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Exploring future flue gas conditions from silicon production through stochastic process simulation

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Abstract – Many industrial producers of metallurgical grade silicon (MG-Si) have a strategy for emission reduction involving biocarbon reductants in the near future, followed by carbon capture on the medium term. Technical and economic challenges in implementing carbon capture are related to flue gas conditions from the submerged arc furnace. This work takes a modelling approach to explore how these conditions will be affected by the upcoming transition to biocarbon.

Two different scenarios are studied, one investigating mixed fossil/bio-reductant charges with increasing use of charcoal, and one investigating selected charge parameters with biocarbon as the only reductant. Six different charcoals, treated at different temperatures and from various wood sources are used in the model. A Monte Carlo approach is taken for simulations, capturing variability and uncertainty in process and furnace parameters.

Results show the significance of volatiles on flue gas conditions. The charcoals contain less volatiles than coal, and thus produce flue gases with significantly lower heat content and temperatures, and with less water and CO_2. There is also a drastic reduction observed on the flue gas sulfur content, although this relies on a mechanism that requires verification. In general, the results indicate that conditions could become more favourable for carbon capture implementation when biocarbon is replacing fossil carbon sources in silicon production.

1. INTRODUCTION

The Norwegian silicon- and ferroalloy-producing industry is aiming at net zero greenhouse gas emissions from their operations by 2050. Current technology for silicon production relies on carbon for reduction of silica and thus inherently produces large amounts of CO_2, with direct emissions around 4.7-5 kg CO_2e/kg Si (Sævarsdottir *et al.*, 2021). While novel, carbon-free technologies are under development, it is necessary to make adaptations to the current processes in the very near future. The strategies shared by major industrial actors Elkem and Eramet (Ravary *et al.*, 2021) highlight both increased use of bio-based carbon materials and implementation of carbon capture (CC) from flue gases as the most viable pathway towards their climate goals.

The carbon capture system needs to be designed for the properties of the furnace flue gas, and some adaptations must likely be made to the furnace operations to make the conditions for carbon capture more economically favourable. Andersen investigated flue gas composition under different conditions for open and semi-closed furnaces, and proposed technology for increasing CO_2 concentration in the flue gas, thus reducing the necessary size and cost of implementing conventional carbon capture equipment (Andersen, 2023). On the other hand, Riboldi et al. has investigated the use of a more novel capture concept based on temperature swing adsorption in a rotary vessel for the conditions from ferroalloy production (Riboldi *et*

al., 2024). There is however a gap in knowledge on how flue gas conditions in silicon production will be impacted by the increasing use of biogenic carbon materials in the furnaces.

The carbon material mixes currently used in silicon producing furnaces can be quite varied, but typically consist mostly of coal together with some coke and woodchips (Myrvågnes, 2008). Reducing the use of fossil carbon entails replacing the coal and coke fractions, usually with woody charcoals and agglomerates thereof. Many technical challenges related to gas flow and reactivity derive from different structural/chemical and mechanical properties of the novel materials, but for flue gas conditions the most important differences are in the amount of fixed carbon, the chemical composition of the ash and volatile fractions, as well as the resulting heating value.

This work explores the impact of these differences through a modelling approach, using mass- and energy balances together with elemental distribution coefficients to relate changes in raw material mix parameters to changes in flue gas conditions. Two case studies are performed, varying both the amount of biocarbon used and specific properties of the biocarbon mix. Six different sets of charcoal analysis data are used, with variation both in pretreatment and wood source. Finally, the findings are discussed with regards to flue gas treatment in general and carbon capture in particular.

2. METHODOLOGY

In this study, a model of material and energy flows in a silicon producing submerged arc furnace was constructed using HSC Sim 10 (Roine, 2025). Distribution coefficients from furnace mass balances (Kamfjord, 2012) were used together with equilibrium calculations to solve the material flows. Heating value correlations and some select temperature specifications were used to solve the energy flows. Being a fully static model, it did not include any dynamics in gas evolution or any accumulation of material in the furnace. This is not to suggest that the furnaces operate in steady state, but rather to limit the scope to operational ranges for parameters instead of studying transients.

2.1 Model details

Starting with a quartz consumption of 2 tonnes/hour, a specified fixed carbon-based raw material mix and a set carbon coverage close to 95 % is used to determine the required carbon material input. Based on the raw material analysis data, these carbon materials are split into fixed carbon, volatile and ash fractions. The volatiles are simplified as N_2, O_2, H_2, and CH_4 or CO only, while all other elements go into the ash as oxides. These volatiles, any moisture, and a small percentage of the fixed carbon, representing carbon losses from fines, are sent to combustion calculations, while the ash, quartz and rest of the carbon is sent down into the furnace. This quartz is assumed to be pure SiO_2. Heating values, calculated from the Dulong formula (Hosokai, 2016), are used to correct the energy content of the volatiles, based on the elemental composition in dry basis. The lower heating values (LHV) are used, which assumes that the energy used for evaporation of water is not recovered through condensation.

