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Modelling Biomass Co-gasification in Downdraft Reactors for Sustainable Heat and Power Production

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ABSTRACT

The development of small-scale modular gasification systems represents one of the several pathways needed to follow to reach a net-zero emission society. Currently, the research is fostering the technology readiness level of those units to achieve clean and sustainable energy production from biomass waste while decreasing the load to the centralized waste treatment facilities. The operability of those conversion systems can be improved with the co-gasification of low-grade residues, like sewage sludge, organic municipal solid waste, nut shells, in wood matrixes.

Downdraft co-gasification is a promising technology that offers competitive conversion efficiencies, reliability, and capillary diffusion especially in the context of renewable energy communities. Still, there are research gaps that must be addressed especially for improving the design and process control.

This work presents a modelling approach that allow for deeper understanding of the treatment and propose improvements for SUPREMAS project. A lumped, steady-state model is developed in Aspen Plus using chemical pseudo-equilibrium and empirical correlations, to replicate the real process. Then, the cleaned syngas is converted to energy with a combined heat and power / solid oxide fuel cell units.

Keywords: Modelling, Co-gasification, Downdraft Reactor, Biomass Residues, CHP.

NOMENCLATURE

Abbreviations	
CFD	Computational Fluid Dynamics
CHP	Combined Heat and Power
CSTR	Continuous Stirred Tank Reactor
DAF	Dry Ash Free Basis
ET	Experimental test
ICE	Internal Combustion Engine
LSM	Lanthanum Strontium Manganite
QET	Quasi-equilibrium temperature
REC	Renewable Energy Community
SMR	Steam Methane Reforming
SOFC	Solid Oxide Fuel Cells
SSM	Steady state model
SUPREMAS	Syngas modular Units Providing Renewable Energy from Multiple wAstes and for different useS
WGS	Water-Gas Shift
WHS	Mixture of Wood and Hazelnut Shells
WSS	Mixture of Wood and Sewage Sludge
YSZ	Yttria-Stabilized Zirconia
Symbols	
C	Carbon content in feedstock [%]
CCE	Carbon Conversion Efficiency [%]
CGE	Cold Gas Efficiency [%]
ER	Equivalence ratio [%]
FC	Fixed Carbon [%]
FU	SOFC utilisation factor [-]
FV	SOFC opening valve [-]
H	Hydrogen content in feedstock [%]
M	Moisture [%]
LHV	Lower Heating Value [MJ/Nm^3] [MJ/kg]
$\dot{m}$	Mass flow rate [kg/s]
η	Efficiency [%]
O	Oxygen content in feedstock [%]
P	Electric Power [kW]
Q	Heat power [kW]
$RMSE$	Root Mean Squared Error [-]
S	Sulphur content in feedstock [%]
T	Temperature [°C]
y	Gas volume fraction [-]
VM	Volatile Matter [%]
Subscripts	
feed	Feedstock
id	Ideal

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od	Off-design
P	Electric Power
Q	Thermal Power
syn	syngas
T	Total Power

1. INTRODUCTION

Biomass gasification is a thermochemical conversion process in which biomass feedstocks are transformed into syngas through high-temperature reactions within a reactor. The efficiency and performance of the gasifier are influenced by multiple interrelated factors, including feedstock properties, reactor design, and operating parameters. A comprehensive understanding of these aspects is essential for various stakeholders: manufacturers focused on optimized reactor designs, end users seeking reliable performance, and planners requiring systems adapted to specific fuel types [1].

In fact, the gasification of biogenic waste materials is of interest for the authorities promoting renewable energy, particularly when such systems can anchor future Renewable Energy Communities (RECs), as foreseen in the SUPREMAS (Syngas modular Units Providing Renewable Energy from Multiple wAstes and for different useS) EU project.

In the framework of the European Green Deal (2020) and the Fit for 55 plan (2021)[2], SUPREMAS will advance the energy transition across diverse contexts (e.g., waste water treatment plants, municipal solid waste plant, etc.) developing sustainable technologies that valorise waste feedstocks into electricity, heat, and cooling at the benefit of local districts energy needs [3]. The SUPREMAS solution is designed for modular deployment and direct combined heat and power (CHP) integration, enabling stable syngas supply and straightforward adaptation to small REC or plants processing residual biomass and other organic wastes. This modular arrangement has been conceived to maximize the flexibility for the management of the system in different configurations according to the variability of the inputs in terms of feedstock and of the demand of energy from the local energy ecosystem, and to enable, in the future, the adaptability of the design to other end uses. To realise these objectives, extensive research and development efforts are to be undertaken in both the experimental and computational R&D in gasification.

