

SIMULATION OF THE GASIFICATION OF AGRICULTURAL RESIDUES USING COCO SIMULATOR

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ABSTRACT: The free simulator COCO has been applied for the study of the gasification of biomass. A Matlab unit operation was included in the model to enable the calculation of equilibrium heterogeneous reactions. The validity of the model has been confirmed by comparing its results with experimental data using sunflower husk as feedstock. Once validated, the model has been applied to the study of the gasification of pruning of apple trees. The influence of excess air and temperature on the efficiency of the process has been analysed. Overall, the model is found to operate stably and consistently over gasification of biomass reactions. The model represents a quick and effective tool to assess the effect of the modification of a variable and its impact on the overall gasification process in an efficient and costless way.

Keywords: agricultural residues, gasification, COCO simulator, spouted bed

1 INTRODUCTION

The use of biomass to produce renewable energy can provide a sustainable and low-carbon alternative to traditional fossil fuels based technologies. In particular, agricultural residues are one of the largest potential feedstock to become an important source of energy [1]. Their wide availability together with their renewable nature provides them with the adequate characteristics to become a new major energy vector. According to FAOSTAT, 2.23 Mton/year of apples are harvested in Italy and, consequently, large quantities of pruning residues need to be managed [2]. Pruning wastes from fruit trees are characterized by low-middle moisture and high cellulose and lignin contents [3]. After being collected, most of these wastes are burnt in the exploitation itself. As an alternative, land disposal of fragmented woody debris for nutrient recycling in soils is being slowly implemented.

The authors have already performed thermo-chemical reactions using pruning of apple trees in a spouted bed reactor at a pilot scale [4]. Despite its promising results, the technology is still far from its implantation at a larger and fully reliable scale. Computer simulations can be very useful to aid the design and scale-up of thermo-chemical conversion reactors. The development of robust mathematical models could provide the necessary tools for a more rapid, efficient and reliable technology development [5]. This arises the need of adequate simulation tools to evaluate, monitor and optimize these complex chemical processes. Different commercial software such as Aspen[®] [6] or Fluent[®] [7] have been already applied for the simulation of the different thermo-chemical reactions. Among them, Aspen[®] is vastly applied in the field of chemical engineering thanks to its complete compound thermodynamic database and its wide range of functionalities [8].

In spite of all the benefits and advantages that commercial software offer for chemical process simulations, a major drawback can be pointed out: commercial process simulators require a license that in most cases is expensive and must be renewed every year. If there is no renewal or purchase of this license it is not possible to develop new simulation projects or to have access to models previously built. This situation generates a problem of technological dependence. In this context, the CO-LaN organization (www.colan.org) has

promoted the creation of the CAPE-OPEN standards, where a set of free-to-use non-proprietary rules are defined. In them, different interfaces allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate. Currently, COCO (CAPE-OPEN to CAPE-OPEN) simulator is the CAPE-OPEN compliant reference tool [9].

COCO simulator is a non-commercial software for process simulation containing a vast database of the most used chemical compounds and a complete set of utilities able to handle almost any chemical engineering process. The simulator entails a set of unit-operations such as stream splitters/mixers, heat-exchangers, compressors, pumps and reactors and features a reaction package to power its simple conversion, equilibrium, CSTR, Gibbs minimization and plug flow reactor models.

For the purpose of this work, the thermodynamic equilibrium unit operation (RGIBBS) [10] based on the calculation of the reaction equilibrium by minimizing the Gibbs free energy is the standard approach. However, this unit is not able to handle reactions occurring in more than one single phase which makes it no adequate to model the gasification of biomass as it is a two-phase reaction. In order to overcome this difficulty and be able to use the whole potentiality of the tool in any context, Matlab/Excel unit operations are available to further personalize the process or overcome the limits of the already defined blocks.

In this context, a free-coded numerical simulation tool for the gasification of pruning of apple trees was developed with the aid of COCO simulator. A Matlab unit operation containing a user-defined code to calculate Gibbs equilibrium was used in order to perform the required two-phase calculations. The results of the new unit were compared with experimental results to validate the simulations. Once the model using COCO was validated, a sensitivity analysis was performed to assess the effect of temperature and equivalence ratio on the efficiency of the gasification of pruning of apple trees.

2 METHODOLOGY

A user-defined Matlab unit operation was introduced in COCO to perform the simulation of the gasification of biomass. The model was firstly validated with experimental data. The gasification of sunflower husk

described by Tasma and Panait [11] was used as the test scenario. Successively, the validated model was applied to evaluate the influence of the temperature and the amount of gasifying agent on the efficiency of the gasification of the pruning of apple trees. The scheme of the methodology of this work is represented in Figure 1.



