Deliverable report

D2.2 – Generation of experimental data for (micro)kinetic modelling

WP2 – Optimization of the reaction of conversion of CO_2 into COS

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Name	Organisation	Role	Action	Date
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Gleb VERYASOV	TotalEnergies OneTech Belgium	Technical Coordinator	Review & approval	27/06/2024
Joris THYBAUT	Universiteit Gent	Project coordinator	Review & approval	30/06/2024

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To request a change to this document, contact the Document Author.

CONFIGURATION MANAGEMENT

Nature of Deliverable		
R	Document, report (excluding the periodic and final reports)	X
DEC	Websites, patents filing, press & media actions, videos, etc.	
DEM	Demonstrator, pilot, prototype, plan designs	
OTHER	Software, technical diagram, algorithms, models, etc.	
ETHICS	Deliverables related to ethics issues.	
DATA	Data sets, microdata, etc.	
DMP	DATA MANAGEMENT PLAN	

Dissemination level		
PU	Public, fully open, e.g., web (Deliverables flagged as public will be automatically published in CORDIS projects.)	X
SEN	Sensitive, limited under the conditions of the Grant Agreement	

ACRONYM/ABBREVIATIONS	
CA	Consortium Agreement (contractual document between members of the consortium)
DoA	Description of Action (technical annex to the Grant Agreement)
EC	European Commission
EU	European Union
FTP	Funding and Tenders Portal: https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/home
GA	Grant Agreement (contractual document between EC and beneficiaries)
IPR	Intellectual Property Rights
KO	Kick Off (meeting)
MC	Management Coordinator
MTA	Milestones Trend Analysis
PC	Project Coordinator
PMO	Project Management Office
TL	Task Leaders
WP	Work Package
WPL	Work Package Leaders

Acknowledgements

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1 EXECUTIVE SUMMARY

1.1 Deliverable content

D2.2 contains information on generating experimental data for converting CO_2 and H_2S into COS to perform (micro)kinetic modelling (WP5). This information comprises the raw catalytic data and the corresponding experimental conditions of the reaction between CO_2 and H_2S to maximize COS production. The raw catalytic data is the results obtained from chromatographic analysis. The data is generated during screening catalytic material, selecting best-performing material, and optimizing reaction conditions.

1.2 Brief description of the state-of-the-art

The key state of the art for the acid gas reaction is reported in the Shell patent (WO2011084973A1), where the reaction between CO_2 and H_2S to produce COS employs different reaction conditions and catalytic materials. However, no literature was explicitly found on employing the results of catalytic conversion of CO_2 and H_2S to COS for the purpose of (micro)kinetic modelling.

1.3 Corrective action (if relevant)

N.A

1.4 IPR issue (if applicable)

N.A.

2 DELIVERABLE REPORT

D2.2 contains raw experimental data for the reaction between CO_2 and H_2S to evaluate COS production and the corresponding catalyst, reactor, pretreatment, and reaction conditions. This data will be employed for the microkinetic modelling of the reaction by WP5. This data has been acquired throughout different tasks of WP2, i.e., pre-screening of available catalytic materials, optimization of reaction and catalyst testing, and selection of best-performing material. Generated data are provided in this deliverable in the form of a table of conditions, while the raw data comprising gas chromatography (GC) analysis of effluent gases is uploaded to the Zenodo platform.

2.1 Context

D2.2 mainly provides a comprehensive collection of raw catalytic data and the corresponding experimental conditions employed for COS production. All the experimental data have been systematically arranged to be used for microkinetic modelling.

2.2 Brief description of the state-of-the-art

See section 1.2.

2.3 Results obtained

This report details the catalyst, reactor dimensions, reaction conditions, and raw catalytic data acquired during the above-mentioned series of events. The results are systematically compiled to be utilized for (micro) kinetic modelling for model development and validation, optimization of reaction conditions, and understanding the mechanism of COS production.

2.3.1 Catalytic setup

The setup used to carry out the experiments is a Micro Catalytic Bed unit from VINCI Technologies. It comprises inlets for the reagent gases (H_2S and CO_2) that come together in a gas mixer and a nitrogen line for additional flow dilution before the reactor. Gas flows are regulated through Mass-Flow Controllers (MFC) to set the desired feed composition. The unit accommodates a fixed bed reactor where the pressure can be controlled via a BackPressure Regulator (BPR) up to 50 bara. A bypass is used to sample the feed concentrations and stabilize flows before feeding the reactor. The catalytic unit is further connected to the Gas Chromatographic (GC) unit, as shown in Figure 1.