Numerical modelling provides substantial benefits by allowing the determination of optimal reactor design and operating conditions without relying on extensive experimentation, which is often costly and time-consuming. In detail, mathematical models support gasifier design and enable the prediction of operational performance, including efficiency and syngas production under steady-state conditions, as well as system behaviour during start-up, shutdown, fuel switching, and load variations [4]. Various modelling strategies can be found in the literature to simulate biomass gasification, with the choice of approach depending on the specific objectives of the applications. Numerical modelling approaches reported in the literature for gasification modelling include thermodynamic equilibrium models and their modifications, kinetic-based models, computational fluid dynamics (CFD) simulations, and process simulation tools such as ASPEN Plus. Each approach offers distinct advantages and limitations depending on the desired level of detail, accuracy, and computational resources. CFD has the advantage to better characterise the gasification physics on a specific 2D-3D reactor geometry. Mass, momentum and energy balance equations are solved in a discretised domain, but a consistent amount of computational time is needed. Alternatively, the simplified process modelling approach can be used as a trade-off between fidelity and time resources. Each approach offers distinct advantages and limitations depending on the desired level of detail, accuracy, and computational resources.

Therefore, the purpose of this paper is to present a modelling approach for steady state gasification, based on chemical equilibrium/quasi-equilibrium.

Equilibrium models are widely used to analyse and predict the thermodynamic constraints of operating parameters in biomass gasification. It assumes that the final product composition attains a stable chemical equilibrium. Based solely on thermodynamic principles, equilibrium modelling does not require detailed information on the gasifier's geometry, capacity, or internal structure, making it particularly suitable for conceptual studies and preliminary design [5]-[6]. Equilibrium modelling is most accurate when reactions approach their equilibrium state, such as under high operating temperatures and when residence times are sufficient for the gasification reactions to reach completion. Its accuracy, however, decreases at lower temperatures (750 – 900 °C) [7], and it is less reliable in predicting light hydrocarbons and residual solid carbon in the product gas. To improve predictive accuracy, semi-empirical modifications of equilibrium modelling have been proposed. For instances, The quasi-equilibrium temperature (QET) method allows to shift the equilibrium of a chemical reaction from the equilibrium at a given reactor temperature [8]-[9]. Moreover,

empirical correlations can be set for a precise prediction of the formation of specific components.

The downstream conversion unit, needed to produce power, is often modelled, too. Centeno et al. [10] developed an integrated downdraft gasification model with syngas-fuelled ignition engine for power production. They showed that the power production is less than the one achieved with traditional fossil fuels due to the low syngas lower heating value (LHV_{syn} [MJ/Nm^3]) and moisture content in the feedstock. The kinetic approach is applied also for sewage sludge gasification and co-gasification with other biomass residues [11]-[12], an operation often needed to raise the feedstock LHV_{feed} [MJ/kg] enough to sustain the gasification reactions.

In summary, equilibrium modelling offers simplicity, minimal input requirements, and suitability for exploratory analyses and design evaluations. Its limitations include reduced accuracy at lower temperatures, inability to reliably predict light hydrocarbons and unconverted solids, and the need for semi-empirical adjustments to improve predictions.

The methodology adopted for the steady state model (SSM) is presented in section 2, together with the models for the power units. The results are presented and compared in section 3.

2. MATERIALS AND METHODS

One way to obtain power from biomass gasification in small-scale RECs is by coupling the gasification unit with power sources, like internal combustion engines (ICE), solid oxide fuel cells (SOFC), or combination of them. For this reason, the power production units are modelled as well, as given in Fig 1.

2.1 Gasification Section

The SSM is a readapted from the QET, lumped model of Biancini et al. [13] used for fluidized bed gasification of waste plastics. The structure of the flowsheet resembles the internal sections of a gasifier, i.e. drying, pyrolysis, combustion and reduction. The conceptual sketch of SSM is reported in Fig 2.

