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Oxygen polishing of chemical looping combustion flue gases

Master's thesis in Sustainable Energy Systems

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CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2016

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Abstract

Chemical looping combustion has arisen as an attractive possible option for carbon capture and storage. With coal as our most abundant fuel type it is of great interest to include it in the process. Chemical looping combustion of solid fuels faces some difficulties, one being unconverted fuel, CO, CH_4 and H_2 leaving the reactor with the flue gas. A possible measure to increase the total efficiency is to oxidize the remaining fuel with pure oxygen in a post oxidation chamber. The aim of this work is to evaluate the performance of such a chamber and to provide recommendations regarding operating conditions.

The project is based on gas reaction modelling in the software CHEMKIN where a thorough simulation setup is established. The importance of operating temperature and mixing of oxygen is analyzed and a sensitivity analysis investigating the importance of different process parameters on the performance is also conducted. In addition to combustion performance a limited study on the fate of NO_x and SO_x in the post oxidation chamber is also performed.

The results from the simulations show that the POC should have a temperature above 800°C and be designed to allow for good mixing with the added oxygen. The vast majority of the remaining fuel from the fuel reactor will be oxidized in the POC but complete oxidation is impossible at stoichiometric conditions. The outlet concentration of oxygen will not be able to meet the guidelines of 100 ppm even at an air to fuel ratio below unity.

Keywords: CLC, oxygen polishing, POC, CCS, CHEMKIN.

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Jakob Johansson, Gothenburg, Oktober 2016

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Introduction

Climate change is arguably one of the more imminent threats to life on earth as we know it. The way of living that the modern society has grown accustomed to is in need of major changes. In the article "A safe operating space for humanity" the authors identified nine processes and thresholds that were believed critical to maintain in order to avoid unacceptable environmental changes [1]. One of the processes identified is global warming, anthropogenic CO_2 is the main contributor.

Carbon dioxide is a natural end-product of combustion between oxygen and carbon based fuel. Since our current energy systems rely heavily on combustion of such fuels a cost-effective solution of how to avoid releasing CO_2 into the atmosphere could have a major impact in reducing emissions [2]. One method of doing this is to separate CO_2 from the flue gas and then store it beneath the earth crust. This is often called carbon capture and storage (CCS). In order to be able to store the CO_2 safely the flue gas flow has to be purified to increase the fraction of CO_2. The operational cost in terms of efficiency loss or monetary investment of this flue gas cleaning is dependent on the flue gas flow and it's composition [3]. There are several ways to clean the flue gas from unwanted species and they can be categorized into measures before, during or after combustion.

The alternative to take action during combustion is commonly known as oxy combustion. When the oxidizer used is air there is a large amount of nitrogen present which has to be removed afterwards. However there are combustion processes that enables the fuel to be burnt without the nitrogen present in air, one which is called chemical looping combustion (CLC). In CLC two separate reactors are present, one air reactor and one fuel reactor. In the air reactor there is an oxygen carrier, possibly a metal oxide (MeO) present. The oxidized MeO is transported over to the second reactor, the fuel reactor, in which the combustion of the selected fuel is taking place. Since the metal is only carrying the oxygen and not the nitrogen the reduction process can be done without excess nitrogen present in air. The metal is then transported back to the air reactor where it is oxidised again.

CLC being a novel technology is still in a developing phase. It is possible to use the technology with gaseous, liquid or solid fuels but the main part of the research has been directed towards gaseous fuels. There has however been an increased amount of research directed towards solid fuels in recent years. One problem that CLC of solid fuels has encountered is that it is difficult to reach full conversion. Unburnt fuel, mainly CO will still be present after combustion which is not desirable in any perspective, additional measures is hence required. One proposed method is to use a post oxidation chamber (POC) with oxy-fuel combustion technology which would keep the flue gases clean and possibly enable complete conversion. There have been a limited amount of studies on how to design such a POC and the chemical compositions inside it in regards of O_2 and CO amount and the possibility of additional fuel required to complete the conversion. This method is called oxy-polishing and is one of the alternatives how to turn the CLC-process into a more attractive option for CCS. This thesis investigates the problems described and primarily uses operation data and reactor geometry from a 100 kW CLC unit at Chalmers university of technology.

1.1 Overview of the 100 kW CLC unit at Chalmers

The 100 kW chemical looping combustor at Chalmers is one of few that use solid fuels. Research has as mentioned earlier mainly been directed towards combustion of gases but since coal is a steadily available resource it is of interest to research how to include it in the CLC process [4]. The combustion of solid fuels is a much more time consuming process than for gaseous fuels since the fuel needs to go through drying, devolatilization and char combustion or gasification. The increased time for char combustion and or gasification requires the combustor to be designed with this in mind. The CLC group at Chalmers designed their CLC to be a circulating fluidized bed (CFB) combustor where both the air- and the fuel reactor is fluidized, the air reactor is fluidized by air and the fuel reactor is fluidized by H_2O. By fluidizing the fuel reactor with H_2O the char present can be gasified to CO and H_2. In addition to the two reactors the combustor also consists of loop seals (LS) that connect the different parts of the unit and serves to avoid mixing of the different gases and two cyclones to separate the moving bed material from the flue gas, see Figure 1.1.

During tests of the unit a number of different oxygen carriers have been used including ilmenite and manganese to study how different bed materials will impact the process. Other important features that have been varied is the type of fuel, ranging from wood char to bituminous coal. The flue gas will have widely varying composition depending on which fuel is used. In measurement data it has also been shown that the combustor does not reach complete conversion but that a significant amount of fuel escapes with the flue gas, somewhere in the order of 20% of the total fuel amount [5]. There is also a problem with unconverted char escaping the fuel reactor. The reactor being relatively small suffers from pressure gradients and slugging which causes some char to escape via the flue gas.

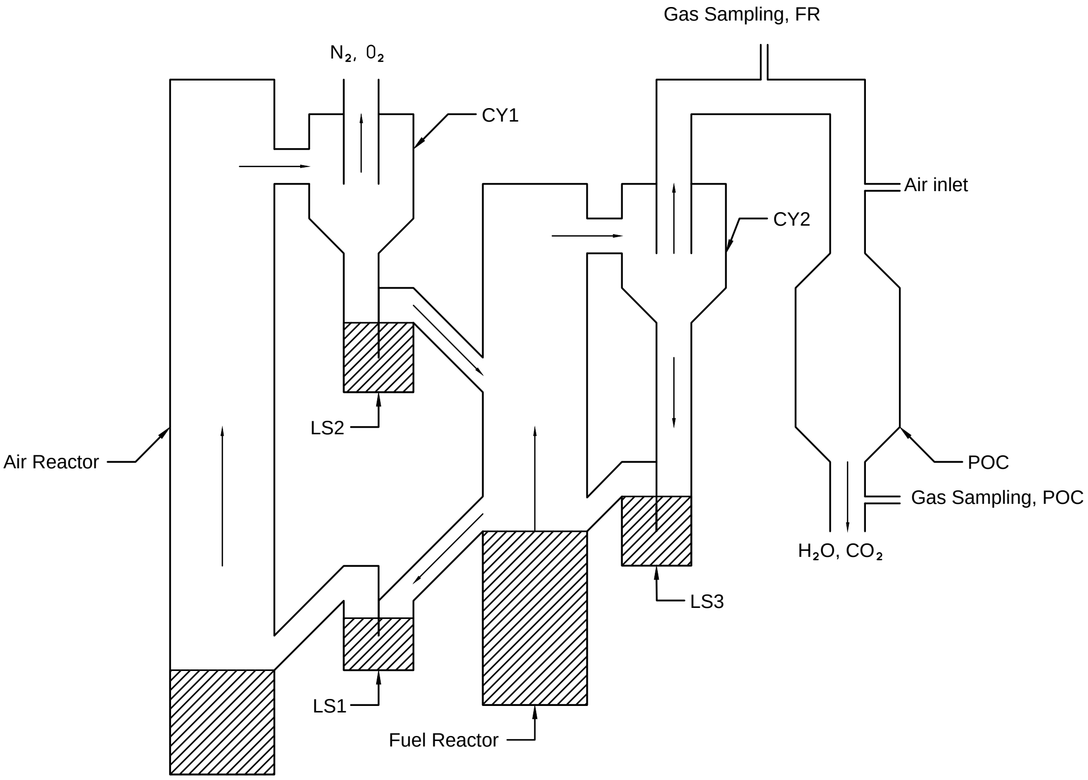

Figure 1.1: Simplified schematic of the 100 kW CLC unit at Chalmers. Loop seals (LS), Air reactor (AR), Fuel reactor (FR), POC, POC air inlet, Gas sampling ports and Cyclones (CY) are displayed.

1.2 Aim and scope

When up-scaling the boiler from it´s current limited size to a proposed 1MWth the problem with the fuel conversion is believed to decrease drastically [6]. By increasing the height of the fuel reactor and improving efficiency of the cyclone most of the char should reach a satisfactory residence time and improving the solid fuel conversion from 80 to 97%. The unburnt syngas and volatiles will however remain and it is by such still of interest. This project aims to give an overview of how a POC with oxy-polishing will perform with the current flue gas composition of the Chalmers 100kW boiler excluding the unburnt char that is currently present. A sensitivity analysis regarding changes in composition as well as temperature and residence time is also in the scope of this work. The project also aims to evaluate which of the parameters that have the largest influence on performance. By investigating all of the above mentioned a simplified layout of a preliminary design of a POC is to be provided.

2

Theory

In the following chapter the theory behind some of the more extensively used concepts are explained to form a basic understanding. The chapter will start with a description of the theory behind chemical looping combustion followed by a description of the post oxidation chamber as it is and the theoretical need for it. The chapter continues with a brief introduction to carbon dioxide capture, transportation and storage and is concluded with some of the more important chemical reactions inside the POC.

2.1 Chemical looping combustion

Chemical looping combustion as such is not a new invention but rather an old concept. The idea to use an oxygen carrier to supply oxygen without using air directly has at least been used since the early twentieth century when Howard Lane used iron oxide to produce hydrogen via steam [7]. Years later in 1954 the technology was studied again by Lewis Gilliland in order to produce CO_2 for the beverage industry and in 1983 Horst Richter and Karl Knoche proposed the technology as a method to increase power plant efficiency [8]. It was first in 1994 that the technology was presented as a way to reduce climate impact by Japanese researchers Ishida, M and Jin, H [9]. Since then the amount of research in the area has increased with a number of Universities including, among others, Chalmers University of technology, Sweden and South East University, China taking interest in the subject [10].

The general chemical reaction taking place in the air reactor can be expressed as

$$\mathrm{Me}_x\mathrm{O}_{\mathrm{y}-1} + \frac{1}{2}\,\mathrm{O}_2 \longrightarrow \mathrm{Me}_x\mathrm{O}_{\mathrm{y}}, \tag{2.1}$$

where MeO denotes metal oxide. This process is highly exothermic and by such produces an extensive amount of heat. In a dual connected fluidized bed reactor system this heat is maintained by transportation of bed material from the air reactor to the fuel reactor which often has a slightly endothermic reaction taking place. The reaction taking place in the fuel reactor can be written as

$$(2\,\mathrm{n}+\mathrm{m})\mathrm{Me}_x\mathrm{O}_{\mathrm{y}} + \mathrm{C}_n\mathrm{H}_{2m} \longrightarrow (2\,\mathrm{n}+\mathrm{m})\mathrm{Me}_x\mathrm{O}_{\mathrm{y}-1} + \mathrm{mH_2O} + \mathrm{nCO_2}, \tag{2.2}$$

where C_nH_{2m} is the fuel fed to the system. The temperature in the air reactor is slightly higher than that in the fuel reactor and can reach around 1000°C [11].

In Figure 2.1 the simplified reactant and product flows are shown. When impurities are neglected the only components exiting the fuel reactor are H_2O and CO_2 which are easily separated through the condensation of water. The stream exiting the air reactor consists of mainly N_2 and some excess O_2, thus a process that inherently separates N_2 from the flue gas stream has been achieved.

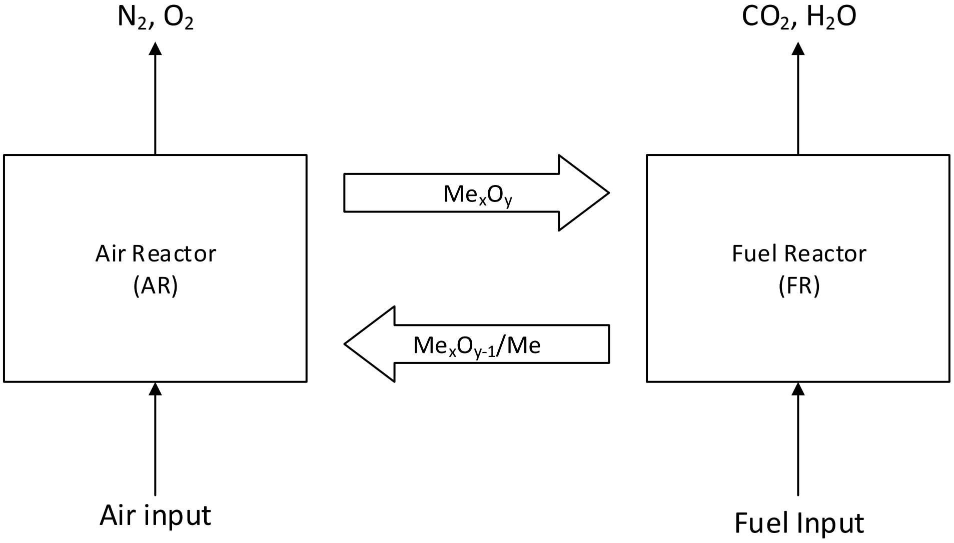

Figure 2.1: Sketch of the reactant and product stream in the two reactors

2.2 Oxygen polishing in a post oxidation chamber

Even though the simplified schematics of the process indicates that complete combustion occur and thus that only CO_2 and H_2O escapes the fuel reactor this is not the case in real operation with solid fuel. While the oxygen carriers would be in direct contact with a gaseous fuel fed from below the syngas released from char particles will in some extent be released in areas with insufficient contact [11]. By such there will always be some amount of CO, CH_4 and H_2 escaping with the flue gas.

Four different possible measures are pointed out by Anders Lyngfelt and Carl Linderholm [11]:
- Oxygen polishing, i.e. introduction of pure oxygen in a post oxidation chamber.
- CO_2 liquefaction and then separate these gases and recirculate them.
- Two fuel reactors in series to convert the gases completely.
- Usage of a different oxygen carrier that can release the oxygen in the fuel reactor, a concept known as Chemical-Looping Oxygen uncoupling, CLOU.

Chemical-Looping Combustion still being a novel technology has received most of the research in areas of different types of oxygen carrier's. The post treatment of unburnt fuel while being noted as an issue has still to be investigated further. All proposed solutions has their advantaged and disadvantages. In the case of oxygen-polishing the disadvantages are among others the cost of an air separation unit, ASU, and the strict requirements of very low concentrations of O_2 in the final product stream to be transported (more about this in Section 2.3).

The separation of oxygen from air in an ASU is highly energy consuming which means that for oxy-polishing to be as profitable as possible no more oxygen than what is required should be added (the amount required is a subject of this report). Reaction kinetics requires that the remaining fuel and the oxygen have a sufficient residence time and temperature to ensure burnout. The increase in residence time can be done via a post oxidation chamber designed to meet the criteria [6].

2.3 CO_2 sequestration, transport and storage

The separation of CO_2 from the rest of the flue gas can be done in different ways. The method is chosen depending on the composition of the flue gas which in the case of CLC will be dominated by CO_2 and H_2O where the latter can be removed via condensation. The flue gas will also contain some amount of impurities such as NO_x, SO_x and N_2 which will have to be removed in order to meet environmental laws. CLC technology will however only leave such small amounts of these as to there will be no need for conventional treatment reducing the cleaning cost [6]. During the cleaning process the CO_2 stream will most often be compressed into a super-critical liquid to simplify transportation.

The required purity of the transported CO_2 stream will vary depending on the application. There are mainly two different alternatives of what to do with CO_2, oil recovery or storage. For the industrial sector most interest has been towards oil recovery where CO_2 can be used both for secondary and tertiary recovery of oil. During primary recovery the natural pressure in the oil well brings the lighter fractions of the oil to the surface, this process will however only recover a small amount of the total reserve [12]. To increase recovery, natural gas or other gases such as CO_2 might be injected in order to push the oil up the well [12]. The final measure to extract remaining heavy oil is to inject solvents or other substances in order to further increase pressure, decrease viscosity or to change the characteristics of the reservoir rock in a beneficial way [12]. This tertiary recovery is also known as enhanced oil recovery, EOR and offers ways to increase the total oil recovered by a significant amount[13].

Enhanced oil recovery is dependent on a chemistry which will vary depending on oil composition. In order to ensure safety and operational success the CO_2 therefore need to meet certain criteria. Much of the EOR takes place in north America and most guidelines and specifications originates from this region. In recent years there has however been studies performed in Europe to establish the requirements. In Table 2.1 the values from the ENCAPCO_2, ENhanced CAPture of CO_2, reference guidelines report can be seen [14].

Table 2.1: Values from ENCAP - WP 1.1 2008 [14]. Maximum limits on impurities often present in CO_2 streams for it to still be used in a safe manner. Non condensable species include N_2, H_2, Ar, CH_4 and O_2

Component	**Concentration**	**Limitation**
H_2O	500 ppm	Should be kept below solubility so there is no free water present because of hydrate formation
H_2S	200 ppm	Health and safety
CO	2000 ppm	Health and safety
O_2	100-1000 ppm	Range for EOR, lack of experimental data on the effect of O_2 underground
CH_4	$<$ 2 vol%	Proposed in ENCAP project
N_2	$<$ 4 vol% (all non condensable gases)	Proposed in ENCAP project
Ar	$<$ 4 vol% (all non condensable gases)	Proposed in ENCAP project
H_2	$<$ 4 vol% (all non condensable gases)	Further reduction recommended because of the high energy content
SO_2	100 ppm	Health and safety
NO_2	100 ppm	Health and safety
CO_2	$>$ 95.5%	Resulting concentration if all other compounds are at their maximum

It is however crucial to note that these values does not set any rules but are mere guidelines. The actual composition being transported and put in to use can vary a lot, especially if it is only intended to be stored. One case where the flue gas composition deviates by a significant amount compared to the one proposed by ENCAPCO_2 can be found in the French Lacq-Rousse CCS project, where the CO_2 concentration can be as low as 90 vol% and the oxygen level up to 7 vol% [15].

The maximum restriction of O_2 level in the super-critical CO_2 is one that has not been well defined yet. This is a problem for the proposed method of oxy-polishing of CLC-flue gas since combustion with O_2 will leave impurities of oxygen in the stream. The amount will vary depending on temperature, air to fuel ratio (lambda) and residence time. There are methods of removing oxygen but these are highly energy intensive.

2.4 Reaction kinetics

Modelling of chemical reactions is complex and there is often a trade off between accuracy and computational time. There has been a substantial amount of experimental studies on combustion reactions in order to determine relevant reaction kinetics. The kinetics of interest to this project are combustion of CH_4, CO and H_2, NH_3 and NO_x chemistry in oxy-fuel combustion and SO_x kinetics. The empirical values for the reactions taking place in the POC are gathered from studies made by Glarborg, P., and Mendiara, T., and the most dominant reaction paths for each specie at the current operating conditions will be presented below [16]. CO will almost solely react via OH through Reaction 2.3 below,

$$\mathrm{CO + OH \rightleftharpoons CO_2 + H.} \tag{2.3}$$

H_2 will also be dominantly oxidized via OH by Reaction 2.4,

$$\mathrm{H_2 + OH \rightleftharpoons H_2O + H.} \tag{2.4}$$

Both of these reactions require OH and will produce H. CH_4 being the only main fuel left in the process has three main reaction paths and will react with OH, H or O, each reaction path is presented below in Reaction 2.5, 2.6 and 2.7,

$$\mathrm{CH_4 + OH \rightleftharpoons CH_3 + H_2O,} \tag{2.5}$$

$$\mathrm{CH_4 + H \rightleftharpoons CH_3 + H_2,} \tag{2.6}$$

$$\mathrm{CH_4 + O \rightleftharpoons CH_3 + OH.} \tag{2.7}$$

The distribution between NO and NO_2 is balanced through Reaction 2.8 and 2.9,

$$\mathrm{NO_2 + H \rightleftharpoons NO + OH,} \tag{2.8}$$

$$\mathrm{NO + HO_2 \rightleftharpoons NO_2 + OH.} \tag{2.9}$$

The net balance of these two reactions are dependent on the temperature and oxygen availability. Both of these reactions are sources of OH. Sulfur in combustion is dominated by SO_2 and H_2S depending on the operating environment. SO_2 can be reduced via H through two paths,

$$\mathrm{SO_2 + H \rightleftharpoons SO + OH,} \tag{2.10}$$

or

$$\mathrm{SO_2 + H \rightleftharpoons HOSO.} \tag{2.11}$$

H_2S is a much more reactive specie and will mainly react via H according to

$$\mathrm{H_2S + H \rightleftharpoons SH + H_2,} \tag{2.12}$$

to eventually form SO which will be oxidized to SO_2.

3

Methods

The work is based on kinetic modelling. In this chapter the setup and work flow will be described in further detail. The first section will give insight into the process model used to simulate gas reactions in a POC. The second section contains information regarding the flue gas composition used. The third and fourth section describes how temperature and mixing distance was varied in order to simulate different operating conditions and the last section aims to explain the method behind the sensitivity analysis.

3.1 POC process model

The reactions in the POC are simulated via the software CHEMKIN. The process layout in CHEMKIN is in form of two separate inlets, one where the flue gas from the fuel reactor enters and one is where the oxidizer enters. Both streams are led to an isothermal plug flow reactor where they will be mixed and allowed to react. In order to establish the importance of mixing of the two streams the oxidizer can be varied in terms of how fast it is inserted, this to simulate a situation where mixing is the rate-limiting factor. Since no empirical data or model is available on the current flow dynamics in the existing POC the effect of perfect contra slow mixing and situations in between has to be simulated in order to determine the effect on the process.

The reaction mechanisms consists of a detailed set of sub reactions described by Mendiara and Glarborg [16]. This set of reactions include the elemental species of oxygen, hydrogen, carbon, nitrogen and sulfur and over a 100 of their radicals and combined molecules. The relevant subsets in this case consists of oxidation of C1 hydrocarbons, CO, H_2 and nitrogen and sulfur kinetics. The sulfur chemistry obtained is from Alzueta, M. U., Bilbao, R., and Glarborg, P. and added to the reaction files. This set of reactions does not involve nitrogen and any interaction between sulfur and nitrogen will therefore only be conducted via the radical pool. This does impose some limitations [17].