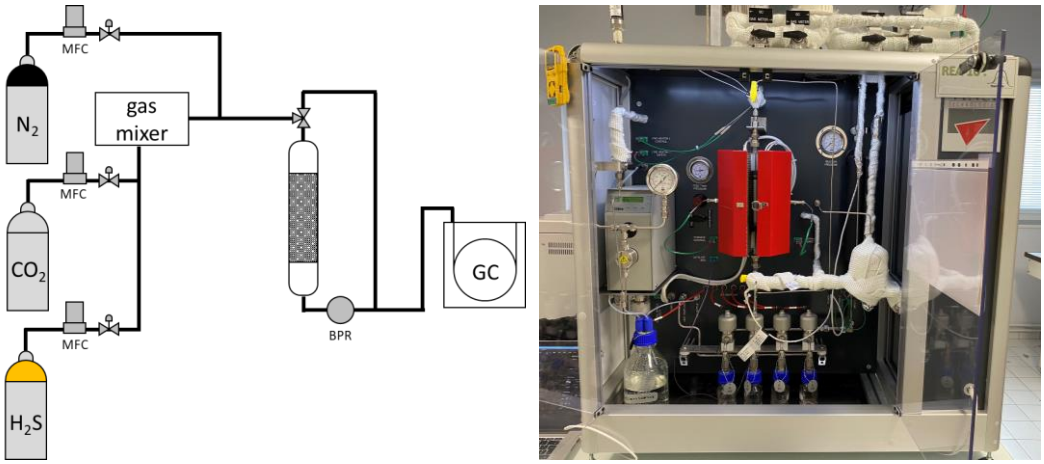

Figure 1 Schematic representation of the unit (left) and photo of the actual unit employed in the project (right).

2.3.2 Data acquisition

The raw catalytic data have been acquired using a Chromatec Crystal9000 GC. The GC is equipped with a split/splitless injector, two capillary columns adapted for acid gas analysis (GS-GasPro (60m) and BP-1 (60m)), two flame detectors (FID, FPD) and two conductivity detectors (TCD-HS, µTCD). This system configuration allows for simultaneously analyzing H_2S, CO_2 and COS. The GC analytical method is developed to ensure sensitivity and separation towards the sulfur compounds and is optimized in the first months of the project with minor changes when needed. The GC oven is kept isothermal at 70°C, which allows for a sampling rate of 15 min in single-injection analysis or 5 min in multi-injection analysis. Two methods have been developed for multi-injection analysis with a run time of one hour and 2 hours, respectively. For long catalytic experiments, a sequence of multiple runs using one or both multi-injection methods are used. A chromatogram of a single injection of 15 minutes with all the components of the reaction i.e. N_2, CO_2, COS, and H_2S is represented in Figure 2.

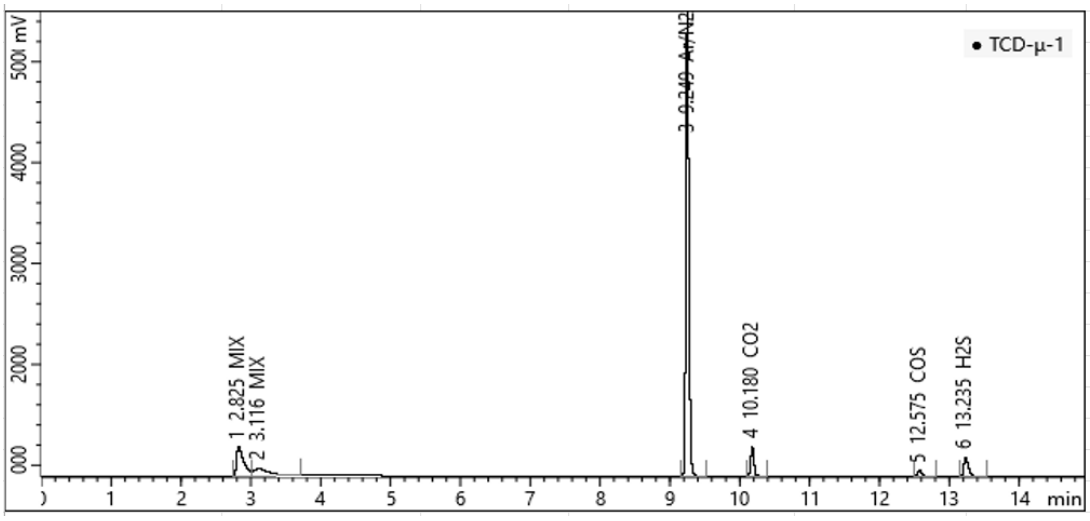

Figure 2 µ-TCD signal of an N_2, H_2S, CO_2, COS mixture for a 15-minute method analysis.

µTCD is used as main detector, while FPD is used to detect the lowest concentrations of sulphur compounds. For the sake of consistency throughout all generated data, only µTCD detector will be used in the writing of this deliverable.

The GC detector is calibrated with H_2S CO_2, and COS in the concentration ranges of interest. Integrated areas of chromatograph peaks as a function of the concentration are reported in Figure 3 for the µTCD detector. The current analytics setup does not allow for the detection of water, which can be separated from the effluent gas before the GC by a condenser element placed after the reactor within the MCB unit.