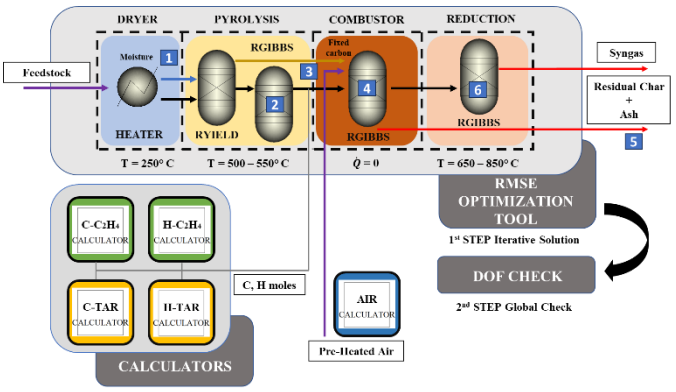

Fig 2. Sketch of SSM.

The following modifications have been done:

- DRYER: in fluidized bed, a fraction of the moisture may exit the reactor right after that the biomass enters the reactor. For downdraft, instead, all steam from dehydration proceeds downdraft to pyrolysis.
- PYROLYSIS: after decomposition (RYIELD), an additional RGIBBS reactor is added to form the typical volatiles compounds expected (H_2, CO, CO_2, H_2O, CH_4, C_2H_4, $C_{10}H_8$, C_6H_6, C_6H_7) assuming that a chemical equilibrium is reached. This is justified by the usually longer residence times of the solids/gas phases in downdraft gasifier.

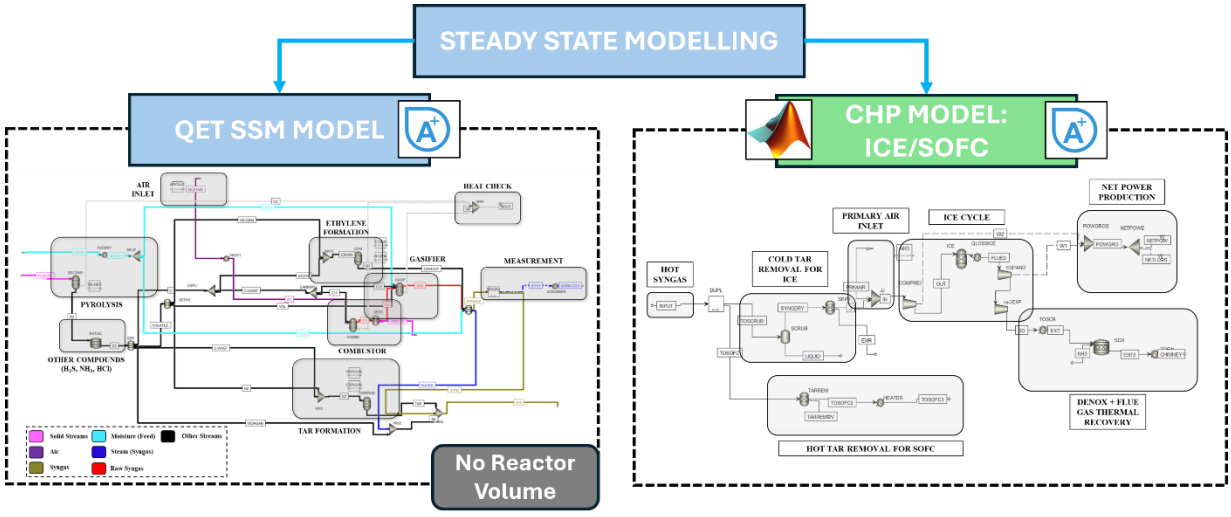

Fig 1. Gasification and CHP models.

• FIXED CARBON: only the fixed carbon of the feedstock moves to the combustion section. No char stream splitting is needed.
• COMBUSTOR: in this reactor, the oxidations reactions occur. CH_4/CO combustion reactions have been added: $CO_{(g)} + 0.5O_{2(g)} \rightarrow CO_{2(g)}$, $CH_{4(g)} + 1.5O_{2(g)} \rightarrow CO_{(g)} + 2H_2O_{(g)}$, $CH_{4(g)} + 2O_{2(g)} \rightarrow CO_{2(g)} + 2H_2O_{(g)}$. Moreover, the temperature of the reactor is calculated automatically such that all of the heat released by the reactions is transferred to the products.
• INERT CARBON: The model uses a calculator block to calculate the fraction of inert carbon, strictly related to the carbon conversion efficiency (CCE [%]). The streams emulate the residual char (assumed as 100% of carbon) that is not converted in the combustor/reduction sections. In general, the char yield is the highest at low ER.
• REDUCTION: the methane formation reaction has been added to the previous ones used for the fluidized model, $C_{(s)} + 2H_{2(g)} \rightarrow CH_{4(g)}$. The reactor temperature is set according to the one measured or reported in literature. At low ER, it is possible that the heat balance of the entire process is negative, meaning that the gasification is endothermic. While this is possible, it is preferable to have it exothermic or self-sustained. When this condition occurs, the temperature of the reactor is set such that almost zero heat is needed for the process.
• OPTIMIZER: for fluidized bed gasification, more parameters were needed to tune the model to match the experimental data of different waste feedstocks. After some preliminary analyses, it was noted that water-gas shift (WGS) and steam methane reforming (SMR) reactions´ equilibrium constant affect the most the model validation. The two temperature approaches are freely varied by the BOBYQA optimizer. The logic about tar and C_2H_4 yield is left untouched.

