Project Title:

Truly Carbon Neutral electricity enhanced Synthesis of Liquefied Natural Gas (LNG) from biomass

Project Acronym:

CarbonNeutralLNG

PUBLIC

Work Package 1

Deliverable D1.1

"Design and Performance Sorption enhanced e-gasifier "

Responsible for Deliverable:

BOKU - University of Natural Resources and Life Sciences, Vienna

April 2024

This project has received funding from Horizon Europe under grant agreement No. 101084066.

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Content

Executive Summary

Deliverable D1.1 in the project "CarbonNeutralLNG" is derived from the work conducted in tasks 1.1-1.3 under the lead of BOKU. D1.1 deals with the design and performance of the sorption enhanced e-gasifier. The ambition of the project task was to develop a reactor concept for dual fluidized bed (DFB) gasification of biomass that allows for the incorporation of renewable electricity sources to enhance the key performance indicators (KPI's) regarding carbon efficiency, cold gas efficiency, and carbon emissions. The original concept was based on the conventional DFB gasification setup, including a gasification reactor coupled with a combustion reactor, with the combustion reactor operating solely as electrically heated calciner of the $CaCO_3$ bed material.

Initially, a novel reactor design was conceptualized to fulfil the criteria outlined as goals in the project proposal. These goals comprise a carbon conversion and a cold gas efficiency of >90%. While this increase in carbon conversion is enabled by including a carbon capture and release cycle that allows for the sequestration of a CO_2-rich "product gas" from the calciner, the increase in cold gas efficiency can be achieved by substituting the char combustion with electrical heating. Recent experiences in experimental DFB gasification studies and process simulation of the underlying reactor system conducted by BOKU showed that these process characteristics are subject to limitations that may be overcome by introducing new functional reactor units. These functional reactor units are the segregator, functioning as a separator of an inlet binary mixture of bed material and char into possibly pure streams of bed material and char, and the converter, gasifying the char-rich outlet stream of the segregator to generate a gasification product gas.

The design of an entirely novel reactor concept with 50 kW_{th} thermal fuel input power (biomass) required additional efforts to determine the functionality of the setup. For computing the mass and energy balances, process simulation with IPSEpro was employed. The results showed, that roughly 80 % (weight based) of the fuel conversion takes place in the gasification reactor and the remaining 20 % are converted in the converter. Under the defined boundary conditions, i.e., maximum fuel-to-product gas conversion, 35 kW electric power are needed to supply the process with heat, 25 kW supplied to the riser and 10 kW supplied to the converter. Theoretically, the electric power supply could be reduced to 25 kW (in case of no heat loss).

Furthermore, experimental studies to determine the control and establishment of suitable fluid dynamics in the novel reactor system required the construction of a cold flow model. Initial studies in the cold flow model showed, that the fundamental principle of creating two solid circulation cycles works. However, challenges regarding the segregation and separation process in the segregator were identified, which require further investigations.

Implications of the necessary adaptations in the work plan for tasks derived from the design of the sorption enhanced e-gasifier are outlined in the report. Furthermore, the current status of the planned data exploitation and knowledge management regarding the design of the novel reactor concept is described.

1. E-gasifier: Initial design considerations and necessary adaptions

1.1 Design and erection of e-gasifier

BOKU's main tasks within the "CarbonNeutralLNG" project are the design, erection, commissioning and operation of a 50 kW_{th} lab-scale dual fluidized bed (DFB) reactor for electrically heated sorption enhanced biomass gasification as it is schematically depicted in Figure 1. These steps are structured into the tasks 1.1, 1.2 and 1.3 of work package (WP) 1. For these tasks BOKU works jointly with the following project partners:

- DIEFFENBACHER GMBH Maschinen- und Anlagenbau (DEA) → Evaluation of different concepts for electrically heated fluidized bed reactors
- RINA-C Consulting SpA (Rina-C) → Elaboration of safety relevant design and control procedures
- BEST – Bioenergy and Sustainable Technologies GmbH (BEST) → Design of control strategy and investigation of dynamic plant behavior

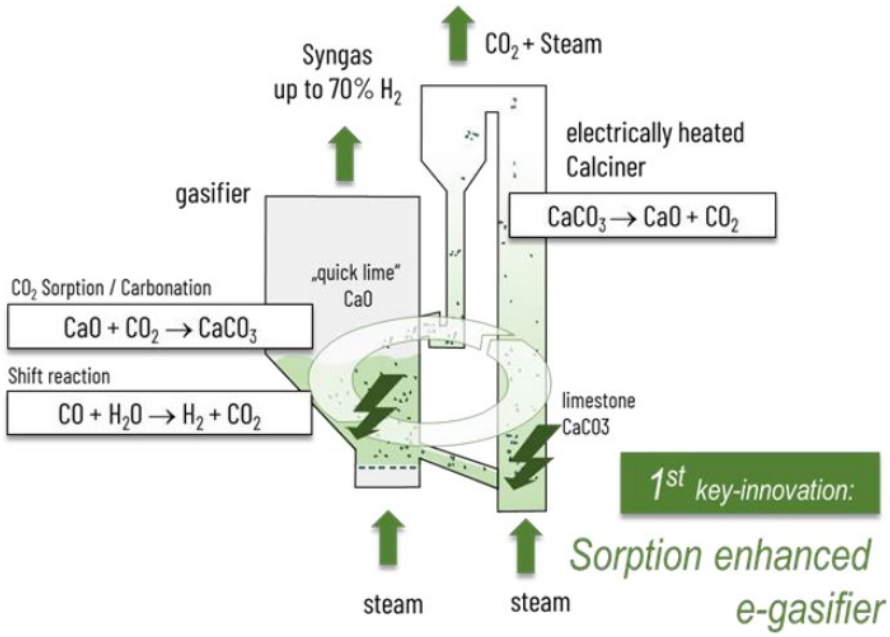


Figure 1 Reactor scheme of the sorption enhanced e-gasifier presented in the proposal.

The elaboration of a suitable reactor design and the subsequent erection of the plant is approached in the following steps:

- Process analysis → Definition of the required reactor properties based on the proposed process specifications
- Basic engineering → Computation of input and output streams via process simulation and subsequent reactor dimensioning according to criteria of fluidized bed reactors
- Detailed engineering → Definition of the required process components (valves, sensors, steam generator, …) and design of a P&I diagram

- Erection → Outsourced to plant construction company

However, this sequence of actions had to be adapted as a matter of research progress, since the originally intended reactor concept (see Figure 1) turned out to have limitations to fully meet the intended performance requirements. The reasons and solutions to even improve the intended gas qualities as well as the consequences for the project are discussed in the following sections.

1.1.1. Process analysis

DFB steam gasification of biomass is an elegant process for generating a high-calorific syngas (no N_2 dilution) which does not need an external energy source. Circulating bed material is used as heat carrier, which supplies heat to the gasification reactor (GR) and is heated itself in the riser (combustion reactor). The idea of the proposed gasification process is based on the sorption enhanced reforming (SER) process, which allows generating an H_2-enriched syngas via in-situ CO_2 capture in the GR through carbonation of the bed material (limestone). The bed material is then reactivated by calcination in the riser releasing CO_2. Due to the temperature dependency of the equilibrium of CO_2 and $CaO/CaCO_3$, it is crucial to establish a high temperature difference between the GR and riser (T_{GR} < 750 °C, T_{riser} > 900 °C) for this process.

