# Prediction Tool for Gasification-produced gas composition Petr SEGHMAN, Tomáš JIROUT, Lukáš KRÁTKÝ

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# Abstract

Gasification is one of the most promising processes to utilize waste and convert it into either directly energy or into chemicals and fuels. The design of such processes requires the knowledge of the produced-gas composition, as it can vary depending not only on the feedstock, but also on the process parameters, reactor type and others. The presented tool including the database of the collected information about gasification outputs allows the user to get a brief estimation of the composition. In the following paper main functionality of the tool is described along with several outcomes showing main composition dependencies.

**Keywords:** Gasification, Produced gas, Composition, Prediction tool, Syngas, Biomass-to-Liquids, Waste Utilization

# Introduction

Biomass and waste gasification has a huge potential when it comes to conversion of waste into chemicals and fuels and thus reducing the amount of CO<sub>2</sub> in the atmosphere. It is a thermo-chemical reaction where feedstock (including carbon) is converted into a mixture of gases consisting of H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> (the product gas, sometimes referred to as syngas or bio-syngas) and other compounds and impurities such as H<sub>2</sub>S, tars and others. The composition of the produced gas can vary. For instance, hydrogen concentration ranges from as low as 9 % mol. during wood gasification using air as agent<sup>1</sup> to over 40 % mol. during wood gasification using steam as agent<sup>2</sup> or even higher when gasifying specific feedstock – producing over 60 % mol. of hydrogen with almond shells steam gasification<sup>3</sup> (all numbers related to dry bio-syngas). Such differences can highly affect the choice of the most suitable technology. Thus, for the purposes of further research including designing suitable technologies for particular scenarios and regions, approximate composition of the produced gas has to be known. This led to collecting data from various sources into a database that has been further developed into the composition predicting tool, allowing simple and quick selection of gasification conditions and separating the data valid for the selected case. Goal of the study was to be able to create a database of the product gas composition data and based on the outcome to evaluate which gasification conditions should be considered for future research.

One of the materials the database proved as reliable when it comes to gas composition is lignocellulosic biomass, especially when narrowed down to woody biomass. World amount of accessible lignocellulosic biomass (or lignocellulosic waste) can reach 20 000 mmt/year<sup>4</sup>. This makes this feedstock accessible and thus suitable for the technology. Typical composition of lignocellulosic biomass is around 35-45 %wt. of cellulose, 25-40 %wt. of hemicellulose, 15-25 %wt. of lignin and the rest composes of protein and ash. Elemental composition of lignocellulosic waste is shown in table below (see Table 1).

Element	Carbon	Hydrogen	Oxygen	Nitrogen	Sulphur	
Abr. / Unit	C [%wt.]	H [%wt.]	O [%wt.]	N [%wt.]	S [%wt.]	
Woody biomass <sup>1</sup>	51,4	6,1	40,8	0,6	0,4	
Straw <sup>5</sup>	44,1	5,3	39,7	0,7	0,1	
Corn stover <sup>5</sup>	49,6	5,4	38,1	0,8	0,1	

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# Methods

The database itself collects information about feedstock, gasification agent, gasifier, some of the gasification conditions, catalyst presence and produced gas composition. Some of the characteristics must be picked from a dropdown list to ensure the macros, that are involved in the tool, work properly. The data were mostly collected from available scientific sources – till 20. 2. 2019 the database contains data from 10 scientific sources with over 80 different gasification configurations. All the references are also stated in the database so that the information can be easily verified.

Not each scenario is represented the same. As can be seen in the figure below, Figure 1, distribution of gathered information is highly unbalanced towards woody biomass. From that reason, many investigations of reliability of the concentration prediction further in this paper were carried out on the cases with woody biomass as feedstock. Therefore, woody biomass along with MSW have been chosen for further studies.



Figure 6: Distribution of feedstock in cases involved in the database.

The main part except for the database containing the data is a simple prediction tool. For the selection of the specified configurations simple dropdown and checking fields were made. After the parameters are set, a simple macro chooses only the correct data as a preparation for the following operations. Then, basic statistical computations (average concentration and standard and relative error of the values for each syngas component) are made. Also, several figures are made from the selected data.

### **Results and discussion**

The first case studied was the possibility to predict product gas composition without specifying any parameter. In this case, relative errors of concentration of H<sub>2</sub> reached almost 60 % (range of H<sub>2</sub> concentration was around 7 – 28 % mol.). Even when agent was specified, the uncertainties still stayed high (relative errors around 35 % for CO and CO<sub>2</sub> concentration).