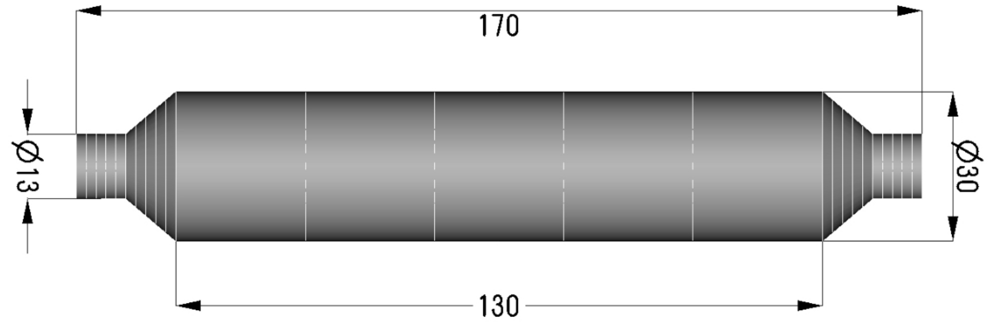

Figure 3.1: Dimensions of the current POC used during gas reaction simulations. Values are in units of cm.

3.2 Flue gas composition and oxygen amount

The flue gas composition is based upon test results of the 100 kW CLC unit at Chalmers during stable operating conditions with coal [18]. Flue gas composition varied during the test because of start up phase and some testing of argon as fluidizer in the middle. The composition chosen is an approximation of the composition during a time window of one hour of operation, from 1.5 to 2.5 hours, see Figure 3.2. The concentrations provided in the figure are dry concentrations. The major part of the flue gas flow is water that has been used as fluidizing agent in the boiler.

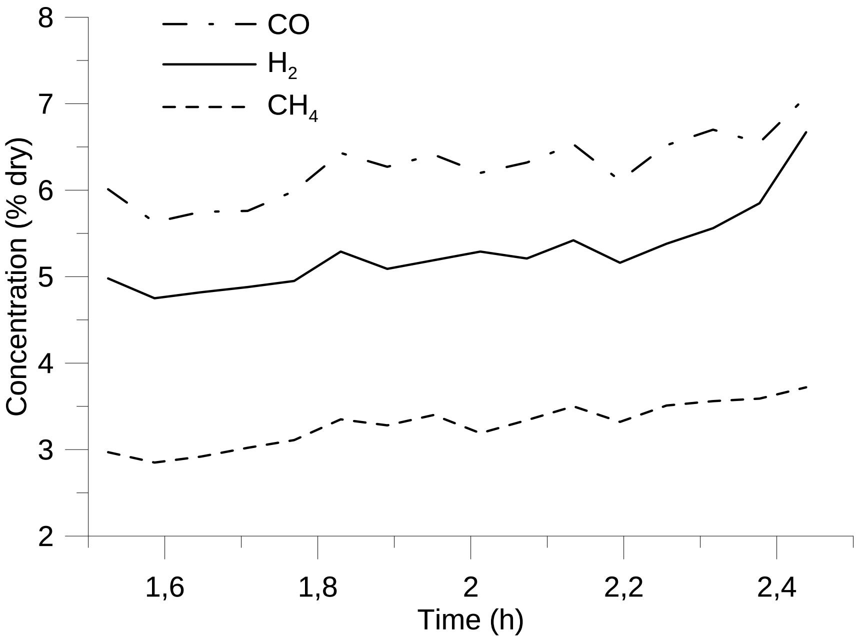

Figure 3.2: Graph of dry flue gas composition at the inlet of the POC during tests at Chalmers 100kW CLC unit, presented for a 1 hour time window of stable operation. Tests carried out in January 2016

The concentrations used as a baseline for each component present in the flue gas can be found in Table 3.1. The presence of N_2 is due to usage as fluidizing agent in some parts of the boiler and possible leakage. The resolution of the test data is low and concentrations can only be assumed to approximately match the actual concentrations.

Table 3.1: Values used in flue gas reaction simulations. Concentrations provided here are the actual wet concentrations that flows through the POC

Component	**Concentration**
CO_2	11.7 %
N_2	4.8 %
CO	1.2 %
H_2	1.1 %
CH_4	0.7 %
H_2O	80.6 %
NO	97 ppm
NH_3	49 ppm
HCN	19 ppm
SO_2	27 ppm
H_2S	51 ppm

The current operation of the POC at Chalmers employs air instead of pure oxygen and at excessive amounts. Since it is of interest to minimize the use of oxygen because of the energy penalty of the ASU and the strict levels of allowed oxygen in the flue gas and to maximize combustion at the same time a stoichiometric condition is used as standard in this project.

3.3 Impact of Temperature

The POC is as stated in Section 3.1 isothermal and neglects all temperature fluctuations in radial and axial position. To establish the importance of the temperature the simulations also consists of a parameter study where different fixed temperatures are tested. The different sets of data are then compared and analyzed to investigate the impact. Temperature affects residence time since the volume of the POC stays constant and this has to be taken into consideration especially at large temperature differences when evaluating results. The minimum temperature tested is 700°C and the maximum is 1000°C which if the flue gas is treated as an ideal gas will yield a difference in residence time of about 30% between the two values.

3.4 Impact of mixing

There is no data available on the flow characteristics inside the POC so a mixing profile has to be guessed. If the POC at Chalmers had dealt with only gases the concentrations could have been matched at the outlet but since there is char burning inside the POC the outlet concentrations are no longer a viable option for modelling mixing. To establish an understanding of how the mixing affect the performance of the POC, a parameter study similar to the temperature study is conducted. Results are evaluated at premixed, 35-, 70-, 105- and 140 cm linear air staging. The choice of a linear profile for the insertion of oxidizer is to simplify calculations. A profile with high availability in the beginning and slow mixing of the last percentage might be more realistic.

The results will as in the case of the temperature study vary in residence time depending on the mixing. When a case with slow mixing is simulated air is added until the vary last parts of the POC which gives a lower average velocity, this difference in time is however only in the order of a few percentage.

3.5 Sensitivity analysis

A sensitivity analysis is performed to evaluate the impact of performance of some of the present parameters. The investigated parameters and the interval of the analysis is displayed in Table 3.2. The flue gas components included are CO_2, CO, H_2, CH_4 and NO. N_2 and the remaining sulfur and nitrogen species are left out, the former because of inert properties at the present temperature level and the latter because of simplicity. The interval for the flue gas concentrations are approximated based on the reported test values in [5]. The residence time interval is based on changed volumetric flow, $\frac{3}{4}$ and $\frac{5}{4}$ of the standard flow. Temperature and Lambda has been increased and decreased slightly to see if there are any immediate effects.

Table 3.2: Dry concentrations, residence time, temperatures and lambda used as maximum and minimum level in the sensitivity analysis

Parameter	Value [low - ref - high]
CO_2	50 - 60 - 65 %
CO	4 - 6 - 8 %
H_2	2 - 5.4 - 8 %
CH_4	1 - 3.6 - 7 %
NO	0 - 500 - 2000 ppm
Residence time	1.00 - 1.33 - 1.77 s
Temperature	800 - 850 - 900°C
Lambda	0.95 - 1.00 - 1.05

The procedure of the sensitivity analysis is to investigate a primary parameter and the affect of a secondary parameter. The primary parameter is fixed while the secondary parameter is changed from the maximum level to the reference level and finally the minimum level *i.e.* three steps. This procedure is then repeated but with the primary parameter set to the reference case and finally repeated once more with it fixed on the minimum level. These nine steps in total are then repeated for the other secondary parameters as well, *i.e.* 54 simulations per parameter are performed, resulting in a total of 378 simulations (since many simulations will be replicas of each other the total of 378 is however reduced to 270).

The impact of lambda is also analyzed to ensure that the fuel can reach full conversion. The method for the analysis of lambda is done through decreasing the amount of flue gas while keeping the oxidizer stream constant. This process will impact residence time approximately by the same percentage as the oxidizer is increased, the residence time will increase due to the lower total flow. The effect of lambda is studied for all the different mixing cases. The air to fuel ratio simulated is from 1 to 1.2 where the 20% excess oxygen is based on common practice in conventional power plants.

4

Results

In this chapter the simulation results are presented. The first section contains results of how the temperature influences the conversion of CO, H_2 and CH_4. The next section contains results of the impact of mixing in the POC, visualized by different mixing distances compared at increasing temperature. The third section contains information about the results of the sensitivity analysis. Impact of lambda and the impact of changing other parameters present in the process is presented. The final section adds results of how the emissions of NO_x and SO_x vary depending on mixing characteristics and temperature.

4.1 Impact of temperature

The temperature has a large impact on the conversion of the fuel. The POC at Chalmers operate at approximately 900°C which according to the results in Figure 4.1 would suggests that CO would have an outlet concentration of approximately 100 ppm and H_2 a concentration of 1000 ppm at premixed and stoichiometric conditions. The concentration of CO drops rapidly from 700 to 800°C and then maintains constant outlet concentration. The outlet concentration of H_2 also drops fast from 700 to 800°C but in difference to CO keeps on decreasing with increased temperature above 800°C. CH_4 is completely converted at premixed conditions for all present temperatures. The residence time is increased with decreasing temperature and stretches from 1.12 seconds to 1.45 seconds due to gas volume variations.

4.2 Impact of mixing

As described in Section 3.4 the impact of mixing is studied via air staging. In Figure 4.3 results from simulations with five different mixing conditions can be seen. Increased mixing distance (*i.e.* slower mixing) yields higher outlet concentration of combustible gases, *i.e.* CH_4, CO and H_2. When increasing temperature beyond 800°C the mixing distance has a larger impact on the outlet concentration than the temperature. The residence time is different depending on mixing condition and temperature as described in Chapter 3 and varies between 1.1 to 1.5 seconds for the two extremes premixed at 1000°C and 140 cm mixing at 700°C. Figure 4.3 is cut off at the y-axis at 2% while the two longest mixing distances would continue beyond this value for the lower temperature range. The 105 cm linear air staging continues up to an outlet concentration of 4% at 700°C and the 140 cm linear air staging increases to almost 8%.

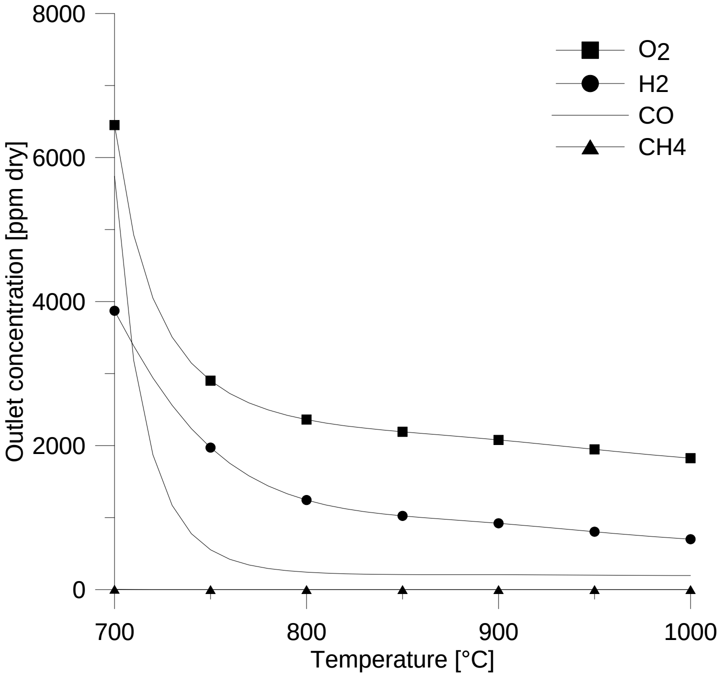

Figure 4.1: Impact of temperature on outlet concentration of combustible gases at premixed conditions and lambda equal to 1. CO and H_2 conversion increase with increasing temperature.

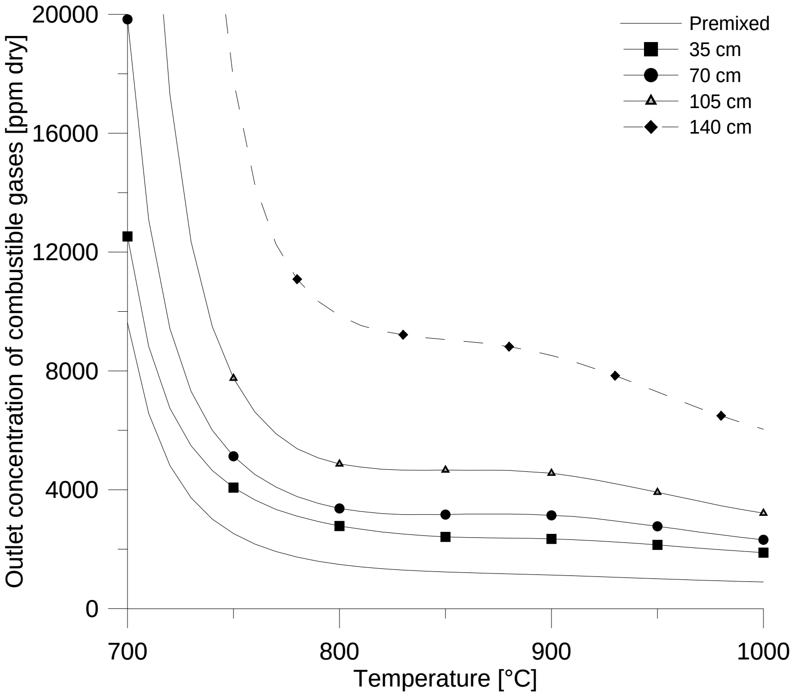

Figure 4.2: Impact of mixing and temperature on outlet concentration of combustible gases (CH_4, CO and H_2) at premixed conditions and lambda equal to 1. CO and H_2 conversion increases with increasing mixing rate and temperature.

4.3 Sensitivity analysis

The method behind the sensitivity analysis is described in Section 3.5. Two separate studies are presented here, one where the amount of oxygen is increased beyond stoichiometric levels to investigate burnout and one to establish the importance of the different parameters of the simulation setup and flue gas composition.

In Figure 4.3 the oxidizer ratio, lambda is increased from 1 to 1.2 as the outlet concentration of combustible gases, CH_4, CO and H_2 under different mixing distances is analyzed. The outlet concentration reaches zero as the amount of oxygen availability is increased. Situations where the mixing characteristics are slower needs a higher lambda to reach complete conversion. The results are depicted for the current operating conditions with standard flue gas composition and at 900°C. Residence time between the different cases vary between 1.21-1.55 seconds from premixed at lambda equal to 1.2 and 140 cm mixing at lambda equal to 1 which are the two extremes. For this simulation it was not possible to have an actual premixed stream due to simulation difficulties. The premixed case is therefore approximated with a mixing distance of 2 cm which is the quickest mixing allowed.

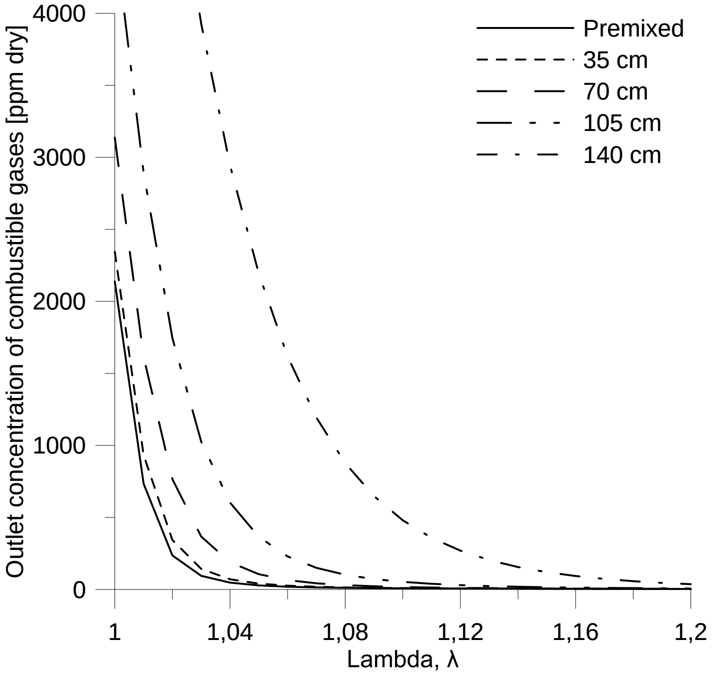

Figure 4.3: Impact of lambda on outlet concentration of combustible gases at 900°C. CO and H_2 reaches complete conversion with excess oxygen, the amount required is decreased with increased mixing rate.

Results from the sensitivity analysis regarding flue gas composition, residence time, temperature and NO concentration are presented in Table 4.1. The original data from where the results are gathered can be found in Appendix A. The base case of the simulations are conducted at a linear air staging profile of 85 cm and a temperature of 850°C. The flue gas composition that is used can be found in Section

3.5. The results for NO variations are large compared to other changes in flue gas composition. The increased conversion of CO and H_2 caused by NO can be traced back to the reaction mechanism involving NO oxidation displayed in Section 2.4 where OH can be supplied in larger amounts at lower temperature levels.

Table 4.1: Results from the sensitivity analysis reported on a parameter basis. The original data is gathered from the tables provided in Appendix A.

Parameter	**Impact on process**
CO_2	Increased combustion efficiency *i.e* lower concentration of combustible species at POC inlet leads to higher CO_2 purity of the product stream
CO	CO concentration does not have any notable effect on the combustion efficiency
H_2	H_2 concentration does not have any notable effect on the combustion efficiency
CH_4	Increased concentration of CH_4 leads to a slight increase of NO reduction and combustion efficiency
NO	NO has a strictly positive impact on the combustion efficiency. NO presence has a larger impact when temperature drops below 850°C
Residence time	Increased residence time compared to base-case has a positive impact on the conversion of H_2 and CO. There is also a slight increase to conversion of NO
Temperature	Increased temperature directly leads to lowered concentrations of combustible gases and NO at the outlet. The outlet concentration of O_2 is unchanged due to the reduction reaction of NO toN_2
Lambda	Increasing lambda will increase the degree of fuel conversion and the concentration of O_2 at the outlet. Decreasing lambda will decrease the degree of fuel conversion (CO & H_2) dramatically. O_2 concentration at the outlet will not drop linearly with 5% due to the decreased degree of fuel conversion.

4.4 Emissions of NO_x and SO_x

This project being a first study of the operational performance of oxygen polishing applied to CLC flue gases is not focused on pollutant reduction and will by such only provide a limited amount of result concerning the topic. Inlet concentration of NO_x (almost solely NO) vary with fuel type and time as described in Section 3.5 but is kept constant at the inlet during these simulations. The concentration of NO at the inlet can not be compared to the outlet concentration due to dilution with air but the molar flows can be compared. The inlet molar flow would compare to an outlet concentration of about 700 ppm which can be traced back as an approximate outlet concentration for the premixed case at 700 °C in Figure 4.4.

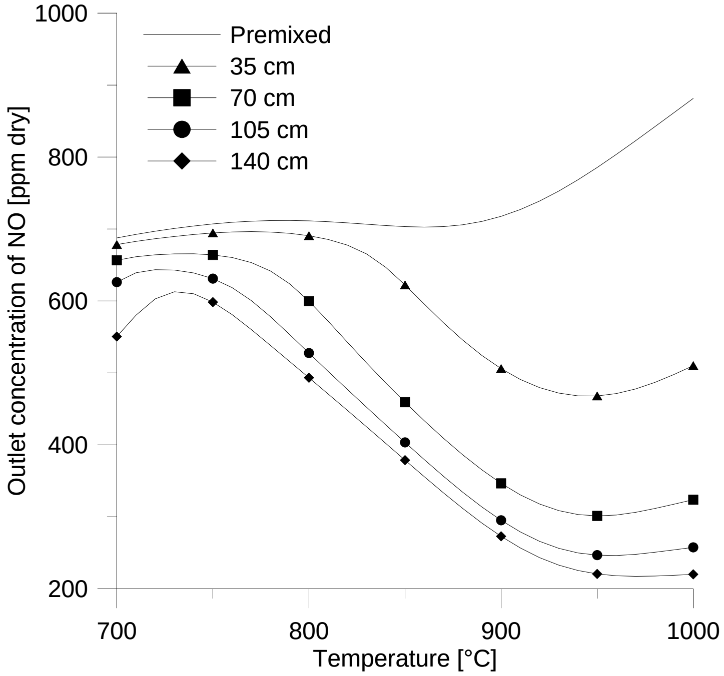

Figure 4.4: Impact of mixing and temperature on the outlet concentration of NO. NO decreases with increasing temperature except at premixed conditions where the high oxygen availability will instead increase the amount of NO.

The temperature and available oxygen amount at the early stages of the POC are the two main factors behind the outlet concentration of NO. For premixed conditions the amount of NO is increased compared to the inlet concentration and the amount increases with increasing temperature. For the remaining mixing cases, total NO flow is lowered and continues dropping hitting a local minimum at about 950°C.

The ratio between NO and total amount of nitrogen species excluding N_2 increases with increasing temperature and is close to unity at 1000°C. For slow mixing cases there is a presence of NH_3 at the outlet while for premixed cases NH_3 is always fully converted. The outlet concentration of HCN appears to not be dependent on mixing but rather requires a temperature of above 900°C to drop below 100 ppm.

Comparisons with the sensitivity analysis where only NO is present as reactive nitrogen specie and at the same inlet concentration show that the presence of HCN, and NH_3 will, as expected, lead to a higher outlet concentration of NO in comparison.

The fate of sulfur in the POC is almost independent of mixing and temperature when the temperature is above 800°C as can be seen in Figure 4.5. At lower temperatures and slow mixing cases the amount of reactive sulfur species, including among others S_2 and SO are slightly higher than for the faster mixing cases, resulting in a lower outlet concentration of SO_2.

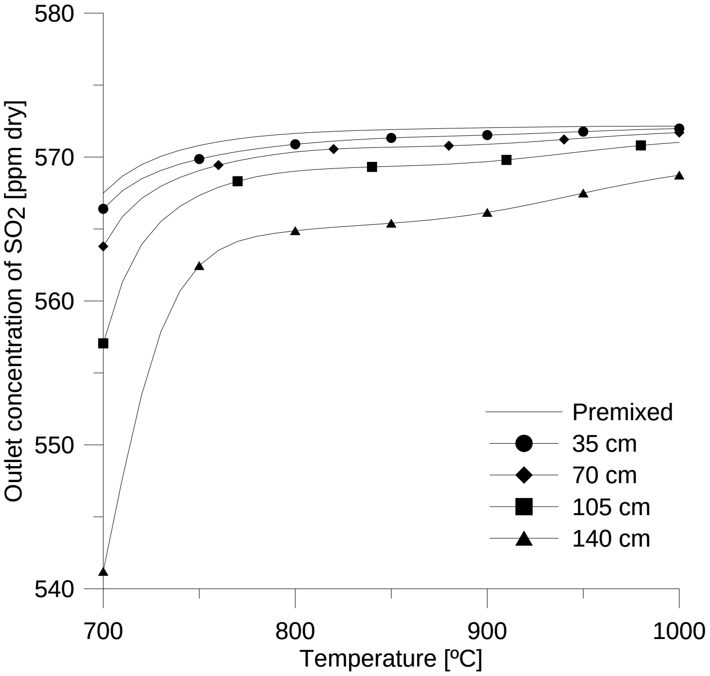

Figure 4.5: Impact of mixing and temperature on the outlet concentration of SO_2. The outlet concentration of SO_2 is almost unchanged for the cases present in this study except for low temperatures and slow mixing when there is a small amount of other sulfur species present.