For this project, the aim is to adapt the SER process in order to enable the following functionalities:

- Electrical heat supply to drive the endothermic gasification reaction → Enhanced feedstock-to-product gas conversion
- Increased carbon and cold gas efficiency compared to classic DFB/SER plants (higher feedstock-to-product gas conversion)
- Flue gas of riser should consist only of CO_2 and H_2O → CO_2 can be directly captured after steam condensation

The latter specification can be either met by fluidizing the riser with steam, pure oxygen or with recycled flue gas (or a mixture of them). However, in contrast to classical SER, it is essential, that no char enters the riser, because it would be gasified in the absence of O_2 and impurify the CO_2/ H_2O flue gas stream. This requirement cannot be met with the traditional DFB reactor concept, as one of its inherent functions is that a part of the feedstock is transported to the riser in the form of unconverted char along with the circulating bed material stream to be burnt and release the heat necessary for the gasification reaction. Therefore, to enable the proposed process characteristics, it is inevitable to change the reactor concept, so that the complete biomass feedstock is converted to product gas (PG) and no char enters the riser. On the other hand, this means that the complete amount of heat required for the gasification process and for heat loss compensation must be supplied electrically. The use of pure oxygen instead of combustion air in the riser requires a complex air separation unit and is therefore not considered.

Furthermore, due to the low temperature level of the GR (determined by the equilibrium of the carbonation reaction), a second high temperature gasification reactor is needed in order to enable complete char conversion within a reasonable timespan (due to the kinetics of the gasification reactions). The functionality of this secondary gasification must guarantee that char conversion may take place fast enough to avoid solids accumulation in an internal gasification loop.

1.1.2. Novel reactor concept

Based on the aforementioned insufficiencies of the DFB system concerning the aspired functionality of the proposed e-gasifier, a novel multi fluidized bed (MFB) reactor system was elaborated which is shown in

Figure 2. The basis for the proposed reactor system is the advanced DFB system invented by TU Wien, in which the GR is divided into two parts, the bubbling fluidized bed (BFB) and the counter-current column (CCC). In the BFB, the biomass conversion takes place and the constrictions along the CCC enhance the solid-gas contact of product gas and hot bed material in order to enhance tar reforming. Properly operated, the increased gas velocity in the constricted cross sections leads to the formation of additional fluidized zones above each constriction (depicted in Figure 2). The functionality of this advanced DFB system was validated over recent years in a 100 kW pilot plant reactor at TU Wien in different operational modes, including SER [1]. The project team at BOKU constitutes a significant share of the researchers involved in the development and scientific exploitation of this advanced DFB system [2], [3].

The novel reactor system extends this DFB system and thereby the functionality of the SER process in the following manner. The solid stream exiting the GR at the bottom consisting of carbonated bed material and residual char must be segregated and split into two streams. One separated char-lean or char-free stream is led to the riser (equipped with additional external heating), where the bed material is calcined. The second separated char-rich solid stream must be further gasified at elevated temperatures in order to enable its fast conversion preventing char accumulation in the system. The proposed capabilities of the plant can be realized by adding two components to the DFB system into the lower connection line between GR and riser. The segregator (labeled SEG) functions as separation unit for the ingoing binary mixture of bed material and char from the GR yielding a char-lean or char-free stream directed to the riser and a stream with high char content transferred to the second new reactor, the converter (labeled CONV). The segregation of the binary mixture is achieved in the only mildly fluidized lower part of the segregator due to the density difference between the two particle types. The floating char particles are subsequently transported through a pipe upwards towards the converter by increasing the gas velocity in the upper part of the segregator via the secondary fluidization stage. Via the two fluidization stages, the separation efficiency can be controlled. In the externally heated converter (bubbling fluidized bed), high-temperature gasification ($T_{conv} > T_{GR}$) with sufficient long residence time for high char conversion. The arising product gas as well as the non-separated bed material and residual char are redirected from the converter to the GR. With this setup, additionally to the global GR-segregator-riser loop, a second (internal) solid circulation loop (GR-segregator-converter) is created.

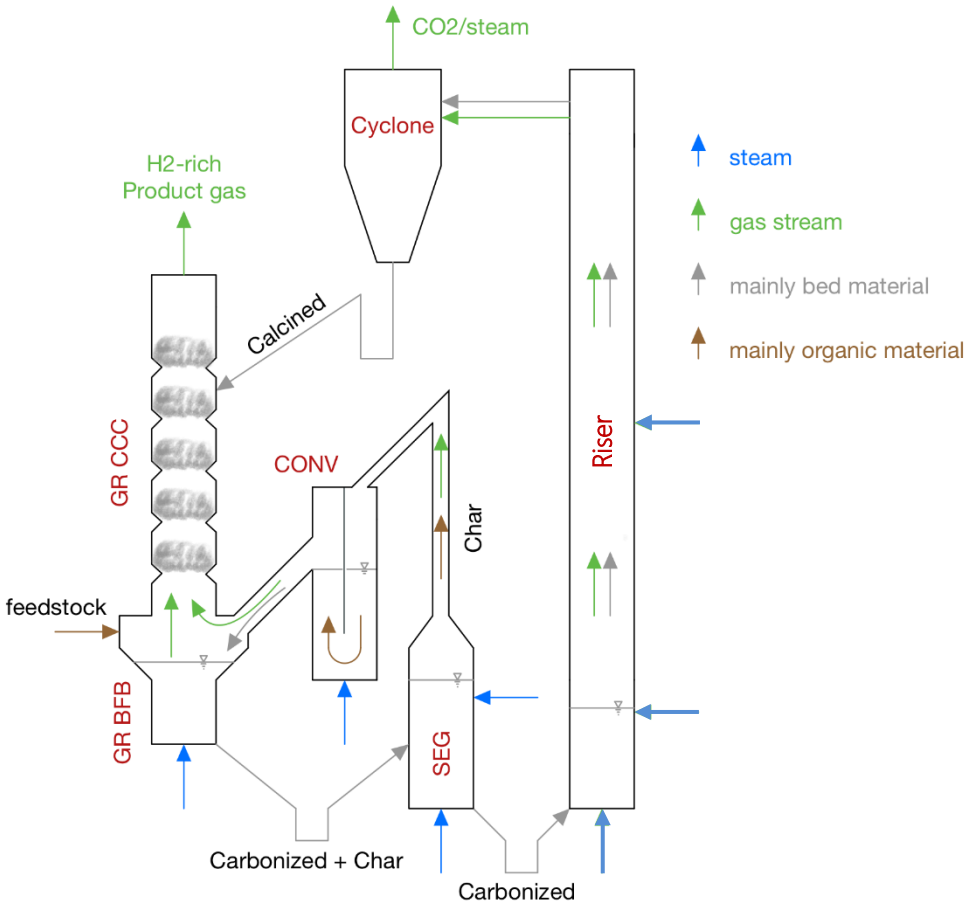


Figure 2 Schematic sketch of the proposed novel fluidized bed reactor system for sorption enhanced steam gasification with the segregator for separating char from the GR solid outlet stream and a second high-temperature gasification stage (converter). The segregator is also fluidized with steam, because the gas input to the segregator mixes eventually with the product gas. Riser and converter are externally heated.

1.1.3. Implications on the design procedure of the e-gasifier

Because of the overall complexity of the new reactor system and the unknown fluid dynamic behavior of the segregator, erecting a reactor based on this concept directly as a hot pilot-scale plant would involve a very high risk. It has been good scientific practice to investigate the fluid dynamic behavior of new fluidized bed reactor systems and specific phenomena in fluidized beds with the help of cold flow models (CFM). A CFM is a fluid dynamically similar scaled version of the actual reactor operated at room temperature without chemical reactions. For this purpose, BOKU proposed at the project meeting in Klaipeda in June 2023 to incorporate the design and erection of a CFM of the new MFB reactor system and conducting pre-engineering studies with it into the project plan. The present representatives of the project partners agreed to this approach.

This means, that afterwards a first design of the hot plant has been developed and based on this a scaled CFM has been built and commissioned. First results have been drawn from CFM tests. These points are addressed in more detail in the following sections.

In addition, the aspect electrical heating of high temperature fluidized beds will be studied separately by upgrading a 20 kW_{th} stationary fluidized gasification/combustion reactor (shown in Figure 3) at BOKU's lab

with heating elements. The details for the approach and major research questions to be addressed for integrating electrical heating elements into fluidized bed reactors are described in in later sections.