Figure 1: Scheme of the methodology of the work

2.1 Feedstock

Sunflower husk (SH) was used as feedstock in the validation of the numerical model with experimental data [11]. Pruning of apple trees (PAT) were studied as potential feedstock for energy recovery purposes [4]. Table I presents the composition of all the tested samples.

Table I: Composition of feedstock

	SH *	PAT **
Proximate analysis (wt%)		
Fixed Carbon	17.00	19.95
Volatile Matter	65.79	77.18
Ash	3.71	2.87
Ultimate analysis (wt%)		
C	49.12	48.88
H	5.90	5.71
O	40.57	42.15
N	0.70	0.26
S	-	0.13
Ash	3.71	2.87

* wet basis (moisture = 13.5%); ** dry basis

2.2 Model development using COCO simulator

COCO is a collection of software components for setting up steady-state chemical engineering flowsheet simulations. It is composed of 4 main components. The CAPE-OPEN flowsheeting engine is called COFE (icon )). The thermodynamic system is called TEA (icon )) (Thermodynamics for Engineering Applications). The collection of unit operations that comes with COCO is called COUSCOUS (icon )). Finally, the CAPE-OPEN Reaction package is called CORN (icon )).

The set-up of the simulation with COCO is performed in two steps: firstly, a property package is created using the library TEA where the compounds involved in the simulation are defined and the property method is chosen. Afterwards, the flowsheet can be drawn through the COFE interface using the unit operations present in COUSCOUS and the reactions, if any, previously defined in CORN.

The thermodynamic library TEA (shown in Figure 2) and its chemical compounds databank are based on ChemSep LITE [12], a free equilibrium column simulator for distillation columns and liquid-liquid extractors.

Configuring TEA property package

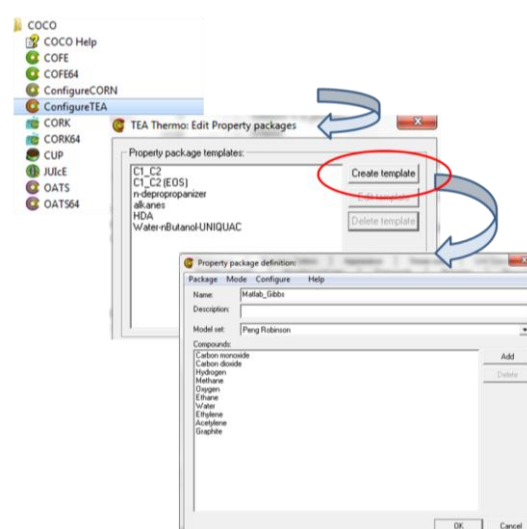


Figure 2: TEA property package

Similarly to commercial tools as Aspen Plus®, a Process Flow Diagram represents the chemical process composed by streams connecting the unit operations [13]. Unit operations are representations of physical equipment (a pump, a valve, a reactor, etc.) and can be coupled with other unit operations by means of material or energy streams. Underlying flowsheet calculations there is a thermodynamic system that represents the material streams and that can be used by the unit operations to perform thermodynamic property calculations [10]. Figure 3 shows the general view of the flowsheet and Figure 4 presents how the property package is added to COFE.

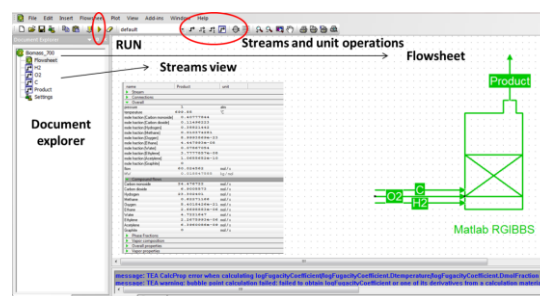


Figure 3: General view of COCO flowsheet

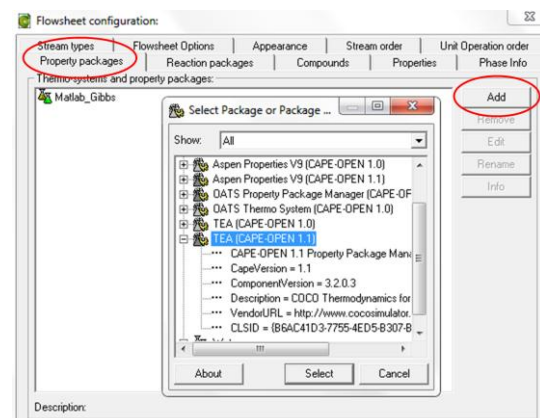


Figure 4: Addition of the property package

As explained before, the RGIBBS reactor in COCO is able to handle single-phase reactions [10]. For that reason, the available block was replaced by a Matlab unit operation in which a code with the same objective (minimizing the Gibbs free energy) was introduced to take into account the existence of the solid phase.