5

Discussion

In this chapter the results and implications of them are assessed. The discussion will begin with a review of the oxidation rate of the fuel in the POC followed by a discussion of the fate of nitrogen and sulfur. To set a frame for what can be considered a good result in terms of performance the outlet concentrations will be compared to guidelines of CO_2 stream quality to establish recommendations. This will in term lead to the following section containing a discussion of how to design a POC in order to achieve desirable performance. To conclude the chapter the test data gathered from the CLC-unit at Chalmers will be reviewed in order to establish sources of possible errors and variations.

5.1 Combustion efficiency

The degree of fuel conversion is increased with increased temperature which is to be expected, the same goes for residence time. There is however only slight benefits when increasing the temperature beyond 800°C and the residence time beyond 1.3 seconds. According to the simulations a vast majority of the incoming fuel will have been oxidized at 800°C, a residence time of 1.33 at all but the absolute worst mixing rate. Since the fuel reactor itself is operating at 950°C it should be of interest to try and maintain as high temperatures as possible on the route to the POC.

The sensitivity analysis provides information on the operational flexibility of the POC and indicates that it should be able to handle relatively large deviations from the flue gas composition tested. The sensitivity analysis is also simulated with lower temperature than the other results which points in the direction that even at reduced temperatures the POC with current residence time should be able to provide a safe operating window.

Temperature and residence time are two operating conditions that are easy to control in the process through correct sizing of the POC and insulation of the pipe together with the possibility of external heating. The mixing rate is however more complex. The simulations suggest that it is of importance that the oxygen is well mixed with the flue gas early in the reactor to ensure maximal oxidation of the fuel. When the mixing rate is high the rate of production of radicals increases and hence the concentration increases early on in the reactor allowing the oxidation process of the fuel to increase in speed.

The reason for the use of stoichiometric condition is explained in Section 3.2 and can be motivated with the energy penalty of the ASU and the strict restrictions of O_2 concentration in the flue gas stream. The complete oxidation of the fuel in the POC however seems to be dependent on a certain partial pressure of O_2 to take place (see Figure 4.3) which means that the operating conditions of a POC is one where benefits and drawbacks of O_2 concentration has to be taken into consideration. Since there are plants where the CO_2 stream transported contains high levels of O_2 without operational malfunctions it is of interest to the CLC-technology for the guidelines to be re-tested.

5.2 Emissions of NO_x and SO_x

The results show no convincing beneficial effect on the emissions of NO or SO_2 in the current setup. The concentration of NO is decreased (see Figure 4.4) almost to the guidelines for NO_2 (found in Table 2.1) at very slow mixing rates and at high temperatures but since the primary purpose of the POC is to increase fuel conversion which according to the reaction sets used will be maximized for a well mixed reactor this is of little practical use. The NO concentration instead seems to remain close to inlet concentrations for situations that are to be regarded as optimal for combustion efficiency. The reason for the drastic decrease in NO emissions at slower mixing conditions is believed to be due to the activation of the NO reburning mechanism where NO is reduced by hydrocarbons and converted to N_2. In case NO emission is an issue, this is something that could be taken into account when designing an oxy-polishing setup.

The inlet concentration of NO varies a lot between different fuels and operating conditions of the CLC-unit. During tests at Chalmers the dry outlet concentration of NO from the fuel reactor has been as low as 100 ppm with operation of wood char and as high as 2500 ppm with operation of petcoke. The sensitivity analysis points towards that the ratio between outlet and inlet molar flow of NO is lower when there is less present at the inlet. The difference is only marginal however and in the order of 5-10% at the tested levels of 500 and 2000 ppm. If this result is valid as a trend for other flue gas compositions and or levels of NO can not be established with current data.

The concentration of NO seems to have significant impact on low temperature (<800°C) oxidation of the fuel and to some extent enhance oxidation even at higher temperatures (see Chapter A). In the case of a low-temperature POC it might by such be of operational interest to use fuel with a specific nitrogen content to ensure some formation of NO in the FR. The NO present in the flue gas can then contribute to increase the fuel oxidation efficiency in the POC. However the actual net benefits of this are of course limited since the need for flue gas cleaning is increased with increasing amount of NO_x.

When focusing on the SO_2 concentration it is evident in the results that the impact under current operating conditions are negligible. SO_2 will be formed from the H_2S

present at the inlet and the ratio of SO_2 and all present sulfur species will be close to unity at the outlet for temperatures between 800-1000°C. In the article that the sulfur chemistry is gathered from the authors states that SO_2 can have both an inhibiting and a sensitizing effect on fuel oxidation. None of these effects are however noted in the present study. The sensitizing reaction of CO oxidation (Reaction 2.10) is not taking place at all in the present simulations. Selectivity towards this reaction is supposed to increase at stoichiometric conditions and at temperatures between 1000 to 1500 kelvin which coincide with this study. One idea to why this is not happening despite stoichiometry and temperature level might be because of a few reasons, some of them noted here. The very high concentrations of steam present in this simulation case but not in the study by Glarborg is one major difference. The level of SO_2 is also significantly lower than the one in the experimental setup used in the article. In the article the CO oxidation is also discovered to increase with increasing temperature from 1200K to 1500K which is higher than the interval in this study.

The flue gas contains some amount of H_2S which is very quick to react to mainly SH which in turn reacts to eventually form SO_2. During this chain of reactions leading to the formation of SO_2 the main products formed include H_2. There is by such reasons to believe that H_2S acts as an inhibitor of fuel oxidation during the conditions of this study.

5.3 CO_2 stream quality standard

The main advantage of CLC as a technology is the possibility to oxidize fuel with low energy penalties and with a reduced flue gas flow containing almost no N_2 as a result. Every new specie introduced to this flue gas stream in need of cleaning is by such an increased cost to the overall process. The results from this study indicates that apart from the N_2 which is supposed to be replaced with recirculated flue gas the species in need of further treatment is H_2O, SO_2, NO and O_2 (see Table 5.1). Since H_2O is part of the process and intended to be a part of any future design it will always need to be condensed and removed. SO_2 and NO are dependent on the type of fuel and although NO is possible to reduce by means of oxidizer staging, the question of emission treatment will be left as a per basis situation.

Table 5.1: Comparison between the dry concentrations reached in different simulations with the guideline values provided in Table 2.1. Concentration range from simulations are based on the maximum and minimum values from the results with a temperature of 900°C and at stoichiometric conditions

Component	Value range in simulations	Guideline limits for EOR
O_2	1700 - 5000 ppm	1000 ppm
NO	270 - 720 ppm	100 ppm
SO_2	565 - 570 ppm	100 ppm

The only remaining specie in need of removal is O_2 and it´s concentration will vary drastically depending on the stoichiometry in the POC. The reference case considering temperature (*i.e.* 900°C) and flue gas composition (see Table 3.1) with a mixing distance of 70 cm and at stoichiometric condition will have a remaining energy content of about 1% compared to the inlet of the POC. This without supplying excess oxygen and since oxygen production is energy intensive it is of interest to keep it down. If lambda would be increased however the remaining energy could be utilized while increasing the outlet concentration of oxygen. The removal of O_2 from the flue gas is however a very energy intensive action when the required purity is in the order of a few hundred ppm. It is not within the scope of this study to evaluate the techno economical benefits of operational parameters but it is noted that to first produce pure O_2 for oxidation purpose in the POC and then subsequently remove O_2 from the flue gas stream is a highly unlikely scenario.

This situation is of significant importance and might be considered as one of the main challenges of CLC. Thermodynamically the complete oxidation of CO and H_2 seems to be impossible at stoichiometric conditions and even at an air to fuel ratio below unity the remaining amount of O_2 will be above the guidelines. Despite a thorough literature study no strict theoretical reason has been given as to why O_2 has to be kept at the very low concentration of 100 ppm. In the co-existence of certain species O_2 can enhance corrosion dramatically but these species can possibly be decreased to lower levels at a much reduced cost compared to O_2. Another reason to why oxygen is out of favor is because of claimed exothermic reactions at oil well heads, reports about the required O_2 concentration for this to happen is how ever hard to come by. There are several reports that states a necessity of further research in the field of how impurities impact each other in order to construct a more well established composition guideline for super critical CO_2-streams.

5.4 Proposed design of a POC

The results of this study is based solely on gas reaction simulations. There are several factors that will have a large impact on performance in the real case operation of a POC compared to the controlled simulation environment employed in this study. Concentration profiles are constant and likewise is the mixing characteristics in each respective case. The gas phase reaction mechanisms are well studied but these are empirical values and can potentially offer sources of error. One known error is the inability for sulfur to react with nitrogen species, the impact of these reactions are however thought to be of lesser importance.

While keeping the information above in mind there are still valuable information to be had from the results in this study. In order to increase oxidation it is necessary to promote a well mixed reactor. Since the real operation of a POC will include heat exchanging in order to extract the energy the temperature will drop in axial direction. With an operational temperature of about 950°C in the FR it should be emphasized on the importance of insulation and limited distance to the POC from the outlet of the FR. The heat exchanging should not extract more than so that the temperature of the POC at the outlet will be maintained above 700°C. The residence time required is in the order of 1.3 seconds but could beneficially be increased to higher values. A higher residence time would impact temperature profile and possibly mixing characteristics (if diameter is increased) why this would have to be kept in mind.

The POC at Chalmers is currently operated with air instead of pure oxygen. This is by far a cheaper option but not one that is proposed for full scale operation since the introduction of N_2 to the flue gas is making the whole CLC-principal of maintaining a flue gas stream free of N_2 obsolete. When the time comes to switch from air it is proposed to be exchanged for O_2 and recirculated flue gas to maintain a certain volumetric flow to enhance mixing at the oxidizer inlets.

Some back of the envelope calculations for the POC at Chalmers show that the pipe flow from the FR is above the border region between laminar and turbulent with an approximate Reynolds number of 3600 before introducing the air and close to 4200 after the air has been added. The jet Reynolds on the other hand is in the lower region and close to laminar with its value of approximately 2400 (calculations available in Appendix B). In literature the recommendation to ensure fully turbulent flow of the jet is to have a jet Reynolds above 4000.[19],[20]

In a study by Forney, L. J., it was established that four jet inlets offered superior mixing compared to 1, 2 and 3 jets [19]. With the operation of 4 jet inlets the volumetric flow would however have to be increased to ensure a fully turbulent flow. This would be possible when switching from air to pure oxygen and recirculated flue gases when the flue gas flow could be increased without increasing the amount of oxygen. The increased flow would impact residence time negatively why the POC would have to be larger.

In Figure 5.1 an idea of how to approach the design criteria of a POC is presented. The main flow is divided into sub-streams in order to create natural circulation zones inside the POC and this is followed by four jet inlets where oxygen and recirculated flue gases can be injected. The design replicates that of a cyclone in order to avoid problems if char will be present in the flue gas flow. A possible alteration to the design would be to place the jet inlets before dividing the flue gas stream which would increase turbulence in the main pipe. There might however be material constraints to this design at inlets and pipe bends.

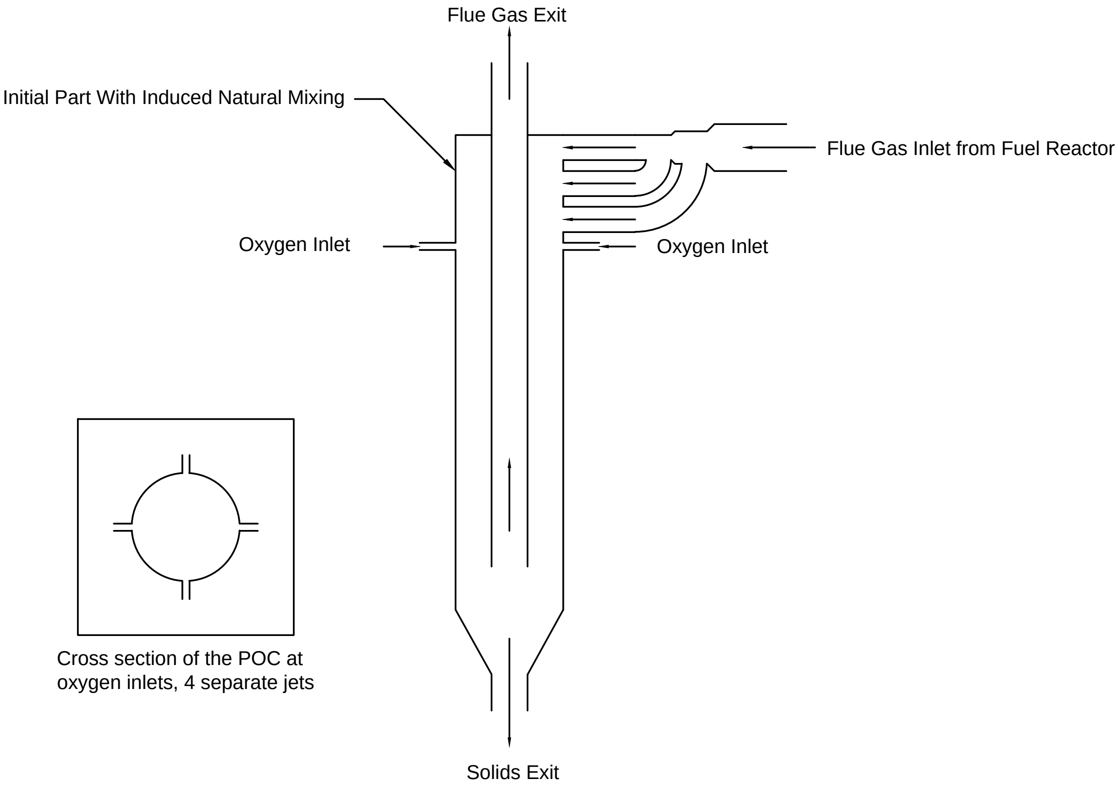

Figure 5.1: Possible design of a POC. Dividing flue gas stream in order to enforce mixing in the reactor before inserting oxygen with recirculated flue gas. With a reactor designed as a cyclone the risk for elutriation is minimized.

5.5 Measurements from Chalmers 100 kW CLC unit

Simulations without experimental data for validation should not be assigned with any higher order of credibility. It is therefore regrettable that the measurement data available from the CLC-unit at Chalmers are not more accurate than they are and that the process it self is not working as good as it is supposed to in terms of solid fuel leaving the fuel reactor. If the POC will have to deal with char as well as the remaining volatiles and syngas the design might have to be altered. Residence time for combustion and design to avoid elutriation might be two factors that will change.

The current measurements from the POC are fluctuating with time and are not designed to be used in the manner that this report is doing. As mentioned earlier the main focus on the research with solid fuels in CLC is in bed material and the fact that the CLC-unit at Chalmers is one of few and the largest at that the data gathered to this report still has to be regarded as the best possible for the time being.

6

Conclusion

This study examines the technical possibilities of oxygen polishing in a post oxidation chamber by means of oxy-combustion as described by *e.g.* Normann, F. [21]. The base case including flue gas concentration, residence time and temperature is gathered from operational data at Chalmers university of technology. Few studies have been made concerning oxygen polishing of CLC flue gases so this report aims to establish a foundation for further research.

The results show that the oxidation of the fuel with current flue gas concentration requires a temperature above 800°C to reach a state that is mostly influenced by air to fuel ratio. In order to increase the oxidation further the temperature can be increased and the mixing of oxygen and flue gas in the POC should be efficient and take place as early on in the POC as possible. H_2 will be the main remaining combustible specie after the POC with a dry concentration in the order of 1000 ppm.

In order to reach complete oxidation of the fuel the air to fuel ratio has to be increased above stoichiometric. Depending on the mixing rate complete oxidation will occur from lambda equal to 1.05 to lambda equal to 1.2 for fast contra slow mixing at an operating temperature of 900°C. The results from the sensitivity analysis also show that the POC with operating conditions similar to those at Chalmers should be able to handle deviations in flue gas composition, temperature and residence time fairly well.

During the simulations it was observed that oxidant staging can have a significant effect on NO_x reduction by means of NO reburning. Although fast mixing between oxidizer and flue gases is beneficial for combustion, this is something that could potentially be taken into consideration when designing an oxy-polishing system in the future. It was also observed that NO has a significant impact on H_2 and CO oxidation especially at temperatures between 700 and 800°C.

The current available transportation guidelines for chemical composition of a super critical CO_2 stream puts severe limitations on O_2 content. In this study there has been no indications towards a result where the O_2 concentration can be beneath the required amount. There is by such a need for additional measures to reduce the outlet O_2 concentration or further research on the impact of impurities in a super critical CO_2 stream to investigate if the limits can be raised.

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Results from the sensitivity analysis

This section includes the numerical values from the sensitivity analysis described in Section 3.5. The values can be found in tables where each main parameter has it's own table. The ordering of the tables (considering main parameters) are CO_2, CO, H_2, CH_4, NO, volumetric flow, lambda and temperature. Values that have been included are the decrease of molar flow going out of the POC compared to that coming in to the POC (conversion), see Equation A.1 below,

$$\left(1 - \frac{\dot{n}_{i,out}}{\dot{n}_{i,in}}\right) * 100 \quad [\%], \tag{A.1}$$

and the dry outlet concentration, where $\dot{n}_i$ represents the molar flow of specie i in moles per second. The column title called "Test case" in the attached tables below refers to the limits explained in Section 3.5. The values for dry outlet concentrations provided in the tables are in percentage for the case of CO_2 and in ppm for all the remaining species.

Table A.1: Results from sensitivity analysis with CO_2 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High CO2 High CO	99.8	93.5	100	10.6	99.6	241	1052	0	2280	2391
High CO2 Ref CO	99.7	96.7	100	17.7	99.6	244	1085	0	2369	2237
High CO2 Low CO	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
Ref CO2 High CO	99.8	98.1	100	23.9	99.6	244	1112	0	2608	2117
Ref CO2 Ref CO	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO2 Low CO	99.6	98.8	100	29.9	99.6	245	1158	0	2840	2019
Low CO2 High CO	99.9	98.9	100	30.5	99.5	252	1218	0	3047	2024
Low CO2 Ref CO	99.8	99.2	100	34.0	99.5	259	1304	0	3261	1996
Low CO2 Low CO	99.7	99.2	100	35.4	99.5	270	1394	0	3318	1992
High CO2 High H2	98.6	99.0	100	11.7	99.6	252	1229	0	2452	2598
High CO2 Ref H2	99.5	98.5	100	21.1	99.6	231	1063	0	2568	2225
High CO2 Low H2	99.6	96.0	100	22.3	99.6	244	1078	0	2465	2105
Ref CO2 High H2	99.6	99.0	100	24.9	99.6	243	1173	0	2762	2205
Ref CO2 Ref H2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO2 Low H2	99.8	95.8	100	25.0	99.6	253	1124	0	2609	2027
Low CO2High H2	99.8	98.9	100	32.4	99.5	265	1293	0	3064	1975
Low CO2 Ref H2	99.8	98.2	100	31.4	99.6	264	1233	0	2998	1922
Low CO2 Low H2	99.9	95.3	100	27.3	99.6	280	1260	0	2821	1956
High CO2 High CH4	98.7	93.7	100	22.0	99.6	272	1203	0	2629	2105
High CO2 Ref CH4	99.5	97.5	100	25.3	99.6	233	1039	0	2623	2055
High CO2 Low CH4	99.6	98.2	100	13.9	99.6	238	1086	0	2418	2402

Table A.2: Results from sensitivity analysis with CO_2 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Ref CO2 High CH4	99.6	97.8	100	29.5	99.6	255	1163	0	2833	1955
Ref CO2 Ref CH4	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO2 Low CH4	99.8	98.8	100	13.2	99.6	250	1187	0	2517	2493
Low CO2 High CH4	99.8	99.0	100	33.5	99.5	265	1305	0	3140	1962
Low CO2 Ref CH4	99.9	99.2	100	27.1	99.5	249	1246	0	3048	2196
Low CO2 Low CH4	99.9	99.2	100	12.4	99.6	266	1370	0	2765	2680
High CO2 High Flow	99.5	97.4	100	20.3	99.6	294	1307	0	2691	2206
High CO2 Ref Flow	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
High CO2 Low Flow	99.7	98.5	100	26.3	99.7	167	755	0	2430	2041
Ref CO2 High Flow	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
Ref CO2 Ref Flow	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO2 Low Flow	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low CO2 High Flow	99.8	98.8	100	28.5	99.5	341	1670	0	3238	2118
Low CO2 Ref Flow	99.8	99.0	100	32.4	99.5	267	1321	0	3075	2006
Low CO2 Low Flow	99.9	99.3	100	37.8	99.6	189	942	0	2939	1848
High CO2 High Lambda	100.0	99.8	100	22.6	99.2	26	77	0	7981	2133
High CO2 Ref Lambda	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
High CO2 Low Lambda	97.1	83.9	100	22.0	99.0	1586	7982	0	710	2149
Ref CO2 High Lambda	100.0	99.9	100	26.8	98.9	18	46	0	11304	2057
Ref CO2 Ref Lambda	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO2 Low Lambda	97.1	83.1	100	26.0	98.4	2453	12802	0	563	2077

Table A.3: Results from sensitivity analysis with CO_2 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Low CO2 High Lambda	100.0	100.0	100	31.4	98.2	14	28	0	18291	2005
Low CO2 Ref Lambda	99.8	99.0	100	32.4	99.5	267	1321	0	3075	2006
Low CO2 Low Lambda	97.0	81.9	100	30.4	97.1	4308	23784	0	443	2027
High CO2 High Temp	99.6	98.2	100	34.3	99.6	219	907	0	2576	1819
High CO2 Ref Temp	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
High CO2 Low Temp	99.5	97.2	100	12.9	99.6	299	1383	0	2658	2408
Ref CO2 High Temp	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref CO2 Ref Temp	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO2 Low Temp	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
Low CO2 High Temp	99.8	99.1	100	51.3	99.5	266	1216	0	3211	1444
Low CO2 Ref Temp	99.8	99.0	100	32.4	99.5	267	1321	0	3075	2006
Low CO2 Low Temp	99.8	98.7	100	17.4	99.5	342	1730	0	3123	2448

Table A.4: Results from sensitivity analysis with CO as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High CO High CO2	99.8	93.5	100	10.6	99.6	241	1052	0	2280	2391
High CO Ref CO2	99.8	98.1	100	23.9	99.6	244	1112	0	2608	2117
High CO Low CO2	99.9	98.9	100	30.5	99.5	252	1218	0	3047	2024
Ref CO High CO2	99.7	96.7	100	17.7	99.6	244	1085	0	2369	2237
Ref CO Ref CO2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO Low CO2	99.8	99.2	100	34.0	99.5	259	1304	0	3261	1996
Low CO High CO2	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
Low CO Ref CO2	99.6	98.8	100	29.9	99.6	245	1158	0	2840	2019
Low CO Low CO2	99.7	99.2	100	35.4	99.5	270	1394	0	3318	1992
High CO High H2	99.8	99.0	100	26.8	99.6	250	1211	0	2838	2144
High CO Ref H2	99.8	98.4	100	26.4	99.6	248	1143	0	2697	2067
High CO Low H2	99.8	95.9	100	23.6	99.6	252	1118	0	2516	2064
Ref CO High H2	99.7	99.0	100	27.6	99.6	250	1208	0	2826	2124
Ref CO Ref H2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO Low H2	99.7	95.9	100	23.6	99.6	252	1118	0	2499	2067
Low COHigh H2	99.6	99.0	100	28.4	99.6	245	1185	0	2840	2103
Low CO Ref H2	99.6	98.4	100	27.7	99.6	243	1120	0	2694	2040
Low CO Low H2	99.5	95.9	100	23.5	99.6	249	1103	0	2502	2074
High CO High CH4	99.8	98.9	100	31.5	99.5	169	729	0	3628	1880
High CO Ref CH4	99.7	98.0	100	26.5	99.6	305	1471	0	2455	2110
High CO Low CH4	99.7	97.6	100	12.4	99.6	385	1975	0	2016	2607