Eventually, based on the findings from studying these two critical aspects, the design of the 50 kW_{th} plant will be adapted and the originally planned schedule for engineering and erection will be continued.

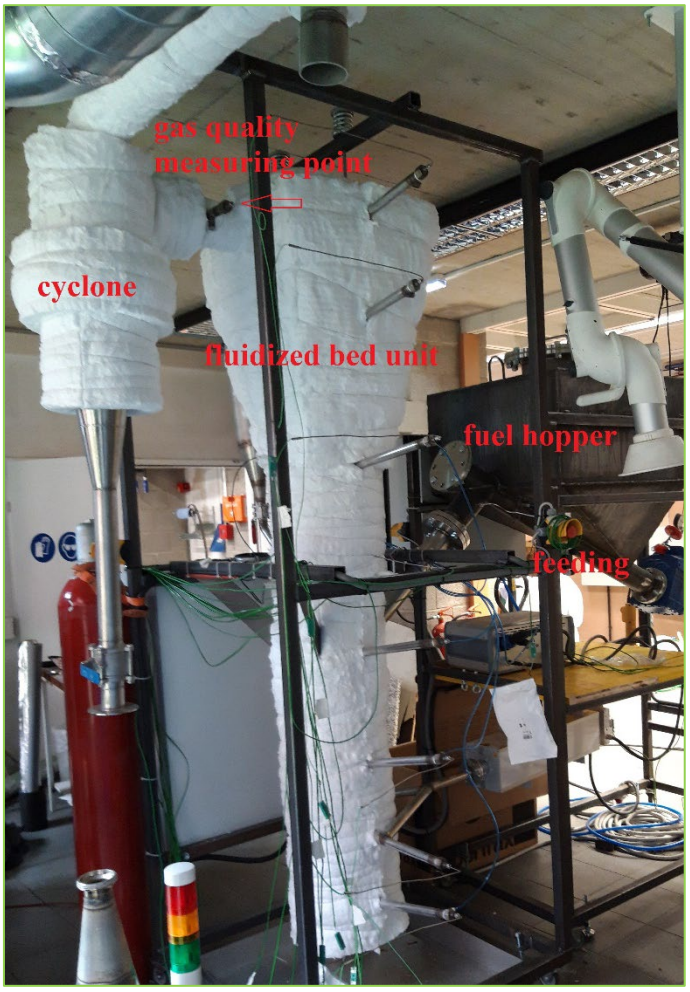


Figure 3 Picture of the 20 kW_{th} stationary fluidized bed that will be used for investigating electrical heating concepts for high-temperature fluidized beds.

1.2 Affected contributions

The new reactor design for the sorption enhanced e-gasifier that is developed in WP1 is more complex than previously anticipated. BOKU therefore designed and built a fluid dynamically scaled cold flow model including the novel reactor units, as discussed and approved by the consortium in the 1st steering committee meeting in Klaipėda in June 2023.

As a consequence, the focus of BOKU's work has been shifted from erecting a slightly adapted version of a well proven gasification system to developing a novel reactor system. For this purpose, additional steps have been and will be necessary:

- Conceptualization of the system (finished)

- Modelling and simulation of the process with IPSEPro (finished)
- Erection of a scaled cold flow model (finished)
- Detailed investigation of the fluid dynamics in the system with the cold flow model – starting in Q1/2024 (ongoing)

These additional steps for establishing the required knowledge about the novel reactor system necessitate an adaptation of the originally anticipated work plan. However, the investigations of the novel concept will provide findings and information vital to the aims of this project and future applications for multi fluidized bed systems targeting similar performance criteria.

Complementary to the cold flow model investigations regarding fluid dynamics, the thermochemical behavior of the individual reactors in the system and electric heating concepts will be studied in a 20 kW_{th} bubbling fluidized bed reactor. Again, the outcome of these studies is essential to provide information for the design of larger scale reactor systems based on the novel reactor concept but will also target future aims for the integration of electrical energy sources in existing or newly-built fluidized bed systems.

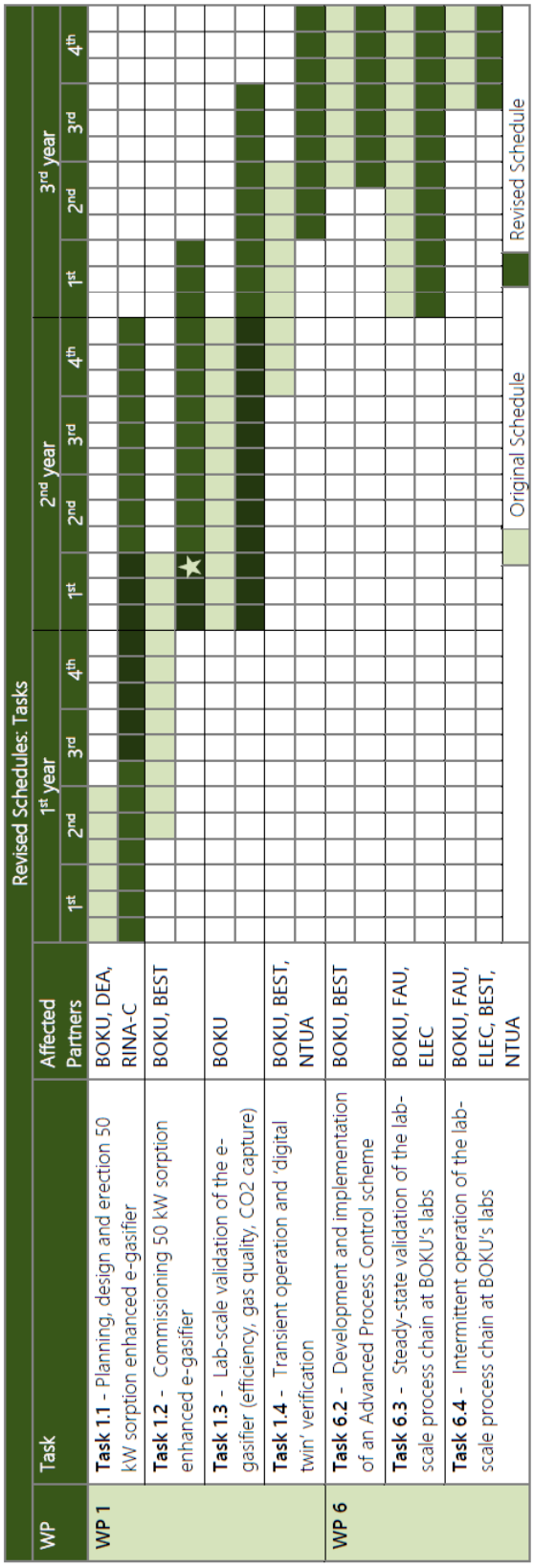
Due to the novel functionalities of the new reactor concept, its development is an iterative process and therefore the time schedule for the process development and final realization of the hot lab-scale model is subject to uncertainties. These additional steps delay the engineering and erection of the hot test plant by up to two years. This alteration of the schedule could exceed the timeframe of the project. However multiple measures are undertaken to ensure that alternative datasets for collaborative tasks are provided. Several project partners and their contributions are affected by this.