Other minor modifications were implemented, especially calculators and design specifications, useful to automate the flowsheet. the tar yield is fixed among the ER range. However, the concentrations are relatively low, and their inclusion is of second importance for this analysis. Hereafter, only C_2H_4 calculators are reported. The modelling sketch of SSM is reported in Fig 3. To optimise the correlation further, the RANSAC method has been used to smooth the trends.

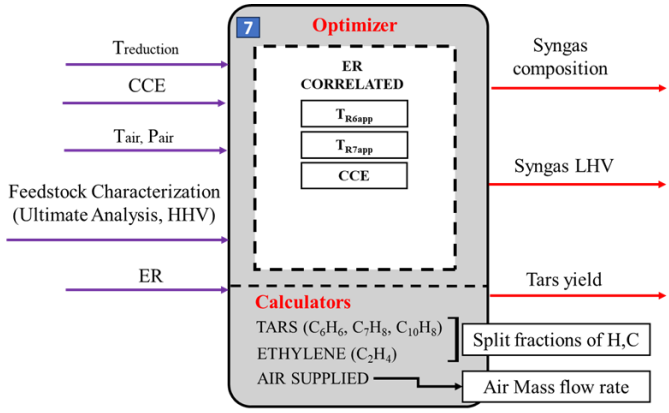

Fig 3. Modelling sketches for SSM.

The objective function $RMSE$ [-] to be minimized is as follows:

$$RMSE = \sqrt{\frac{\Delta LHV_{syn}}{LHV_{syn}} + \sum_{j=1}^{4} \frac{\Delta y_j}{y_j}}$$

where j denotes the element CO, H_2, CH_4, and C_2H_4. CO_2 is not considered since the precise volume fraction in the syngas is unknown. The syngas LHV_{syn} on a volumetric basis is calculated as follows [15] for SSM:

$$LHV_{syn} = 10{,}779 \times y_{H_2} + 12{,}621 \times y_{CO} + 35{,}874 \times y_{CH_4} + 59{,}483 \times y_{C_2H_4}$$

where y [-] denotes the element volume fraction in the gas phase. The air flow rate is calculated as following:

$$\dot{m}_{air} = \left[0.1153 \times C + 0.3434 \times \left(H - \frac{O}{8}\right) + 0.0434 \times S\right]/100 \times \dot{m}_{feed,dry} \times ER/100$$

where C, H, O and S denotes the mass fractions from the ultimate analysis [%], and $\dot{m}_{feed,dry}$ [kg/s] is the dry feedstock mass flow rate.

2.2 CHP Models

The ICE unit is modelled in Aspen Plus according to the typical transformations of an Otto cycle with controlled ignition. Data from manufacturer is not available, therefore a list of assumptions are stated and listed below:

• The clean syngas is blended with air in a lean mixture. The air flow rate is calculated by setting an equivalence

ratio of 1.6. A calculator block with FORTRAN code is used;

• Isentropic compression (efficiency 85 %), isochoric combustion with heat losses (10 % of LHV_{syn}), isentropic expansion (efficiency 90 %). Compressor blocks have been used for the compression and expansion, whereas the RGIBBS block simulates the combustion in the chamber. The fuel/air mixture is compressed up to 20 bar. The maximum pressure of the cycle is 50 bar, and the flue gases are discharged at 3 bar.

• DeNO$_x$ system for flue gases treatment, priorly to their release into environment. The unit operates at 350 °C, where the following reactions occur: $4NH_{3(g)} + 4NO_{(g)} + O_{2(g)} \rightarrow 4N_{2(g)} + 6H_2O_{(g)}$ (for NO) and $4NH_{3(g)} + 2NO_{(g)} + 2NO_{2(g)} \rightarrow 4N_{2(g)} + 6H_2O_{(g)}$ (for NO_2) [17]. The fractional conversion assumed for the two reactions is 95 %;

• Sensible heat is recovered from flue gas cooling (before and after the DeNO$_x$) and engine cooling;

• Implementation of a simplified off-design performance to scale the electric power production only. The characteristic curve is defined in a way that, at half load, the power produced is 40 % of the rated one (200 kW). Electric and mechanical conversion efficiencies, respectively of 97 % and 90 %, were defined to get the net power of the engine.