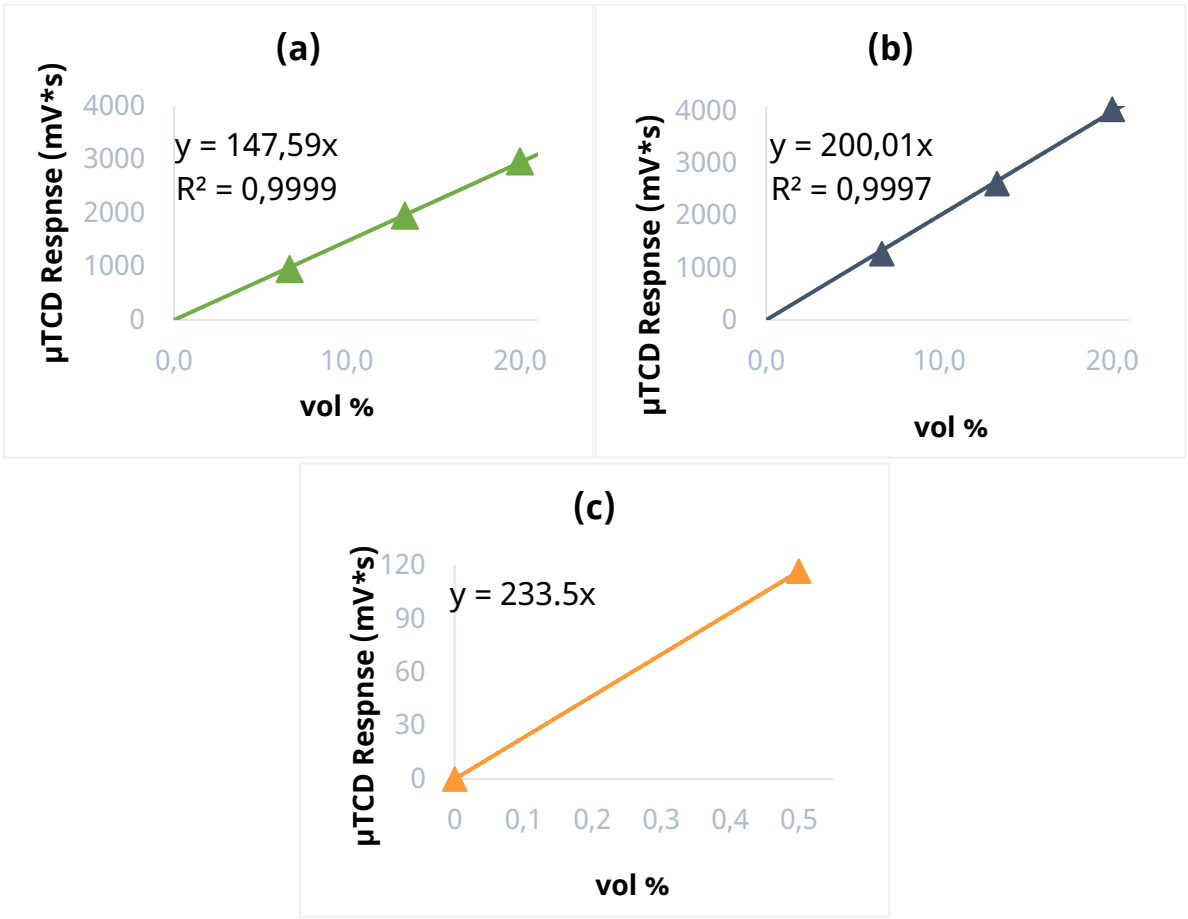

Figure 3 H_2S (a), CO_2 (b) and COS (c)calibration curves for µTCD detector. Curve equations, error bars and R^2 values are reported.

The obtained data are extracted from the GC computer through a report generated by the analytics software. Each report contains a table, with the signals of detectors (in mV), for each analysis that is carried out. For the sake of readability, we collected all the reports for a single experiment in one file/folder containing every analysis.

2.3.3 Experimental Conditions

The information about the dimensions of the reactor (reactor length, catalytic bed diameter, reactor internal diameter) used for catalytic experiments is presented in Table 1. The reactor

specifications remain the same in all the catalytic tests. Different catalysts have been used to screen catalytic materials and identify the best-performing catalyst. These include FAU, LTA, and MFI-type zeolites. Most of these chosen catalysts are microsized materials. Some nanosized materials have also been tested whose names are indicated with the prefix 'nano.' For some experiments, 13X (FAU) zeolite was stored in a 75% Relative Humidity chamber before the analysis, and this material was labelled as 13X-75%RH (as listed in Table 1).

Some zeolites are shaped into extrudates (EXT) and employed for the catalytic tests. The nomenclature as well as the composition of these extrudates has been discussed in detail in deliverable D2.6 as follows.

The experiments were conducted on pure zeolite powders pressed and sieved to attain the desired particle fraction. Extrudates were also subjected to the same sieving to keep the same particle size ratio with respect to the reactor. Tests on uncrushed extrudes are being performed during the writing of the deliverable. The relative raw data will not be part of this deliverable but will be part of the available shared data later.

Table 1 presents the list of tested catalytic materials with their respective physicochemical properties.