The work packages as well as project partners and their contributions, which are affected by these changes and the adaption of time and work schedule are listed below:

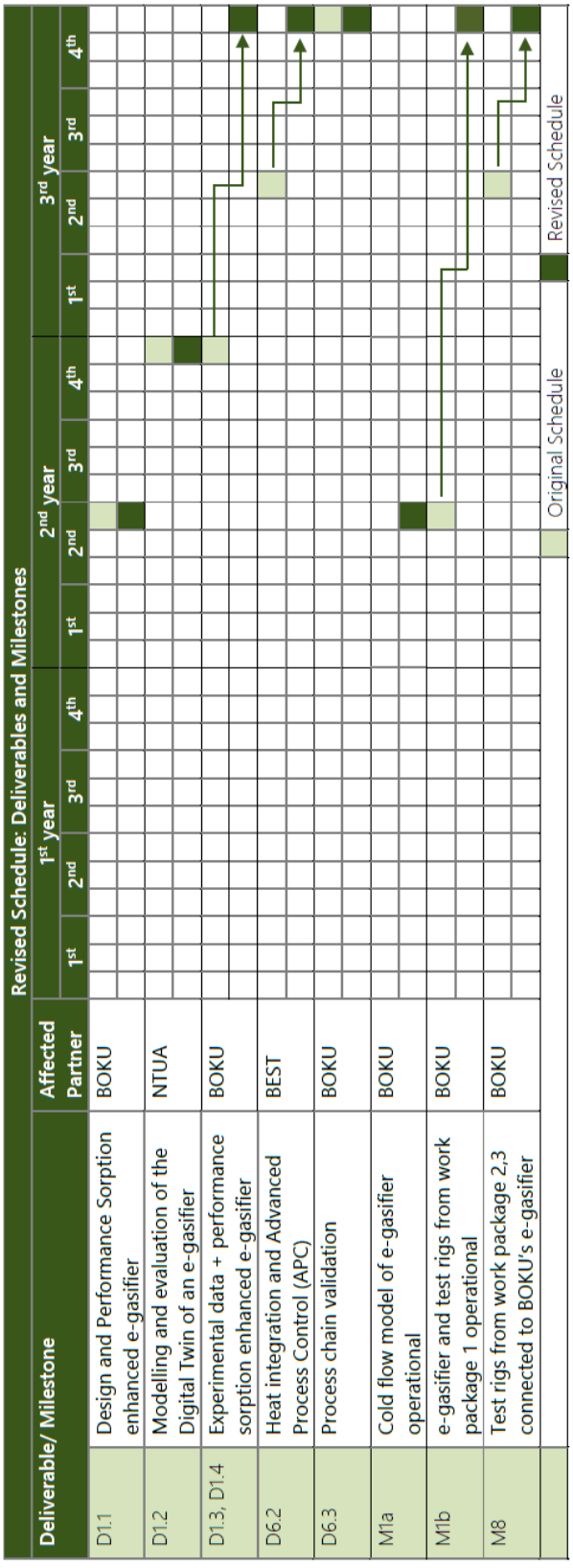
Affected Contributions			
WP	Task	Affected Partners	Changes
WP1	Task 1.1	**BOKU, DEA, RINA-C**	Planning, design and erection of a 50 kW_{th} sorption enhanced e-gasifier • New subtasks: Conceptualization and simulation of the new gasification system, Erection of a cold flow model, Cold flow model studies • The planning, design and erection of the hot test plant are delayed. **(D1.1, due April 30th 2024)** • The elaboration of safety relevant design and control procedures which is supported by RINA-C and DEA will also be delayed, because the design process of the hot test plant is delayed. However, it is planned to provide a concept for the plant within Q1/2025 to provide input for RINA-C and DEA.
	Task 1.2	**BOKU, BEST**	Commissioning of the 50 kW_{th} sorption enhanced e-gasifier • New subtasks: Commissioning of the cold flow model **(M1a, due February 29th 2024)** • The commissioning of the hot test plant will be delayed, since previous steps are delayed **(M1b, due October 31th 2025)**
	Task 1.3	**BOKU**	Lab-scale validation of the e-gasifier (efficiency, gas quality, CO_2 capture) • New subtasks: Lab-scale evaluation of different electric heating concepts, investigation of thermochemical behaviour of the individual reactors of the new system • The lab-scale validation of the hot test plant will be delayed, since previous steps are delayed **(D1.3 and D1.4, due October 31st 2025)**
	Task 1.4	**BOKU, BEST, NTUA**	Transient operation and 'digital twin' verification

			• New subtasks: Investigation of transient behaviour of stationary fluidized bed with focus on electrical heating • The data base conceived by NTUA and BEST could be developed at a later stage • The CFD model of the gasifier developed by NTUA will focus on the gasification reactor and riser. **(D1.2, due April 30st 2025)** • The CFD model will be validated with SER data from literature respectively from experience of BOKU team members who did significant research on SER.
WP6	Task 6.2	**BOKU, BEST**	Heat integration and implementation of an Advanced Process Control (APC) scheme • The heat integration of the complex process chain might be delayed, due to the delay of the hot test plant design, especially when considering the implementation of the electrical heating **(D6.2, due April 30th 2025)** • BEST's simulation builds on using the optimized process chain, and is therefore delayed if the optimization of heat integration is delayed
	Task 6.3	**BOKU, FAU, ELEC**	Steady-state validation of the lab-scale process chain at BOKU's labs • The implementation of the whole process chain could take place using a substitute gasifier in another lab of one of the project partners (BEST, Simmering; FAU, Heatpipe Reformer), if the hot test plant will not be ready in time **(M8, due October 31th 2025)**
	Task 6.4	**BOKU, FAU, ELEC, BEST, NTUA**	Intermittent operation of the lab-scale process chain at BOKU's labs • The transient operation of the whole process chain could take place using a substitute gasifier in another lab of one of the project partners (BEST, Simmering; FAU, Heatpipe Reformer), if the hot test plant will not be ready in time **(D6.3, due October 31st 2025)** • BEST's comparison of the process behaviour with the artificial siblings and the publishing of processed data by NTUA depends on whether the gasifier is ready or not for the validation of the lab-scale process chain

1.3 Revised Schedule for each affected task



1.4 Proposed shift in deliverables and milestones



2. Design of e-gasifier

2.1 Critical process characteristics

In section 1.1.2, the key properties of the novel reactor concept including the functions of the newly introduced reactors (segregator and converter) are described. The purpose of the gasification reactor (GR), namely partial conversion of feedstock (drying, devolatilization and partial gasification) and partial carbonation of the bed material at a temperature < 750 °C, does not change in the new concept. The lower part of the GR is realized as bubbling fluidized bed (BFB). However, for the dimensioning of the counter-current column (CCC) it must be considered, that the additional product gas (PG) from the converter (which is mixed with the PG from the GR in the freeboard below the CCC) significantly increases the volume flow rate. In classical DFB gasification processes, the riser (also labeled as combustion reactor) must be designed to match specifications regarding the air-to-fuel ratio (λ) as well as fluidization (U/U_{mf}, U/U_t), where U_{mf} represents the minimum fluidization velocity and U_t represents the terminal velocity where drag forces balance the gravimetric forces of the bed material particles. Circulating fluidized beds (fast fluidization regime) are typically operated with a superficial gas velocity of 4-8 m/s [4]. In the proposed concept, the fluidization medium of the riser does not take part in any chemical reaction, but only serves the proper fluidization of the reactor. Staging of the fluidization medium is required in order to have additional control of the bed material entrainment and thereby the global solid circulation. The necessary heat for the calcination of the bed material and the high reactor temperature (> 900 °C due to the equilibrium of CO_2 and $CaO/CaCO_3$) must be maintained by electrical heating. Therefore, heating elements with a sufficiently large surface area and capable to endure the thermal and mechanical stress in the circulating fluidized bed must be installed (the larger the heat exchange area, the smaller the required temperature difference between the bed and the heating elements). The segregator has two functions: First, segregation at slow fluidization conditions and second, transport of the char into the converter. To keep the required mass flow of fluidization medium (steam, that does not directly take part in chemical reactions) relatively low, the cross-section area of the segregator should be kept small. In order to change the fluidization regime within the segregator from a mildly bubbling (segregation) to an entraining fluidized bed (transport of char), a second fluidization stage and a reduction of the reactor cross section in the upper part of the segregator are necessary. The converter must be designed to provide high temperature (> 850 °C) and a long residence time of the char particles to ensure sufficiently fast char conversion and avoid its accumulation in the loop GR-segregator-converter. Due to the slower kinetics of the gasification reactions (compared to devolatilization or combustion), the converter is realized as BFB. Analogously to the riser, the surface area of the heating elements in the converter must be appropriately designed. Because of the higher feedstock conversion compared to classic DFB gasification, more gasification agent (steam) must be supplied. This additional amount of steam is supplied to the converter. From a global perspective, the plant must be able to handle different load scenarios. This means, that the BFB reactors (GR and converter) must be operable with lower steam mass flows, and the circulating solid mass flow rates must be controllable via the fluidization of the transporting fluidized bed reactors (riser and segregator).

