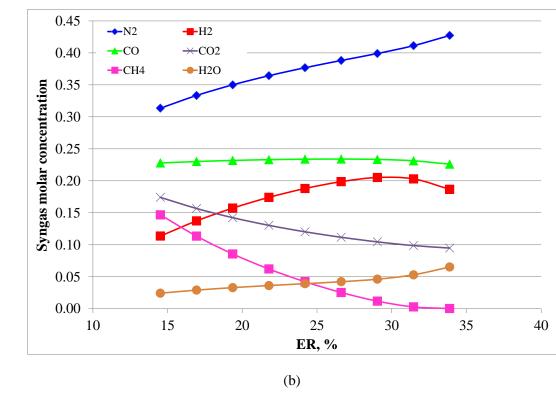
adoption of low ER could be reasonable. Actually the model-does not take into consideration

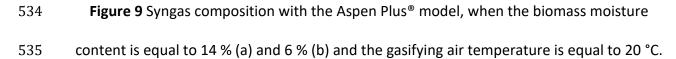
tar production which drastically increases at the lowest ER. Usually, an ER around 25-30 % is
adopted during operative conditions.

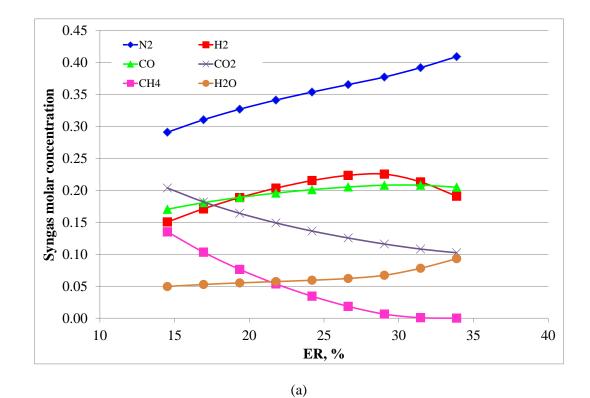
519 The effect of the gasifying air temperature on the gasifier performance is more relevant in 520 comparison with the MC (Figures 9, 10, 11, 12). On average, the change of the gasifying air 521 temperature from 20 °C to 300 °C implies the increase of the gasification efficiency by about 522 two percentage points. High values of the temperature assure an effective heating of the 523 biomass bed within the reactor and a more efficient development of the gasification reactions 524 with a higher syngas outlet temperature, as shown in Figure 13, and consequently higher 525 biomass conversion into syngas. Moreover, the syngas outlet temperature (Figure 13) can be 526 higher when the biomass has a low MC and, consequently, a higher LHV. With a low value of 527 MC it is possible to obtain higher gasification efficiencies as it happens increasing the air inlet 528 temperature. In particular, the change of MC from 6 % to 14 % implies the increase of the 529 gasification efficiency by about one percentage point.