The Matlab CAPE-OPEN unit operation (Figure 5) can implement the functionalities of COCO while enabling a further personalization of the process through the insertion of an own-developed Matlab code. The script is inserted as shown in Figure 5 with the specific commands *getFeedProp* to pass the inlet data from COCO to the Matlab block and *setProduct* to restore the obtained results from Matlab back to COCO simulator.

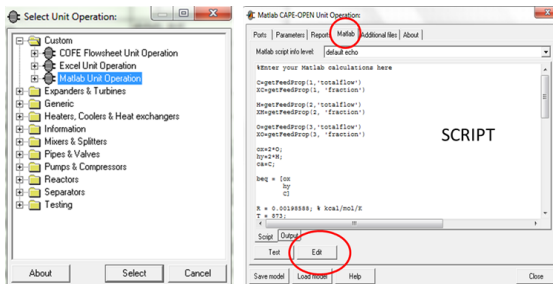


Figure 5: Set-up of the Matlab block

The code to calculate the equilibrium of two-phase reactions was inserted following the procedure described above. In it, the values of Gibbs free energy of the single components at the different temperatures of reaction were specified with data from the NIST Database [14].

Finally, the report with the main results can be shown directly in the flowsheet as shown as an example in Figure 6.

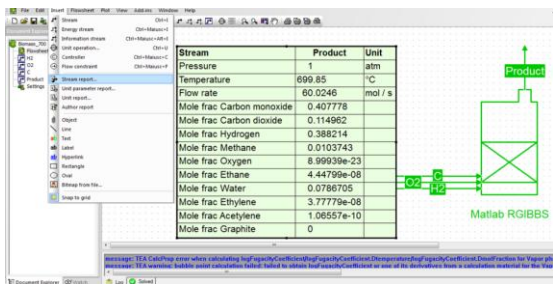


Figure 6: Main results report

2.3 Modelling approach

Different approaches have been applied to simulate the gasification of biomass. The use of equilibrium models is useful in a number of cases [15]. For example, when reaction kinetics are fast enough to assume the reactions are in equilibrium; or to study the limit-case of a process design: the reaction equilibrium represents the best-case scenario for the operation of a real reactor. The equilibrium approach [6] was used for the validation.

In order to specify the desired gasification conditions, the amount of additional air introduced in the system (ER) was calculated as:

$$ER = \frac{\dot{m}_{air}}{ER_{st} \cdot \dot{m}_{biomass}} \quad (1)$$

with $\dot{m}_{air}$ and $\dot{m}_{biomass}$ the mass flow rate of air and biomass respectively and ER_{st} the stoichiometric quantity of air required for the complete oxidation of biomass. ER_{st} was calculated on the basis of the ultimate analysis of the main components defined in Table I.

3 RESULTS

3.1 Validation of COCO model with experimental results

Sunflower husk was used as feedstock to perform the validations of the COCO model [11]. The flow rate of the inlet biomass (defined according to its ultimate analysis) was held constant for all simulations. For simplicity, only C, H and O were considered as representative elements, introduced in a mol of C basis.

Figure 7 shows the experimental results against those provided by COCO simulator. The good agreement confirms the validity of the model to study the gasification of biomass.

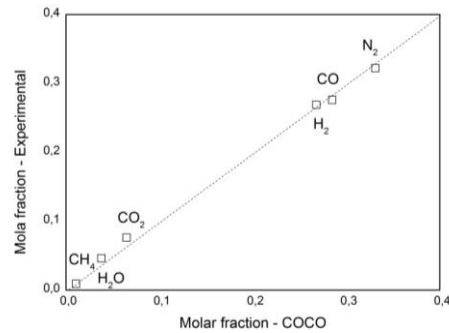


Figure 7: Validation with experimental data

3.2 Sensitivity analysis

Once the model was proved valid for the study of the gasification of sunflower husk, it was further applied to the evaluation of the gasification of the pruning of apple trees. In order to account for the un-reacted fraction of carbon in the biomass, a specified carbon fraction was separated from the main gas stream following the approach described in [16].

The effect of the Equivalence Ratio (ER) on the composition of the producer gas is shown in Figure 8 (T=700°C).

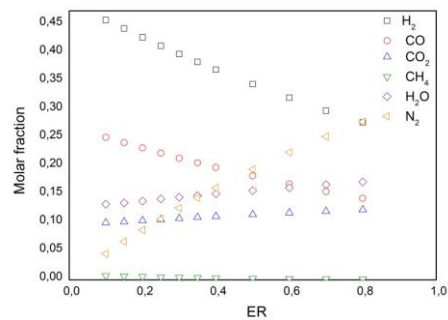


Figure 8: Influence of ER on gas composition

As expected, the concentration of CO decreases with ER due to the increased oxidation of the feed whereas CO₂ shows a slight increase as a consequence of the predominance of the reactions of oxidation. For the entire range of ER, the concentration of H₂ decreases in contrast with that of H₂O that increases and CH₄ remains very low with a decreasing trend. N₂ presented an obvious increasing trend with ER in all cases causing a diluent effect in the produced gas.