2.2 Process simulation

Simulation of the process is needed for computing the required flow rates of input and output streams and the required electrical power supplies for the reactors. These process parameters are essential for dimensioning the reactors and heating elements as well as for defining specifications of actuators (valves, pumps, compressors, …) and sensors.

2.2.1. Model description

The steady state model for simulating the proposed gasification system (sketched in Figure 2) is derived from a modelling approach described in detail in [5]. It contains different units in which conservation of mass (elements) and energy is preserved and certain physical phenomena are modelled (chemical reactions, heat transfer, …). These units are connected with different types of material streams (water/steam, gaseous, organic solid and inorganic solid). Modelling and simulation of the process are conducted with the commercial steady-state equation solver for mass- and energy balances IPSEpro. Formulation and implementation of energy balances as well as the used sources for property data can be inferred from [5]. The flowchart of the presented model is depicted in Figure 4. The main units are the gasification reactor (GR), the calcination reactor (riser), the segregator and the converter. The counter-current column (CCC) of the GR is not modelled. This means that the product gases (PG) from the GR and the converter are mixed as output of the individual reactor units and the final PG is not in chemical equilibrium (not relevant for the plant design). The modelled fluidized bed reactors are treated as ideally mixed vessels with uniform bed temperatures. The solid circulation rate is assumed to be controllable via adjustments of the gas staging in the riser.

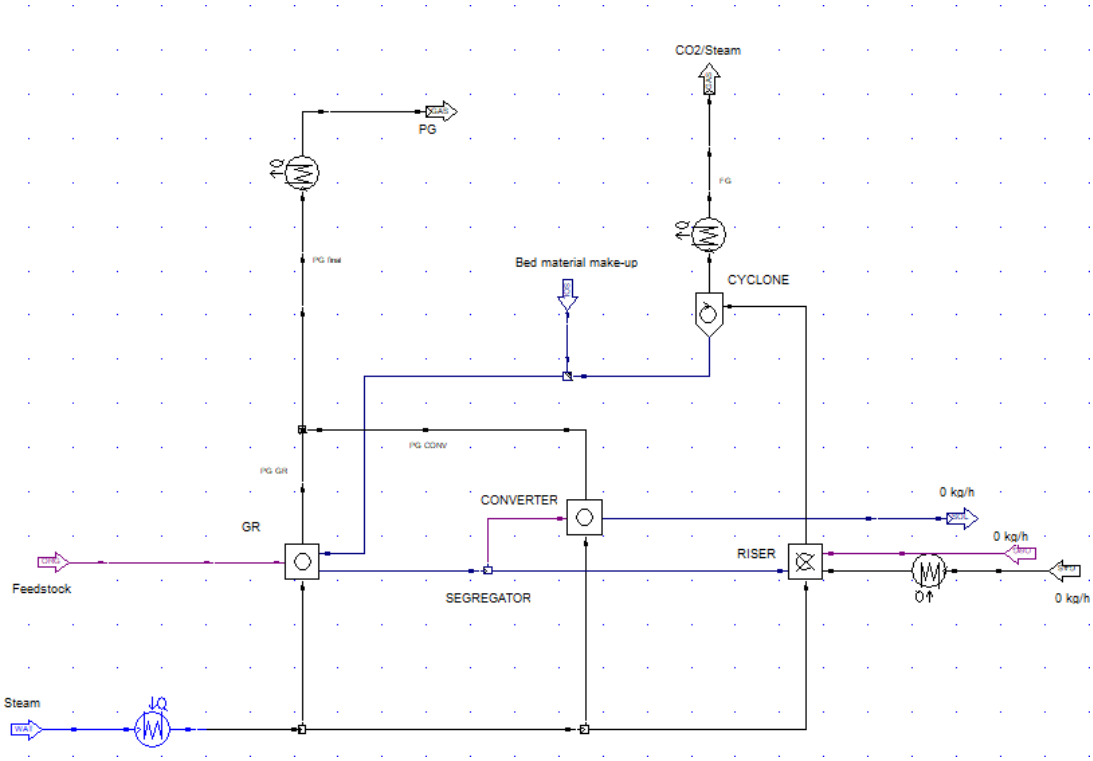


Figure 4 Screenshot of the process flowsheet in IPSE. Some material streams are set to 0 and can be ignored (indicated with 0 kg/h).

The temperatures of the individual fluidized bed reactors are set as parameter input. Except for the GR, material streams exit the reactors with these predefined reactor temperatures. The energy balance of the GR determines the necessary circulating bed material flow rate. The bed material supplies energy by entering the GR with elevated temperature and via the carbonation reaction it partially undergoes in the GR. The energy balances of the riser and converter are closed via the electrical power input. A detailed description of the unit models of the individual reactors (GR, segregator, converter and riser) and the compositions of the material streams can be found in the Appendix.

2.2.2. Parameter settings

In order to run the simulation, a set of parameters must be defined, e.g., composition and state of input streams and heat losses of reactors. These parameters are derived from a defined operating point that is used for designing the plant. Converter and segregator are modelled as ideal reactors for the design case. This means, that the segregator perfectly separates the two particle types (bed material and char) and the separated char is completely converted to PG in the converter. The heat loss of lab-scale DFB reactors is typically within the range of 20-30 % of the design value of thermal fuel input power [1]. Because of the lower GR temperature in case of the SER process, a heat loss at the lower bound of this range can be estimated. However, due to the additional reactors of the proposed concept, a global heat loss of 30 % (15 kW) is considered, roughly allocated to the reactors according to their temperatures and approximated surface areas. The bed material inventory of the GR is estimated according to the reactor volume. For the GR and the converter, the steam-to-fuel ratio $\varphi_{S/F}$ is defined as the steam input to the reactor (steam + water content of fuel) divided by the organic fuel input. For the GR it is set slightly lower than for common DFB biomass gasification because of the lower biomass conversion in the SER process. For the converter it is set with the aim to provide a considerable steam excess for the gasification. For the riser and the segregator, the required steam mass flow is not determined chemically (it only serves as fluidization agent). The parameter values of the design case are shown Table 1. This includes also the representative compositions of the material input streams. The composition of the feedstock (softwood) used for the simulation is taken from the Phyllis 2 database (https://phyllis.nl). The CaO-content of the ash is contributing to the carbonation-calcination cycle while the rest of it is treated as chemically inert (SiO_2). Fresh limestone is assumed to be 100 % $CaCO_3$. The energy demand for generating the 450 °C steam needed for the process and the thermal energy content of the product gas and flue gas are not considered in the simulation.

Table 1 Simulation parameters for the design case.