The ICE is fed with tar-free syngas. For this reason, a cold treatment with web scrubbing is needed between the gasifier and the ICE. The flowsheet of the entire system can be visualised in Fig 4.

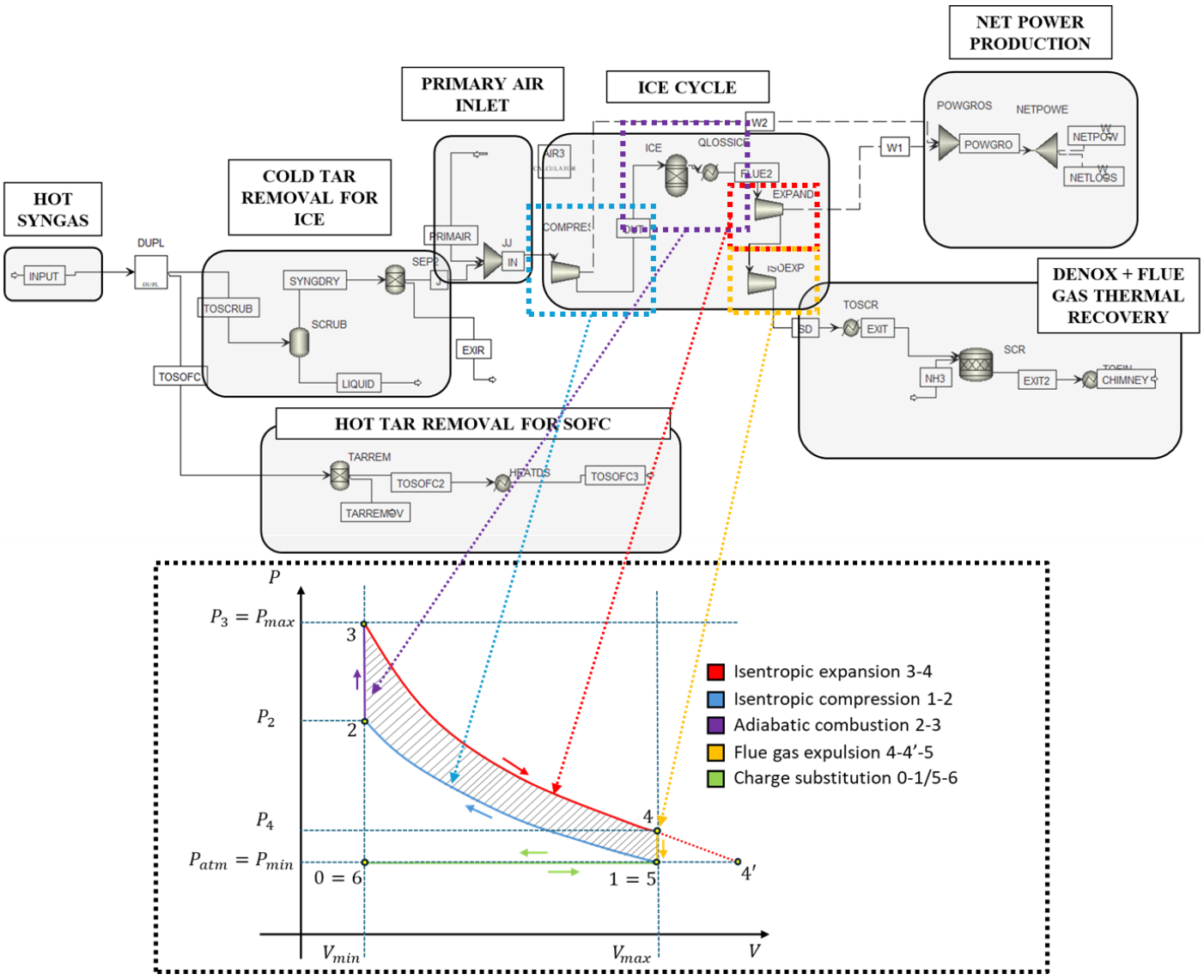

Fig 4. Visualisation of the ICE cycle in Aspen Plus.