Table 1 List of the experimental conditions (a) Specifications of the reactor used for catalytic experiments and (b) Information about the catalysts employed.

Reactor Specifications[a]							
	Reactor Length					300 mm	
	Catalytic Bed Active length					100 mm	
	Reactor Internal Diameter					9.1 mm	
Catalyst Information[b]							
#	Material	Topology	Quantity (g)	Pellet Diameter (µm)	Si/Al Ratio	Surface area (m^2/g)	Density (g/ml)
1	**13X**	FAU	2-8	250-500	1.2	900	0.65
2	**13X-75%RH**	FAU	2-8	250-500	1.2	900	0.65
3	**4A**	LTA	2-8	250-500	0.97	20	0.4
4	**Y**	FAU	2-8	250-500	2.5	700	-
5	**nanoX**	FAU	2-8	250-500	1.2	900	0.65
6	**nanoA**	LTA	2-8	250-500	0.97	20	0.4
7	**ZSM5**	MFI	2-8	250-500	45	-	-
8	**13X(80)a**	FAU	2-8	250-500	1.2	-	-
9	**13X(90)a**	FAU	2-8	250-500	1.2	-	-
10	**13X(90)b**	FAU	2-8	250-500	1.2	-	-
11	**13X(90)c**	FAU	2-8	250-500	1.2	-	-
12	**EXT-nanoX**	FAU	2-8	250-500	1.2	900	0.65
14	**ZSM5-Cl-Na**	MFI	2-8	250-500	45	-	-
15	**13X-K**	FAU	2-8	250-500	1.2	900	0.65

All the experiments and the corresponding operating conditions employed are listed in Table 2.

Each experiment is subdivided into sections where the feed flow remains constant throughout the whole time:

- Preloading: pre-adsorption of one reactant prior to the reaction.
- Purge: flushing of reactive gases from the system by means of an inert gas.
- Temperature Programmed Desorption (TPD).
- Catalytic reaction.

Each experiment is labeled with a sequential number (1, 2, 3 etc.) followed by the section name (a, b, c, etc.). Table 2 also lists the most significant parameters used in each experimental section. These parameters refer to:

(i) set of conditions at which the catalyst is treated before performing the experiment (i.e., Pretreatment conditions, Table 2)

(ii) set of conditions at which each section of the experiment is performed (i.e., weight hourly space velocity WHSV, feed composition, temperature, pressure, total flow).

The catalyst material does not change within the different sections of an experiment. Any information specific to a particular experiment, i.e., additional steps performed/conditions applied, is given as comments on the experiment. The formulas used to calculate the partial pressure of the feed in the reactor and the WHSV are given below.

$$\text{Mole fraction } \mathbf{x_i} = \frac{\mathbf{n_i}}{\mathbf{n_{total}}}$$

$$\text{Partial Pressure } = \mathbf{x_i}.\boldsymbol{P_{total}}$$

$$\text{WHSV } (\text{h}^{-1}) = \left(\frac{\frac{\text{Flow rate of feed gas}}{\text{Molar volume}} \text{ x molar mass of gas}}{\text{mass of catalyst}} \right) / 60$$

Table 2 List of the catalytic experiments with the corresponding information about (a) pre-treatment and (b) reaction conditions used and (c) comments (if any) specific to each experiment. The WHSV values are given relative to H_2S component of the feed.

Label	Material	Experiment Type	Pretreatment Conditions[a]			Reaction Conditions[b]								Comments[c]
			Temperature(°C)	Duration (h)	Atmosphere	Temperature (°C)	Pressure (bar)	WHSV (h^{-1})	Total Flow (mL/min)	H_2S (v%)	CO_2 (v%)	N_2 (v%)	Ar (v%)	
1a	13X	Preloading	450	10	air	45	1.1	0.0061	12	16	-	84	-	H_2S adsorption
1b		Purge	-	-	-	45	1.1	-	10	-	-	100	-	H_2S desorption
1c		TPD	-	-	-	450	1.1	-	10	-	-	100	-	H_2S TPD
2a	13X	Preloading	450	5	air	45	1.1	-	12	-	16	84	-	CO_2 adsorption
2b		Purge	-	-	-	45	1.1	-	10	-	-	100	-	CO_2 desorption
2c		TPD	-	-	-	450	1.1	-	10	-	-	100	-	CO_2 TPD
3a	13X	Preloading	350	6	N_2	45	1.1	0.0061	32	6	-	94	-	H_2S adsorption
3b		Purge	-	-	-	45	1.1	-	30	-	-	100	-	H_2S desorption
3c		Catalytic Reaction	-	-	-	45	1.1	-	32	-	6	94	-	CO_2 on chemisorbed H_2S
3d		Purge	-	-	-	45	1.1	-	30	-	-	100	-	purge
3e		TPD	-	-	-	450	1.1	-	30	-	-	100	-	TPD after reaction
4a	13X	Preloading	350	6	N_2	60	1.1	0.0061	32	6	-	94	-	H_2S adsorption
4b		Purge	-	-	-	60	1.1	-	30	-	-	100	-	H_2S desorption
4c		Catalytic Reaction	-	-	-	60	1.1	-	30	-	6	94	-	CO_2 pulse
4d		Purge	-	-	-	60	1.1	-	30	-	-	100	-	purge
4e		TPD	-	-	-	450	1.1	-	30	-	-	100	-	TPD after reaction
5a	13X	Preloading	350	6	N_2	45	1.1	0.0061	32	-	6	94	-	CO_2 adsorption
5b		Purge	-	-	-	45	1.1	-	30	-	-	100	-	CO_2 desorption
5c		Catalytic Reaction	-	-	-	45	1.1	-	30	6	-	94	-	H_2S pulse
5d		Purge	-	-	-	45	1.1	-	30	-	-	100	-	purge
5e		TPD	-	-	-	450	1.1	-	30	-	-	100	-	TPD after reaction
6a	13X	Preloading	45	12	N_2	45	1.1	0.0228	30	12	-	88	-	H_2S adsorption on non-activated 13X
6b		Purge	-	-	-	45	1.1	-	30	-	-	100	-	H_2S desorption