To lower the uncertainties, it was necessary to fix more of the gasification parameters. The easiest and probably most common fixation would be picking a specific feedstock (input). For this purpose, woody biomass and MSW were selected, as most data cover those cases.

### Woody biomass as feedstock

Two main cases inspected are oxy-gasification and steam gasification of woody biomass. In those cases, lower uncertainties compared to those from mixed input gasification were obtained. In the following table, Table 4, data for comparison of the cases are stated.

Table 4: Syngas composition from oxy- and steam gasification of woody biomass, independent on gasification time and reactor type.

Oxy- and Air- gasification (Temperature between 690 – 820 °C)							
Compound	Abr.	Average c <sub>i</sub> [%mol]	St. error [%mol]	Relative error [%]			
Hydrogen	H <sub>2</sub>	12,1	2,8	22,8			
Carbon Monoxide	CO	36,5	6,8	18,5			
Carbon Dioxide	CO <sub>2</sub>	44,3	7,8	17,7			
Methane CH <sub>4</sub> 7,0 1,8 25,7				25,7			
Steam gasification (Temperature between 800 – 950 °C)							
Compound	Abr.	Average c <sub>i</sub> [%mol]	St. error [%mol]	Relative error [%]			
Hydrogen	H <sub>2</sub>	39,8	4,6	11,5			
Carbon Monoxide	CO	24,3	4,6	19,2			
Carbon Dioxide	CO <sub>2</sub>	24,7	4,8	19,4			
Methane	CH <sub>4</sub>	11,3	2,0	17,7			

As seen in the table above, the range for each concentration is smaller than it is for the gasification of mixed inputs. In this more specified case better optimization can be achieved. In the following figures, Figure 1-4, several scenarios have been chosen to demonstrate the range of concentration (shown on the figures depending on temperature) for woody biomass gasification.



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Figure 1: Concentration of  $H_2$  and CO in wood-gasification, reactor and gasification agent not specified, without catalyst specification.

Figure 2: Concentration of  $CH_4$  and  $CO_2$  in wood-gasification, reactor and gasification agent not specified, without catalyst specification.



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Figure 4: Composition of biosyngas (H<sub>2</sub> and CO concentrations shown) for woody biomass, only steam gasification, reactor not specified.

### Mixed solid waste as feedstock

For MSW only data for steam gasification have been obtained. Therefore, all the following data are for that case. As seen in the following table, Table 5, concentrations along with their uncertainties for MSW steam gasification are shown.

Table	5:	Syngas	composition	from	steam	gasification	of	mixed	solid	waste	(MSW),
Tempera	ture	ranged f	rom 700 – 900	°C.							

Compound	Abr.	Average c <sub>i</sub> [%mol]	St. error [%mol]	Relative error [%]
Hydrogen	H <sub>2</sub>	45,4	8,4	18,6
Carbon Monoxide	CO	28,8	12,5	43,4
Carbon Dioxide	CO <sub>2</sub>	22,3	8,9	39,7
Methane	$CH_4$	3,4	4,6	135,6

As seen in the table, even after close specification (MSW as feedstock, steam as agent) the ranges of each concentration are wide. Especially values for CO and CO<sub>2</sub> have uncertainty close around 40 % and can range from 16 to over 40 % mol. for CO and from 14 to over 31 % mol. for CO<sub>2</sub>. This is caused by the nature of mixed solid waste – its composition can vary greatly. The results for CO and H<sub>2</sub> concentration for steam gasification of MSW are shown in the following figure, Figure 5.

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Figure 5: Syngas composition (shown only on  $H_2$  and CO) from steam gasification of mixed solid waste (MSW).

### Fixed feedstock and agent results

As seen in the figures above, after a close specification of parameters (fixing both feedstock and agent), a narrower dataset is obtained, and thus downstream technology is easier to be designed. Unfortunately, composition of MSW can vary a lot, thus the composition of produced syngas varies as well.

#### **Fixed temperature**

In the cases above, temperature dependency was chosen to demonstrate the variety of data. However, temperature control in practice would not allow to gasify the inputs at a constant temperature. Also, most of the times, the temperature is dependent on the gasifier type and highly dependent on the gas. agent (steam gasifiers involved in the database have been operated at higher temperatures than the air- and oxy-gasifiers). Furthermore, based on experimental experience, the temperature is in most cases different in the upper and the lower part of the gasifier. Therefore, having temperature as a fixed parameter would not be realisable in practise and thus will not be concerned in the further studies.