The effect of the temperature of the gasifier on the mole fraction of the components present in the produced gas is shown in Figure 9 (ER=0,25). All results are in wet basis. As shown from the figure, the concentration of H₂ increases sharply with the increasing temperature as well as that of CO whereas CO₂ reveals an opposite trend. CH₄ decreases steadily within the entire range of temperature. At relatively low temperatures (T=600°C) endothermic reactions are limited by the lack of energy and pyrolysis plays a more dominant role yielding more CH₄ at the initial stages of the reaction. As the temperature increases, endothermic reactions are strengthened in accordance to Le Chatelier's principle obtaining higher concentrations of CO and H₂. Moreover, due to the water gas shift reaction ($CO + H_2O \leftrightarrow CO_2 + H_2$) and its tendency to shift towards reactants as temperature increases, H₂ is further converted to CO and so, a faster growth rate of CO is observed at temperatures over 800 °C.

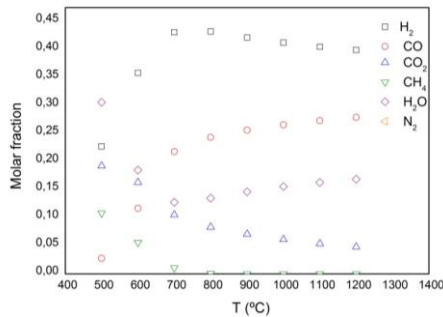


Figure 9: Influence of T on the gas composition

The performance of the gasification process was evaluated through the Cold Gas Efficiency (CGE).

$$CGE(\%) = \frac{\dot{m}_{gas} \cdot HHV_{gas}}{\dot{m}_{biomass} \cdot HHV_{biomass}} \cdot 100 \quad (2)$$

with $\dot{m}_{gas}$ and $\dot{m}_{biomass}$ being the mass flow rates of the produced gas and fed biomass respectively, and HHV_{gas} and $HHV_{biomass}$ the high heating values of the produced gas and fed biomass respectively, defined as:

$$HHV_{gas} (MJ / kg) = \sum_i x_i \cdot HHV_i \quad (3)$$

with x_i being the mass fraction of each combustible gas in the produced gas and HHV_i its corresponding high heating value in MJ/kg [17].

Table II presents the effect of ER (at T=700°C) and T (at ER=0,25) on the efficiency of the gasification of pruning of apple trees.

Table II: Effect of ER on the efficiency of the process

ER	CGE (%)	ER	CGE (%)
0,1	72,51	0,4	65,34
0,15	71,44	0,5	62,91
0,2	70,26	0,6	60,53
0,25	69,00	0,7	57,97
0,3	67,75	0,8	55,70
0,35	66,54		

At a fixed temperature, the CGE decreases with the ER as a consequence of the decrease on the molar fraction of the combustible gases (Figure 8).

Table III: Effect of T on the efficiency of the process

T (°C)	CGE (%)	T (°C)	CGE (%)
500	49,19	900	74,11
600	61,68	1000	74,11
700	69,00	1100	74,10
800	74,05	1200	74,09

On the contrary, as shown in Table III, the increase in temperature (at a fixed ER) leads to an increase in the CGE as a result of the increase of CO and H₂ at the initial phase (Figure 9) followed by a constant trend from 800°C on. From these results it can be stated that lower ER values and temperatures above 800°C would be optimum to perform the gasification of pruning of apple trees.

The obtained values using pruning of apple trees as feedstock are in line with other types of feedstock as rice straw or kaki leaves and stems with CGE around 70% at optimum gasification conditions [16].

4 CONCLUSIONS

A model for the simulation of the gasification of biomass has been developed using the free tool COCO. A Matlab unit operation has been included in order to perform the calculation of the two-phase equilibrium reactions. The validity of the model has been confirmed by comparing its results with experimental data using sunflower husk as feedstock. The high degree of agreement has proved valid the model using COCO. Afterwards, the model has been applied to the study of the gasification of pruning of apple trees. The influence of excess air and temperature has been evaluated confirming the suitability of the feedstock as energy vector.

In summary, the developed model is found to operate stably and consistently over gasification of biomass reactions. This represents a quick and effective tool to assess the effect of the modification of a variable and its impact on the overall process in an efficient and costless way. An upgrade to consider minor elements (S, N) will be included in the model to complete the scheme.

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7 LOGO SPACE