Label	Material	Experiment Type	Pretreatment Conditions[a]			Reaction Conditions[b]								Comments[c]
			Temperature(°C)	Duration (h)	Atmosphere	Temperature (°C)	Pressure (bar)	WHSV (h^{-1})	Total Flow (mL/min)	H_2S (v%)	CO_2 (v%)	N_2 (v%)	Ar (v%)	
6c		Catalytic Reaction	-	-	-	45	1.1	-	30	-	6	94	-	CO_2 reaction on chemisorbed H_2S
6d		Purge	-	-	-	45	1.1	-	30	-	-	100	-	desorption after reaction
6e		TPD	-	-	-	450	1.1	-	30	-	-	100	-	TPD
7a	13X	Preloading	350	6	N_2	45	1.1	0.1902	30	100	-	-	-	Pure H_2S adsorption
7b		Purge	-	-	-	45	1.1	-	30	-	-	100	-	H_2S desorption
7c		TPD	-	-	-	450	1.1	-	30	-	-	100	-	H_2S TPD
8a	13X-75%RH	Catalytic Reaction	45	12	N_2	45	1.1	0.0247	30	13	13	74	-	reaction on water-saturated 13X
8b		Catalytic Reaction	350	12	N_2	45	1.1	0.0247	30	13	13	74	-	-
8c		Purge	-	-	-	45	1.1	-	30	-	-	100	-	purge
8d		Catalytic Reaction	-	-	-	45	1.1	0.0247	30	13	13	74	-	Reaction after reactivation at 350°C
9a	13X	Preloading	350	6	N_2	45	1.1	0.0494	30	13	-	74	13	screening 13X
9b		Catalytic Reaction	-	-	-	45	1.1	0.0494	30	13	13	74	-	-
10a	4A	Preloading	350	6	N_2	45	1.1	0.0247	30	13	-	74	13	screening 4A
10b		Catalytic Reaction	-	-	-	45	1.1	0.0247	30	13	13	74	-	-
11a	Y	Preloading	350	6	N_2	45	1.1	0.0247	30	13	-	74	13	screening Y
11b		Catalytic Reaction	-	-	-	45	1.1	0.0247	30	13	13	74	-	-
12a	nanoX	Preloading	350	6	N_2	45	1.1	0.0247	30	13	-	74	13	screening nanoX
12b		Catalytic Reaction	-	-	-	45	1.1	0.0247	30	13	13	74	-	-
13a	nanoA	Preloading	350	6	N_2	45	1.1	0.0247	30	13	-	74	13	screening nanoX
13b		Catalytic Reaction	-	-	-	45	1.1	0.0247	30	13	13	74	-	-
14a	13X	Preloading	350	6	N_2	45	1.1	0.0247	30	13	-	87	-	Temperature optimization 45°C on 13X
14b		Catalytic Reaction	-	-	-	45	1.1	0.0247	30	13	13	74	-	-