#### **Fixed gasifier type**

In the following figure, Figure 6, distribution of concentration at air, oxy-, air-steam and oxy-steam gasification to gasifier types is shown. As can be seen, in circulating fluidised bed gasifiers, the least concentration of  $H_2$  is reached whereas the concentrations of both CO and CO<sub>2</sub> are higher. This might also reflect the fact that not all feedstock has been gasified in each reactor. Some reactor types involved in the database have been used only for steam-gasification and thus are not involved in the following charts (EF - Entrained Flow and DFB - Dual Fluidised Bed gasifiers). However, conclusions about syngas composition based on reactor type are not quite reliable as both temperature and agent can differ in those cases and most often are the main cause of the differences.

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Figure 6: Syngas composition (shown only on  $H_2$  and CO) from oxy-, air, oxy-steam and airsteam gasification of various feedstock data contained in the database. FB – fluidised bed, EF – entrained flow, CFB – circulating fluidised bed, FIX – fixed bed, DFB – dual fluidised bed

### Conclusions

Gasification is a promising method and depending on the particular gasification conditions, its product – the product gas or biosyngas – can be suitable for various technologies that convert it into valuable chemicals or fuels. However, its composition depends on many gasification parameters. Some of those parameters must be defined in advance to designing the utilization technologies to ensure a stable composition and thus allow picking the most suitable technology and its optimization.

As seen in the table below, Table 6, fixing both feedstock and agent narrows the standard deviations (and uncertainties) the most so that the range of the concentrations. Other parameters were not fixed as in some cases it would reduce the amount of data under the specified criteria to as low as a set of 3 or 4 values for the narrowest specification. That would lead to distortion of the deviations and would not provide reliable information.

Table 6: Standard deviation of	f concentration of H₂ and CO in cases with no specification, with
feedstock specified and with both	h feedstock and agent specified (respectively).

Feedstock	Agent	Standard dev. CO [%mol]	Standard. dev. H <sub>2</sub> [%mol]	Temperature range [°C]*
-	-	8,9	14,7	690 – 1000
Woody	-	8,6	13,9	690 – 950
Woody	Oxygen + air	6,8	2,8	690 - 820
Woody	Steam	4,6	4,6	800 - 950

\*Temperature range was not specified but resulted from the chosen scenario

When woody biomass being the feedstock and either air, oxygen or steam being the gasification agent, reliable information about concentration is achieved. For comparison, values for MSW are shown as well. The approximate concentration of the main components –  $H_2$ , CO, CO<sub>2</sub> and CH<sub>4</sub> are as follows, with standard deviations:

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Table 7: Values of main components concentrations and deviations for gasification of woody biomass by oxygen/air and steam and gasification of MSW by steam (\*irrational value as returns negative values of concentration, shown for demonstration of the variety).

Feedstock	Agent	H <sub>2</sub> [%mol]	CO [%mol]	CO <sub>2</sub> [%mol]	CH₄ [%mol]
Woody	Oxygen + air	12 ± 3	37 ± 7	44 ± 8	7 ± 2
Woody	Steam	40 ± 5	24 ± 5	25 ± 5	11 ± 2
MSW	Steam	45 ± 8	29 ± 13	22 ± 9	3 ± 5*

The future goals for the research are:

- to collect wider information of the data and fill gaps in feedstock types
- to gather information about impurities (such as H<sub>2</sub>S, halogens and other) and involve it into the database
- to study possibilities of woody-biomass gasification-produced syngas utilization
- to compare feasibility of the produced fuels and chemicals to conventionally produced ones

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# Nástroj pro odhad složení plynu produkovaného gasifikací

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### Souhrn

Zplyňování je jedním ze slibných způsobů pro využívání odpadu a jeho konverzi na energii či na paliva a cenné chemikálie. Návrh takovýchto technologií vyžaduje znalost složení plynu vznikajícího gasifikací, protože se toto složení liší v závislosti na různých parametrech, zejména pak na vstupním materiálu a zplyňovacím médiu. Představený násrtroj umožnil posouzení závislosti na jednotlivých parametrech. Zahrnuje databází sebraných informací ohledně zplyňování a umožňuje jednoduchý odhad složený produkované směsi. V tomto textu je popsána funkce tohoto nástroje spolu se zhodnocením závislosti na vybraných parametrech.

Klíčová slova: zplyňování, gasifikace, produktový plyn, složení, biomass-to-liquids.