Table A.5: Results from sensitivity analysis with CO as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Ref CO High CH4	99.8	98.9	100	31.8	99.6	177	773	0	3526	1885
Ref CO Ref CH4	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO Low CH4	99.6	97.7	100	12.8	99.6	373	1917	0	2042	2611
Low CO High CH4	99.7	98.9	100	32.0	99.6	183	804	0	3457	1889
Low CO Ref CH4	99.5	98.2	100	27.4	99.6	306	1490	0	2430	2110
Low CO Low CH4	99.4	97.9	100	13.3	99.6	353	1820	0	2094	2613
High CO High Flow	99.7	98.1	100	23.5	99.5	312	1429	0	2871	2156
High CO Ref Flow	99.8	98.5	100	26.5	99.6	245	1134	0	2726	2072
High CO Low Flow	99.8	98.9	100	30.7	99.6	175	818	0	2591	1954
Ref CO High Flow	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
Ref CO Ref Flow	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO Low Flow	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low CO High Flow	99.4	98.2	100	24.8	99.5	315	1453	0	2836	2136
Low CO Ref Flow	99.6	98.5	100	27.9	99.6	247	1148	0	2701	2047
Low CO Low Flow	99.7	98.9	100	32.4	99.6	178	834	0	2563	1922
High CO High Lambda	100.0	99.9	100	26.1	98.8	17	42	0	11733	2067
High CO Ref Lambda	99.8	98.5	100	26.5	99.6	245	1134	0	2726	2072
High CO Low Lambda	97.7	81.4	100	25.3	98.3	2624	13651	0	541	2086
Ref CO High Lambda	100.0	99.9	100	26.8	98.9	18	46	0	11304	2057
Ref CO Ref Lambda	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO Low Lambda	97.1	83.1	100	26.0	98.4	2453	12802	0	563	2077

Table A.6: Results from sensitivity analysis with CO as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Low CO High Lambda	100.0	99.9	100	27.5	98.9	20	51	0	10737	2045
Low CO Ref Lambda	99.6	98.5	100	27.9	99.6	247	1148	0	2701	2047
Low CO Low Lambda	95.9	84.5	100	26.6	98.5	2325	12171	0	580	2067
High CO High Temp	99.8	98.6	100	40.8	99.6	235	1003	0	2787	1668
High CO Ref Temp	99.8	98.5	100	26.5	99.6	245	1134	0	2726	2072
High CO Low Temp	99.7	98.0	100	14.7	99.5	314	1490	0	2810	2403
Ref CO High Temp	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref CO Ref Temp	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CO Low Temp	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
Low CO High Temp	99.6	98.7	100	43.5	99.6	239	1022	0	2769	1605
Low CO Ref Temp	99.6	98.5	100	27.9	99.6	247	1148	0	2701	2047
Low CO Low Temp	99.4	98.1	100	15.4	99.5	320	1527	0	2778	2401

Table A.7: Results from sensitivity analysis with H_2 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High H2 High CO2	98.6	99.0	100	11.7	99.6	252	1229	0	2452	2598
High H2 Ref CO2	99.6	99.0	100	24.9	99.6	243	1173	0	2762	2205
High H2 Low CO2	99.8	98.9	100	32.4	99.5	265	1293	0	3064	1975
Ref H2 High CO2	99.5	98.5	100	21.1	99.6	231	1063	0	2568	2225
Ref H2 Ref CO2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref H2 Low CO2	99.8	98.2	100	31.4	99.6	264	1233	0	2998	1922
Low H2 High CO2	99.6	96.0	100	22.3	99.6	244	1078	0	2465	2105
Low H2 Ref CO2	99.8	95.8	100	25.0	99.6	253	1124	0	2609	2027
Low H2 Low CO2	99.9	95.3	100	27.3	99.6	280	1260	0	2821	1956
High H2 High CO	99.8	99.0	100	26.8	99.6	250	1211	0	2838	2144
High H2 Ref CO	99.7	99.0	100	27.6	99.6	250	1208	0	2826	2124
High H2 Low CO	99.6	99.0	100	28.4	99.6	245	1185	0	2840	2103
Ref H2 High CO	99.8	98.4	100	26.4	99.6	248	1143	0	2697	2067
Ref H2 Ref CO	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref H2 Low CO	99.6	98.4	100	27.7	99.6	243	1120	0	2694	2040
Low H2High CO	99.8	95.9	100	23.6	99.6	252	1118	0	2516	2064
Low H2 Ref CO	99.7	95.9	100	23.6	99.6	252	1118	0	2499	2067
Low H2 Low CO	99.5	95.9	100	23.5	99.6	249	1103	0	2502	2074
High H2 High CH4	99.7	98.9	100	33.7	99.5	255	1238	0	3125	1945
High H2 Ref CH4	99.7	99.0	100	28.1	99.6	240	1158	0	2901	2110
High H2 Low CH4	99.7	99.0	100	13.4	99.6	249	1212	0	2572	2538

Table A.8: Results from sensitivity analysis with H_2 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Ref H2 High CH4	99.7	98.4	100	31.8	99.6	256	1199	0	2945	1931
Ref H2 Ref CH4	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref H2 Low CH4	99.7	98.5	100	13.5	99.6	246	1147	0	2454	2446
Low H2 High CH4	99.7	95.7	100	25.5	99.6	263	1174	0	2692	2017
Low H2 Ref CH4	99.7	96.1	100	23.4	99.6	242	1068	0	2547	2073
Low H2 Low CH4	99.7	96.0	100	13.1	99.6	244	1078	0	2299	2351
High H2 High Flow	99.6	98.8	100	24.7	99.5	307	1465	0	3036	2209
High H2 Ref Flow	99.7	99.0	100	27.7	99.6	239	1154	0	2892	2121
High H2 Low Flow	99.8	99.3	100	31.9	99.6	171	833	0	2747	1998
Ref H2 High Flow	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
Ref H2 Ref Flow	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref H2 Low Flow	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low H2 High Flow	99.6	94.7	100	20.5	99.6	324	1424	0	2616	2149
Low H2 Ref Flow	99.7	95.8	100	23.6	99.6	256	1138	0	2479	2067
Low H2 Low Flow	99.8	96.9	100	28.1	99.7	186	830	0	2349	1947
High H2 High Lambda	100.0	100.0	100	27.2	98.8	17	43	0	12426	2117
High H2 Ref Lambda	99.7	99.0	100	27.7	99.6	239	1154	0	2892	2121
High H2 Low Lambda	96.8	87.6	100	26.3	98.2	2649	14416	0	559	2140
Ref H2 High Lambda	100.0	99.9	100	26.8	98.9	18	46	0	11304	2057
Ref H2 Ref Lambda	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref H2 Low Lambda	97.1	83.1	100	26.0	98.4	2453	12802	0	563	2077

Table A.9: Results from sensitivity analysis with H_2 as main parameter.

Test case	**Component conversion** [%]				**Dry outlet concentration** [%, ppm]					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Low H2 High Lambda	100.0	99.8	100	23.3	99.0	19	50	0	9779	2062
Low H2 Ref Lambda	99.7	95.8	100	23.6	99.6	256	1138	0	2479	2067
Low H2 Low Lambda	97.3	58.5	100	22.7	98.6	2260	11177	0	567	2077
High H2 High Temp	99.7	99.1	100	42.2	99.6	232	1032	0	2950	1697
High H2 Ref Temp	99.7	99.0	100	27.7	99.6	239	1154	0	2892	2121
High H2 Low Temp	99.6	98.7	100	15.5	99.5	309	1523	0	2972	2477
Ref H2 High Temp	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref H2 Ref Temp	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref H2 Low Temp	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
Low H2 High Temp	99.7	96.3	100	38.1	99.6	244	993	0	2530	1676
Low H2 Ref Temp	99.7	95.8	100	23.6	99.6	256	1138	0	2479	2067
Low H2 Low Temp	99.6	94.4	100	12.9	99.6	330	1507	0	2579	2354

Table A.10: Results from sensitivity analysis with CH_4 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High CH4 High CO2	98.7	93.7	100	22.0	99.6	272	1203	0	2629	2105
High CH4 Ref CO2	99.6	97.8	100	29.5	99.6	255	1163	0	2833	1955
High CH4 Low CO2	99.8	99.0	100	33.5	99.5	265	1305	0	3140	1962
Ref CH4 High CO2	99.5	97.5	100	25.3	99.6	233	1039	0	2623	2055
Ref CH4 Ref CO2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CH4 Low CO2	99.9	99.2	100	27.1	99.5	249	1246	0	3048	2196
Low CH4 High CO2	99.6	98.2	100	13.9	99.6	238	1086	0	2418	2402
Low CH4 Ref CO2	99.8	98.8	100	13.2	99.6	250	1187	0	2517	2493
Low CH4 Low CO2	99.9	99.2	100	12.4	99.6	266	1370	0	2765	2680
High CH4 High CO	99.8	98.9	100	31.5	99.5	169	729	0	3628	1880
High CH4 Ref CO	99.8	98.9	100	31.8	99.6	177	773	0	3526	1885
High CH4 Low CO	99.7	98.9	100	32.0	99.6	183	804	0	3457	1889
Ref CH4 High CO	99.7	98.0	100	26.5	99.6	305	1471	0	2455	2110
Ref CH4 Ref CO	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CH4 Low CO	99.5	98.2	100	27.4	99.6	306	1490	0	2430	2110
Low CH4High CO	99.7	97.6	100	12.4	99.6	385	1975	0	2016	2607
Low CH4 Ref CO	99.6	97.7	100	12.8	99.6	373	1917	0	2042	2611
Low CH4 Low CO	99.4	97.9	100	13.3	99.6	353	1820	0	2094	2613
High CH4 High H2	99.7	98.9	100	33.7	99.5	255	1238	0	3125	1945
High CH4 Ref H2	99.7	98.4	100	31.8	99.6	256	1199	0	2945	1931
High CH4 Low H2	99.7	95.7	100	25.5	99.6	263	1174	0	2692	2017

Table A.11: Results from sensitivity analysis with CH_4 as main parameter.

Test case	**Component conversion** [%]				**Dry outlet concentration** [%, ppm]					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Ref CH4 High H2	99.7	99.0	100	28.1	99.6	240	1158	0	2901	2110
Ref CH4 Ref H2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CH4 Low H2	99.7	96.1	100	23.4	99.6	242	1068	0	2547	2073
Low CH4 High H2	99.7	99.0	100	13.4	99.6	249	1212	0	2572	2538
Low CH4 Ref H2	99.7	98.5	100	13.5	99.6	246	1147	0	2454	2446
Low CH4 Low H2	99.7	96.0	100	13.1	99.6	244	1078	0	2299	2351
High CH4 High Flow	99.6	97.9	100	27.3	99.5	329	1516	0	3075	2051
High CH4 Ref Flow	99.7	98.4	100	31.5	99.6	255	1185	0	2941	1932
High CH4 Low Flow	99.8	98.8	100	37.5	99.6	180	843	0	2817	1766
Ref CH4 High Flow	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
Ref CH4 Ref Flow	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CH4 Low Flow	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low CH4 High Flow	99.7	98.2	100	12.1	99.6	304	1403	0	2629	2490
Low CH4 Ref Flow	99.7	98.6	100	13.5	99.6	244	1139	0	2478	2453
Low CH4 Low Flow	99.8	98.9	100	15.4	99.7	180	849	0	2329	2400
High CH4 High Lambda	100.0	100.0	100	30.6	98.4	15	30	0	15943	1935
High CH4 Ref Lambda	99.7	98.4	100	31.5	99.6	255	1185	0	2941	1932
High CH4 Low Lambda	95.2	72.2	100	29.6	97.6	3808	19880	0	450	1956
Ref CH4 High Lambda	100.0	99.9	100	26.8	98.9	18	46	0	11304	2057
Ref CH4 Ref Lambda	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CH4 Low Lambda	97.1	83.1	100	26.0	98.4	2453	12802	0	563	2077

Table A.12: Results from sensitivity analysis with CH_4 as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Low CH4 High Lambda	100.0	99.9	100	13.5	99.2	26	85	0	7547	2441
Low CH4 Ref Lambda	99.7	98.6	100	13.5	99.6	244	1139	0	2478	2453
Low CH4 Low Lambda	98.3	90.1	100	13.1	99.0	1514	7813	0	757	2452
High CH4 High Temp	99.7	98.5	100	51.8	99.6	252	1081	0	3097	1360
High CH4 Ref Temp	99.7	98.4	100	31.5	99.6	255	1185	0	2941	1932
High CH4 Low Temp	99.6	97.8	100	16.7	99.5	336	1594	0	2981	2349
Ref CH4 High Temp	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref CH4 Ref Temp	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref CH4 Low Temp	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
Low CH4 High Temp	99.7	98.7	100	17.5	99.6	232	994	0	2418	2340
Low CH4 Ref Temp	99.7	98.6	100	13.5	99.6	244	1139	0	2478	2453
Low CH4 Low Temp	99.7	98.2	100	8.5	99.6	304	1458	0	2639	2591

Table A.13: Results from sensitivity analysis with NO as main parameter. These are the only simulations where the concentration of NO has been varied.

Test case	**Component conversion** [%]				**Dry outlet concentration** [%, ppm]					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High NO High CO2	99.6	98.0	100	22.8	99.6	224	1008	0	2549	2137
Ref NO High CO2	99.1	95.2	100	18.2	99.5	498	2375	0	2007	567
Low NO High CO2	97.7	88.7	100	100.0	98.9	1290	5598	1	4219	0
High NO Ref CO2	99.7	98.6	100	27.3	99.6	230	1067	0	2754	2058
Ref NO Ref CO2	99.4	96.6	100	20.9	99.5	523	2573	0	2187	560
Low NO Ref CO2	98.6	93.0	100	100.0	98.8	1218	5361	2	4923	0
High NO Low CO2	99.8	99.1	100	32.4	99.5	255	1265	0	3081	2004
Ref NO Low CO2	99.6	97.7	100	23.9	99.4	578	3040	0	2494	564
Low NO Low CO2	99.3	96.4	100	100.0	98.7	1083	4796	4	6918	0
High NO High CO	99.8	98.5	100	26.6	99.6	235	1087	0	2731	2071
Ref NO High CO	99.5	96.5	100	20.4	99.5	531	2608	0	2170	561
Low NOHigh CO	98.9	92.7	100	100.0	98.9	1218	5361	2	4872	0
High NO Ref CO	99.7	98.6	100	27.3	99.6	230	1067	0	2754	2058
Ref NO Ref CO	99.4	96.6	100	20.9	99.5	523	2573	0	2187	560
Low NO Ref CO	98.6	93.0	100	100.0	98.8	1218	5361	2	4923	0
High NO Low CO	99.6	98.6	100	28.0	99.6	238	1111	0	2694	2046
Ref NO Low CO	99.1	96.6	100	21.5	99.5	538	2658	0	2134	558
Low NO Low CO	97.8	93.0	100	100.0	98.8	1241	5478	2	4854	0
High NO High H2	99.7	99.1	100	27.7	99.6	231	1115	0	2886	2120
Ref NO High H2	99.4	97.7	100	21.6	99.4	528	2707	0	2297	575
Low NO High H2	98.6	95.2	100	100.0	98.8	1215	5553	2	5198	0

Table A.14: Results from sensitivity analysis with NO as main parameter. These are the only simulations where the concentration of NO has been varied.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High NO Ref H2	99.7	98.6	100	27.3	99.6	230	1067	0	2754	2058
Ref NO Ref H2	99.4	96.6	100	20.9	99.5	523	2573	0	2187	560
Low NO Ref H2	98.6	93.0	100	100.0	98.8	1218	5361	2	4923	0
High NO Low H2	99.7	95.9	100	23.7	99.6	248	1100	0	2473	2066
Ref NO Low H2	99.1	84.5	100	16.0	99.3	858	4459	0	1427	604
Low NO Low H2	98.5	79.9	100	100.0	98.9	1310	5406	1	4572	0
High NO High CH4	99.7	98.4	100	31.6	99.6	245	1141	0	2937	1931
Ref NO High CH4	99.3	96.3	100	21.7	99.4	549	2713	0	2377	553
Low NO High CH4	98.6	93.6	100	100.0	98.8	1114	4602	3	6575	0
High NO Ref CH4	99.7	98.6	100	27.3	99.6	230	1067	0	2754	2058
Ref NO Ref CH4	99.4	96.6	100	20.9	99.5	523	2573	0	2187	560
Low NO Ref CH4	98.6	93.0	100	100.0	98.8	1218	5361	2	4923	0
High NO Low CH4	99.7	98.6	100	13.5	99.6	236	1105	0	2469	2452
Ref NO Low CH4	99.4	97.0	100	10.6	99.5	491	2414	0	1960	634
Low NO Low CH4	98.5	92.5	100	100.0	98.9	1311	5961	0	3970	0
High NO High Flow	99.7	98.2	100	24.2	99.5	294	1349	0	2894	2145
Ref NO High Flow	99.3	96.1	100	17.7	99.4	624	3013	0	2437	582
Low NO High Flow	98.3	92.2	100	100.0	98.7	1415	5948	-1	5389	0
High NO Ref Flow	99.7	98.6	100	27.3	99.6	230	1067	0	2754	2058
Ref NO Ref Flow	99.4	96.6	100	20.9	99.5	523	2573	0	2187	560
Low NO Ref Flow	98.6	93.0	100	100.0	98.8	1218	5361	2	4923	0

Table A.15: Results from sensitivity analysis with NO as main parameter. These are the only simulations where the concentration of NO has been varied.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High NO Low Flow	99.8	99.0	100	31.6	99.6	163	762	0	2632	1936
Ref NO Low Flow	99.5	97.3	100	25.6	99.6	417	2090	0	1914	527
Low NO Low Flow	98.8	93.9	100	100.0	99.0	1009	4651	2	4370	0
High NO High Temp	99.7	98.8	100	42.2	99.6	221	944	0	2818	1636
Ref NO High Temp	99.3	96.7	100	34.9	99.5	575	2555	0	2214	461
Low NO High Temp	98.9	94.7	100	100.0	99.2	917	4036	1	3166	0
High NO Ref Temp	99.7	98.6	100	27.3	99.6	230	1067	0	2754	2058
Ref NO Ref Temp	99.4	96.6	100	20.9	99.5	523	2573	0	2187	560
Low NO Ref Temp	98.6	93.0	100	100.0	98.8	1218	5361	2	4923	0
High NO Low Temp	99.6	98.2	100	15.1	99.5	298	1416	0	2833	2401
Ref NO Low Temp	99.4	96.5	100	9.6	99.5	520	2686	0	2200	640
Low NO Low Temp	92.3	87.4	100	100.0	97.3	6476	9544	23	10606	0

Table A.16: Results from sensitivity analysis with volumetric flow as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Flow High CO2	99.5	97.4	100	20.3	99.6	294	1307	0	2691	2206
High Flow Ref CO2	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
High Flow Low CO2	99.8	98.8	100	28.5	99.5	341	1670	0	3238	2118
Ref Flow High CO2	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
Ref Flow Ref CO2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref Flow Low CO2	99.8	99.0	100	32.4	99.5	267	1321	0	3075	2006
Low Flow High CO2	99.7	98.5	100	26.3	99.7	167	755	0	2430	2041
Low Flow Ref CO2	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Flow Low CO2	99.9	99.3	100	37.8	99.6	189	942	0	2939	1848
High Flow High CO	99.7	98.1	100	23.5	99.5	312	1429	0	2871	2156
High Flow Ref CO	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
High Flow Low CO	99.4	98.2	100	24.8	99.5	315	1453	0	2836	2136
Ref Flow High CO	99.8	98.5	100	26.5	99.6	245	1134	0	2726	2072
Ref Flow Ref CO	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref Flow Low CO	99.6	98.5	100	27.9	99.6	247	1148	0	2701	2047
Low FlowHigh CO	99.8	98.9	100	30.7	99.6	175	818	0	2591	1954
Low Flow Ref CO	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Flow Low CO	99.7	98.9	100	32.4	99.6	178	834	0	2563	1922
High Flow High H2	99.6	98.8	100	24.7	99.5	307	1465	0	3036	2209
High Flow Ref H2	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
High Flow Low H2	99.6	94.7	100	20.5	99.6	324	1424	0	2616	2149

Table A.17: Results from sensitivity analysis with volumetric flow as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Ref Flow High H2	99.7	99.0	100	27.7	99.6	239	1154	0	2892	2121
Ref Flow Ref H2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref Flow Low H2	99.7	95.8	100	23.6	99.6	256	1138	0	2479	2067
Low Flow High H2	99.8	99.3	100	31.9	99.6	171	833	0	2747	1998
Low Flow Ref H2	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Flow Low H2	99.8	96.9	100	28.1	99.7	186	830	0	2349	1947
High Flow High CH4	99.6	97.9	100	27.3	99.5	329	1516	0	3075	2051
High Flow Ref CH4	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
High Flow Low CH4	99.7	98.2	100	12.1	99.6	304	1403	0	2629	2490
Ref Flow High CH4	99.7	98.4	100	31.5	99.6	255	1185	0	2941	1932
Ref Flow Ref CH4	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref Flow Low CH4	99.7	98.6	100	13.5	99.6	244	1139	0	2478	2453
Low Flow High CH4	99.8	98.8	100	37.5	99.6	180	843	0	2817	1766
Low Flow Ref CH4	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Flow Low CH4	99.8	98.9	100	15.4	99.7	180	849	0	2329	2400
High Flow High Lambda	100.0	99.9	100	23.9	98.9	25	65	0	11279	2137
High Flow Ref Lambda	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
High Flow Low Lambda	97.0	82.9	100	23.2	98.4	2526	13005	0	661	2155
Ref Flow High Lambda	100.0	99.9	100	26.8	98.9	18	46	0	11304	2057
Ref Flow Ref Lambda	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref Flow Low Lambda	97.1	83.1	100	26.0	98.4	2453	12802	0	563	2077

Table A.18: Results from sensitivity analysis with volumetric flow as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
Low Flow High Lambda	100.0	100.0	100	30.8	98.9	12	30	0	11349	1944
Low Flow Ref Lambda	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Flow Low Lambda	97.2	83.5	100	29.9	98.5	2370	12542	0	460	1968
High Flow High Temp	99.6	98.4	100	38.2	99.5	298	1262	0	2954	1748
High Flow Ref Temp	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
High Flow Low Temp	99.5	97.6	100	13.2	99.5	396	1805	0	3016	2452
Ref Flow High Temp	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Flow Ref Temp	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Ref Flow Low Temp	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
Low Flow High Temp	99.8	99.1	100	47.4	99.6	159	682	0	2709	1490
Low Flow Ref Temp	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Flow Low Temp	99.7	98.6	100	17.7	99.6	226	1106	0	2667	2328