Label	Material	Experiment Type	Pretreatment Conditions[a]			Reaction Conditions[b]								Comments[c]
			Temperature(°C)	Duration (h)	Atmosphere	Temperature (°C)	Pressure (bar)	WHSV (h^{-1})	Total Flow (mL/min)	H_2S (v%)	CO_2 (v%)	N_2 (v%)	Ar (v%)	
15a	13X	Preloading	350	6	N_2	60	1.1	0.0247	30	13	-	87	-	Temperature optimization 60°C on 13X
15b		Catalytic Reaction	-	-	-	60	1.1	0.0247	30	13	13	74	-	-
16a	13X	Preloading	350	6	N_2	80	1.1	0.0247	30	13	-	87	-	Temperature optimization 80°C on 13X
16b		Catalytic Reaction	-	-	-	80	1.1	0.0247	30	13	13	74	-	-
17a	13X	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	Temperature optimization 100°C on 13X
17b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
18a	13X	Preloading	350	6	N_2	120	1.1	0.0247	30	13	-	87	-	Temperature optimization 120°C on 13X
18b		Catalytic Reaction	-	-	-	120	1.1	0.0247	30	13	13	74	-	-
19a	ZSM5-Cl	Preloading	350	6	N_2	120	1.1	0.0247	30	13	-	87	-	test on ZSM-5 H-form
19b		Catalytic Reaction	-	-	-	120	1.1	0.0247	30	13	13	74	-	-
20a	13X	Preloading	350	6	N_2	80	1.1	0.0247	30	13	-	87	-	-
20b		Catalytic Reaction	-	-	-	80	1.1	0.0247	30	13	13	74	-	-
21a	13X	Preloading	350	6	N_2	110	1.1	0.0247	30	13	-	87	-	-
21b		Catalytic Reaction	-	-	-	110	1.1	0.0247	30	13	13	74	-	-
22a	13X(80)a	Preloading	350	6	N_2	110	1.1	0.0198	30	13	-	87	-	test on SG extrudate1 fraction
22b		Catalytic Reaction	-	-	-	110	1.1	0.0198	30	13	13	74	-	-
23a	13X(90)a	Preloading	350	6	N_2	100	1.1	0.0225	30	13	-	87	-	test on SG extrudate2 fraction
23b		Catalytic Reaction	-	-	-	100	1.1	0.0225	30	13	13	74	-	-

Label	Material	Experiment Type	Pretreatment Conditions[a]			Reaction Conditions[b]								Comments[c]
			Temperature(°C)	Duration (h)	Atmosphere	Temperature (°C)	Pressure (bar)	WHSV (h^{-1})	Total Flow (mL/min)	H_2S (v%)	CO_2 (v%)	N_2 (v%)	Ar (v%)	
24a	13X(90)b	Preloading	350	6	N_2	100	1.1	0.0225	30	13	-	87	-	test on SG extrudate3 fraction
24b		Catalytic Reaction	-	-	-	100	1.1	0.0225	30	13	13	74	-	-
25a	13X(90)c	Preloading	350	6	N_2	100	1.1	0.0225	30	13	-	87	-	test on SG extrudate4 fraction
25b		Catalytic Reaction	-	-	-	100	1.1	0.0225	30	13	13	74	-	-
26a	13X	Preloading	350	6	N_2	100	1.1	0.0494	30	13	-	87	-	contact time on 13X
26b		Catalytic Reaction	-	-	-	100	1.1	0.0494	30	13	13	74	-	
27a	13X	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	contact time on 13X
27b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
28a	EXT-nanoX	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on LCS extrudate nanoX fraction
28b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
29a	ZSM5-Cl-Na	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on ZSM-5 Na-form
29b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
30a	13X	Preloading	350	6	N_2	100	1.1	0.0330	30	13	-	87	-	contact time on 13X
30b		Catalytic Reaction	-	-	-	100	1.1	0.0330	30	13	13	74	-	-
31a	13X-75%RH	Preloading	100	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on 13X pretreated at 100°C
31b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
32a	13X-75%RH	Preloading	150	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on 13X pretreated at 150°C
32b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-

Label	Material	Experiment Type	Pretreatment Conditions[a]			Reaction Conditions[b]								Comments[c]
			Temperature(°C)	Duration (h)	Atmosphere	Temperature (°C)	Pressure (bar)	WHSV (h^{-1})	Total Flow (mL/min)	H_2S (v%)	CO_2 (v%)	N_2 (v%)	Ar (v%)	
33a	13X-75%RH	Preloading	200	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on 13X pretreated at 200°C
33b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
34c	13X-75%RH	Preloading	250	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on 13X pretreated at 250°C
34c		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
35a	13X-75%RH	Preloading	300	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on 13X pretreated at 300°C
35b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
36a	13X-75%RH	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	test on 13X pretreated at 350°C
36b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	-
37a	13X	Catalytic Reaction	350	6	N_2	100	1.1	0.0247	30	13	13	74	-	test on 13X regenerated at 200°C
37b		Catalytic Reaction	200	6	N_2	100	1.1	0.0247	30	13	13	74	-	
38a	4A	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	test 4A in optimized conditions
38b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	18h experiment, pretreated at 350°C
38c		Preloading	200	6	N_2	100	1.1	0.0247	30	13	-	87	-	
38d		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	18h experiment, pretreated at 200°C
39a	13X	Preloading	350	6	N_2	100	1.1	0.0247	30	13	-	87	-	H_2S adsorption on 13X exchanged-K
39b		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	18h experiment, pretreated at 350°C