The SOFC model was realised in MATLAB, modelled as a co-flow, anode-supported, planar configuration with stainless steel 441 used as the interconnect material. The electrolyte consisted of yttria-stabilized zirconia (YSZ), the cathode was composed of YSZ–lanthanum strontium manganite (LSM), and the anode was nickel-doped YSZ (Ni–YSZ). A one-dimensional (1D) dynamic model was developed to calculate the distributed temperature profile, localized current density, electrochemical losses, and Nernst potential across the cell using the finite volume method. The 1D framework allowed simplified calculations of flow and heat transfer, while chemical kinetic models were applied to evaluate the reactions along the cell length. The pressure drops in both the cathode and anode channels were assumed to be negligible. A detailed description and validation of this model are provided by Hughes et al [16].

3. RESULTS

3.1 Validation

The study of Barontini et al. [12] is used as a starting point, since it summarises the outcome of several experiments conducted with a similar downdraft gasifier, where the gasification of low feedstock LHV_{feed} was achieved by blending it with organic matter with higher LHV. In detail, the tests were conducted with woodchips and mixtures of organic fraction of municipal solid waste, sewage sludge (30 %), and hazelnut shells (53.5 %). The thermal power of the gasifier is around 800 kW. The conditions, tests and results are reported in Table 1 for the two feedstocks (WSS-WHS).

Table 1. Experimental data used for validation [12].

Parameter	Sewage sludge / Woodchips + Sewage sludge (WSS)	Hazelnut shells / Woodchips + Hazelnut shells (WHS)
Proximate analysis (blended feedstock)		
M (wt %. ar)	15.6	20.3
VM (wt %. dry)	-	-
FC (wt %. dry)	-	-
ASH (wt %. dry)	20	1.15
Ultimate analysis (blended feedstock) DAF		
C (wt %. dry)	39.89	50.48
H (wt %. dry)	4.93	5.92
N (wt %. dry)	0.42	0.27
O (wt %. dry)	34.61	42.14
Cl (wt %. dry)	0.06	0.02
S (wt %. dry)	0.07	0.02
LHV (MJ/kg dry)	15.05	19.26
Process parameters		
Fuel feeding rate (kg_{ar}/h)	226	191
Air flow rate (Nm^3/h)	250	247
Equivalence ratio (ER [%])	35.1	34.7
Syngas properties and gasification performance		
Gasification temperature (°C)	642	848
H_2 (vol %)	16.4	15.5
CO (vol %)	20.6	20
CO_2 (vol %)	11.3	12.3
CH_4 (vol %)	1.83	2.46
C_2H_6 (vol %)	0.02	0.07
C_2H_4 (vol %)	0.23	0.51
C_2H_2 (vol %)	0.01	0.03
N_2 (vol %)	49.6	49.1
Syngas LHV (MJ/Nm^3 dry)	5.18	5.44
Syngas flow rate (Nm^3/h^1)	415	415
Gas Yield (Nm^3/kg^1 fuel)	1.84	2.18
CGE (%)	71.9	73.8

The most important aspect to consider for the validation of SSM is not only the replication of the syngas properties, but also how they vary with different process conditions, especially the ER. Therefore, the validation of SSM will consider six experimental tests (ET1, ET6) for WSS and five for WHS (ET1, ET5), which offer an insight of the gasifier response between the ER range of 32 – 38 %. In general, with increasing ERs, the syngas yield increases but its LHV decreases due to the high nitrogen and low flammable gas contents. It is in fact recognised that such systems are designed to operate at an optimal ER. The maximum cold gas efficiency (CGE [%]) is reached around 32 – 34 %. The reference does not provide detailed data for the carbon conversion efficiency (CCE [%]) and CO_2 content. The validation of the model is reported in Table 2. A $RMSE$ below 0.30 is to be considered acceptable.

Table 2. Validation of SSM.