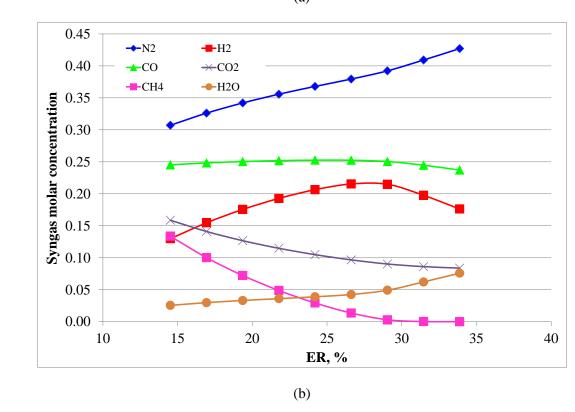


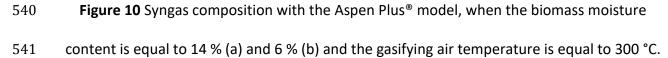


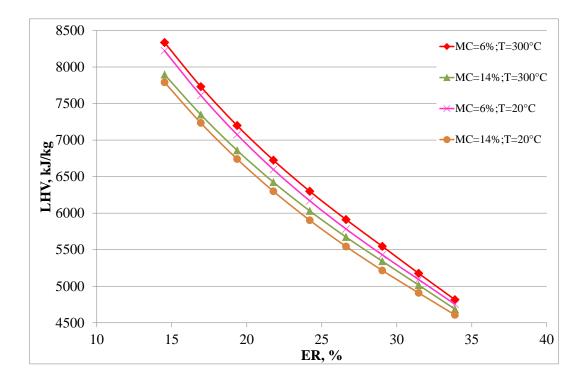




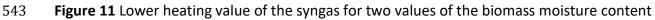




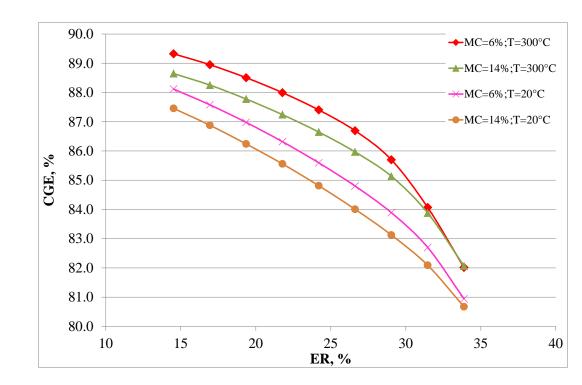




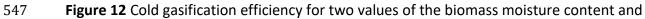




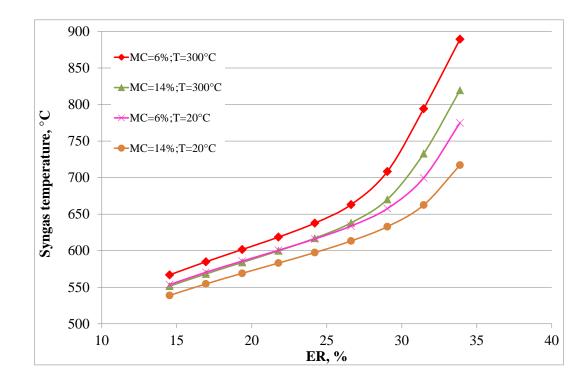
and gasifying air temperature.



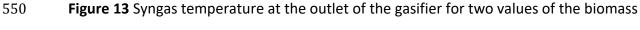




gasifying air temperature.







moisture content and gasifying air temperature.

552

553 **5.3 Comparison of the simulated results with literature data**

554 It is interesting to compare the simulated results presented in the previous section with the 555 data that are available in the wide scientific literature. In order to avoid the use of 556 heterogeneous results achieved with markedly different hypotheses, we have taken into 557 account only results that are obtained with equilibrium mathematical modelling and concern 558 explicitly small scale biomass downdraft gasifiers [23]. In order to make a reasonable 559 comparison, we have taken into account only results that are obtained with equilibrium 560 mathematical modelling and concern explicitly small-scale biomass downdraft gasifiers [23]. 561 Moreover, further experimental reference [42] has been taken into account for the 562 comparison. As previously mentioned the simulations have been performed considering 563 biomass characteristics, gasifying air temperature and ER (see Table 4).

565 **Table 4** Ultimate and proximate analyses of biomass for the literature comparison

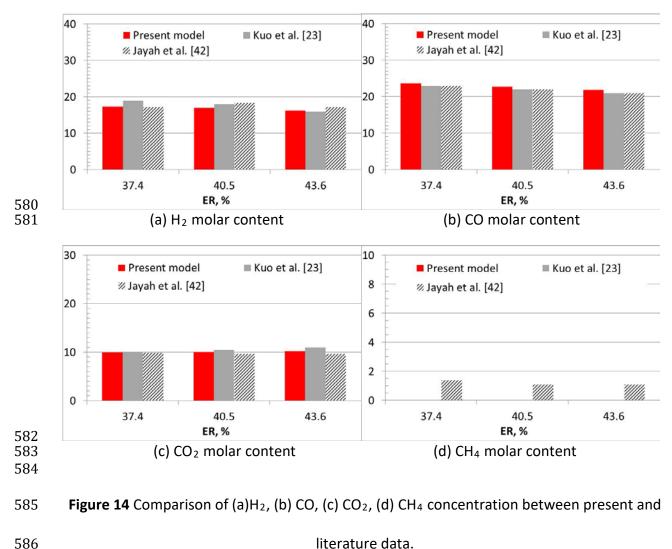
[42].