$$LHV\ [kWh/kg] = 33.8m_C + 122.3\left(m_H - \frac{m_O}{8}\right) + 9.4m_S \quad [1]$$

The descending reactants are first heated by ascending process gases. Then, distribution coefficients are used on the elements in the ash to determine how much should enter the metal and slag phases. Any remaining material enters the rising process gas phase. To maintain the oxygen balance when elemental vapours form from the ash oxides, some of the SiO in the process gas reacts to SiO_2 and enters the oxide phase with the remaining ash. These oxides

then react to equilibrium at 2000 °C with the fixed carbon to form metal and slag, which is tapped, and the CO- and SiO-containing process gas. It is here assumed that all fixed carbon eventually reacts to CO. A small percentage of this gas, on CO basis with a set SiO/CO ratio, is removed as tapping gas at 1800 °C before the addition of vapours from the ash.

Power is supplied to the furnace based on the energy balance of the equilibrium reaction. A small but proportional amount of carbon is also added as electrode consumption. The degree of reactant heating and remaining energy flows are then determined by fixing the temperature of the process gas in both the lower and upper part of the furnace. Any difference in process gas heat content between the slag/metal equilibrium calculation and the lower part of the furnace is taken as diffuse heat loss.

The combustion step is also solved as an equilibrium. Here, process gas and volatiles combine with large amounts of air, and are allowed to react to form gaseous oxides. The temperature is controlled to maintain the energy balance. For simplicity, it is assumed that all particles combust to gases in this step. In the next step SiO_2(s) fumes are condensed and removed from the gas, and other elements also enter the solid fume phase according to their distribution coefficients. A simplification is made specifying only a single solid compound per element in the fumes, either an oxide, sulphide or hydroxide, according to predominance. The amount of sulfides formed determines how much SO_x(g) is left in the gas, and as such the distribution coefficient for sulfur is not used. An exception is made for calcium, which forms both CaO(s) and $CaSO_4$(s) depending on stoichiometry and availability of sulfur. Lastly, an equilibrium is solved in the remaining gas phase, allowing for the formation of CO and H_2 if conditions allow. The temperature is again controlled to maintain the energy balance, and the final flue gas conditions are obtained.

2.2 Simulation strategy

Any simplified model of complex systems like a silicon furnace will heavily depend on the values set for innate and operational parameters, such as electrode consumption, carbon coverage and the aforementioned process gas temperatures. Many of these are difficult to know accurately, and they will also vary between furnaces and with time. In order to capture this uncertainty and variability in the results, a Monte Carlo simulation strategy is adopted. Here, most parameters are given a probability distribution around a typical value, and results are aggregated from a large number of simulations where the actual parameter values are randomly drawn each time. The probabilities are distributed normally, with mean values and standard deviations derived both from open literature and discussion with industry. An illustration of the simulation framework is included in Figure 1, together with an overview of process parameters in Table 1.

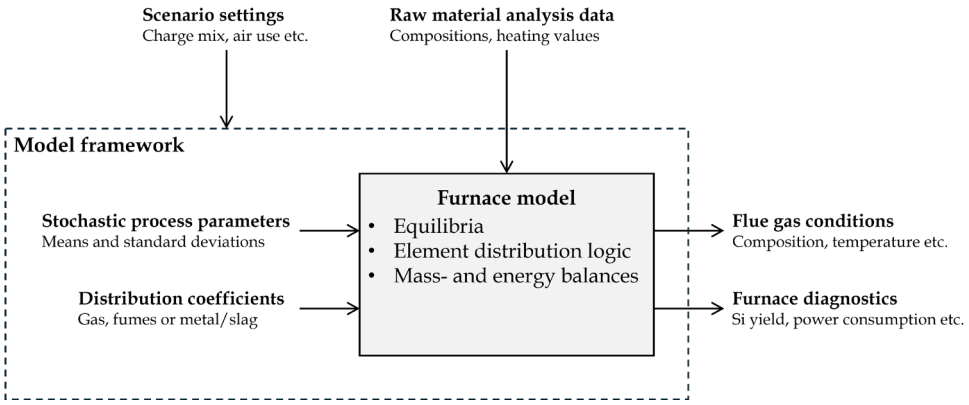

Figure 1: Illustration of model framework and boundaries.

Table 1: Model input parameters with their mean values and standard deviations. Parameters without st.d. values are kept constant in the current iteration of the model.