PAR.	POINTS WSS						POINTS WHS				
	ET 1	ET 2	ET 3	ET 4	ET 5	ET 6	ET 1	ET 2	ET 3	ET 4	ET 5
ER [%]	32.83	33.26	35.06	35.56	36.15	37.13	32.19	33.15	33.92	36.50	37.53
CO [% v/v]	22.35	22.14	20.75	20.26	19.61	18.44	20.38	20.13	20.10	19.36	19.08
CO_2 [% v/v]	10.75	10.82	11.50	11.77	12.14	12.83	12.57	12.55	12.46	12.50	12.53
H_2 [% v/v]	16.84	16.69	16.24	16.17	16.10	16.03	14.71	14.86	15.03	15.32	15.44
CH_4 [% v/v]	2.02	1.97	1.81	1.78	1.76	1.73	3.10	2.84	2.73	2.10	1.90
C_2H_4 [% v/v]	0.27	0.27	0.26	0.25	0.25	0.24	0.92	0.79	0.61	0.41	0.30
LHV [MJ/Nm^3]	5.52	5.46	5.17	5.09	4.99	4.82	5.81	5.63	5.5	5.09	4.94
Syngas Yield [Nm^3/h]	388	390	400	404	407	413	377	384	391	411	419
CGE MODEL [%]	74.68	74.23	72.13	71.51	70.74	69.42	74.81	73.85	73.46	71.36	70.55
CGE EXP [%]	75.66	75.63	71.28	70.06	69.93	69.51	74.88	74.52	73.77	72.53	72.14
RMSE [-]	**0.075**	**0.077**	**0.117**	**1.830**	**0.016**	**0.029**	**0.055**	**0.184**	**0.06**	**0.089**	**0.07**

PAR.	POINTS WSS						POINTS WHS				
	ET 1	ET 2	ET 3	ET 4	ET 5	ET 6	ET 1	ET 2	ET 3	ET 4	ET 5
RMSE (No C_2H_4) [-]	**ND**	**ND**	**ND**	**0.031**	**ND**	**ND**	**ND**	**ND**	**ND**	**ND**	**ND**

Sufficient accuracy has been achieved in the tight ER range. The $RMSE$ for ET4 is acceptable if ethylene is excluded. The predicted CGE for SSM is close to real data, with minor deviations. This result has been achieved by considering a constant CCE of 97 % for WSS, and 99 % for WHS, for the entire ER range. The following correlations, valid for WSS, have been obtained (x = ER):

- WGS T_{WGS}(x) = + 0.972x^3 - 108.62x^2 + 3991x - 47887 (cubic, for additional accuracy);
- SMR T_{SMR}(x) = - 0.729x - 47.959 (linear);
- C_2H_4, C fraction = - 0.0004x + 0.0519 (linear);
- C_2H_4, H fraction = - 0.0002x + 0.0284 (linear);

The following correlations, valid for WHS, have been obtained (x = ER):

- WGS T_{WGS}(x) = - 13.67x + 633.17 (linear);
- SMR T_{SMR}(x) = + 3.109x - 394.15 (linear);
- C_2H_4, C fraction = - 0.012x + 0.051 (linear);
- C_2H_4, H fraction = - 0.008x + 0.336 (linear);

3.2 CHP results

Table 3 and Fig 5 reports the heat and power produced with the ICE, after the tar removal with wet scrubber. The SSM and ICE flowsheets were linked. Three points were selected, to represent the performance at the minimum, medium and maximum values of ER in the validation range.

Table 3. CHP production with ICE.

Parameter	POINTS WSS			POINTS WHS		
	ET1	ET3	ET6	ET1	ET3	ET5
P_{id} [kW]	163	155	148	170	165	154
P_{od} [kW]	150	141	132	160	153	140
Q_{id} [kW]	411	394	375	427	415	392
Q_{syn} [kW]	596	575	554	609	598	574
$\eta_{P,syn}$ [%]	25	25	24	26	26	24
$\eta_{Q,syn}$ [%]	44	44	44	44	44	44
$\eta_{T,syn}$ [%]	69	69	68	70	69	68
$\eta_{P,feed}$ [%]	19	18	17	20	19	17
$\eta_{Q,feed}$ [%]	33	32	30	33	32	31
$\eta_{T,feed}$ [%]	52	49	47	52	51	48