Parameter	Value	Unit	Reference
	GR		
$P_{th,fuel}$	50	kW	
$\varphi_{S/F,GR}$	0.7	kg/kg	
$w_{H2O,feedstock}$	0.15	kg/kg	
T_{GR}	700	°C	
$T_{PG,GR}$	800	°C	
$m_{bed,GR}$	7	kg	assumption
$\dot{Q}_{loss,GR}$	3.75	kW	assumption
$y_{CH4,PG,GR,wf}$	13.8	$vol\%_{wf}$	[1]

$y_{C2H4,PG,GR,wf}$	1.8	vol%$_{wf}$	[1]
$y_{C2H6,PG,GR,wf}$	0.7	vol%$_{wf}$	[1]
$\beta_{tar,PG,GR,wf}$	4	g/Nm$^3_{wf}$	[1]
$\beta_{dust,PG,GR,wf}$	0	g/Nm$^3_{wf}$	simplified assumption
$\beta_{char,PG,GR,wf}$	0	g/Nm$^3_{wf}$	simplified assumption
	Segregator		
$\dot{Q}_{loss,SEG}$	0	kW	assumption
$\eta_{bed,SEG}$	1	-	simplified assumption
$\eta_{char,SEG}$	1	-	simplified assumption
	Converter		
$\varphi_{S/F,CONV}$	2	kg/kg	
T_{CONV}	900	°C	
$\dot{Q}_{loss,CONV}$	5	kW	assumption
$y_{CH4,PG,CONV,wf}$	0	vol%$_{wf}$	[6]
$y_{C2H4,PG,CONV,wf}$	0	vol%$_{wf}$	[6]
$y_{C2H6,PG,CONV,wf}$	0	vol%$_{wf}$	[6]
$\beta_{tar,PG,CONV,wf}$	0	g/Nm$^3_{wf}$	[6]
$\beta_{dust,PG,CONV,wf}$	0	g/Nm$^3_{wf}$	simplified assumption
$\beta_{char,PG,CONV,wf}$	0	g/Nm$^3_{wf}$	simplified assumption
	Complete char conversion (long enough residence time is supposed)		
	Riser		
T_{RIS}	900	°C	
U_{RIS}	7	m/s	[4]
$\dot{Q}_{loss,RIS}$	6.25	kW	assumption
$\eta_{cyclone}$	0.995	-	assumption
	Global		
$T_{steam,in}$	450	°C	
	Woody feedstock (spruce)		
$w_{ash,wf}$	0.7	wt%$_{wf}$	
$w_{C,wf}$	48.4	wt%$_{wf}$	
$w_{H,wf}$	5.9	wt%$_{wf}$	
$w_{O,wf}$	44.675	wt%$_{wf}$	
$w_{N,wf}$	0.3	wt%$_{wf}$	
$w_{S,wf}$	0.02	wt%$_{wf}$	
$w_{Cl,wf}$	0.005	wt%$_{wf}$	
$LHV_{wf,Boie}$	17.6	MJ/kg$_{wf}$	
	Ash		

$w_{CaO,ash}$	27	wt%	[7]
$w_{SiO2,ash}$	73	wt%	

2.2.1. Simulation results

The resulting volume flow rates of fluidization agent and PG as well as the required heat supplies to the riser and the converter, which are relevant for dimensioning the reactors and heating elements are presented in Table 2.

Table 2 Design-relevant results of the simulation of the design operating point.

Reactor	Parameter	Parameter symbol	Unit	Value
GR	Steam to GR	$\dot{V}_{steam,GR,in}$	Nm^3/h	6.8
GR	PG from GR	$\dot{V}_{PG,GR,out}$	Nm^3/h	15.4
Converter	Steam to converter	$\dot{V}_{steam,CONV,in}$	Nm^3/h	5.0
Converter	PG from converter	$\dot{V}_{PG,CONV,out}$	Nm^3/h	8.6
Converter	El. heating converter	$P_{el,CONV}$	kW	10.5
Riser	El. heating riser	$P_{el,RIS}$	kW	25.3

2.3 Reactor geometries

The cross-sectional areas of the reactors have to be chosen based on the computed volume flow rates and the limitations of the desired fluidization regimes. The state of fluidization strongly depends on the bed material properties. According to [8], the limestone particles have a density of 1600 kg/m^3 in the fully calcined state and 2650 kg/m^3 in the fresh carbonated state. Therefore, a mean particle density of 2000 kg/m^3 is taken for the calculation of the fluidization regime. As mean diameter d_{sv}, 350 µm is chosen. Definitions of dimensionless numbers and correlations for the boundaries of the fluidization regimes can be inferred from [9]. The chosen reactor cross sections and the resulting fluidization numbers are presented in Table 3. The fluids and the temperatures used for calculating these operating points are also stated in the table. Additionally, the operating points are indicated in the Grace diagram shown in Figure 5.

The BFB gasification reactors (GR and converter) are designed to realize a fluidization number U/U_{mf} of about 10 for the inlet steam flow rate. This value is chosen, because it enables part load operation of the plant with lower steam supply (for a well-mixed BFB U/U_{mf} needs to be > 5). Based on this criterion, the cross section of the GR and the converter are set to 0.15 x 0.1 m and 0.15 x 0.08 m, respectively. Due to the biomass conversion, the volume flow rate increases along the reactor height, which also increases the fluidization number accordingly. The GR has an expanded freeboard that ensures, that no bed material is transported from the BFB upwards into the CCC.

In case of the riser and the segregator, the volume flow rates are not determined by chemical reactions. Therefore, these reactors theoretically could be designed deliberately small in order to minimize the steam

demand and thereby the energy consumption of the plant. However, the diameter of the riser is set to 0.08 m in order to ensure broad applicability of the plant (for classic DFB gasification and chemical looping combustion). The diameter of the upper transport pipe of the segregator must be bigger than the char particles and is therefore set to 0.04 m. The lower rectangular part of the segregator has a cross section of 0.07 x 0.06 m in order to provide a sufficiently long residence time for the segregation process. However, the design and dimensions of the segregator is the biggest unknown of the reactor system and these geometries are only a first attempt, that must be investigated and optimized in cold flow model studies (addressed later in this report). The loop seals have a cross section of 0.12 x 0.05 m and are fluidized with $U/U_{mf} = 3$.

Table 3 Overview of the fluidization regimes in the individual reactors for the design case.

Reactor	Zone	Cross section	Medium	T / °C	Flow rate / Nm^3/h	U / m/s	Fluidization number
GR	BFB inlet	0.15 x 0.1 m	Steam	700	6.8	0.449	$U/U_{mf} = 9.12$
GR	BFB outlet	0.15 x 0.1 m	PG	700	15.4	1.016	$U/U_{mf} = 17.72$
CCC	free	D = 0.11 m	PG	800	27.2	3.123	$U/U_t = 1.16$
CCC	constricted	D = 0.06 m	PG	800	27.2	10.411	$U/U_{se} = 1.17$
Segregator	lower zone	0.07 x 0.06 m	Steam	700	0.31	0.074	$U/U_{mf} = 1.5$
Segregator	upper zone	0.07 x 0.06 m	Steam	700	3.20	0.754	$U/U_{mf} = 15.33$
Segregator	transport zone	D = 0.04 m	Steam	700	3.20	2.519	$U/U_t = 1$
Converter	inlet	0.15 x 0.08 m	Steam	900	5.0	0.497	$U/U_{mf} = 12.21$
Converter	outlet	0.15 x 0.08 m	PG	900	8.6	0.855	$U/U_{mf} = 17.29$
Riser		D = 0.08 m	Steam	900	29.5	7	$U/U_{se} = 0.76$

The relevant volume flow rate for the CCC is the sum of the gas streams exiting the GR, the converter and the segregator. Based on the findings from [9], the ratio of the constricted cross sections along the CCC to the free cross section is set to 30 %. In the constriction U/U_{se} should be about 1 and in the free section U/U_t should be about 1. Based on this, the diameter of the CCC is set to 0.11 m. Four constrictions are arranged equidistantly below the bed material input.

The heights of the BFB's (and thereby the reactor heights) were chosen to realize bed pressure drops of about 100 mbar. The vertical positions of the reactors with respect to each other were chosen under the consideration that the reactors behave similar to communicating vessels and the transporting pipes and loop seals cause pressure drops.