Process parameters in model	**Mean**	**St.d.**
Carbon coverage (%)	95	2
Carbon loss, all materials (% of fix. C)	2,5	1
Woodchips moisture content (wt %)	45	5
Charcoal moisture content (wt %)	25	8
Coke moisture content (wt %)	3	0,5
Coal moisture content (wt %)	25	5
Metal/slag equilibrium temperature (°C)	2000	-
Lower furnace gas temperature (°C)	1750	50
Tapping gas temperature (°C)	1800	-
Upper furnace gas temperature (°C)	1550	50
Ambient air temperature (°C)	15	5
Tapping gas amount (% of CO)	1	-
Tapping gas SiO content (vol %)	40	-
Electrode consumption (kg/MWh)	0,15	0,01
SO2 to SO3 conversion rate (%)	3	0,5
CaO to CaSO4 conversion rate (%, also limited by available sulfur)	50	-

Two case studies were conducted for this work, one investigating the impact of increasing the charcoal use, and one investigating the impact of selected charcoal parameters when using only biocarbon. For these studies, some parameters of interest were given uniform distributions over a wider range, while others were kept constant as listed in Table 2.

Table 2: Parameter specifications for simulation cases.

	Uniformly distributed parameters		**Constants**	
	Parameter	**Range**	**Parameter**	**Value**
Case 1	Charcoal use (% of fix.C)	0-85	Woodchips use (% of fix.C)	15
	Coke use (% of fossil fix.C)	0-34	Air flow (Nm^3/h)	36 000
Case 2	Woodchips use (% of fix.C)	5-25	Coke use (% of fix.C)	0
	Charcoal moisture (wt %)	5-45	Coal use (% of fix.C)	0
	Charcoal carbon loss (wt %)	2-15	Air flow (Nm^3/h)	36 000

Case 1 examines the effects of gradually removing the fossil reductants, a random mix of coal and coke, and replacing them with charcoal. This represents the path the industry is taking, and should reveal the main trends in flue gas conditions in the near future.

Case 2 examines a scenario where the fossil reductants are no longer in use. It studies the effects of woodchips/charcoal ratio in the charge, moisture content of the charcoal, and the amount of fixed carbon burning off at the top of the charge instead of contributing to reduction. The moisture content is of interest because while freshly produced charcoal contains very little of it, environmental conditions during storage can cause them to absorb large amounts. The carbon loss from charcoal is included in the study because it primarily depends on the strength of the material and how much fines it produces during charging. This is a known issue with charcoal specifically. Outside of case 2, this parameter is kept normally distributed around 2,5 % for all carbon materials.

2.3 Charcoal materials

Six different charcoal materials were used in the simulations. These were chosen simply due to availability of complete analysis data. Two were sourced from Wang et al., who produced charcoal at high temperatures specifically with the metal industry in mind (Wang *et al.*, 2024). Two were sourced from the Phyllis2 open database (TNO, 2026), originally uploaded by the Energy Research Centre of the Netherlands. The last two were unpublished analysis data on charcoals used by SINTEF and NTNU in pilot experiments, originally received from industry. Woodchips, coal and coke data was also sourced from materials used for pilot experiments. Table 3 below gives an overview of the charcoals used in this study.

Table 3: Data source, wood type and pyrolysis temperature for charcoal materials.

Charcoal material	Wood source	Pyrolysis temperature	Data source
Char O Char W	Oak Willow	400 °C 550 °C	Phyllis2 database
Char B Char S	Birch Spruce	1000 °C	Wang et al.
Char P Char Z	Unknown	Unknown	Unpublished analyses

The charcoals differ in their proximate analysis, showing a range of volatile and ash content. There is also variation in composition for some key elements such as sulphur and calcium. Heating values also differ, but this was derived from the composition for comparisons sake, even though it was included in some data sets. Figures 2-4 show these differences compared to the other carbon materials.

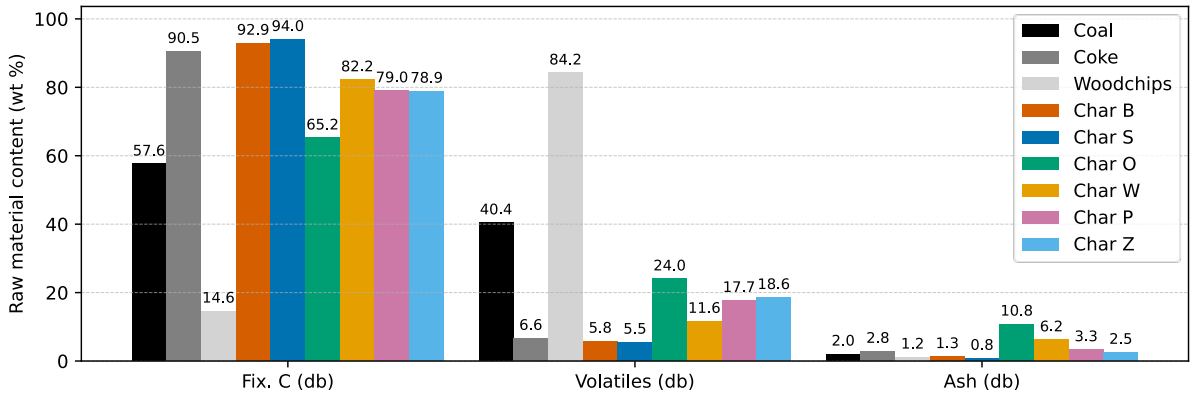

Figure 2: Proximate analysis data for the carbon materials in the study, on dry basis.