Table A.19: Results from sensitivity analysis with lambda as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Lambda High CO2	100.0	99.8	100	23	99.2	26	77	0	7981	2133
Ref Lambda High CO2	99.6	97.9	100	23	99.6	231	1040	0	2557	2138
Low Lambda High CO2	97.1	83.9	100	22	99.0	1586	7982	0	710	2149
High Lambda Ref CO2	100.0	99.9	100	27	98.9	18	46	0	11304	2057
Ref Lambda Ref CO2	99.7	98.6	100	27	99.6	238	1102	0	2762	2059
Low Lambda Ref CO2	97.1	83.1	100	26	98.4	2453	12802	0	563	2077
High Lambda Low CO2	100.0	100.0	100	31	98.2	14	28	0	18291	2005
Ref Lambda Low CO2	99.8	99.0	100	32	99.5	267	1321	0	3075	2006
Low Lambda Low CO2	97.0	81.9	100	30	97.1	4308	23784	0	443	2027
High Lambda High CO	100.0	99.9	100	26	98.8	17	42	0	11733	2067
Ref Lambda High CO	99.8	98.5	100	27	99.6	245	1134	0	2726	2072
Low LambdaHigh CO	97.7	81.4	100	25	98.3	2624	13651	0	541	2086
High Lambda Ref CO	100.0	99.9	100	27	98.9	18	46	0	11304	2057
Ref Lambda Ref CO	99.7	98.6	100	27	99.6	238	1102	0	2762	2059
Low Lambda Ref CO	97.1	83.1	100	26	98.4	2453	12802	0	563	2077
High Lambda Low CO	100.0	99.9	100	27	98.9	20	51	0	10737	2045
Ref Lambda Low CO	99.6	98.5	100	28	99.6	247	1148	0	2701	2047
Low Lambda Low CO	95.9	84.5	100	27	98.5	2325	12171	0	580	2067
High Lambda High H2	100.0	100.0	100	27	98.8	17	43	0	12426	2117
Ref Lambda High H2	99.7	99.0	100	28	99.6	239	1154	0	2892	2121
Low Lambda High H2	96.8	87.6	100	26	98.2	2649	14416	0	559	2140

Table A.20: Results from sensitivity analysis with lambda as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Lambda Ref H2	100.0	99.9	100	27	98.9	18	46	0	11304	2057
Ref Lambda Ref H2	99.7	98.6	100	27	99.6	238	1102	0	2762	2059
Low Lambda Ref H2	97.1	83.1	100	26	98.4	2453	12802	0	563	2077
High Lambda Low H2	100.0	99.8	100	23	99.0	19	50	0	9779	2062
Ref Lambda Low H2	99.7	95.8	100	24	99.6	256	1138	0	2479	2067
Low Lambda Low H2	97.3	58.5	100	23	98.6	2260	11177	0	567	2077
High Lambda High CH4	100.0	100.0	100	31	98.4	15	30	0	15943	1935
Ref Lambda High CH4	99.7	98.4	100	32	99.6	255	1185	0	2941	1932
Low Lambda High CH4	95.2	72.2	100	30	97.6	3808	19880	0	450	1956
High Lambda Ref CH4	100.0	99.9	100	27	98.9	18	46	0	11304	2057
Ref Lambda Ref CH4	99.7	98.6	100	27	99.6	238	1102	0	2762	2059
Low Lambda Ref CH4	97.1	83.1	100	26	98.4	2453	12802	0	563	2077
High Lambda Low CH4	100.0	99.9	100	14	99.2	26	85	0	7547	2441
Ref Lambda Low CH4	99.7	98.6	100	13	99.6	244	1139	0	2478	2453
Low Lambda Low CH4	98.3	90.1	100	13	99.0	1514	7813	0	757	2452
High Lambda High Flow	100.0	99.9	100	24	98.9	25	65	0	11279	2137
Ref Lambda High Flow	99.6	98.2	100	24	99.5	304	1393	0	2904	2146
Low Lambda High Flow	97.0	82.9	100	23	98.4	2526	13005	0	661	2155
High Lambda Ref Flow	100.0	99.9	100	27	98.9	18	46	0	11304	2057
Ref Lambda Ref Flow	99.7	98.6	100	27	99.6	238	1102	0	2762	2059
Low Lambda Ref Flow	97.1	83.1	100	26	98.4	2453	12802	0	563	2077

Table A.21: Results from sensitivity analysis with lambda as main parameter.

Test case	**Component conversion** [%]				**Dry outlet concentration** [%, ppm]					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Lambda Low Flow	100.0	100.0	100	31	98.9	12	30	0	11349	1944
Ref Lambda Low Flow	99.8	99.0	100	32	99.6	170	792	0	2631	1938
Low Lambda Low Flow	97.2	83.5	100	30	98.5	2370	12542	0	460	1968
High Lambda High Temp	100.0	99.9	100	41	98.9	13	41	0	11443	1663
Ref Lambda High Temp	99.7	98.7	100	42	99.6	229	979	0	2828	1637
Low Lambda High Temp	96.9	84.0	100	41	98.5	2603	12165	0	447	1644
High Lambda Ref Temp	100.0	99.9	100	27	98.9	18	46	0	11304	2057
Ref Lambda Ref Temp	99.7	98.6	100	27	99.6	238	1102	0	2762	2059
Low Lambda Ref Temp	97.1	83.1	100	26	98.4	2453	12802	0	563	2077
High Lambda Low Temp	99.9	99.9	100	15	98.9	42	75	0	11200	2374
Ref Lambda Low Temp	99.6	98.1	100	15	99.5	308	1462	0	2837	2402
Low Lambda Low Temp	96.8	82.4	100	14	98.3	2664	13362	1	790	2399

Table A.22: Results from sensitivity analysis with temperature as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Temp High CO2	99.6	98.2	100	34.3	99.6	219	907	0	2576	1819
Ref Temp High CO2	99.6	97.9	100	22.8	99.6	231	1040	0	2557	2138
Low Temp High CO2	99.5	97.2	100	12.9	99.6	299	1383	0	2658	2408
High Temp Ref CO2	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Temp Ref CO2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Low Temp Ref CO2	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
High Temp Low CO2	99.8	99.1	100	51.3	99.5	266	1216	0	3211	1444
Ref Temp Low CO2	99.8	99.0	100	32.4	99.5	267	1321	0	3075	2006
Low Temp Low CO2	99.8	98.7	100	17.4	99.5	342	1730	0	3123	2448
High Temp High CO	99.8	98.6	100	40.8	99.6	235	1003	0	2787	1668
Ref Temp High CO	99.8	98.5	100	26.5	99.6	245	1134	0	2726	2072
Low TempHigh CO	99.7	98.0	100	14.7	99.5	314	1490	0	2810	2403
High Temp Ref CO	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Temp Ref CO	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Low Temp Ref CO	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
High Temp Low CO	99.6	98.7	100	43.5	99.6	239	1022	0	2769	1605
Ref Temp Low CO	99.6	98.5	100	27.9	99.6	247	1148	0	2701	2047
Low Temp Low CO	99.4	98.1	100	15.4	99.5	320	1527	0	2778	2401
High Temp High H2	99.7	99.1	100	42.2	99.6	232	1032	0	2950	1697
Ref Temp High H2	99.7	99.0	100	27.7	99.6	239	1154	0	2892	2121
Low Temp High H2	99.6	98.7	100	15.5	99.5	309	1523	0	2972	2477

Table A.23: Results from sensitivity analysis with temperature as main parameter.

Test case	**Component conversion [%]**				**Dry outlet concentration [%, ppm]**					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Temp Ref H2	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Temp Ref H2	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Low Temp Ref H2	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
High Temp Low H2	99.7	96.3	100	38.1	99.6	244	993	0	2530	1676
Ref Temp Low H2	99.7	95.8	100	23.6	99.6	256	1138	0	2479	2067
Low Temp Low H2	99.6	94.4	100	12.9	99.6	330	1507	0	2579	2354
High Temp High CH4	99.7	98.5	100	51.8	99.6	252	1081	0	3097	1360
Ref Temp High CH4	99.7	98.4	100	31.5	99.6	255	1185	0	2941	1932
Low Temp High CH4	99.6	97.8	100	16.7	99.5	336	1594	0	2981	2349
High Temp Ref CH4	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Temp Ref CH4	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Low Temp Ref CH4	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
High Temp Low CH4	99.7	98.7	100	17.5	99.6	232	994	0	2418	2340
Ref Temp Low CH4	99.7	98.6	100	13.5	99.6	244	1139	0	2478	2453
Low Temp Low CH4	99.7	98.2	100	8.5	99.6	304	1458	0	2639	2591
High Temp High Flow	99.6	98.4	100	38.2	99.5	298	1262	0	2954	1748
Ref Temp High Flow	99.6	98.2	100	24.1	99.5	304	1393	0	2904	2146
Low Temp High Flow	99.5	97.6	100	13.2	99.5	396	1805	0	3016	2452
High Temp Ref Flow	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Temp Ref Flow	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Low Temp Ref Flow	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402

Table A.24: Results from sensitivity analysis with temperature as main parameter.

Test case	**Component conversion** [%]				**Dry outlet concentration** [%, ppm]					
	CO	H_2	CH_4	NO	CO_2	CO	H_2	CH_4	O_2	NO
High Temp Low Flow	99.8	99.1	100	47.4	99.6	159	682	0	2709	1490
Ref Temp Low Flow	99.8	99.0	100	31.6	99.6	170	792	0	2631	1938
Low Temp Low Flow	99.7	98.6	100	17.7	99.6	226	1106	0	2667	2328
High Temp High Lambda	100.0	99.9	100	40.8	98.9	13	41	0	11443	1663
Ref Temp High Lambda	100.0	99.9	100	26.8	98.9	18	46	0	11304	2057
Low Temp High Lambda	99.9	99.9	100	15.5	98.9	42	75	0	11200	2374
High Temp Ref Lambda	99.7	98.7	100	42.2	99.6	229	979	0	2828	1637
Ref Temp Ref Lambda	99.7	98.6	100	27.2	99.6	238	1102	0	2762	2059
Low Temp Ref Lambda	99.6	98.1	100	15.1	99.5	308	1462	0	2837	2402
High Temp Low Lambda	96.9	84.0	100	41.5	98.5	2603	12165	0	447	1644
Ref Temp Low Lambda	97.1	83.1	100	26.0	98.4	2453	12802	0	563	2077
Low Temp Low Lambda	96.8	82.4	100	14.4	98.3	2664	13362	1	790	2399

B

Concentration and flow calculations including Matlab code

This section includes the calculations used to determine the molar fractions and volumetric flows. Matlab has been used as the main calculation option and the code used is provided in the following subsections. This section also includes the calculations for Reynolds number mentioned in Section 5.4.

B.1 Main file

```
% Flue gas composition calculations with air staging

clear all; clc;
Ln_FR = 200;                  % [Ln/min] of C+H2 from FR
m_dot_H2O = 40*1000/60/60; % Fluidizing agent, FR 40 kg/h
lambda = 1.0;                 % Oxygen excess in POC
n_dot_CO_char = 0;            % Possibility to add CO to
% simulate char combustion in POC in mol/s,
% Assumed condition from balance is 0.0098 mol/s
%Returns composition of the wet fluegas
[nchem,Mchem,Ln_tot] = composition_mod(1,Ln_FR,m_dot_H2O);
% function for returning the governing flows
% in liter normal /min and g/sec
[n_dot_FR,n_dot_dry_FR,n_dot_O2,A] = ...
    flow_mod(nchem,Mchem,lambda,Ln_FR,m_dot_H2O,...
    Ln_tot,n_dot_CO_char);
%Displays values for oxidizer flow
disp('O2␣g/s␣Air␣g/s␣O2␣Ln/min␣Air␣Ln/min')
disp(A)
%Molar flow of each specie from FR before POC
molfloden=n_dot_FR.*nchem;

%%
% Flue gas composition calculations

% with plug flow, no staging
clear all; clc;
% Ln/min of C+H2 flow from FR
```

```
Ln_FR = 200;
% Fluidizing agent in FR 40 kg/h
m_dot_H2O = 40*1000/60/60;
% Oxygen excess in POC
lambda = 1.0;
% Possibility to add CO to simulate char combustion in POC
% in mol/s, Assumed condition from balance is 0.0098 mol/s
n_dot_CO_char = 0;
%Returns composition of the wet fluegas
[nchem,Mchem,Ln_tot] = composition_mod(1,Ln_FR,m_dot_H2O);

% function for returning the governing flows in liter
% normal /min and g/sec
% alternative function when plug flow is used
[n_dot_FR,n_dot_dry_FR,n_dot_O2,A,Ln_tot,nchemplug] = ...
    flow_plug(nchem,Mchem,lambda,...
    Ln_FR,m_dot_H2O,Ln_tot,n_dot_CO_char);
%Displays values for oxidizer flow
disp('O2␣g/s␣Air␣g/s␣O2␣Ln/min␣Air␣Ln/min')
disp(A)
%Molar flow of each specie from FR before POC
molfloden=n_dot_FR.*nchem;

%% Mixing calculations, Reynolds

rho_fluegas = 0.223; % kg/m3
rho_air = 0.233;     % kg/m3
% approximate [my] at 900deg C for air/water vapor [Pa*s]
my = 4.4E-5;
n = 2;                          % number of inlets
d_pipe = 0.13;                  % main pipe d [m]
d_air = 0.0125;                 % pipe d of air inlet(s)
                                % [m], 0.0125 = current
d_POC = 0.3;                    % POC diameter [m]
A_inlet = pi*(d_pipe/2)^2;      % Cross area of main pipe[m2]
A_airinlet = pi*(d_air/2)^2;    % Cross area of jet inlet[m2]
A_POC = pi*(d_POC/2)^2;         % Cross area of POC[m2]
T = 900;                        % Temperature [deg C]
% Velocitys @ T [m/s]
velocity_fluegas = sum(molfloden)*...
    8.314*(T+273.15)/1.013e5/A_inlet;
velocity_air = n_dot_O2/0.21*8.314*...
    (T+273.15)/1.013e5/A_airinlet/n;
velocity_O2 = n_dot_O2*8.314*(T+273.15)/...
    1.013e5/A_airinlet/n;
velocity_mixed = (sum(molfloden)+n_dot_O2/0.21)*8.314...
    *(T+273.15)/1.013e5/A_inlet;
velocity_POC =  (sum(molfloden)+n_dot_O2/0.21)*8.314...
    *(T+273.15)/1.013e5/A_POC;
```

```
% Reynolds numbers for different segments of the pipe
% Main pipe
Re_fluegas = rho_fluegas*velocity_fluegas*d_pipe/my;
% Air inlet
Re_air = rho_fluegas*velocity_air*d_air/my;
% Main pipe after mixing
Re_mix = rho_fluegas*velocity_mixed*d_pipe/my;
% POC
Re_POC = rho_fluegas*velocity_POC*d_POC/my;
```

B.2 Composition file

```
function [nchem,Mchem,Ln_tot] = composition_mod(n,Ln_FR,m_dot_H2O)
% Gives the chemical composition of the flue gas in a matrix nchem
MCO2 = 12.01+16*2;              %g/mol
MN2 = 14.01*2;                  %g/mol
MCO = 12.01+16;                 %g/mol
MH2 = 1.008*2;                  %g/mol
MCH4 = 12.01+1.008*4;           %g/mol
MH2O = 1.008*2+16;              %g/mol
MC2H4 = 12.01*2+1.008*4;        %g/mol
MNO2 = 14.01+16*2;              %g/mol
MNO = 14.01+16;                 %g/mol
MH2S = 1.008*2+32.07;           %g/mol
MHCN = 1.008+12.01+14.01;       %g/mol
MSO2 = 32.07+16*2;              %g/mol
MNH3 = 14.01+1.008*3;           %g/mol
%matrix with molarmass
Mchem = [MCO2;MN2;MCO;MH2;MCH4;MH2O;...
    MC2H4;MNO2;MNO;MH2S;MHCN;MSO2;MNH3];
%Dry molefraction (based on test data)
nCO2 = 0.60;                    %mole fraction
nN2 = 0.2481;                   %mole fraction
nCO = 0.06;                     %mole fraction
nH2 = 0.054;                    %mole fraction
nCH4 = 0.036;                   %mole fraction
nH2O = 0;                       %mole fraction
nC2H4 = 0.0;                    %mole fraction
nNO2 = 0.0;                     %mole fraction
nNO = 0.0005;                   %mole fraction
nH2S = 0.00026;                 %mole fraction
nHCN = 0.0001;                  %mole fraction
nSO2 = 0.00014;                 %mole fraction
nNH3 = 0.000250;                %mole fraction
% Flow of H2O from fluidizing Ln/min
Ln_H2O = m_dot_H2O/Mchem(6)*22.414*60;
% Flow from FR, wet. [Ln/min]
Ln_tot = Ln_FR+Ln_H2O;
%Wet molefraction (based on test data)
```

```
nCO2=nCO2*Ln_FR/Ln_tot;               % mole fraction
nN2=nN2*Ln_FR/Ln_tot;                 % mole fraction
nCO=nCO*Ln_FR/Ln_tot;                 % mole fraction
nH2=nH2*Ln_FR/Ln_tot;                 % mole fraction
nCH4=nCH4*Ln_FR/Ln_tot;               % mole fraction
nH2O=(nH2O*Ln_FR+Ln_H2O)/Ln_tot;      % mole fraction
nC2H4=nC2H4*Ln_FR/Ln_tot;             % mole fraction
nNO2=nNO2*Ln_FR/Ln_tot;               % mole fraction
nNO=nNO*Ln_FR/Ln_tot;                 % mole fraction
nH2S=nH2S*Ln_FR/Ln_tot;               % mole fraction
nHCN=nHCN*Ln_FR/Ln_tot;               % mole fraction
nSO2=nSO2*Ln_FR/Ln_tot;               % mole fraction
nNH3=nNH3*Ln_FR/Ln_tot;               % mole fraction
nchem = [nCO2;nN2;nCO;nH2;nCH4;nH2O;...
    nC2H4;nNO2;nNO;nH2S;nHCN;nSO2;nNH3];
normalize = 1/sum(nchem);    % Normalizing
nCO2=nCO2*normalize;         % normalized mole fraction
nN2=nN2*normalize;           % normalized mole fraction
nCO=nCO*normalize;           % normalized mole fraction
nH2=nH2*normalize;           % normalized mole fraction
nCH4=nCH4*normalize;         % normalized mole fraction
nH2O=nH2O*normalize;         % normalized mole fraction
nC2H4=nC2H4*normalize;       % normalized mole fraction
nNO2=nNO2*normalize;         % normalized mole fraction
nNO=nNO*normalize;           % normalized mole fraction
nH2S=nH2S*normalize;         % normalized mole fraction
nHCN=nHCN*normalize;         % normalized mole fraction
nSO2=nSO2*normalize;         % normalized mole fraction
nNH3=nNH3*normalize;         % normalized mole fraction
nchem = [nCO2;nN2;nCO;nH2;nCH4;nH2O;...
    nC2H4;nNO2;nNO;nH2S;nHCN;nSO2;nNH3];
end
```

B.3 Flow file with air staging

```
function [n_dot_FR,n_dot_dry_FR,n_dot_O2,A] = ...
    flow_mod( nchem,Mchem,lambda,Ln_FR,...
    m_dot_H2O,Ln_tot,n_dot_CO_char)
% Calculations of the flow in different
% parts of the reactor system and POC
% V/n = TR/P
% Liter normal per mole
Vn = 273.15*8.3144598/101325*1000;
% Flow of H2O from fluidizing
Ln_H2O = m_dot_H2O/Mchem(6)*Vn*60;
n_dot_FR = Ln_tot/Vn/60;                  % [mole/s]
n_dot_dry_FR = (Ln_FR)/Vn/60;             % [mole/s]
m_dot_FR = n_dot_FR*sum(nchem.*Mchem);   % [g/s]
% Stochiometric coefficients for combustion
```

```
Oxydemand = [0;0;0.5;0.5;2;0;3;0;0.5;3/2;9/4;0;7/4];
n_dot_O2 = (sum(nchem(1:13).*Oxydemand(1:13))*n_dot_FR...
    +n_dot_CO_char*0.5)*lambda; % Moles of O2 [mole/s]
MO2 = 16*2;                    % g/mol
m_dot_O2 = n_dot_O2*MO2;       % Mass flow of O2 [g/s]
n_dot_air = n_dot_O2/0.21;     % [mole/s] if air is used
m_dot_air = n_dot_air*0.79*Mchem(2)+m_dot_O2; % Air [g/s]
Ln_air = n_dot_air*60*Vn;      % Ln of Air
Ln_O2 = n_dot_O2*60*Vn;        % Ln of O2
Ln_POC_air = Ln_air+Ln_tot;    % Ln, POC after mixing (Air)
Ln_POC_O2 = Ln_O2+Ln_tot;      % Ln, POC after mixing (O2)
Ln_char = 273.15*8.3144598/101325*1000*n_dot_CO_char...
    *60;                       %Flow of char if it is used
A=[m_dot_O2,m_dot_air,Ln_O2,Ln_air]; % Matrix to view values
end
```

B.4 Flow file without air staging

```
function [n_dot_FR,n_dot_dry_FR,n_dot_O2,A,...
    Ln_tot,nchemplug] = flow_plug( nchem,Mchem,...
    lambda,Ln_FR,m_dot_H2O,Ln_tot,n_dot_CO_char)
% Calculations of the flow in different
% parts of the reactor system and POC
% V/n = TR/P
% Liter normal per mole
Vn = 273.15*8.3144598/101325*1000;
% Flow of H2O from fluidizing
Ln_H2O = m_dot_H2O/Mchem(6)*Vn*60;
n_dot_FR = Ln_tot/Vn/60;                  % [mole/s]
n_dot_dry_FR = (Ln_FR)/Vn/60;             % [mole/s]
m_dot_FR = n_dot_FR*sum(nchem.*Mchem);    % [g/s]
% Stochiometric coefficients for combustion
Oxydemand = [0;0;0.5;0.5;2;0;3;0;0.5;3/2;9/4;0;7/4];
n_dot_O2 = (sum(nchem(1:13).*Oxydemand(1:13))*n_dot_FR...
    +n_dot_CO_char*0.5)*lambda; % Moles of O2 [mole/s]
MO2 = 16*2;                     % g/mol
m_dot_O2 = n_dot_O2*MO2;        % Mass flow of O2 g/s
n_dot_air = n_dot_O2/0.21;      % [mole/s] if air is used
m_dot_air = n_dot_air*0.79*...
    Mchem(2)+m_dot_O2;     % Air [g/s]
Ln_air = n_dot_air*60*Vn;           % Ln of Air
Ln_O2 = n_dot_O2*60*Vn;             % Ln of O2
Ln_POC_air = Ln_air+Ln_tot;         % Ln, POC mixed (Air)
Ln_POC_O2 = Ln_O2+Ln_tot;           % Ln, POC mixed (O2)
A=[m_dot_O2,m_dot_air,Ln_O2,Ln_air]; % Disp-Value matrix
% Dry molefraction (based on test data)
% needs to be the same as in flow_mod
nCO2 = 0.60;             %mole fraction
nN2 = 0.2481;            %mole fraction
```

```
nCO = 0.06;             %mole fraction
nH2 = 0.054;            %mole fraction
nCH4 = 0.036;           %mole fraction
nH2O = 0;               %mole fraction
nC2H4 = 0.0;            %mole fraction
nNO2 = 0.0;             %mole fraction
nNO = 0.0005;           %mole fraction
nH2S = 0.00026;         %mole fraction
nHCN = 0.0001;          %mole fraction
nSO2 = 0.00014;         %mole fraction
nNH3 = 0.000250;        %mole fraction
% same as above but with H2O
nCO2=nCO2*Ln_FR/Ln_POC_air;
nN2=(nN2*Ln_FR+Ln_air*0.79)/Ln_POC_air;
nCO=nCO*Ln_FR/Ln_POC_air;
nH2=nH2*Ln_FR/Ln_POC_air;
nCH4=nCH4*Ln_FR/Ln_POC_air;
nH2O=(nH2O*Ln_FR+Ln_H2O)/Ln_POC_air;
nC2H4=nC2H4*Ln_FR/Ln_POC_air;
nNO2=nNO2*Ln_FR/Ln_POC_air;
nNO=nNO*Ln_FR/Ln_POC_air;
nH2S=nH2S*Ln_FR/Ln_POC_air;
nHCN=nHCN*Ln_FR/Ln_POC_air;
nSO2=nSO2*Ln_FR/Ln_POC_air;
nNH3=nNH3*Ln_FR/Ln_POC_air;
nO2=Ln_O2/Ln_POC_air;
nchem = [nCO2;nN2;nCO;nH2;nCH4;nH2O;...
    nC2H4;nNO2;nNO;nH2S;nHCN;nSO2;nNH3;nO2];
normalize = 1/sum(nchem);    % Normalizing
nCO2=nCO2*normalize;         % normalized mole fraction
nN2=nN2*normalize;           % normalized mole fraction
nCO=nCO*normalize;           % normalized mole fraction
nH2=nH2*normalize;           % normalized mole fraction
nCH4=nCH4*normalize;         % normalized mole fraction
nH2O=nH2O*normalize;         % normalized mole fraction
nC2H4=nC2H4*normalize;       % normalized mole fraction
nNO2=nNO2*normalize;         % normalized mole fraction
nNO=nNO*normalize;           % normalized mole fraction
nH2S=nH2S*normalize;         % normalized mole fraction
nHCN=nHCN*normalize;         % normalized mole fraction
nSO2=nSO2*normalize;         % normalized mole fraction
nNH3=nNH3*normalize;         % normalized mole fraction
nO2=nO2*normalize;           % normalized mole fraction
nchemplug = [nCO2;nN2;nCO;nH2;nCH4;nH2O;...
    nC2H4;nNO2;nNO;nH2S;nHCN;nSO2;nNH3;nO2];
end
```

C

Simulation information

This sections provides information about the choices made in Chemkin for the basic simulations and the sensitivity analysis. Remaining parts required for simulation setup to be complete include thermodynamic data for the species present and their reaction sets the latter which will be provided in the next section of this Appendix.