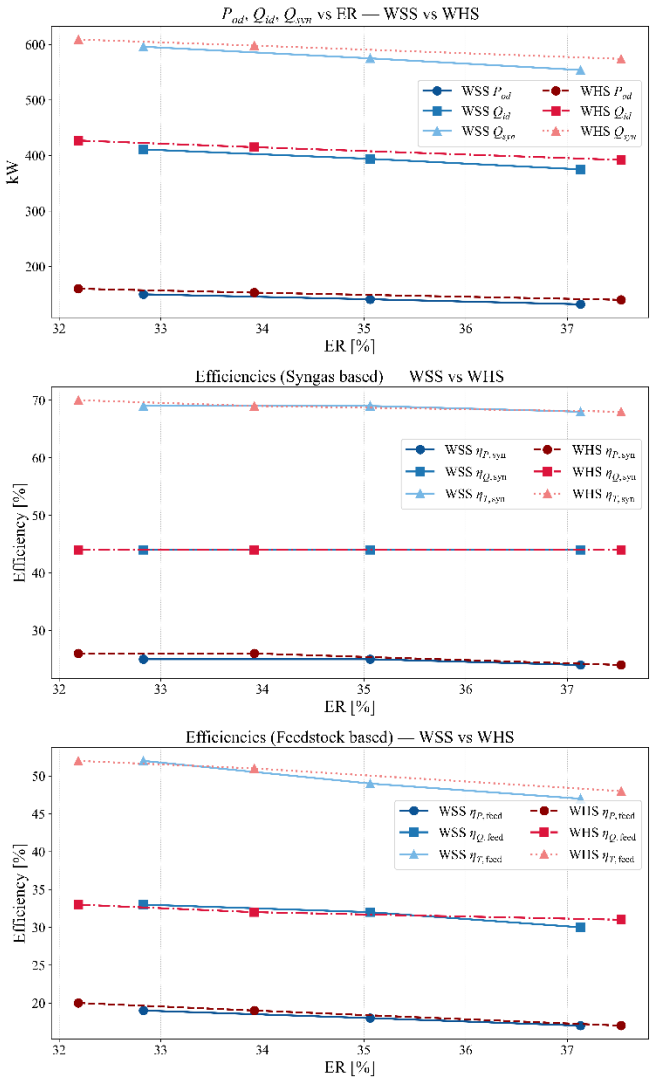

Fig 5. Power production and efficiency of the ICE, SSM1, in the validation range.

The combined recovery efficiency, comprehensive of the gasification CGE, is at maximum 52 % for both feedstocks, at the lowest ER (32 %). The maximum power efficiency is 20 %, while the heat one is 33 %. The trend decreases with ER, due to the syngas dilution with nitrogen.

Table 4 reports the power production with SOFC. The syngas enters at 600 °C and tars are removed with catalytic cracking.

Table 4. Power production with SOFC.

Parameter	POINTS WSS			POINTS WHS		
	ET1	ET3	ET6	ET1	ET3	ET5
Inlet flow [kg/s]	0.135	0.141	0.146	0.135	0.139	0.148
syngas thermal power [kW]	596	575	554	427	415	392
Stack power [kW]	280	266	253	270	271	259
FU [-]	0.8	0.8	0.8	0.8	0.8	0.8
cell number [-]	1600	1550	1490	1570	1580	1530
Efficiency [%]	47	46	46	44	45	45

Parameter	POINTS WSS			POINTS WHS		
	ET1	ET3	ET6	ET1	ET3	ET5
SOFC Temperature [°C]	835	835	835	850	850	850
FV opening [-]	55.8	56.65	57.41	55.4	56.18	57.8
Airflow [kg/s]	0.188	0.08	0.08	0.07	0.07	0.07
Air Temperature [°C]	771.5	692	695	683	678	670

The table shows the efficiencies of the SOFC unit when the gasifier operates at different ERs for the sewage sludges blended gasification. The SOFC efficiency stays around 45 %. The SOFC performs better with a higher hydrogen concentration, which variations are tight in this ER range. The power output of the SOFC stack reaches 280 kW, i.e. higher than the ICE (160 kW). Additional power can be recovered downstream the SOFC, with either combustion in an ICE or with sensible heat recovery with heat exchangers.

4. CONCLUSIONS AND FUTURE WORKS

The steady-state models successfully predict syngas composition, lower heating value (LHV), and cold gas efficiency (CGE) across a range of operating conditions and feedstock mixtures. Empirical correlations incorporated into the equilibrium model improved accuracy, while the kinetic model captured detailed reaction mechanisms and reactor hydrodynamics. Validation against experimental data from the literature confirmed the reliability of these models for subsequent design and techno-economic analysis.

Results show that co-gasification of sewage sludge with biomass enhances process stability and syngas quality, mitigating the limitations of sludge-only gasification. The modelling framework also highlighted the importance of controlling key parameters, such as equivalence ratio and temperature profiles, to maximize efficiency and syngas yield while maintaining operational flexibility. SSM has also prediction of the CGE.

The models used for power production are useful to address the overall efficiency of the system, crucial for supporting the REC.

Under SUPREMAS project, a real gasification unit will be constructed, and the models will be validated with in-field experimental data. They will be used for optimisation of the reactor and of the process, as a starting point for the algorithms of multi predictive control.

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