As could be expected, the proximate analysis data show less volatiles in the charcoals produced at higher temperatures. Seeing the same trend in the ash fraction is surprising, but this could be due to difference in wood source, or analysis method.

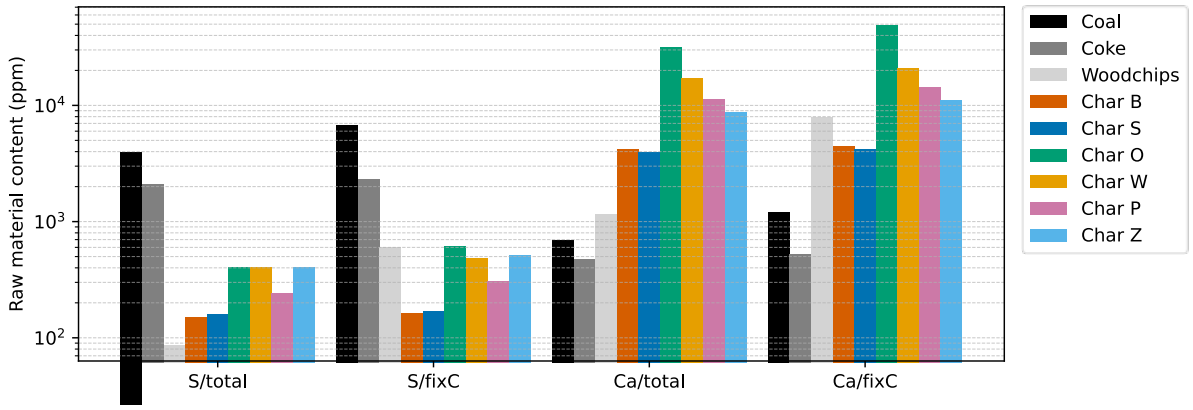

Figure 3: Content of sulphur and calcium in the carbon materials.

Compared to the fossil reductants, the charcoals contain less sulphur and more calcium by an order of magnitude. There is also significant differences between the charcoals, especially between those treated at high temperatures and the rest.

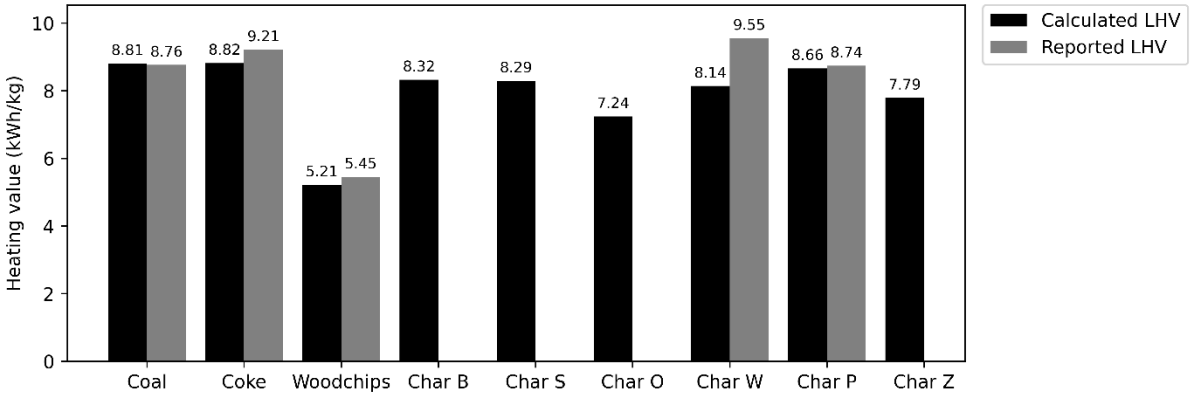

Figure 4: Lower heating values for the carbon materials. Calculated values were used for simulations, reported values from original data source shown for comparison.

With the calculated heating values used in this work, there is a slight decrease in energy input when using charcoal instead of fossil reductants. This is amplified by higher fix. C content, giving lower total amount of carbon material added. Using calculated values seem less

consistent for charcoals than for other materials, which motivates including calorimetric heating value determination in raw material analysis.

3. RESULTS

The simulation strategy produces one large dataset for each case, containing randomly drawn input parameters and resulting output parameters. They are made up of six subsets, one for each charcoal material. The following statistical methods are used to explore relations between parameters: First, locally weighted linear regression (Cleveland and Devlin, 1988) is performed on the entire dataset, giving a smooth trendline. This is plotted along with a shaded prediction interval capturing the variability of the data, calculated using conditional quantile regression with the same local weighting. Lastly, the same regression is performed on each subset. Subset quantiles are not included for visibility.