C.1 CHEMKIN input parameter

Choices made for the plug flow reactor:

Problem type: Fix gas temperature
Turn on momentum equation: Yes
Turn on residence time calculations: Yes
Starting axial position: 0.0 cm
Ending axial position: 170 cm
Diameter: Defined geometry from POC design
Internal surface area per unit length: Empty
External surface area per unit length: Empty
Temperature: Defined for each case
Pressure: 1 atm
Surface temperature same as gas temperature: Yes
Mixture viscosity at inlet: 0.0 g/cm-sec
Gas reaction rate multiplier: 1.0

Choices made for the primary inlet (flue gas):

Volumetric flow rate in SCCM: Varying dependent on simulation type, @ 273.15K
Species: Composition dependent on simulation case

Choices made for the secondary inlet (air):

Distance profile: Depending on simulation type, @ 273.15K
Species: N_2=0.79 and O_2=0.21

C.2 Sensitivity analysis

Distance profile: Linear staging from 1-85 cm inside POC, @ 273.15K
Remaining input parameters varied as explained in Section 3.5

D

Reaction sets

D.1 H_2 subset

$$\begin{gathered}
H + O_2 \rightleftharpoons O + OH \\
H + H + M \rightleftharpoons H_2 + M \\
H + H + N_2 \rightleftharpoons H_2 + N_2 \\
H + H + H_2 \rightleftharpoons H_2 + H_2 \\
H + H + H_2O \rightleftharpoons H_2 + H_2O \\
H + O + M \rightleftharpoons OH + M \\
H + O_2(+M) \rightleftharpoons HO_2(+M) \\
H + O_2(+AR) \rightleftharpoons HO_2(+AR) \\
H + O_2(+N_2) \rightleftharpoons HO_2(+N_2) \\
O + O + M \rightleftharpoons O_2 + M \\
O + H_2 \rightleftharpoons OH + H \\
OH + OH \rightleftharpoons O + H_2O \\
OH + H + M \rightleftharpoons H_2O + M \\
OH + H_2 \rightleftharpoons H + H_2O \\
H_2 + O_2 \rightleftharpoons HO_2 + H \\
HO_2 + H \rightleftharpoons OH + OH \\
HO_2 + H \rightleftharpoons H_2O + O \\
HO_2 + O \rightleftharpoons OH + O_2 \\
HO_2 + OH \rightleftharpoons H_2O + O_2 \\
HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2 \\
H_2O_2(+M) \rightleftharpoons OH + OH(+M) \\
H_2O_2 + H \rightleftharpoons H_2O + OH \\
H_2O_2 + H \rightleftharpoons HO_2 + H_2 \\
H_2O_2 + O \rightleftharpoons HO_2 + OH \\
H_2O_2 + OH \rightleftharpoons H_2O + HO_2
\end{gathered}$$

D.2 CO subset

$$\begin{gathered}
CO + O(+M) \rightleftharpoons CO_2(+M) \\
CO + O_2 \rightleftharpoons CO_2 + O \\
CO + HO_2 \rightleftharpoons CO_2 + OH \\
CO + OH \rightleftharpoons CO_2 + H \\
CO + OH \rightleftharpoons HOCO \\
HOCO \rightleftharpoons CO_2 + H
\end{gathered}$$

$$HOCO + OH \leftrightharpoons CO_2 + H_2O$$
$$HOCO + OH \leftrightharpoons CO + H_2O_2$$
$$HOCO + O_2 \leftrightharpoons CO_2 + HO_2$$

D.3 $\mathbf{CH_2O}$ subset

$$CH_2O(+M) \leftrightharpoons HCO + H(+M)$$
$$CH_2O(+M) \leftrightharpoons CO + H_2(+M)$$
$$CH_2O + H \leftrightharpoons HCO + H_2$$
$$CH_2O + O \leftrightharpoons HCO + OH$$
$$CH_2O + O_2 \leftrightharpoons HCO + HO_2$$
$$CH_2O + OH \leftrightharpoons HCO + H_2O$$
$$CH_2O + HO_2 \leftrightharpoons HCO + H_2O_2$$
$$CH_2O + CH_3 \leftrightharpoons HCO + CH_4$$
$$HCO \leftrightharpoons H + CO$$
$$HCO + H \leftrightharpoons CO + H_2$$
$$HCO + O \leftrightharpoons CO + OH$$
$$HCO + O \leftrightharpoons CO_2 + H$$
$$HCO + OH \leftrightharpoons CO + H_2O$$
$$HCO + O_2 \leftrightharpoons CO + HO_2$$
$$HCO + HO_2 \leftrightharpoons CO_2 + OH + H$$
$$HCO + HCO \leftrightharpoons CO + CH_2O$$

D.4 $\mathbf{CH_4}$ subset

$$CH_3 + H(+M) \leftrightharpoons CH_4(+M)$$
$$CH_4 + H \leftrightharpoons CH_3 + H_2$$
$$CH_4 + O \leftrightharpoons CH_3 + OH$$
$$CH_4 + OH \leftrightharpoons CH_3 + H_2O$$
$$CH_4 + HO_2 \leftrightharpoons CH_3 + H_2O_2$$
$$CH_4 + O_2 \leftrightharpoons CH_3 + HO_2$$
$$CH_4 + CH_2 \leftrightharpoons CH_3 + CH_3$$
$$CH_4 + CH_2(S) \leftrightharpoons CH_3 + CH_3$$
$$CH_2 + H(+M) \leftrightharpoons CH_3(+M)$$
$$CH_3 + H \leftrightharpoons CH_2 + H_2$$
$$CH_2(S) + H_2 \leftrightharpoons CH_3 + H$$
$$CH_3 + O \leftrightharpoons CH_2O + H$$
$$CH_3 + O \leftrightharpoons H_2 + CO + H$$
$$CH_3 + OH \leftrightharpoons CH_2 + H_2O$$
$$CH_3 + OH \leftrightharpoons CH_2(S) + H_2O$$
$$CH_2(S) + H_2O \leftrightharpoons CH_3 + OH$$
$$CH_3 + HO_2 \leftrightharpoons CH_4 + O_2$$
$$CH_3 + HO_2 \leftrightharpoons CH_3O + OH$$
$$CH_3 + O_2 \leftrightharpoons CH_3O + O$$
$$CH_3 + O_2 \leftrightharpoons CH_2O + OH$$

$$CH_3 + O_2 + M \leftrightharpoons CH_3OO + M$$
$$CH_3 + O_2 \leftrightharpoons CH_3OO$$
$$CH_3 + HCO \leftrightharpoons CH_4 + CO$$
$$CH_3 + CH_3 \leftrightharpoons C_2H_5 + H$$
$$CH_3 + CH_3(+M) \leftrightharpoons C_2H_6(+M)$$
$$CH_2 + M \leftrightharpoons CH + H + M$$
$$CH_2 + M \leftrightharpoons C + H_2 + M$$
$$CH_2 + H \leftrightharpoons CH + H_2$$
$$CH_2 + O \leftrightharpoons CO + H + H$$
$$CH_2 + O \leftrightharpoons CO + H_2$$
$$CH_2 + OH \leftrightharpoons CH_2O + H$$
$$CH_2 + OH \leftrightharpoons CH + H_2O$$
$$CH_2 + O_2 \leftrightharpoons CO + H_2O$$
$$CH_2 + O_2 \leftrightharpoons CO_2 + H + H$$
$$CH_2 + O_2 \leftrightharpoons CH_2O + O$$
$$CH_2 + O_2 \leftrightharpoons CO_2 + H_2$$
$$CH_2 + O_2 \leftrightharpoons CO + OH + H$$
$$CH_2 + CO_2 \leftrightharpoons CO + CH_2O$$
$$CH_2(S) + M \leftrightharpoons CH_2 + M$$
$$CH_2(S) + N_2 \leftrightharpoons CH_2 + N_2$$
$$CH_2(S) + AR \leftrightharpoons CH_2 + AR$$
$$CH_2(S) + H \leftrightharpoons CH_2 + H$$
$$CH_2(S) + H \leftrightharpoons CH + H_2$$
$$CH_2(S) + O \leftrightharpoons CO +_2 H$$
$$CH_2(S) + OH \leftrightharpoons CH_2O + H$$
$$CH_2(S) + O_2 \leftrightharpoons CH_2 + O_2$$
$$CH_2(S) + H_2O \leftrightharpoons CH_2 + H_2O$$
$$CH_2(S) + CO_2 \leftrightharpoons CH_2O + CO$$
$$CH + H \leftrightharpoons C + H_2$$
$$CH + O \leftrightharpoons CO + H$$
$$CH + OH \leftrightharpoons HCO + H$$
$$CH + OH \leftrightharpoons C + H_2O$$
$$CH + O_2 \leftrightharpoons HCO + O$$
$$CH + H_2O \leftrightharpoons CH_2O + H$$
$$CH + CO_2 \leftrightharpoons HCO + CO$$
$$C + OH \leftrightharpoons CO + H$$
$$C + O_2 \leftrightharpoons CO + O$$
$$CH_3OH(+M) \leftrightharpoons CH_3 + OH(+M)$$
$$CH_3OH(+M) \leftrightharpoons CH_2(S) + H_2O(+M)$$
$$CH_3OH + H \leftrightharpoons CH_2OH + H_2$$
$$CH_3OH + H \leftrightharpoons CH_3O + H_2$$
$$CH_3OH + O \leftrightharpoons CH_2OH + OH$$
$$CH_3OH + O \leftrightharpoons CH_3O + OH$$
$$CH_3OH + OH \leftrightharpoons CH_2OH + H_2O$$
$$CH_3OH + OH \leftrightharpoons CH_3O + H_2O$$
$$CH_3OH + HO_2 \leftrightharpoons CH_2OH + H_2O_2$$

$$CH_3OH + O_2 \rightleftharpoons CH_2OH + HO_2$$
$$CH_3OH + O_2 \rightleftharpoons CH_3O + HO_2$$
$$CH_2OH(+M) \rightleftharpoons CH_2O + H(+M)$$
$$CH_2OH + H \rightleftharpoons CH_2O + H_2$$
$$CH_2OH + H \rightleftharpoons CH_3 + OH$$
$$CH_2OH + H(+M) \rightleftharpoons CH_3OH(+M)$$
$$CH_2OH + O \rightleftharpoons CH_2O + OH$$
$$CH_2OH + OH \rightleftharpoons CH_2O + H_2O$$
$$CH_2OH + HO_2 \rightleftharpoons CH_2O + H_2O_2$$
$$CH_2OH + O_2 \rightleftharpoons CH_2O + HO_2$$
$$CH_2OH + HCO \rightleftharpoons CH_3OH + CO$$
$$CH_2OH + HCO \rightleftharpoons CH_2O + CH_2O$$
$$CH_2OH + CH_2O \rightleftharpoons CH_3OH + HCO$$
$$CH_2OH + CH_2OH \rightleftharpoons CH_3OH + CH_2O$$
$$CH_2OH + CH_3O \rightleftharpoons CH_3OH + CH_2O$$
$$CH_2OH + CH_4 \rightleftharpoons CH_3OH + CH_3$$
$$CH_3O(+M) \rightleftharpoons CH_2O + H(+M)$$
$$CH_3O + H \rightleftharpoons CH_2O + H_2$$
$$CH_3O + H \rightleftharpoons CH_3 + OH$$
$$CH_3O + H(+M) \rightleftharpoons CH_3OH(+M)$$
$$CH_3O + O \rightleftharpoons CH_2O + OH$$
$$CH_3O + OH \rightleftharpoons CH_2O + H_2O$$
$$CH_3O + HO_2 \rightleftharpoons CH_2O + H_2O_2$$
$$CH_3O + O_2 \rightleftharpoons CH_2O + HO_2$$
$$CH_3O + CO \rightleftharpoons CH_3 + CO_2$$
$$CH_3O + CH_3 \rightleftharpoons CH_2O + CH_4$$
$$CH_3O + CH_4 \rightleftharpoons CH_3OH + CH_3$$
$$CH_3O + CH_2O \rightleftharpoons CH_3OH + HCO$$
$$CH_3O + CH_3O \rightleftharpoons CH_3OH + CH_2O$$
$$CH_3OOH \rightleftharpoons CH_3O + OH$$
$$CH_3OOH + H \rightleftharpoons CH_2OOH + H_2$$
$$CH_3OOH + H \rightleftharpoons CH_3OO + H_2$$
$$CH_3OOH + H \rightleftharpoons CH_3O + H_2O$$
$$CH_3OOH + O \rightleftharpoons CH_2OOH + OH$$
$$CH_3OOH + O \rightleftharpoons CH_3OO + OH$$
$$CH_3OOH + OH \rightleftharpoons CH_3OO + H_2O$$
$$CH_3OOH + OH \rightleftharpoons CH_2OOH + H_2O$$
$$CH_3OOH + HO_2 \rightleftharpoons CH_3OO + H_2O_2$$
$$CH_3OO + H \rightleftharpoons CH_3O + OH$$
$$CH_3OO + O \rightleftharpoons CH_3O + O_2$$
$$CH_3OO + OH \rightleftharpoons CH_3OH + O_2$$
$$CH_3OO + OH \rightleftharpoons CH_3O + HO_2$$
$$CH_3OO + HO_2 \rightleftharpoons CH_3OOH + O_2$$
$$CH_3OO + CH_3 \rightleftharpoons CH_3O + CH_3O$$
$$CH_3OO + CH_4 \rightleftharpoons CH_3OOH + CH_3$$
$$CH_3OO + HCO \rightleftharpoons CH_3O + H + CO_2$$

$$CH_3OO + CO \rightleftharpoons CH_3O + CO_2$$
$$CH_3OO + CH_2O \rightleftharpoons CH_3OOH + HCO$$
$$CH_3OO + CH_3O \rightleftharpoons CH_2O + CH_3OOH$$
$$CH_3OO + CH_3OH \rightleftharpoons CH_3OOH + CH_2OH$$
$$CH_3OO + CH_3OO \rightleftharpoons CH_3O + CH_3O + O_2$$
$$CH_3OO + CH_3OO \rightleftharpoons CH_3OH + CH_2O + O_2$$
$$CH_3OO + C_2H_5 \rightleftharpoons CH_3O + CH_3CH_2O$$
$$CH_3OO + C_2H_6 \rightleftharpoons CH_3OOH + C_2H_5$$
$$CH_2OOH \rightleftharpoons CH_2O + OH$$

D.5 C_2 subset

$$C_2H_6 + H \rightleftharpoons C_2H_5 + H_2$$
$$C_2H_6 + O \rightleftharpoons C_2H_5 + OH$$
$$C_2H_6 + OH \rightleftharpoons C_2H_5 + H_2O$$
$$C_2H_6 + HO_2 \rightleftharpoons C_2H_5 + H_2O_2$$
$$C_2H_6 + O_2 \rightleftharpoons C_2H_5 + HO_2$$
$$C_2H_6 + CH_3 \rightleftharpoons C_2H_5 + CH_4$$
$$C_2H_6 + CH_2(S) \rightleftharpoons C_2H_5 + CH_3$$
$$C_2H_4 + H(+M) \rightleftharpoons C_2H_5(+M)$$
$$C_2H_5 + H(+M) \rightleftharpoons C_2H_6(+M)$$
$$C_2H_5 + O \rightleftharpoons CH_3 + CH_2O$$
$$C_2H_5 + O \rightleftharpoons CH_3CHO + H$$
$$C_2H_5 + O \rightleftharpoons C_2H_4 + OH$$
$$C_2H_5 + OH \rightleftharpoons C_2H_4 + H_2O$$
$$C_2H_5 + HO_2 \rightleftharpoons CH_3CH_2O + OH$$
$$C_2H_5 + O_2 \rightleftharpoons C_2H_4 + HO_2$$
$$C_2H_5 + O_2(+M) \rightleftharpoons C_2H_4 + HO_2(+M)$$
$$C_2H_5 + CH_2O \rightleftharpoons C_2H_6 + HCO$$
$$C_2H_5 + HCO \rightleftharpoons C_2H_6 + CO$$
$$C_2H_5 + CH_3 \rightleftharpoons C_2H_4 + CH_4$$
$$C_2H_5 + C_2H_5 \rightleftharpoons C_2H_6 + C_2H_4$$
$$C_2H_3 + H(+M) \rightleftharpoons C_2H_4(+M)$$
$$C_2H_4(+M) \rightleftharpoons H_2CC + H_2(+M)$$
$$C_2H_4 + H \rightleftharpoons C_2H_3 + H_2$$
$$CH_4 + CH \rightleftharpoons C_2H_4 + H$$
$$CH_3 + CH_2 \rightleftharpoons C_2H_4 + H$$
$$CH_3 + CH_2(S) \rightleftharpoons C_2H_4 + H$$
$$C_2H_4 + O \rightleftharpoons CH_3 + HCO$$
$$C_2H_4 + O \rightleftharpoons CH_2CHO + H$$
$$C_2H_4 + OH \rightleftharpoons C_2H_3 + H_2O$$
$$C_2H_4 + OH \rightleftharpoons CH_3 + CH_2O$$
$$C_2H_4 + OH \rightleftharpoons CH_3CHO + H$$
$$C_2H_4 + OH \rightleftharpoons CH_2CHOH + H$$
$$C_2H_4 + OH \rightleftharpoons CH_2CH_2OH$$
$$C_2H_4 + HO_2 \rightleftharpoons cC_2H_4O + OH$$

$$C_2H_4 + O_2 \leftrightharpoons C_2H_3 + HO_2$$
$$C_2H_4 + CH_3 \leftrightharpoons C_2H_3 + CH_4$$
$$C_2H_2 + H(+M) \leftrightharpoons C_2H_3(+M)$$
$$C_2H_3 + H \leftrightharpoons C_2H_2 + H_2$$
$$CH_3 + CH \leftrightharpoons C_2H_3 + H$$
$$C_2H_3 + O \leftrightharpoons CH_2CO + H$$
$$C_2H_3 + OH \leftrightharpoons C_2H_2 + H_2O$$
$$C_2H_3 + HO_2 \leftrightharpoons CH_2CHO + OH$$
$$C_2H_3 + O_2 \leftrightharpoons CH_2CHOO$$
$$C_2H_3 + O_2 \leftrightharpoons CH_2O + HCO$$
$$C_2H_3 + O_2 \leftrightharpoons CH_2CHO + O$$
$$C_2H_3 + O_2 \leftrightharpoons C_2H_2 + HO_2$$
$$C_2H_3 + O_2 \leftrightharpoons CH_3O + CO$$
$$C_2H_3 + O_2 \leftrightharpoons CH_3 + CO_2$$
$$C_2H_3 + CH_2O \leftrightharpoons C_2H_4 + HCO$$
$$C_2H_3 + HCO \leftrightharpoons C_2H_4 + CO$$
$$C_2H_3 + CH_3 \leftrightharpoons C_2H_2 + CH_4$$
$$C_2H_3 + CH \leftrightharpoons CH_2 + C_2H_2$$
$$C_2H_3 + C_2H_3 \leftrightharpoons C_2H_4 + C_2H_2$$
$$C_2H_3 + C_2H \leftrightharpoons C_2H_2 + C_2H_2$$
$$C_2H_2 + M \leftrightharpoons C_2H + H + M$$
$$CH_3 + C \leftrightharpoons C_2H_2 + H$$
$$CH_2 + CH \leftrightharpoons C_2H_2 + H$$
$$CH_2 + CH_2 \leftrightharpoons C_2H_2 + H + H$$
$$CH_2 + CH_2 \leftrightharpoons C_2H_2 + H_2$$
$$C_2H_2 + O \leftrightharpoons HCCO + H$$
$$C_2H_2 + O \leftrightharpoons CH_2 + CO$$
$$C_2H_2 + O \leftrightharpoons C_2H + OH$$
$$C_2H_2 + OH \leftrightharpoons CH_3 + CO$$
$$C_2H_2 + OH \leftrightharpoons HCCOH + H$$
$$C_2H_2 + OH \leftrightharpoons CHCHOH$$
$$C_2H_2 + OH \leftrightharpoons CH_2CO + H$$
$$C_2H_2 + HO_2 \leftrightharpoons CH_2O + HCO$$
$$C_2H_2 + HO_2 \leftrightharpoons CH_2CHO + O$$
$$C_2H_2 + O_2 \leftrightharpoons HCO + HCO$$
$$C_2H_2 + CH_2(S) \leftrightharpoons C_2H_2 + CH_2$$
$$H_2CC \leftrightharpoons C_2H_2$$
$$H_2CC + H \leftrightharpoons C_2H_2 + H$$
$$H_2CC + OH \leftrightharpoons CH_2CO + H$$
$$H_2CC + O_2 \leftrightharpoons CH_2 + CO_2$$
$$C_2 + H_2 \leftrightharpoons C_2H + H$$
$$CH_2 + C \leftrightharpoons C_2H + H$$
$$C_2H + O \leftrightharpoons CH + CO$$
$$C_2H + OH \leftrightharpoons HCCO + H$$
$$C_2H + OH \leftrightharpoons C_2 + H_2O$$
$$C_2H + H_2 \leftrightharpoons C_2H_2 + H$$