A CAD drawing has been generated for the scaled CFM and is presented in Chapter 3 and the Appendix. The main reactor dimensions of the E-Gasifier and its CFM are presented in Table 5. The experimental

findings of the CFM studies will be the basis for the reactor design in the engineering phase of the 50 kW_{th} reactor system.

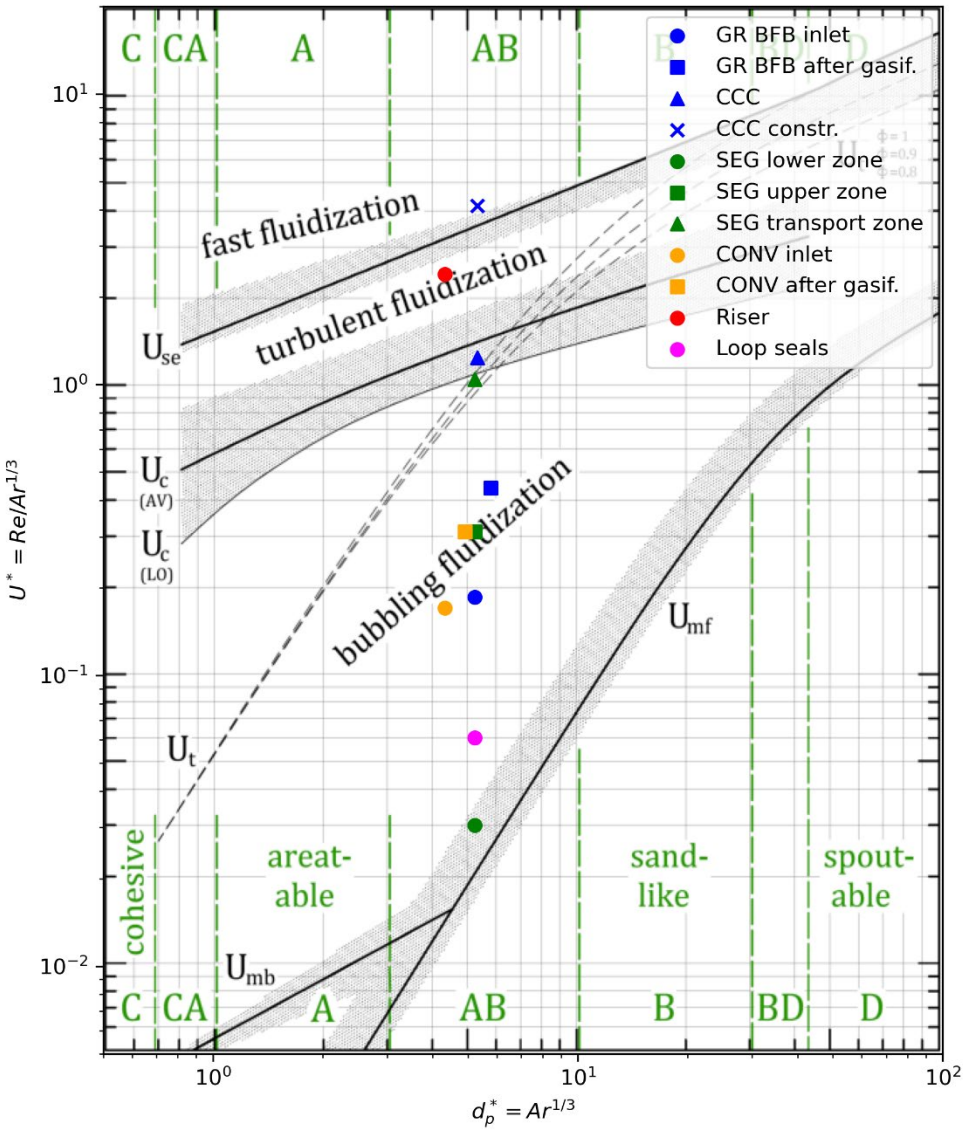


Figure 5 Operating points of the individual fluidized bed reactors of the e-gasifier for the design case indicated in the dimensionless Grace diagram.

2.4 Heating elements

In addition to the process simulation regarding the goal of creating a synergy between DFB biomass gasification with renewable electricity, a practical concept for supplying the heat in fluidized bed systems needs to be developed. The topic of heating fluidized beds by means of electrical energy has gained increased interest in recent years due to the industrial requirements for decarbonization and future perspectives for making use of peak electricity capacities in an energy market increasingly relying on renewable energy resources [10]. However, heating concepts for fluidized bed systems are subject to several limitations and have to be comparably resistant to withstand the thermal and mechanical stress in

DFB gasification systems. The primary considerations for the development of heating elements suitable for the novel reactor concept outlined above are:

- Heat transfer: Although fluidized beds in general are characterized by highly homogenous temperature distribution, the heat transfer from electrical heating sources may be limited by the interplay of conductive and convective transport in the fluid dynamics. Furthermore, the applicability of external heating elements, e.g., heating shells on the reactor walls, may create radial temperature gradients and are limited in their scaling capacity due to the functional correlations of reactor surface and volume.
- Mechanical resistance: Reactor-internal heating elements have to be highly resistant to the erosive environment in the fluidized bed.
- Chemical resistance: Reactor-internal heating elements should be highly chemically inert to the chemical environment in the reactors. This also includes the chemical inertia towards reactions that may degrade the heating elements by means of reduction in the steam-fluidized and sub-stoichiometric ($\lambda<1$) systems.
- Cyclic stability: Variations in process load and operational modes require the material of the heating elements to be highly resistant to thermal cycles. The mounting and heating elements configurations in the reactor also need to consider the thermal expansion of the material. Furthermore, the control of the reactor temperature by means of electrical load should target a minimum response time.
- Process interference: The geometry and local temperature gradients close to the heating elements should not inflict changes on the overall DFB gasification process. It must be considered that reactor-internal heating elements may work as baffles for the fluid dynamics and create local areas with elevated temperature that may overheat individual particles and reactor zones and influence the kinetics of chemical reactions.

Based on these considerations, the development of suitable heating elements for implementation in the novel reactor concept is conducted. The application in the calciner and in the converter requires similar specifications for the material and geometry of the heating elements. Due to the planned implementation of the heating elements in large-scale facilities, reactor-internal heating elements are considered advantageous for the evaluation. An experimental evaluation of suitable heating concepts and elements is planned to be conducted in a 20 kW_{th} lab-scale fluidized bed at BOKU. The experimental findings will provide the basis for the incorporation of electrical heating elements in the engineering of the 50 kW_{th} reactor system.

3. Cold flow model of e-gasifier

3.1 Purpose

Cold flow models (CFM) are fluid dynamically scaled versions of hot reactors that allow investigating their fluid dynamic behavior at ambient temperatures. This has the advantage, that test campaigns are cheaper, faster and easier to conduct. CFMs made of acrylic glass have the convenience of being transparent, and therefore the fluid dynamic behavior can be qualitatively assessed by eye. Moreover, values that cannot

be easily obtained from the operation of a hot reactor unit such as the solid circulation rates can be measured in the CFM. However, CFM's do not give insights into the thermochemical processes of the studied reactor. Furthermore, the bed material and the fluidization settings must be appropriately chosen in order to produce data transferable to the hot plant.

In case of the presented novel electrically driven multi fluidized bed (MFB) reactor concept, the CFM is needed for studying the segregation and separation behavior inside the Segregator and for studying the controllability of the overall process (solid flow rates, separation efficiencies, pressure loops, bed levels relative to each other).