3.1 From fossil to biocarbon

As can be interpreted from the proximate analysis, replacing fossil carbon materials with charcoal primarily has the effect of reducing the amount of volatiles and ash added to the furnace. Figure 5 shows how this reduces the concentration of CO_x, SO_x and water in the flue gas. Both CO_2 and CO is included in the CO_x number, but the model predicts close to no CO after combustion. Due to the simulated formation of $CaSO_4$, additional Ca in the charcoals also contributes to a predicted reduced SO_x content.

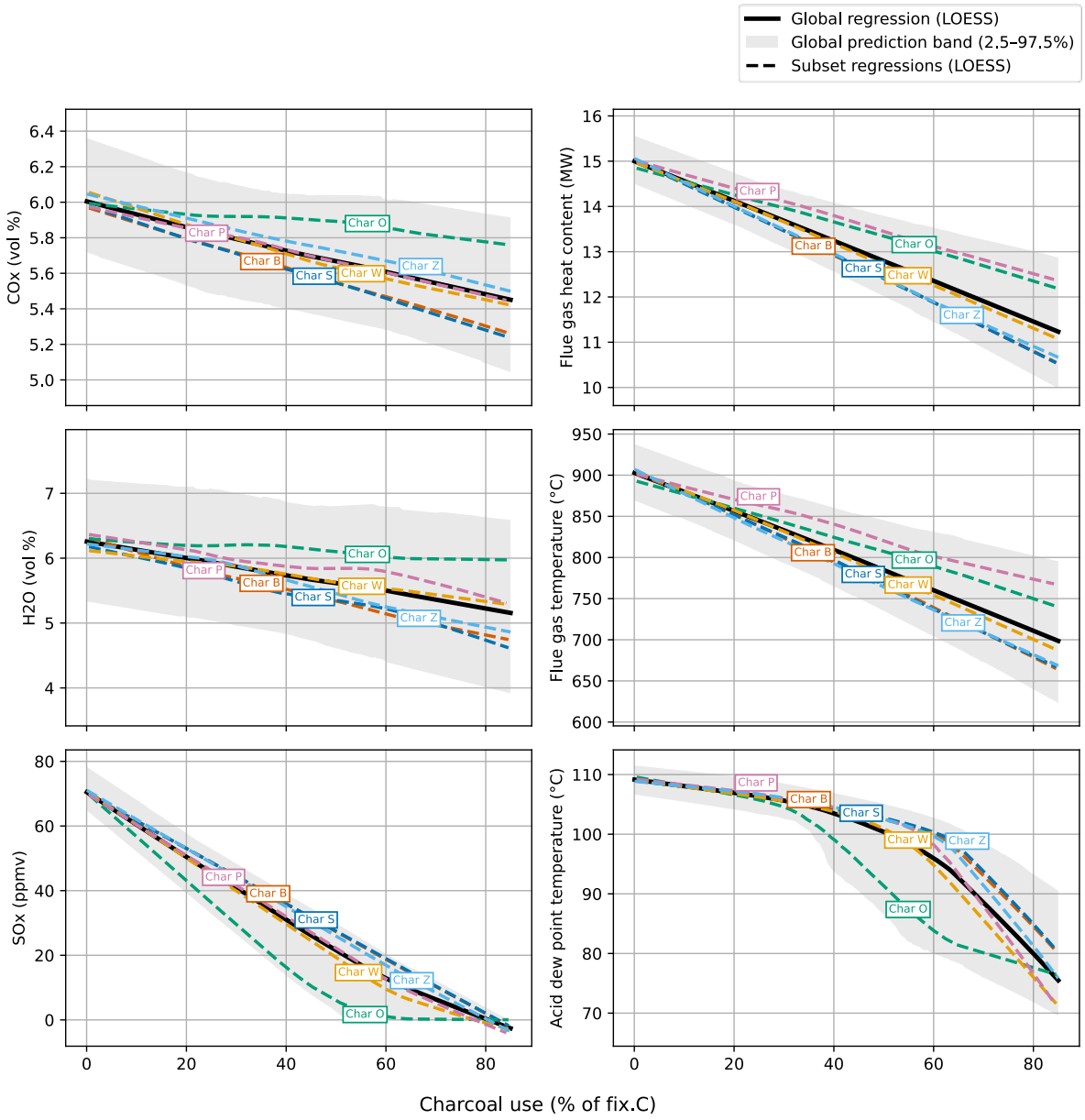

Figure 5: Effect of increased charcoal use on CO_x, water and SO_x content of the flue gas, along with temperature, heat content, and predicted sulfuric acid dew point temperature.

Also shown in Figure 5 is the effect on heat content and flue gas temperature. A reduced amount of combustible volatiles significantly reduces the energy of the flue gas, by around 15-30 %. With the amount of air used in these simulations, this corresponds to a temperature drop of around 200 °C.