$$C_2H + O_2 \rightleftharpoons CO + CO + H$$
$$C_2H + CH_4 \rightleftharpoons CH_3 + C_2H_2$$
$$C_2 + M \rightleftharpoons C + C + M$$
$$C_2 + O \rightleftharpoons C + CO$$
$$C_2 + OH \rightleftharpoons C_2O + H$$
$$C_2 + O_2 \rightleftharpoons CO + CO$$
$$CH_3CHO(+M) \rightleftharpoons CH_3 + HCO(+M)$$
$$CH_3CHO + H \rightleftharpoons CH_3CO + H_2$$
$$CH_3CHO + H \rightleftharpoons CH_2CHO + H_2$$
$$CH_3CHO + O \rightleftharpoons CH_3CO + OH$$
$$CH_3CHO + O \rightleftharpoons CH_2CHO + OH$$
$$CH_3CHO + OH \rightleftharpoons CH_3CO + H_2O$$
$$CH_3CHO + OH \rightleftharpoons CH_2CHO + H_2O$$
$$CH_3CHO + HO_2 \rightleftharpoons CH_3CO + H_2O_2$$
$$CH_3CHO + HO_2 \rightleftharpoons CH_2CHO + H_2O_2$$
$$CH_3CHO + O_2 \rightleftharpoons CH_3CO + HO_2$$
$$CH_3CHO + CH_3 \rightleftharpoons CH_3CO + CH_4$$
$$CH_3CHO + CH_3 \rightleftharpoons CH_2CHO + CH_4$$
$$CH_2CHOH + H \rightleftharpoons CHCHOH + H_2$$
$$CH_2CHOH + H \rightleftharpoons CH_2CHO + H_2$$
$$CH_2CHOH + O \rightleftharpoons CH_2OH + HCO$$
$$CH_2CHOH + O \rightleftharpoons CH_2CHO + OH$$
$$CH_2CHOH + OH \rightleftharpoons CHCHOH + H_2O$$
$$CH_2CHOH + OH \rightleftharpoons CH_2CHO + H_2O$$
$$CH_2CHOH + O_2 \rightleftharpoons CH_2O + HCO + OH$$
$$CHCHOH \rightleftharpoons HCCOH + H$$
$$CHCHOH + H \rightleftharpoons CH_2CHO + H$$
$$CHCHOH + O \rightleftharpoons OCHCHO + H$$
$$CHCHOH + O_2 \rightleftharpoons HCCOH + HO_2$$
$$CHCHOH + O_2 \rightleftharpoons OCHCHO + OH$$
$$cC_2H_3O \rightleftharpoons CH_2CHO$$
$$cC_2H_3O \rightleftharpoons CH_2CO + H$$
$$cC_2H_3O \rightleftharpoons CH_3 + CO$$
$$CH_2CHO \rightleftharpoons CH_2CO + H$$
$$CH_2CHO \rightleftharpoons CH_3 + CO$$
$$CH_2CHO + H \rightleftharpoons CH_3 + HCO$$
$$CH_2CHO + H \rightleftharpoons CH_3CO + H$$
$$CH_2CHO + H \rightleftharpoons CH_2CO + H_2$$
$$CH_2CHO + O \rightleftharpoons CH_2CO + OH$$
$$CH_2CHO + OH \rightleftharpoons CH_2CO + H_2O$$
$$CH_2CHO + OH \rightleftharpoons CH_2OH + HCO$$
$$CH_2CHO + O_2 \rightleftharpoons CH_2O + CO + OH$$
$$CH_2CHO + CH_3 \rightleftharpoons C_2H_5 + CO + H$$
$$CH_2CHO + HO_2 \rightleftharpoons CH_2O + HCO + OH$$
$$CH_2CHO + HO_2 \rightleftharpoons CH_3CHO + O_2$$
$$CH_2CHO + CH_2 \rightleftharpoons C_2H_4 + HCO$$

$$CH_2CHO + CH \rightleftharpoons C_2H_3 + HCO$$
$$CH_3CO \rightleftharpoons CH_3 + CO$$
$$CH_2CO + H \rightleftharpoons CH_3CO$$
$$CH_3CO + H \rightleftharpoons CH_3 + HCO$$
$$CH_3CO + H \rightleftharpoons CH_2CO + H_2$$
$$CH_3CO + O \rightleftharpoons CH_3 + CO_2$$
$$CH_3CO + O \rightleftharpoons CH_2CO + OH$$
$$CH_3CO + OH \rightleftharpoons CH_2CO + H_2O$$
$$CH_3CO + CH_3OO \rightleftharpoons CH_3 + CO_2 + CH_3O$$
$$CH_3CO + CH_3 \rightleftharpoons C_2H_6 + CO$$
$$CH_3CO + CH_3 \rightleftharpoons CH_2CO + CH_4$$
$$CH_3CO + O_2 \rightleftharpoons CH_2O + CO + OH$$
$$CH_2 + CO(+M) \rightleftharpoons CH_2CO(+M)$$
$$CH_2CO + H \rightleftharpoons CH_3 + CO$$
$$CH_2CO + H \rightleftharpoons HCCO + H_2$$
$$CH + CH_2O \rightleftharpoons CH_2CO + H$$
$$CH_2CO + O \rightleftharpoons CO_2 + CH_2$$
$$CH_2CO + O \rightleftharpoons HCCO + OH$$
$$CH_2CO + OH \rightleftharpoons CH_2OH + CO$$
$$CH_2CO + OH \rightleftharpoons CH_3 + CO_2$$
$$CH_2CO + OH \rightleftharpoons HCCO + H_2O$$
$$CH_2CO + CH_2(S) \rightleftharpoons C_2H_4 + CO$$
$$HCCOH + H \rightleftharpoons HCCO + H_2$$
$$HCCOH + O \rightleftharpoons HCCO + OH$$
$$HCCOH + OH \rightleftharpoons HCCO + H_2O$$
$$CH + CO(+M) \rightleftharpoons HCCO(+M)$$
$$HCCO + H \rightleftharpoons CH_2(S) + CO$$
$$HCCO + O \rightleftharpoons CO + CO + H$$
$$HCCO + OH \rightleftharpoons HCO + HCO$$
$$HCCO + OH \rightleftharpoons C_2O + H_2O$$
$$HCCO + O_2 \rightleftharpoons CO_2 + CO + H$$
$$HCCO + O_2 \rightleftharpoons CO + CO + OH$$
$$HCCO + O_2 \rightleftharpoons HCO + CO + O$$
$$HCCO + CH_2 \rightleftharpoons C_2H_3 + CO$$
$$HCCO + CH \rightleftharpoons C_2H_2 + CO$$
$$HCCO + HCCO \rightleftharpoons C_2H_2 + CO + CO$$
$$C_2O + M \rightleftharpoons C + CO + M$$
$$C_2O + H \rightleftharpoons CH + CO$$
$$C_2O + O \rightleftharpoons CO + CO$$
$$C_2O + OH \rightleftharpoons CO + CO + H$$
$$C_2O + O_2 \rightleftharpoons CO + CO + O$$
$$C_2O + O_2 \rightleftharpoons CO + CO_2$$
$$C_2O + C \rightleftharpoons CO + C_2$$
$$OCHCHO(+M) \rightleftharpoons CO + CO + H_2(+M)$$
$$OCHCHO + H \rightleftharpoons CH_2O + HCO$$
$$OCHCHO + OH \rightleftharpoons HCO + CO + H_2O$$

D.6 Nitrogen subset

$$HNO + H \leftrightharpoons NO + H_2$$
$$HNO + O \leftrightharpoons NO + OH$$
$$HNO + OH \leftrightharpoons NO + H_2O$$
$$HNO + O_2 \leftrightharpoons HO_2 + NO$$
$$HNO + HNO \leftrightharpoons N_2O + H_2O$$
$$HNO + NO_2 \leftrightharpoons HONO + NO$$
$$NO + H(+M) \leftrightharpoons HNO(+M)$$
$$NO + O(+M) \leftrightharpoons NO_2(+M)$$
$$NO + O(+AR) \leftrightharpoons NO_2(+AR)$$
$$NO + OH(+M) \leftrightharpoons HONO(+M)$$
$$NO + HO_2 \leftrightharpoons NO_2 + OH$$
$$NO_2 + H \leftrightharpoons NO + OH$$
$$NO_2 + O \leftrightharpoons NO + O_2$$
$$NO_2 + O(+M) \leftrightharpoons NO_3(+M)$$
$$NO_2 + OH(+M) \leftrightharpoons HONO_2(+M)$$
$$NO_2 + HO_2 \leftrightharpoons HONO + O_2$$
$$NO_2 + HO_2 \leftrightharpoons HNO_2 + O_2$$
$$NO_2 + H_2 \leftrightharpoons HONO + H$$
$$NO_2 + H_2 \leftrightharpoons HNO_2 + H$$
$$NO_2 + NO_2 \leftrightharpoons NO + NO + O_2$$
$$NO_2 + NO_2 \leftrightharpoons NO_3 + NO$$
$$HONO + H \leftrightharpoons HNO + OH$$
$$HONO + H \leftrightharpoons NO + H_2O$$
$$HONO + O \leftrightharpoons NO_2 + OH$$
$$HONO + OH \leftrightharpoons NO_2 + H_2O$$
$$HONO + NO_2 \leftrightharpoons HONO_2 + NO$$
$$HONO + HONO \leftrightharpoons NO + NO_2 + H_2O$$
$$HNO_2(+M) \leftrightharpoons HONO(+M)$$
$$HNO_2 + O \leftrightharpoons NO_2 + OH$$
$$HNO_2 + OH \leftrightharpoons NO_2 + H_2O$$
$$NO_3 + H \leftrightharpoons NO_2 + OH$$
$$NO_3 + O \leftrightharpoons NO_2 + O_2$$
$$NO_3 + OH \leftrightharpoons NO_2 + HO_2$$
$$NO_3 + HO_2 \leftrightharpoons NO_2 + O_2 + OH$$
$$NO_3 + NO_2 \leftrightharpoons NO + NO_2 + O_2$$
$$HONO_2 + H \leftrightharpoons H_2 + NO_3$$
$$HONO_2 + H \leftrightharpoons H_2O + NO_2$$
$$HONO_2 + H \leftrightharpoons OH + HONO$$
$$HONO_2 + OH \leftrightharpoons H_2O + NO_3$$
$$N_2O(+M) \leftrightharpoons N_2 + O(+M)$$
$$N_2O + H \leftrightharpoons N_2 + OH$$
$$N_2O + O \leftrightharpoons NO + NO$$
$$N_2O + O \leftrightharpoons N_2 + O_2$$
$$N_2O + OH \leftrightharpoons N_2 + HO_2$$

$$N_2O + OH \leftrightharpoons HNO + NO$$
$$N_2O + NO \leftrightharpoons NO_2 + N_2$$
$$NH_3 + M \leftrightharpoons NH_2 + H + M$$
$$NH_3 + H \leftrightharpoons NH_2 + H_2$$
$$NH_3 + O \leftrightharpoons NH_2 + OH$$
$$NH_3 + OH \leftrightharpoons NH_2 + H_2O$$
$$NH_3 + HO_2 \leftrightharpoons NH_2 + H_2O_2$$
$$NH_2 + H \leftrightharpoons NH + H_2$$
$$NH_2 + O \leftrightharpoons HNO + H$$
$$NH_2 + O \leftrightharpoons NH + OH$$
$$NH_2 + OH \leftrightharpoons NH + H_2O$$
$$NH_2 + HO_2 \leftrightharpoons H_2NO + OH$$
$$NH_2 + HO_2 \leftrightharpoons NH_3 + O_2$$
$$NH_2 + O_2 \leftrightharpoons H_2NO + O$$
$$NH_2 + O_2 \leftrightharpoons HNO + OH$$
$$NH_2 + NH_2 \leftrightharpoons NH_3 + NH$$
$$NH_2 + NH \leftrightharpoons N_2H_2 + H$$
$$NH_2 + NH \leftrightharpoons NH_3 + N$$
$$NH_2 + HNO \leftrightharpoons NH_3 + NO$$
$$NH_2 + NO \leftrightharpoons N_2 + H_2O$$
$$NH_2 + NO \leftrightharpoons NNH + OH$$
$$NH_2 + HONO \leftrightharpoons NH_3 + NO_2$$
$$NH_2 + NO_2 \leftrightharpoons N_2O + H_2O$$
$$NH_2 + NO_2 \leftrightharpoons H_2NO + NO$$
$$NH + H \leftrightharpoons N + H_2$$
$$NH + O \leftrightharpoons NO + H$$
$$NH + OH \leftrightharpoons HNO + H$$
$$NH + OH \leftrightharpoons N + H_2O$$
$$NH + O_2 \leftrightharpoons HNO + O$$
$$NH + O_2 \leftrightharpoons NO + OH$$
$$NH + NH \leftrightharpoons N_2 + H + H$$
$$NH + N \leftrightharpoons N_2 + H$$
$$NH + NO \leftrightharpoons N_2O + H$$
$$NH + NO \leftrightharpoons N_2 + OH$$
$$NH + HONO \leftrightharpoons NH_2 + NO_2$$
$$NH + NO_2 \leftrightharpoons N_2O + OH$$
$$N + OH \leftrightharpoons NO + H$$
$$N + O_2 \leftrightharpoons NO + O$$
$$N + NO \leftrightharpoons N_2 + O$$
$$NNH \leftrightharpoons N_2 + H$$
$$NNH + H \leftrightharpoons N_2 + H_2$$
$$NNH + O \leftrightharpoons N_2O + H$$
$$NNH + O \leftrightharpoons N_2 + OH$$
$$NNH + O \leftrightharpoons NH + NO$$
$$NNH + OH \leftrightharpoons N_2 + H_2O$$
$$NNH + O_2 \leftrightharpoons N_2 + HO_2$$

$$NNH + O_2 \leftrightharpoons N_2 + H + O_2$$
$$NNH + NH_2 \leftrightharpoons N_2 + NH_3$$
$$NNH + NO \leftrightharpoons N_2 + HNO$$
$$NH_2 + NH_2 \leftrightharpoons N_2H_4$$
$$N_2H_4 + H \leftrightharpoons N_2H_3 + H_2$$
$$N_2H_4 + O \leftrightharpoons NH_2OH + NH$$
$$N_2H_4 + O \leftrightharpoons N_2H_3 + OH$$
$$N_2H_4 + OH \leftrightharpoons N_2H_3 + H_2O$$
$$N_2H_4 + NH_2 \leftrightharpoons N_2H_3 + NH_3$$
$$N_2H_3 \leftrightharpoons N_2H_2 + H$$
$$NH_2 + NH_2 \leftrightharpoons N_2H_3 + H$$
$$N_2H_3 + H \leftrightharpoons N_2H_2 + H_2$$
$$N_2H_3 + O \leftrightharpoons N_2H_2 + OH$$
$$N_2H_3 + O \leftrightharpoons NH_2 + HNO$$
$$N_2H_3 + O \leftrightharpoons NH_2 + NO + H$$
$$N_2H_3 + OH \leftrightharpoons N_2H_2 + H_2O$$
$$N_2H_3 + OH \leftrightharpoons H_2NN + H_2O$$
$$N_2H_3 + OH \leftrightharpoons NH_3 + HNO$$
$$N_2H_3 + HO_2 \leftrightharpoons N_2H_2 + H_2O_2$$
$$N_2H_3 + HO_2 \leftrightharpoons N_2H_4 + O_2$$
$$N_2H_3 + NH_2 \leftrightharpoons N_2H_2 + NH_3$$
$$N_2H_3 + NH_2 \leftrightharpoons H_2NN + NH_3$$
$$N_2H_3 + NH \leftrightharpoons N_2H_2 + NH_2$$
$$N_2H_2 + M \leftrightharpoons NNH + H + M$$
$$N_2H_2 + H \leftrightharpoons NNH + H_2$$
$$N_2H_2 + O \leftrightharpoons NNH + OH$$
$$N_2H_2 + O \leftrightharpoons NH_2 + NO$$
$$N_2H_2 + OH \leftrightharpoons NNH + H_2O$$
$$N_2H_2 + NH_2 \leftrightharpoons NNH + NH_3$$
$$N_2H_2 + NH \leftrightharpoons NNH + NH_2$$
$$N_2H_2 + NO \leftrightharpoons N_2O + NH_2$$
$$NH_2 + NH_2 \leftrightharpoons H_2NN + H_2$$
$$H_2NN \leftrightharpoons NNH + H$$
$$H_2NN + H \leftrightharpoons NNH + H_2$$
$$H_2NN + H \leftrightharpoons N_2H_2 + H$$
$$H_2NN + O \leftrightharpoons NNH + OH$$
$$H_2NN + O \leftrightharpoons NH_2 + NO$$
$$H_2NN + OH \leftrightharpoons NNH + H_2O$$
$$H_2NN + OH \leftrightharpoons NH_2 + NO + H$$
$$H_2NN + HO_2 \leftrightharpoons NH_2 + NO + OH$$
$$H_2NN + HO_2 \leftrightharpoons NNH + H_2O_2$$
$$H_2NN + O_2 \leftrightharpoons NH_2 + NO_2$$
$$H_2NN + NH_2 \leftrightharpoons NNH + NH_3$$
$$H_2NO + M \leftrightharpoons HNO + H + M$$
$$H_2NO + M \leftrightharpoons HNOH + M$$
$$H_2NO + H \leftrightharpoons HNO + H_2$$

$$
\begin{gathered}
H_2NO + H \leftrightharpoons NH_2 + OH \\
H_2NO + O \leftrightharpoons HNO + OH \\
H_2NO + OH \leftrightharpoons HNO + H_2O \\
H_2NO + HO_2 \leftrightharpoons HNO + H_2O_2 \\
H_2NO + O_2 \leftrightharpoons HNO + HO_2 \\
H_2NO + NH_2 \leftrightharpoons HNO + NH_3 \\
H_2NO + NO \leftrightharpoons HNO + HNO \\
H_2NO + NO_2 \leftrightharpoons HONO + HNO \\
HNOH + M \leftrightharpoons HNO + H + M \\
HNOH + H \leftrightharpoons NH_2 + OH \\
HNOH + H \leftrightharpoons HNO + H_2 \\
HNOH + O \leftrightharpoons HNO + OH \\
HNOH + OH \leftrightharpoons HNO + H_2O \\
HNOH + HO_2 \leftrightharpoons HNO + H_2O_2 \\
HNOH + HO_2 \leftrightharpoons NH_2OH + O_2 \\
HNOH + O_2 \leftrightharpoons HNO + HO_2 \\
HNOH + NH_2 \leftrightharpoons N_2H_3 + OH \\
HNOH + NH_2 \leftrightharpoons H_2NN + H_2O \\
HNOH + NH_2 \leftrightharpoons NH_3 + HNO \\
HNOH + NO_2 \leftrightharpoons HONO + HNO \\
HCN + M \leftrightharpoons H + CN + M \\
HCN + N_2 \leftrightharpoons H + CN + N_2 \\
HCN + M \leftrightharpoons HNC + M \\
CN + H_2 \leftrightharpoons HCN + H \\
HCN + O \leftrightharpoons NCO + H \\
HCN + O \leftrightharpoons CN + OH \\
HCN + O \leftrightharpoons NH + CO \\
HCN + OH \leftrightharpoons CN + H_2O \\
HCN + OH \leftrightharpoons HOCN + H \\
HCN + OH \leftrightharpoons HNCO + H \\
HCN + OH \leftrightharpoons NH_2 + CO \\
HCN + O_2 \leftrightharpoons CN + HO_2 \\
HCN + CN \leftrightharpoons NCCN + H \\
HNC + H \leftrightharpoons HCN + H \\
HNC + O \leftrightharpoons NH + CO \\
HNC + OH \leftrightharpoons HNCO + H \\
HNC + CN \leftrightharpoons NCCN + H \\
CN + O \leftrightharpoons CO + N \\
CN + OH \leftrightharpoons NCO + H \\
CN + O_2 \leftrightharpoons NCO + O \\
CN + O_2 \leftrightharpoons NO + CO \\
CN + NO \leftrightharpoons NCO + N \\
CN + NO_2 \leftrightharpoons NCO + NO \\
CN + NO_2 \leftrightharpoons CO + N_2O \\
CN + NO_2 \leftrightharpoons N_2 + CO_2 \\
CN + HNO \leftrightharpoons HCN + NO
\end{gathered}
$$

$$CN + HONO \leftrightharpoons HCN + NO_2$$
$$CN + N_2O \leftrightharpoons NCN + NO$$
$$CN + HNCO \leftrightharpoons HCN + NCO$$
$$CN + NCO \leftrightharpoons NCN + CO$$
$$HNCO + M \leftrightharpoons CO + NH + M$$
$$HNCO + H \leftrightharpoons NH_2 + CO$$
$$HNCO + H \leftrightharpoons NCO + H_2$$
$$HNCO + O \leftrightharpoons NCO + OH$$
$$HNCO + O \leftrightharpoons NH + CO_2$$
$$HNCO + O \leftrightharpoons HNO + CO$$
$$HNCO + OH \leftrightharpoons NCO + H_2O$$
$$HNCO + HO_2 \leftrightharpoons NCO + H_2O_2$$
$$HNCO + O_2 \leftrightharpoons HNO + CO_2$$
$$HNCO + NH \leftrightharpoons NH_2 + NCO$$
$$HOCN + H \leftrightharpoons HNCO + H$$
$$HOCN + H \leftrightharpoons NH_2 + CO$$
$$HOCN + H \leftrightharpoons H_2 + NCO$$
$$HOCN + O \leftrightharpoons OH + NCO$$
$$HOCN + OH \leftrightharpoons H_2O + NCO$$
$$HOCN + NH_2 \leftrightharpoons NCO + NH_3$$
$$HCNO \leftrightharpoons HCN + O$$
$$HCNO + H \leftrightharpoons HCN + OH$$
$$HCNO + O \leftrightharpoons HCO + NO$$
$$HCNO + OH \leftrightharpoons CH_2O + NO$$
$$HCNO + O \leftrightharpoons NCO + OH$$
$$HCNO + OH \leftrightharpoons NO + CO + H_2$$
$$HCNO + OH \leftrightharpoons NCO + H + OH$$
$$HCNO + OH \leftrightharpoons NCO + H_2O$$
$$HCNO + OH \leftrightharpoons HCO + HNO$$
$$HCNO + CN \leftrightharpoons HCN + NCO$$
$$NCO + M \leftrightharpoons N + CO + M$$
$$NCO + H \leftrightharpoons CO + NH$$
$$NCO + O \leftrightharpoons NO + CO$$
$$NCO + OH \leftrightharpoons HON + CO$$
$$NCO + OH \leftrightharpoons H + CO + NO$$
$$NCO + HO_2 \leftrightharpoons HNCO + O_2$$
$$NCO + O_2 \leftrightharpoons NO + CO_2$$
$$NCO + NO \leftrightharpoons N_2O + CO$$
$$NCO + NO \leftrightharpoons N_2 + CO_2$$
$$NCO + NO_2 \leftrightharpoons CO + NO + NO$$
$$NCO + NO_2 \leftrightharpoons CO_2 + N_2O$$
$$NCO + HNO \leftrightharpoons HNCO + NO$$
$$NCO + HONO \leftrightharpoons HNCO + NO_2$$
$$NCO + NH_3 \leftrightharpoons HNCO + NH_2$$
$$NCO + N \leftrightharpoons N_2 + CO$$
$$NCO + NCO \leftrightharpoons CO + CO + N_2$$