Label	Material	Experiment Type	Pretreatment Conditions[a]			Reaction Conditions[b]								Comments[c]
			Temperature(°C)	Duration (h)	Atmosphere	Temperature (°C)	Pressure (bar)	WHSV (h^{-1})	Total Flow (mL/min)	H_2S (v%)	CO_2 (v%)	N_2 (v%)	Ar (v%)	
39c		Preloading	200	6	N_2	100	1.1	0.0247	30	13	-	87	-	H_2S adsorption on 13X exchanged-K
39d		Catalytic Reaction	-	-	-	100	1.1	0.0247	30	13	13	74	-	18h experiment, pretreated at 200°C
40a		Preloading	350	6	N_2	45	1.1	0.0317	10	50	-	50	-	H_2S adsorption
40b	13X	Purge	-	-	-	45	1.1		10	-	-	100	-	desorption
40c		TPD	-	-	-	350	1.1		10	-	-	100	-	H_2S TPD 45°C-350 °C, 2°/min
41a		Preloading	350	6	N_2	120	1.1	0.0317	10	50	-	50	-	H_2S adsorption
41b	13X	Purge	-	-	-	120	1.1	-	10	-	-	100	-	desorption
41c		TPD	-	-	-	350	1.1	-	10	-	-	100	-	H_2S TPD 120°C-350 °C, 2°/min
42a		Preloading	350	6	N_2	45	1.1	-	10	-	50	50	-	CO_2 adsorption
42b	13X	Purge	-	-	-	45	1.1	-	10	-	-	100	-	desorption
42c		TPD	-	-	-	350	1.1	-	10	-	-	100	-	CO_2 TPD 45°C-350 °C, 2°/min
43a		Preloading	350	6	N_2	100	1.1	-	10	-	50	50	-	CO_2 adsorption
43b	13X	Purge	-	-	-	100	1.1	-	10	-	-	100	-	desorption
43c		TPD	-	-	-	350	1.1	-	10	-	-	100	-	CO_2 TPD 100°C-350 °C, 2°/min
44a		Preloading	350	6	N_2	120	1.1	-	10	-	50	50	-	CO_2 adsorption
44b	13X	Purge	-	-	-	120	1.1	-	10	-	-	100	-	desorption
44c		TPD	-	-	-	350	1.1	-	10	-	-	100	-	CO_2 TPD 120°C-350 °C, 2°/min

The raw data obtained from the GC analysis of the effluent gases is the Micro Thermal Conductivity Detector (μ-TCD) response in milli volts (mV) as a function of time in minutes (min). The raw GC data from the most straightforward experiment comprises more than 200,000 GC points. Therefore, due to the large data size, the Excel files containing raw GC data of all catalytic tests are uploaded on the Zenodo platform within the project directory (e-CODUCT GA101058100 Horizon Europe project) and protected by a Digital Object Identifier (DOI) for the use in further dissemination activities, namely publication of academic articles (see next section).

As an example, the first 100 GC points of experiment # 19 as a function of time are presented in Table 3.

Table 3 Raw experimental data showing time and corresponding GC response for 100 (out of 224346) datapoints from the experiment No. 19.

#	Time (min)	TCD-μ Response (mV)	#	Time (min)	TCD-μ Response (mV)
1	0.0000	799.0722	51	0.0333	799.8738
2	0.0007	799.0893	52	0.0340	799.8738
3	0.0013	799.1063	53	0.0347	799.8908
4	0.0020	799.1404	54	0.0353	799.9079
5	0.0027	799.1404	55	0.0360	799.9249
6	0.0033	799.1575	56	0.0367	799.9420
7	0.0040	799.1916	57	0.0373	799.9590
8	0.0047	799.2086	58	0.0380	799.9761
9	0.0053	799.2257	59	0.0387	799.9932
10	0.0060	799.2257	60	0.0393	800.0103
11	0.0067	799.2427	61	0.0400	800.0273
12	0.0073	799.2598	62	0.0407	800.0444
13	0.0080	799.2769	63	0.0413	800.0614
14	0.0087	799.2769	64	0.0420	800.0785
15	0.0093	799.2939	65	0.0427	800.0956
16	0.0100	799.3110	66	0.0433	800.0785
17	0.0107	799.3110	67	0.0440	800.1126
18	0.0113	799.3110	68	0.0447	800.1467
19	0.0120	799.3280	69	0.0453	800.1638
20	0.0127	799.3450	70	0.0460	800.1638
21	0.0133	799.3621	71	0.0467	800.1808
22	0.0140	799.3792	72	0.0473	800.1979
23	0.0147	799.4133	73	0.0480	800.2321
24	0.0153	799.4303	74	0.0487	800.2491
25	0.0160	799.4474	75	0.0493	800.2491
26	0.0167	799.4644	76	0.0500	800.2662
27	0.0173	799.4815	77	0.0507	800.2832
28	0.0180	799.4985	78	0.0513	800.2832
29	0.0187	799.5156	79	0.0520	800.3003
30	0.0193	799.5327	80	0.0527	800.3174
31	0.0200	799.5497	81	0.0533	800.3174
32	0.0207	799.5838	82	0.0540	800.3344
33	0.0213	799.6009	83	0.0547	800.3515
34	0.0220	799.6179	84	0.0553	800.3685