Proximate Analys	sis (wt%)	Ultimate Analysis (wt%)		
Moisture	5.76 %	Carbon	48.64 %	
Fixed Carbon	14.4 %	Hydrogen	5.64 %	
Volatile Matter	78.76 %	Nitrogen	0.52 %	
Ash	1.08 %	Sulphur	0.03 %	
		Oxygen	44.09 %	
Higher heating value (MJ/kg) 18.94				
Gasifying air temperature (°C) 20				

567

568 The results of the comparison, executed considering three values of ER, are summarized in 569 Figure 14, where it is possible to note a good agreement between current simulated results 570 and the references ones. The maximum relative error of H₂, CO and CO₂ molar concentration 571 on dry basis between the current results and those of [23] is about 9 %, 4 % and 7 %, 572 respectively. If the comparison is executed with the experimental reference [42], the 573 maximum relative error is about 7 %, 4 % and 5.5 %, respectively. As previously mentioned in 574 section 5.1, large differences are present concerning methane whose simulated predictions is 575 close to zero. This depends on the fact that the hypothesis of equilibrium for large values of 576 ER (as those used in this comparison) practically implies the complete conversion of methane into hydrogen and carbon monoxide [38-39], even if some incomplete conversion of pyrolysis 577 products can occur in real operative conditions [23]. 578

579



586

6. CONCLUSIONS AND FUTURE REMARKS 588

In this paper, a detailed numerical model developed with Aspen Plus[®] for an experimental 589 590 full-scale biomass gasification plant has been proposed, simulating the gasification process 591 with a kinetic free equilibrium approach.

592 The model has been implemented with all the measured plant data, such as the exact 593 geometrical and performance characteristics of the plant equipment and the control 594 operative logics. This approach assured to obtain a good matching between the simulation 595 results and the plant data in terms of syngas composition and energy performance of the 596 gasification process. In particular, the syngas composition is well simulated and predicted

except for the hydrogen and methane components, because the equilibrium assumption of
the model implies the complete conversion of methane into hydrogen. The other parameters,
such as the LHV of the syngas and the CGE, are estimated by the simulation model with an
average percentage error lower than 7 %.

Once the reliability of the simulation model has been demonstrated with the experimental results, it has been used to analyse the operative behavior and energy performance with respect to some important plant parameters. The most meaningful results are summarized below:

605 - By by recovering the sensible heat of the syngas at the outlet of the gasifier, it is possible
 606 to obtain high values of the gasifying air temperature and an improvement of the overall

- 607 gasification performances.
- The adoption of dried biomass with higher LHV assures higher gasification efficiencies with
 larger production of CO.

610 - The decrease of ER from about 35 % to about 15 % implies an increase of the gasification

611 efficiency by about 6-7 % in function of MC and gasifying air temperature.

612 - An increase of about 300 °C of the gasifying air temperature assures an improvement of

613 two percentage points of the gasification efficiency.

As a whole, the influence of MC on the gasifier performance is lower than that of the
gasifying air temperature.

- 616 The simulation model here presented allows to develop other investigations about some 617 modified layouts of the experimental gasification plant:
- 618 the syngas suction fan can be moved upstream the gasifier in order to obtain a pressurized
- 619 gasification process;

620 - the insertion within the simulation model of a specific external routine for the performance

assessment of the internal combustion engine;

622 - the flowing of some syngas through the gasifier to combine air gasification with CO₂
623 gasification.

624

625 **APPENDIX A**

626 A.1 Calculation of the pressure drop of the syngas across the gasifier

627 The pressure drop of the air/syngas across the gasifier (ΔP [Pa]) has been estimated with the

628 Ergun equation for flow through a randomly packed bed of spheres as follows [43]:

629

630
$$\Delta P = \left(150 \frac{\left(1-\varepsilon\right)^2}{\varepsilon^3} \frac{\mu_i}{d_\rho^2} u_i + 1.75 \frac{\left(1-\varepsilon\right)}{\varepsilon^3} \frac{\rho_i}{d_\rho} u_i^2\right) I$$
(A.1)