Lastly, a drastic effect on the H_2SO_4 Acid Dew Point (ADP) temperature is observed, which is calculated using the following empirical correlation from Okkes (Okkes, 1987):

$$T_{ADP}[°C] = 203.25 + 27.6 \log_{10} p_{H_2O} + 10.83 \log_{10} p_{SO_3} + 1.06 (\log_{10} p_{SO_3} + 8)^{2.19} \quad [2]$$

The acid dew point depends both on the moisture content of the gas and the amount of SO_3 present. While the rate of reaction to form SO_3 from SO_2 is typically kinetically limited, this model instead has the SO_3/SO_x rate in the flue gas as a stochastic input parameter around 3 % for simplicity.

Both Char O and Char P behave noticeably different than the global trend. Char O contains more volatiles than the rest, thus adding more carbon, hydrogen and energy to the system. It also has more calcium, which explains the more rapid drop in SO_x. Char P has a slightly higher heating value than the other charcoals, giving a smaller drop in temperature and heat levels.

3.2 Biocarbon charge mix properties

This set of simulations studies the conditions at 100 % biocarbon more intently, and investigates the effect of woodchips use, moisture content, and carbon loss. These parameters are varied simultaneously, which increases the variability of results, but regression trends are still clearly identifiable.

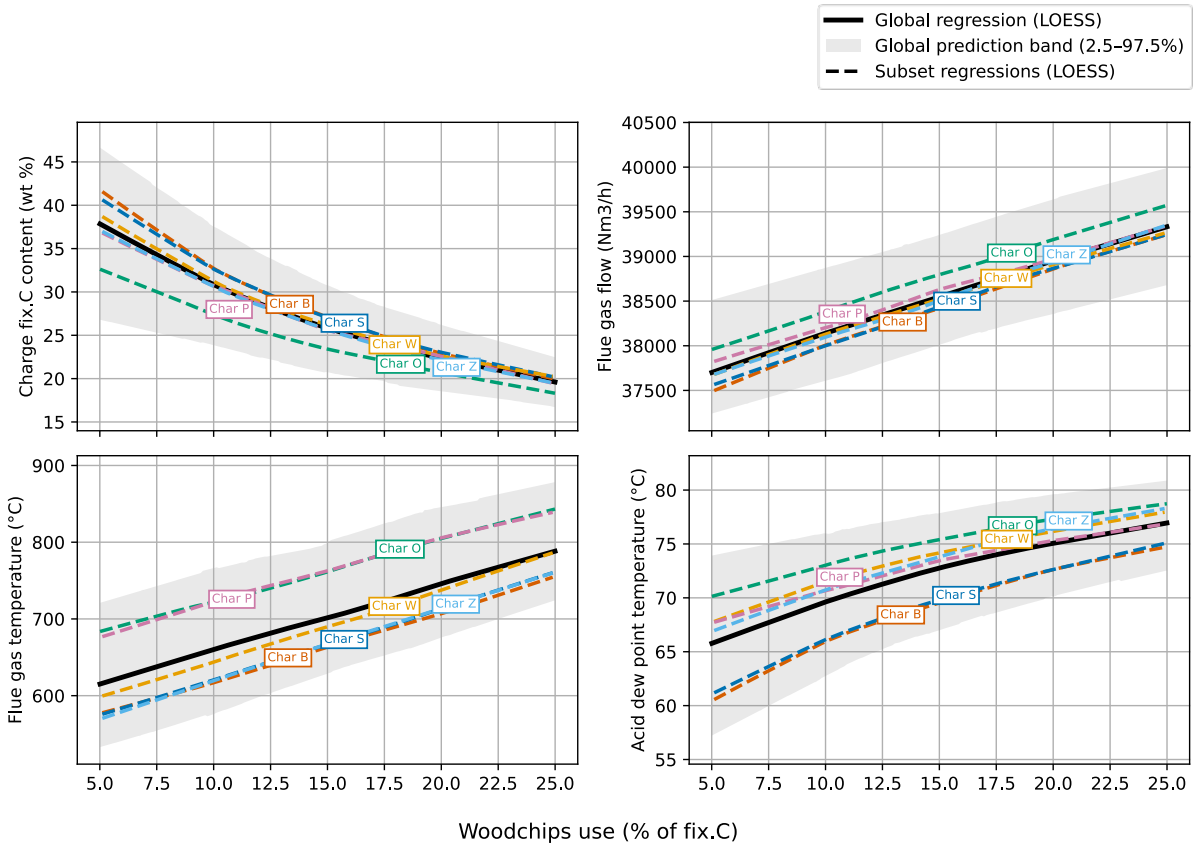

Figure 6: Effect of woodchips amount at 100 % biocarbon use on fixed carbon content in charge, flue gas production, temperature and acid dew point.

Figure 6 shows the effect of varying the woodchip amount at the cost of charcoal. More woodchips significantly increases the amount of volatiles in the charge, leading to more flue gas and higher flue gas temperatures at fixed air intake. There is also a clear increase in the acid dew point temperature. Woodchips has less sulphur than charcoal, but this could be explained by increased moisture content or the reduced fixed C content leading to more carbon material used overall. The dew point remains lower than when using fossil reductants, however.