#	Time (min)	TCD-μ Response (mV)	#	Time (min)	TCD-μ Response (mV)
35	0.0227	799.6179	**85**	0.0560	800.3685
36	0.0233	799.6349	**86**	0.0567	800.3685
37	0.0240	799.6520	**87**	0.0573	800.3856
38	0.0247	799.6520	**88**	0.0580	800.3856
39	0.0253	799.6520	**89**	0.0587	800.4026
40	0.0260	799.6691	**90**	0.0593	800.4197
41	0.0267	799.6691	**91**	0.0600	800.4197
42	0.0273	799.6862	**92**	0.0607	800.4368
43	0.0280	799.7032	**93**	0.0613	800.4539
44	0.0287	799.7203	**94**	0.0620	800.4539
45	0.0293	799.7373	**95**	0.0627	800.4709
46	0.0300	799.7714	**96**	0.0633	800.4880
47	0.0307	799.7885	**97**	0.0640	800.5051
48	0.0313	799.8055	**98**	0.0647	800.5222
49	0.0320	799.8397	**99**	0.0653	800.5392
50	0.0327	799.8567	**100**	0.0660	800.5563

The raw GC data is exploited for (micro)kinetic modelling purposes as follows.

Peak integration is performed for every peak of each separated component (i.e. H_2S, CO_2, COS, N_2) resulting in the peak area in millivolt seconds (mV*s). This quantity is directly proportional to the concentration of the identified specie. The evolution of this value is followed throughout the entire experiment and often expressed relative to the value of the initial feed concentration (C_0). For the COS the evolution is shown as the value relative to maximum theoretical production from the feed composition used. These quantities are plotted as a function of time for each component. Figure 3 presents an example of raw catalytic data exploitation for (micro)kinetic modelling where the catalytic data of the benchmark reaction on 13X demonstrates the evolution of the relative concentrations of different components as a function of the time of stream.

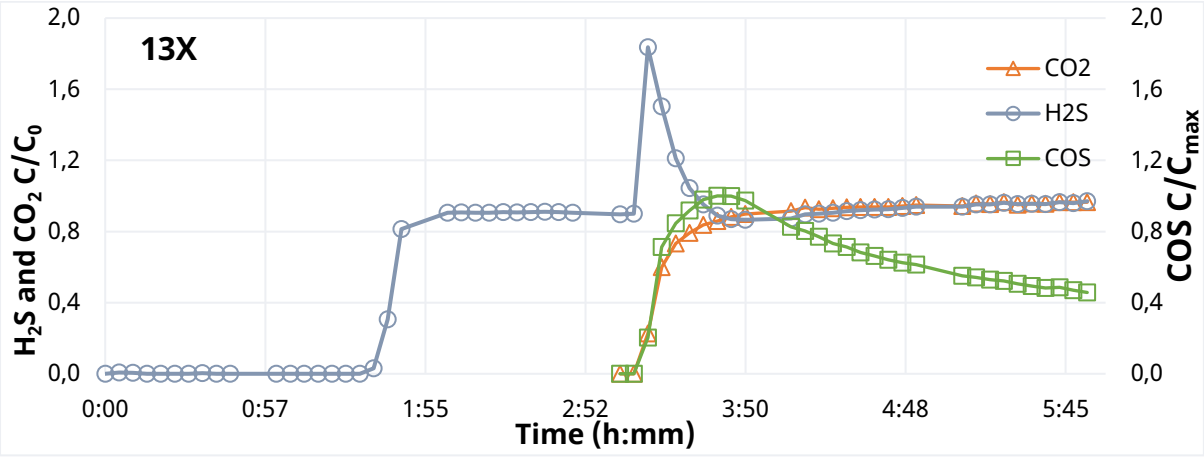

Figure 4 Relative concentrations evolution for the benchmark reaction.

2.4 Data Availability

The raw GC data of all catalytic tests are uploaded on the Zenodo platform within the project community and protected by a Digital Object Identifier () for the use in further dissemination activities, namely publication of academic article:

- Repository: https://zenodo.org/
- Community: e-CODUCT GA101058100 Horizon Europe project
- DOI: https://doi.org/10.5281/zenodo.12581428

2.5 Impact of the results

The experimental data impacts the microkinetic modelling in several ways, serving as the backbone for developing, validating, and refining kinetic models. The set of experimental data and reaction conditions presented in this report will be utilized to construct a suitable kinetic model for converting CO_2 and H_2S to COS, providing deeper insights into the reaction mechanism. This also will help estimate kinetic parameters and determine rate laws. The refined and customized (micro)kinetic models based on these experimental results will help predict optimal conditions for maximizing COS yield and selectivity.

2.6 Related IPR

N/A

3 CONCLUSION

This report compiles the raw experimental data generated by catalytic tests and the associated reactor, reaction and catalyst conditions for the purpose of (micro)kinetic modeling. This data is generated during pre-screening of available materials for the reaction of CO_2 with H_2S for COS production), optimization of reaction conditions and catalyst testing, and selection of best performing material. These results will be employed to construct an appropriate (micro)kinetic model to get deeper insights into the reaction mechanism and optimize the reaction conditions. The experimental conditions and the raw data, together with a refined kinetic model, will help to optimize the reaction conditions and maximize COS production.