D.7 C_xH_y interactions with Nitrogen

$$CO + NO_2 \leftrightharpoons NO + CO_2$$
$$CO + N_2O \leftrightharpoons N_2 + CO_2$$
$$HOCO + NO \leftrightharpoons CO + HONO$$
$$CH_2O + NO_2 \leftrightharpoons HONO + HCO$$
$$CH_2O + NO_2 \leftrightharpoons HNO_2 + HCO$$
$$HCO + NO \leftrightharpoons HNO + CO$$
$$HCO + NO_2 \leftrightharpoons NO + CO_2 + H$$
$$HCO + NO_2 \leftrightharpoons HONO + CO$$
$$HCO + NO_2 \leftrightharpoons NO + CO + OH$$
$$HCO + HNO \leftrightharpoons NO + CH_2O$$
$$CH_4 + NO_2 \leftrightharpoons HONO + CH_3$$
$$CH_4 + NO_2 \leftrightharpoons HNO_2 + CH_3$$
$$CH_3 + NO(+M) \leftrightharpoons CH_3NO(+M)$$
$$CH_3 + NO_2 \leftrightharpoons CH_3O + NO$$
$$CH_3 + HNO \leftrightharpoons NO + CH_4$$
$$CH_3OH + NO_2 \leftrightharpoons HONO + CH_2OH$$
$$CH_3OH + NO_2 \leftrightharpoons HNO_2 + CH_2OH$$
$$CH_3O + NO \leftrightharpoons HNO + CH_2O$$
$$CH_3O + NO(+M) \leftrightharpoons CH_3ONO(+M)$$
$$CH_3O + NO_2 \leftrightharpoons HONO + CH_2O$$
$$CH_3O + NO_2(+M) \leftrightharpoons CH_3ONO_2(+M)$$
$$CH_3O + HNO \leftrightharpoons NO + CH_3OH$$
$$CH_2OH + NO \leftrightharpoons CH_2O + HNO$$
$$CH_2OH + NO_2 \leftrightharpoons HONO + CH_2O$$
$$CH_2OH + HNO \leftrightharpoons NO + CH_3OH$$
$$CH_3OO + NO \leftrightharpoons NO_2 + CH_3O$$
$$C_2H_6 + NO_2 \leftrightharpoons HONO + C_2H_5$$
$$C_2H_6 + NO_2 \leftrightharpoons HNO_2 + C_2H_5$$
$$C_2H_5 + NO_2 \leftrightharpoons CH_3CH_2O + NO$$
$$C_2H_4 + NO_2 \leftrightharpoons C_2H_3 + HONO$$
$$C_2H_4 + NO_2 \leftrightharpoons C_2H_3 + HNO_2$$
$$C_2H_3 + NO \leftrightharpoons C_2H_2 + HNO$$
$$C_2H_3 + NO_2 \leftrightharpoons CH_2CHO + NO$$
$$CH_3CH_2O + NO \leftrightharpoons CH_3CHO + HNO$$
$$CH_3CH_2O + NO(+M) \leftrightharpoons CH_3CH_2ONO(+M)$$
$$CH_3CH_2O + NO_2 \leftrightharpoons CH_3CHO + HONO$$
$$CH_3CH_2O + NO_2(+M) \leftrightharpoons CH_3CH_2ONO_2(+M)$$
$$CH_2CHO + NO_2 \leftrightharpoons CH_2CO + HONO$$
$$CH_2CHO + NO_2 \leftrightharpoons CHOCH_2O + NO$$
$$CH_2CHO + NO_2 \leftrightharpoons CHOCH_2NO_2$$
$$CH_3CO + NO_2 \leftrightharpoons CH_3 + CO_2 + NO$$
$$CH_2CH_2OH + NO_2 \leftrightharpoons CH_2O + CH_2OH + NO$$
$$CH_3NO_2(+M) \leftrightharpoons CH_3 + NO_2(+M)$$
$$CH_3NO_2 + H \leftrightharpoons CH_3 + HONO$$

$$CH_3NO_2 + H \rightleftharpoons CH_3NO + OH$$
$$CH_3NO_2 + H \rightleftharpoons CH_2NO_2 + H_2$$
$$CH_3NO_2 + O \rightleftharpoons CH_2NO_2 + OH$$
$$CH_3NO_2 + O_2 \rightleftharpoons CH_2NO_2 + HO_2$$
$$CH_3NO_2 + OH \rightleftharpoons CH_3OH + NO_2$$
$$CH_3NO_2 + OH \rightleftharpoons CH_2NO_2 + H_2O$$
$$CH_3NO_2 + HO_2 \rightleftharpoons CH_2NO_2 + H_2O_2$$
$$CH_3NO_2 + CH_3 \rightleftharpoons CH_2NO_2 + CH_4$$
$$CH_3NO_2 + CH_3O \rightleftharpoons CH_2NO_2 + CH_3OH$$
$$CH_3NO_2 + NO_2 \rightleftharpoons CH_2NO_2 + HONO$$
$$CH_2NO_2 \rightleftharpoons CH_2O + NO$$
$$CH_2NO_2 + H \rightleftharpoons CH_3 + NO_2$$
$$CH_2NO_2 + O \rightleftharpoons CH_2O + NO_2$$
$$CH_2NO_2 + OH \rightleftharpoons CH_2OH + NO_2$$
$$CH_2NO_2 + OH \rightleftharpoons CH_2O + HONO$$
$$CH_3ONO + H \rightleftharpoons CH_3OH + NO$$
$$CH_3ONO + H \rightleftharpoons CH_2O + H_2 + NO$$
$$CH_3ONO + O \rightleftharpoons CH_3O + NO_2$$
$$CH_3ONO + OH \rightleftharpoons CH_3OH + NO_2$$
$$CH_3ONO_2 + H \rightleftharpoons CH_3O + HONO$$
$$CH_3ONO_2 + O \rightleftharpoons CH_3O + NO_3$$
$$CH_3ONO_2 + OH \rightleftharpoons CH_3O + HONO_2$$
$$CO_2 + N \rightleftharpoons NO + CO$$
$$CO_2 + CN \rightleftharpoons NCO + CO$$
$$CH_2O + CN \rightleftharpoons HCO + HCN$$
$$CH_2O + NCO \rightleftharpoons HNCO + HCO$$
$$HCO + NCO \rightleftharpoons HNCO + CO$$
$$CH_4 + NH_2 \rightleftharpoons CH_3 + NH_3$$
$$CH_4 + CN \rightleftharpoons CH_3 + HCN$$
$$CH_4 + NCO \rightleftharpoons CH_3 + HNCO$$
$$CH_3 + NH_2 \rightleftharpoons CH_3NH_2$$
$$CH_3 + NH_2 \rightleftharpoons CH_2NH_2 + H$$
$$CH_3 + NH_2 \rightleftharpoons CH_3NH + H$$
$$CH_3 + NH_2 \rightleftharpoons CH_2NH + H_2$$
$$CH_3 + NH_2 \rightleftharpoons CH_4 + NH$$
$$CH_4 + NH \rightleftharpoons CH_3 + NH_2$$
$$CH_3 + NH_2 \rightleftharpoons CH_2 + NH_3$$
$$CH_3 + NH \rightleftharpoons CH_2NH + H$$
$$CH_3 + NH \rightleftharpoons N + CH_4$$
$$CH_3 + N \rightleftharpoons H_2CN + H$$
$$CH_3 + N_2H_2 \rightleftharpoons NNH + CH_4$$
$$CH_3 + H_2NN \rightleftharpoons CH_4 + NNH$$
$$CH_3 + N_2H_4 \rightleftharpoons N_2H_3 + CH_4$$
$$CH_3 + N_2H_3 \rightleftharpoons N_2H_2 + CH_4$$
$$CH_3 + N_2H_3 \rightleftharpoons H_2NN + CH_4$$
$$CH_3 + NO \rightleftharpoons HCN + H_2O$$

$$CH_3 + NO \leftrightharpoons H_2CN + OH$$
$$CH_3 + H_2NO \leftrightharpoons CH_3O + NH_2$$
$$CH_3 + H_2NO \leftrightharpoons CH_4 + HNO$$
$$CH_3 + CN \leftrightharpoons CH_2CN + H$$
$$CH_3 + HOCN \leftrightharpoons CH_3CN + OH$$
$$CH_2 + N \leftrightharpoons HCN + H$$
$$CH_2 + NO \leftrightharpoons HCNO + H$$
$$CH_2 + NO \leftrightharpoons HCN + OH$$
$$CH_2 + NO_2 \leftrightharpoons CH_2O + NO$$
$$CH_2 + N_2 \leftrightharpoons HCN + NH$$
$$CH_2(S) + NO \leftrightharpoons HCN + OH$$
$$CH_2(S) + NO \leftrightharpoons CH_2 + NO$$
$$CH_2(S) + N_2O \leftrightharpoons CH_2O + N_2$$
$$CH_2(S) + NH_3 \leftrightharpoons CH_2NH_2 + H$$
$$CH_2(S) + HCN \leftrightharpoons CH_2CN + H$$
$$CH + NH_3 \leftrightharpoons H_2CN + H + H$$
$$CH + N \leftrightharpoons CN + H$$
$$CH + NO \leftrightharpoons CO + NH$$
$$CH + NO \leftrightharpoons NCO + H$$
$$CH + NO \leftrightharpoons HCN + O$$
$$CH + NO \leftrightharpoons CN + OH$$
$$CH + NO \leftrightharpoons HCO + N$$
$$CH + NO_2 \leftrightharpoons HCO + NO$$
$$CH + N_2O \leftrightharpoons HCN + NO$$
$$CH + N_2 \leftrightharpoons NCN + H$$
$$C + NO \leftrightharpoons CN + O$$
$$C + NO \leftrightharpoons CO + N$$
$$C + N_2O \leftrightharpoons CN + NO$$
$$C + N_2 \leftrightharpoons CN + N$$
$$CN + N \leftrightharpoons C + N_2$$
$$C_2H_6 + NH_2 \leftrightharpoons C_2H_5 + NH_3$$
$$C_2H_6 + CN \leftrightharpoons C_2H_5 + HCN$$
$$C_2H_6 + NCO \leftrightharpoons C_2H_5 + HNCO$$
$$C_2H_5 + N \leftrightharpoons C_2H_4 + NH$$
$$C_2H_5 + N \leftrightharpoons CH_3 + H_2CN$$
$$C_2H_4 + NH_2 \leftrightharpoons C_2H_3 + NH_3$$
$$C_2H_4 + CN \leftrightharpoons CH_2CHCN + H$$
$$C_2H_3 + NO \leftrightharpoons HCN + CH_2O$$
$$C_2H_2 + NH_2 \leftrightharpoons NH_2C_2H_2$$
$$C_2H_2 + NCO \leftrightharpoons HCCO + HCN$$
$$C_2H_2 + CN \leftrightharpoons C_2HCN + H$$
$$C_2H + NH_3 \leftrightharpoons C_2H_2 + NH_2$$
$$C_2H + NO \leftrightharpoons HCN + CO$$
$$C_2 + NO \leftrightharpoons C_2O + N$$
$$C_2 + NO \leftrightharpoons CCN + O$$
$$C_2 + N_2 \leftrightharpoons CN + CN$$

$$
\begin{gathered}
HCCO + N \leftrightharpoons HCN + CO \\
HCCO + NO \leftrightharpoons HCNO + CO \\
HCCO + NO \leftrightharpoons HCN + CO_2 \\
HCCO + NO_2 \leftrightharpoons HCNO + CO_2 \\
C_2O + NO \leftrightharpoons CO + NCO \\
C_2O + NO_2 \leftrightharpoons CO_2 + NCO \\
H_2CCCH + N \leftrightharpoons HCN + C_2H_2 \\
NCN + H \leftrightharpoons HCN + N \\
NCN + O \leftrightharpoons CN + NO \\
NCN + OH \leftrightharpoons HCN + NO \\
NCN + O_2 \leftrightharpoons NO + NCO \\
CH_3NH_2 + M \leftrightharpoons CHNH_2 + H_2 + M \\
CH_3NH_2 + M \leftrightharpoons CH_2NH + H_2 + M \\
CH_3NH_2 + M \leftrightharpoons CH_3N + H_2 + M \\
CH_3NH_2 + H \leftrightharpoons CH_2NH_2 + H_2 \\
CH_3NH_2 + H \leftrightharpoons CH_3NH + H_2 \\
CH_3NH_2 + O \leftrightharpoons CH_2NH_2 + OH \\
CH_3NH_2 + O \leftrightharpoons CH_3NH + OH \\
CH_3NH_2 + OH \leftrightharpoons CH_2NH_2 + H_2O \\
CH_3NH_2 + OH \leftrightharpoons CH_3NH + H_2O \\
CH_3NH_2 + CH_3 \leftrightharpoons CH_2NH_2 + CH_4 \\
CH_3NH_2 + CH_3 \leftrightharpoons CH_3NH + CH_4 \\
CH_3NH_2 + NH_2 \leftrightharpoons CH_2NH_2 + NH_3 \\
CH_3NH_2 + NH_2 \leftrightharpoons CH_3NH + NH_3 \\
CH_2NH_2 \leftrightharpoons CH_2NH + H \\
CH_2NH_2 + H \leftrightharpoons CH_2NH + H_2 \\
CH_2NH_2 + O \leftrightharpoons CH_2O + NH_2 \\
CH_2NH_2 + O \leftrightharpoons CH_2NH + OH \\
CH_2NH_2 + OH \leftrightharpoons CH_2OH + NH_2 \\
CH_2NH_2 + OH \leftrightharpoons CH_2NH + H_2O \\
CH_2NH_2 + O_2 \leftrightharpoons NH_2CH_2O + O \\
CH_2NH_2 + O_2 \leftrightharpoons CH_2NH + HO_2 \\
CH_2NH_2 + CH_3 \leftrightharpoons C_2H_5 + NH_2 \\
CH_2NH_2 + CH_3 \leftrightharpoons CH_2NH + CH_4 \\
CH_3NH \leftrightharpoons CH_2NH + H \\
CH_3NH + H \leftrightharpoons CH_2NH + H_2 \\
CH_3NH + O \leftrightharpoons CH_2NH + OH \\
CH_3NH + OH \leftrightharpoons CH_2NH + H_2O \\
CH_3NH + CH_3 \leftrightharpoons CH_2NH + CH_4 \\
CH_2NH + H \leftrightharpoons H_2CN + H_2 \\
CH_2NH + H \leftrightharpoons HCNH + H_2 \\
CH_2NH + O \leftrightharpoons H_2CN + OH \\
CH_2NH + O \leftrightharpoons HCNH + OH \\
CH_2NH + O \leftrightharpoons CH_2O + NH \\
CH_2NH + OH \leftrightharpoons H_2CN + H_2O \\
CH_2NH + OH \leftrightharpoons HCNH + H_2O
\end{gathered}
$$

$$
\begin{gathered}
CH_2NH + CH_3 \leftrightharpoons H_2CN + CH_4 \\
CH_2NH + CH_3 \leftrightharpoons HCNH + CH_4 \\
CH_2NH + NH_2 \leftrightharpoons H_2CN + NH_3 \\
CH_2NH + NH_2 \leftrightharpoons HCNH + NH_3 \\
H_2CN \leftrightharpoons HCN + H \\
H_2CN + H \leftrightharpoons HCN + H_2 \\
H_2CN + O \leftrightharpoons HCN + OH \\
H_2CN + OH \leftrightharpoons HCN + H_2O \\
H_2CN + O_2 \leftrightharpoons CH_2O + NO \\
H_2CN + NH_2 \leftrightharpoons HCN + NH_3 \\
H_2CN + N \leftrightharpoons CH_2 + N_2 \\
HCNH \leftrightharpoons HCN + H \\
HCNH + H \leftrightharpoons H_2CN + H \\
HCNH + H \leftrightharpoons HCN + H_2 \\
HCNH + O \leftrightharpoons HNCO + H \\
HCNH + O \leftrightharpoons HCN + OH \\
HCNH + OH \leftrightharpoons HCN + H_2O \\
HCNH + CH_3 \leftrightharpoons HCN + CH_4 \\
CH_3CN + H \leftrightharpoons HCN + CH_3 \\
CH_3CN + H \leftrightharpoons CH_2CN + H_2 \\
CH_3CN + O \leftrightharpoons NCO + CH_3 \\
CH_3CN + OH \leftrightharpoons CH_2CN + H_2O \\
CH_2CN + O \leftrightharpoons CH_2O + CN \\
CH_2OH + CN \leftrightharpoons CH_2CN + OH
\end{gathered}
$$

D.8 Sulfur subset

$$
\begin{gathered}
H_2S + M \leftrightharpoons S + H_2 + M \\
H_2S + H \leftrightharpoons SH + H_2 \\
H_2S + O \leftrightharpoons SH + OH \\
H_2S + OH \leftrightharpoons SH + H_2O \\
H_2S + S \leftrightharpoons SH + SH \\
H_2S + S \leftrightharpoons HS_2 + H \\
S + H_2 \leftrightharpoons SH + H \\
SH + O \leftrightharpoons H + SO \\
SH + OH \leftrightharpoons S + H_2O \\
SH + HO_2 \leftrightharpoons HSO + OH \\
SH + O_2 \leftrightharpoons HSO + O \\
S + OH \leftrightharpoons H + SO \\
S + O_2 \leftrightharpoons SO + O \\
SH + SH \leftrightharpoons S_2 + H_2 \\
SH + S \leftrightharpoons S_2 + H \\
S_2 + M \leftrightharpoons S + S + M \\
S_2 + H + M \leftrightharpoons HS_2 + M \\
S_2 + O \leftrightharpoons SO + S \\
HS_2 + H \leftrightharpoons S_2 + H_2
\end{gathered}
$$

$$
\begin{gathered}
HS_2 + O \leftrightharpoons S_2 + OH \\
HS_2 + OH \leftrightharpoons S_2 + H_2O \\
HS_2 + S \leftrightharpoons S_2 + SH \\
HS_2 + H + M \leftrightharpoons H_2S_2 + M \\
H_2S_2 + H \leftrightharpoons HS_2 + H_2 \\
H_2S_2 + O \leftrightharpoons HS_2 + OH \\
H_2S_2 + OH \leftrightharpoons HS_2 + H_2O \\
H_2S_2 + S \leftrightharpoons HS_2 + SH \\
SO_3 + H \leftrightharpoons HOSO + O \\
SO + O(+M) \leftrightharpoons SO_2(+M) \\
SO_2 + OH \leftrightharpoons HOSO + O \\
SO_2 * + M \leftrightharpoons SO_2 + M \\
SO_2 * + SO_2 \leftrightharpoons SO_3 + SO \\
SO + M \leftrightharpoons S + O + M \\
SO + OH(+M) \leftrightharpoons HOSO(+M) \\
SO + O_2 \leftrightharpoons SO_2 + O \\
HSO + H \leftrightharpoons HSOH \\
HSO + H \leftrightharpoons SH + OH \\
HSO + H \leftrightharpoons S + H_2O \\
HSO + H \leftrightharpoons H_2SO \\
HSO + H \leftrightharpoons H_2S + O \\
HSO + H \leftrightharpoons SO + H_2 \\
HSO + O + M \leftrightharpoons HSO_2 + M \\
HSO + O \leftrightharpoons SO_2 + H \\
HSO + O + M \leftrightharpoons HOSO + M \\
HSO + O \leftrightharpoons O + HOS \\
HSO + O \leftrightharpoons OH + SO \\
HSO + OH \leftrightharpoons HOSHO \\
HSO + OH \leftrightharpoons HOSO + H \\
HSO + OH \leftrightharpoons SO + H_2O \\
HSO + O_2 \leftrightharpoons SO_2 + OH \\
HSOH \leftrightharpoons SH + OH \\
HSOH \leftrightharpoons S + H_2O \\
HSOH \leftrightharpoons H_2S + O \\
H_2SO \leftrightharpoons H_2S + O \\
HOSO(+M) \leftrightharpoons HSO_2(+M) \\
HOSO + M \leftrightharpoons O + HOS + M \\
HOSO + OH \leftrightharpoons SO_2 + H_2O \\
HSO_2 + OH \leftrightharpoons SO_2 + H_2O \\
HOSO_2 \leftrightharpoons HOSO + O \\
HOSO_2 \leftrightharpoons SO_3 + H \\
HOSO_2 + H \leftrightharpoons SO_2 + H_2O \\
HOSO_2 + O \leftrightharpoons SO_3 + OH \\
HOSO_2 + OH \leftrightharpoons SO_3 + H_2O \\
HOSO_2 + O_2 \leftrightharpoons HO_2 + SO_3 \\
HOSHO \leftrightharpoons HOSO + H
\end{gathered}
$$

$$
\begin{gathered}
HOSHO \leftrightharpoons SO + H_2O \\
HOSHO + H \leftrightharpoons HOSO + H_2 \\
HOSHO + O \leftrightharpoons HOSO + OH \\
HOSHO + OH \leftrightharpoons HOSO + H_2O \\
H + SO_2(+M) \leftrightharpoons HSO_2(+M) \\
H + SO_2(+M) \leftrightharpoons HOSO(+M) \\
H + SO_2(+M) \leftrightharpoons OH + SO(+M) \\
HOSO + O_2 \leftrightharpoons SO_2 + HO_2 \\
HOSO + H \leftrightharpoons SO(S) + H_2O \\
HOSO + H \leftrightharpoons SO_2 + H_2 \\
SO_2 + O(+M) \leftrightharpoons SO_3(+M) \\
SO_2 + O(+N_2) \leftrightharpoons SO_3(+N_2) \\
SO_3 + H \leftrightharpoons SO_2 + OH \\
SO_3 + O \leftrightharpoons SO_2 + O_2 \\
SO_3 + OH \leftrightharpoons SO_2 + HO_2 \\
SO_2 + OH(+M) \leftrightharpoons HOSO_2(+M) \\
HSO + M \leftrightharpoons SO + H + M \\
SO_2 + S \leftrightharpoons SO + SO \\
SO_3 + SO \leftrightharpoons SO_2 + SO_2 \\
HSO_2 + H \leftrightharpoons SO_2 + H_2 \\
HSO_2 + O_2 \leftrightharpoons HO_2 + SO_2 \\
SO + HO_2 \leftrightharpoons SO_2 + OH \\
SO(S) + M \leftrightharpoons SO + M \\
SO(S) + O_2 \leftrightharpoons SO_2 + O \\
SO_2 + CO \leftrightharpoons SO + CO_2 \\
CO + SO \leftrightharpoons CO_2 + S
\end{gathered}
$$