Varying the charcoal moisture content has a less pronounced effect, as shown in Figure 7. The water content and acid dew point temperature both increase predictably, while the flue gas temperature decreases from the increased use of energy for vaporisation.

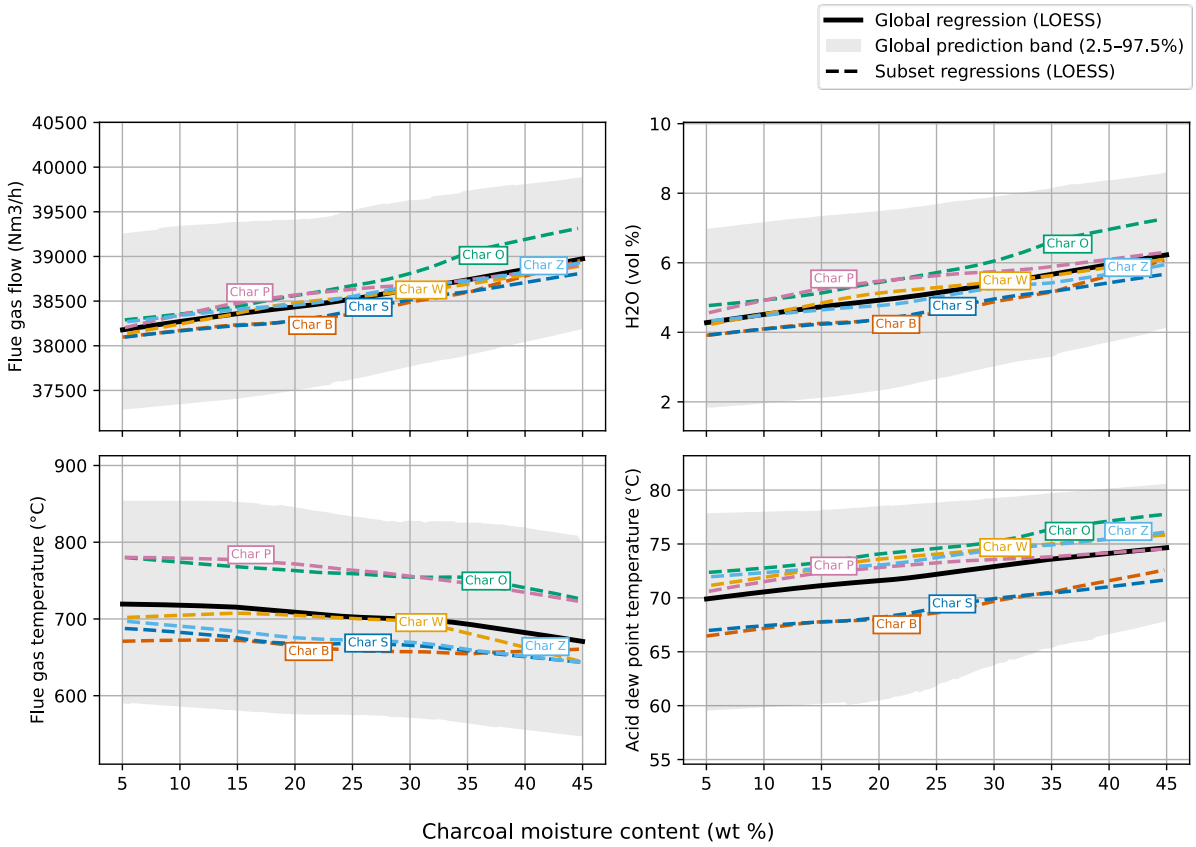

Figure 7: Effect of increasing moisture in charcoal at 100 % biocarbon use on flue gas production, water content, acid dew point, and temperature.

When the carbon loss was varied, the mean value for carbon coverage was also adjusted to maintain the silicon yield. This is shown in Figure 8. While this increases the carbon material need of the furnace, it also has the direct effect of increasing flue gas energy content, temperature and CO_2 content.