631

632 A.2 Calculation of the heat loss of the gasifier to the environment

The reactor is constituted by a stainless steel shell, which is internally protected by a refractory layer. The external surface of the reactor is insulated by ceramic fiber insulation that is protected by an aluminum cover. The procedure for the estimation of the thermal losses from the gasifier into the environment is described below [44-46]:

637

638

$$\dot{Q} = \frac{T_r - T_e}{R_{tot}} \tag{A.2}$$

639

640 *R*_{tot} can be calculated as follows:

642
$$R_{tot} = R_i + R_{c1} + R_{c2} + R_{c3} + \left(\frac{1}{R_e} + \frac{1}{R_r}\right)$$
(A.3)

644 where the thermal resistances are summarized in Table A1.

645

646

Table A1 Thermal resistances of the gasifier.

$$R_{i} = \frac{1}{\alpha_{i}\pi D_{i}L}$$

$$R_{c1} = \frac{ln\left(\frac{D_{e_refractory}}{D_{i}}\right)}{2\pi k_{refractory}L}$$

$$R_{c2} = \frac{ln\left(\frac{D_{e_shell}}{D_{e_refractory}}\right)}{2\pi k_{shell}L}$$

$$R_{c3} = \frac{ln\left(\frac{D_{e_shell}}{D_{e_shell}}\right)}{2\pi k_{insulation}L}$$

$$R_{e} = \frac{1}{\alpha_{e}\pi D_{e_insulation}L}$$

$$R_{r} = \frac{1}{\alpha_{r}\pi D_{e_insulation}L}$$

647

648 The evaluation of α_i [W/m² K] for the convective heat exchange between the air/syngas and 649 the internal surface of the refractory layer is executed with the following expression:

$$\alpha_i = \frac{Nu_i k_i}{D_i}$$
(A.4)

651 where

652
$$Nu_i = 0.023 Re_i^{0.8} Pr_i^{1/3}$$
 (A.5)

$$Re_{i} = \frac{\rho_{i} u_{i} D_{i}}{\mu_{i}}$$
(A.6)

$$Pr_{i} = \frac{C\rho_{i} \mu_{i}}{k_{i}}$$
(A.7)

655 α_e [W/m² K] is calculated considering the wind flow across the cylindrical shell using the 656 relation of Churchill-Bernstein:

657
$$\alpha_e = \frac{Nu_a k_a}{D_{e_insulation}}$$
(A.8)

658 where

659
$$Nu_{a} = 0.3 + 0.62 \frac{Re_{a}^{0.5} Pr_{a}^{1/3}}{\left[1 + \left(0.4 / Pr_{a}^{2/3}\right)\right]^{0.25}} \left[1 + \left(\frac{Re_{a}}{282000}\right)^{5/8}\right]^{0.8}$$
(A.9)

$$Re_{a} = \frac{\rho_{a}u_{a}D_{e_insulation}}{\mu_{a}}$$
(A.10)

$$Pr_a = \frac{Cp_a \ \mu_a}{k_a} \tag{A.11}$$

662

The evaluation of the radiative heat exchange between the cover of the external thermal insulation of the gasifier and the environment has been executed considering an equivalent coefficient of convective heat exchange. Hence, the evaluation of α_r is obtained with the following expression:

667

$$\alpha_r = E_m \sigma \left(T_\rho + T_e \right) \left(T_\rho^2 + T_e^2 \right) \tag{A.12}$$

Appendix B

- 671 The experimental data that have been used for the simulation with the Aspen Plus[®] model
- are summarized in Table B1.

Table B1 Experimental data used in the Aspen Plus[®] simulation

	_	
ER, %	Gasifying air temperature at the inlet of the reactor, °C	Biomass moisture content, %
34.9	252	5.6
33.2	280	5.6
33.7	328	6.5
28.9	375	6.5
34.0	414	6.5
28.9	284	8.3
32.0	351	8.3
31.3	401	7.4
33.6	422	7.4
20.4	427	4.8
36.9	350	9.8
35.2	491	7.9
38.1	292	7.9
36.8	384	10.1
38.1	206	4.7
37.9	362	7.1
35.4	362	7.6
35.5	400	7.6
37.3	425	5.5
30.4	321	8.7
37.4	394	8.7
37.9	434	6.2
37.2	450	6.2

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- 680

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