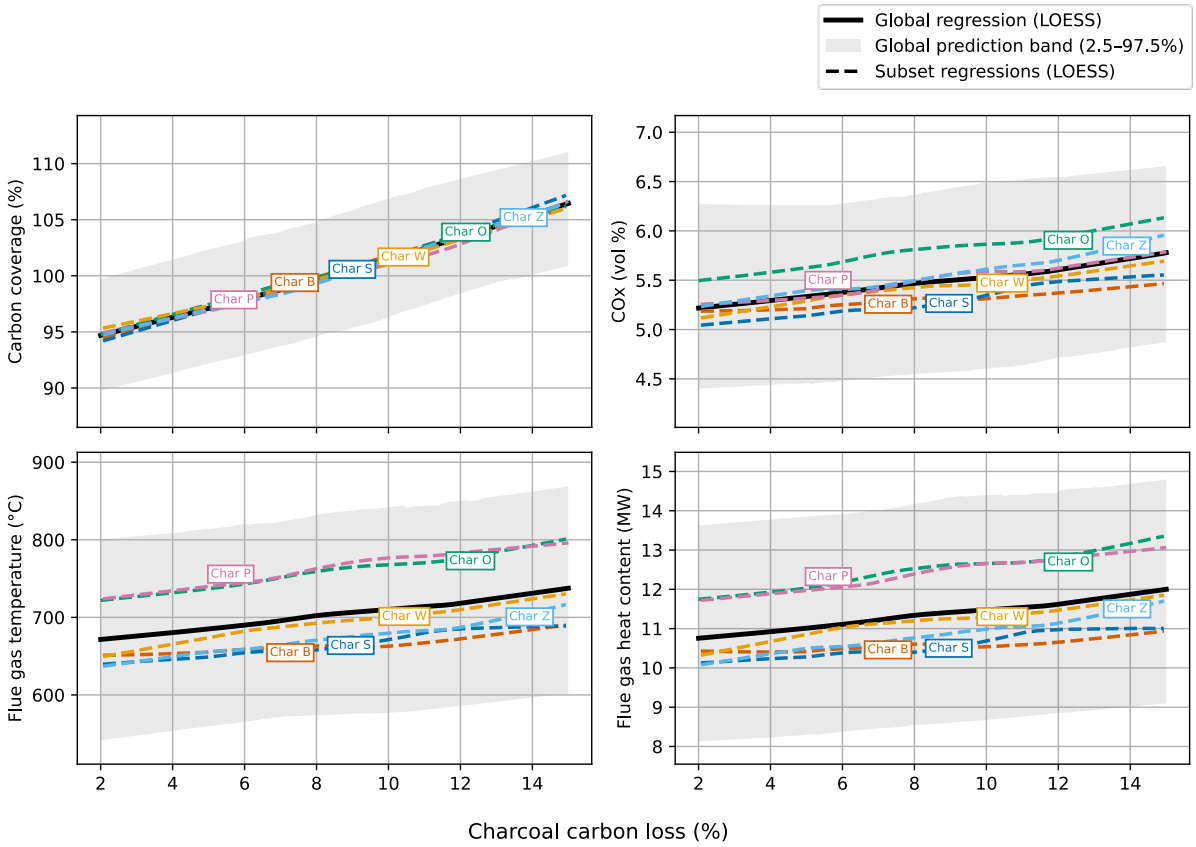

Figure 8: Effect of increasing carbon loss for charcoal at 100 % biocarbon use on required carbon coverage, flue gas CO_x concentration, temperature and heat content.

4. DISCUSSION

The simulations carried out in the current work show the importance of volatiles in the carbon materials for the characteristics of the flue gas. Charcoals contain less volatiles than fossil coal, and thus produce flue gas with drastically lower heat content and temperature. Woodchips contain more volatiles and has the opposite effect. Combustion products from charcoal volatiles such as water and CO_2 has their concentrations noticeably reduced. Further studies could verify if this holds true for more complex combustion products not included in this model, such as NO_x and PAHs.

Furthermore, the results indicate that the issues of SO_x and sulphuric acid in the flue gas system could be almost entirely removed. This relies heavily on the formation of $CaSO_4$ in the flue gas from CaO, originating from ash or mineral impurities in quartz, and as such the mechanisms behind this should be studied and verified experimentally. The potential for detrimental effects on silica fume quality should also be addressed.

There are significant differences between the charcoal materials used in this study, again mostly related to volatile content. Those pyrolysed at higher temperatures contain less volatiles, and thus behave most differently from the fossil reductants. With regards to heat content and temperature, these results heavily rely on the correlation for heating value, which was developed for coal and could be inconsistent depending on the actual volatile compounds present. Calorimetry should therefore be included in any analysis of carbon materials for use in furnaces if energy balance is of concern.

Considering how much the flue gas conditions are predicted to change when transitioning to biocarbon, there are some significant effects that should be taken into account should CC be implemented: Firstly, while the reduction in CO_2 concentration is bad for equipment sizing, it is a minor effect and could be compensated for by other means, such as the reduction in overall gas production. Next, sulphur removal might not be necessary, which could simplify the entire process. Lastly, the reduced heat content of the flue gas is unfortunate for energy recovery systems, and reduces the potential benefits of using thermally driven carbon capture processes. However, the reduced temperatures might also be beneficial, as this would reduce the need for air dilution on top of the furnace. This could increase the CO_2 concentration and reduce the gas volume significantly, which would benefit carbon capture implementation greatly.

While these simulations give good insights into how flue gas conditions are related to raw materials and process parameters, they are the result of a model that is yet to be validated. Verification of mechanisms and calibration of furnace parameters by use of actual furnace data is a necessary next step to enable trust in the findings. If successful, this modelling approach has potential for investigating even more scenarios and raw materials, or even other furnace systems besides silicon.

4. ACKNOWLEDGEMENTS

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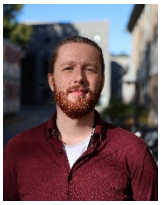

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