3.2 Scaling

For the design of the CFM, a geometric scaling factor of 1:2 was chosen, which is a compromise in order to reduce the reactor heights without generating reactors with very small cross sections, which would increase the interaction between particles and walls unrepresentatively. Not only the reactors, but also the cyclones, connection pipes and loop seals are scaled according to this ratio. In order to establish fluid dynamic similarity of the designed hot lab-plant and the CFM, the scaling laws of Glicksman are used for calculating the required bed material properties and volume flow rates [11]. These scaling criteria state, that the following dimensionless numbers must be equal for the hot plant and the CFM: Reynolds particle number Re_p, Archimedes number Ar, density ratio of particle and gas, Froude number Fr, geometric ratio of reactor and particle, height-to-diameter ratio of reactor, particle sphericity and particle size distribution. However, under the limitations of reality, it is not possible to perfectly match these numbers. Furthermore, the reactors of the E-Gasifier are operated at different temperatures and even the bed material changes its properties in the SER process, therefore it is not possible to comply with the scaling laws for all reactors at the same time. For reasons of practicability, humidified air at room temperature is used as fluidization medium. Based on that, the required bed material properties and superficial gas velocity can be calculated with the similarity laws of Glicksman. However, the desired particle properties cannot be matched due to the limitations of reality. Bronze particles, which are a good approximation of the ideal bed material due to its high density, are chosen as bed material for the CFM. Also, the reactor diameters calculated via the Glicksman laws are not sensible to realize, because they would become very small causing unwanted wall effects (significantly lower volume-to-wall surface ratio of the reactors compared to the hot plant). In Table 4 the bed material and fluidization parameters of the hot plant (exemplary for steam with 700 °C) are compared with those calculated according to the scaling laws and the actually implemented ones. In Figure 6, the vertical line in the Grace diagram is indicated, on which operating points of the CFM lay on (d_p^* only depends on the fluid and particle properties and is therefore fixed for the CFM). With the bed material and the fluidization medium being defined, the superficial gas velocity is the remaining parameter that has to be set in a reasonable manner to replicate the fluidization regime in the hot plant. This is done by choosing the relevant fluidization numbers (U/U_{mf}, U/U_{se} or U/U_t) for the individual reactor zones as the parameter, which is kept constant.

Table 4 Comparison of the geometry and material properties of the hot plant, the ideally scaled CFM (according to Glicksman laws) and the actual CFM.

Parameter	Unit	Hot	Glicksman [11]		Used	
			abs. value	ratio	abs. value	ratio
Fluid		Steam	Air	-	Air	-
Bed material		$CaO/CaCO_3$	-	-	Bronze	-
$\boldsymbol{T}$	°C	700	22	-	22	-
$\boldsymbol{\rho_f}$	kg/m3	2.26e-1	1.20e+0	5.30	1.20e+0	5.30
$\boldsymbol{\mu_f}$	Pa·s	3.66e-5	1.83e-5	0.50	1.83e-5	0.50
$\boldsymbol{d_{sv}}$	µm	3.50e+2	7.26e+1	0.21	8.00e+1	0.23
$\boldsymbol{\rho_p}$	kg/m3	2.00e+3	1.06e+4	5.30	8.72e+3	4.36
$\boldsymbol{Ar}$	-	1.42e+2	1.42e+2	1	1.56e+2	1.1
$\boldsymbol{\rho_p/\rho_f}$	-	8.86e+3	8.86e+3	1	7.29e+3	0.82
Geometric ratio	-	D_{hot}	$0.21 \cdot D_{hot}$	0.21	$0.5 \cdot D_{hot}$	0.5

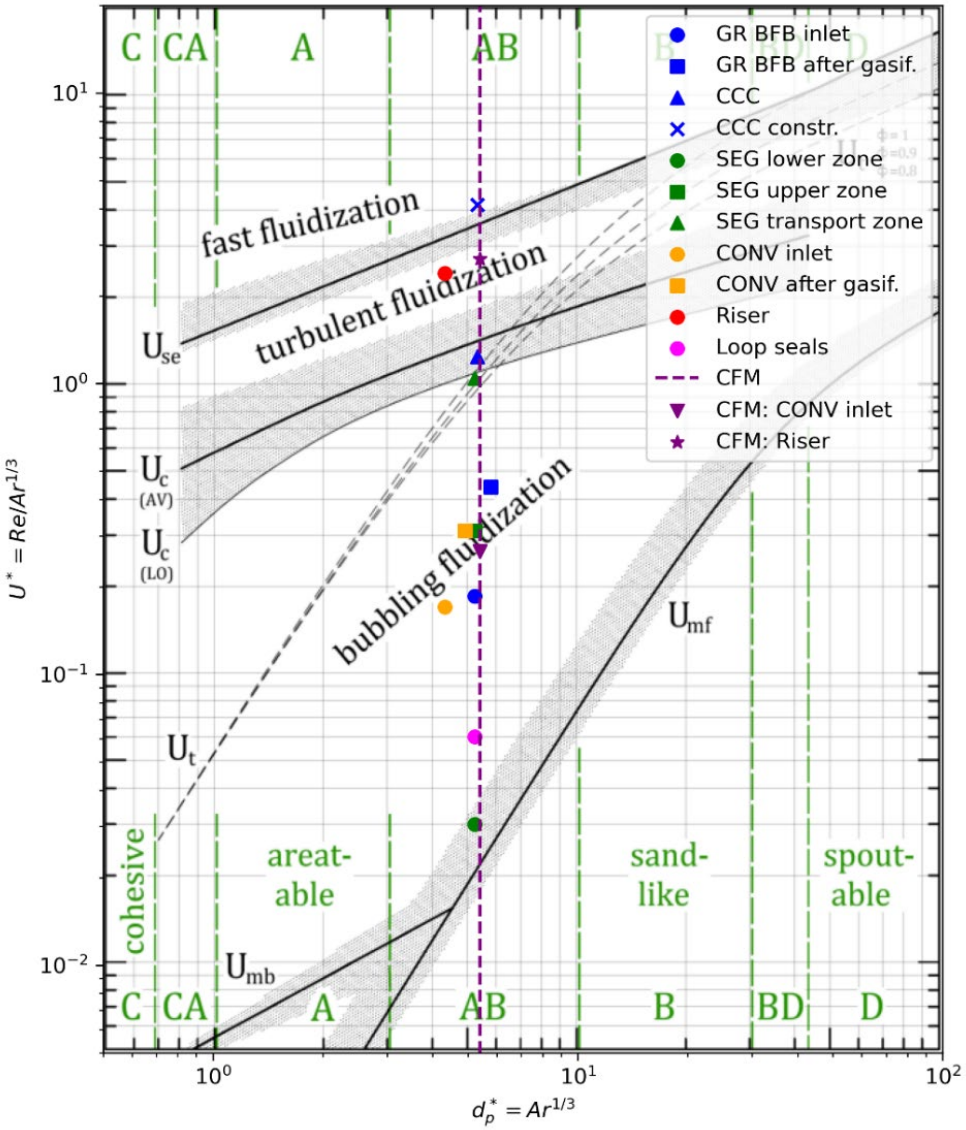


Figure 6 Comparison of fluid dynamic operating points in the hot plant and in the CFM. The vertical line for the CFM is determined by the choice of fluid and bed material. The position on this point depends on the superficial gas velocity. To avoid overcrowding the diagram, only two exemplary operating points of the hot plant are also indicated for the CFM. Scaling criteria: Converter inlet → U/U_{mf} = const., Riser → U/U_{se} = const.

3.3 Model description

The reactors, loop seals, cyclones and connecting tubes of the CFM are made of acrylic glass. Tubes and reactors are connected to each other via flexible silicone tubes to prevent tension-caused breakings. Furthermore, this allows uncomplicated adaptations of certain reactor parts. Local sinks at low points are equipped with ball valves which enable fast discharge of the complete bed material. Figure 7 shows the CFM as 3D CAD drawing and in real life. Furthermore, 2D technical drawings of the individual CFM-parts can be found in the Appendix. In order to decrease electrical charging of the CFM, it was wrapped with a grounded copper band that allows electrically charged particles to be conducted away.

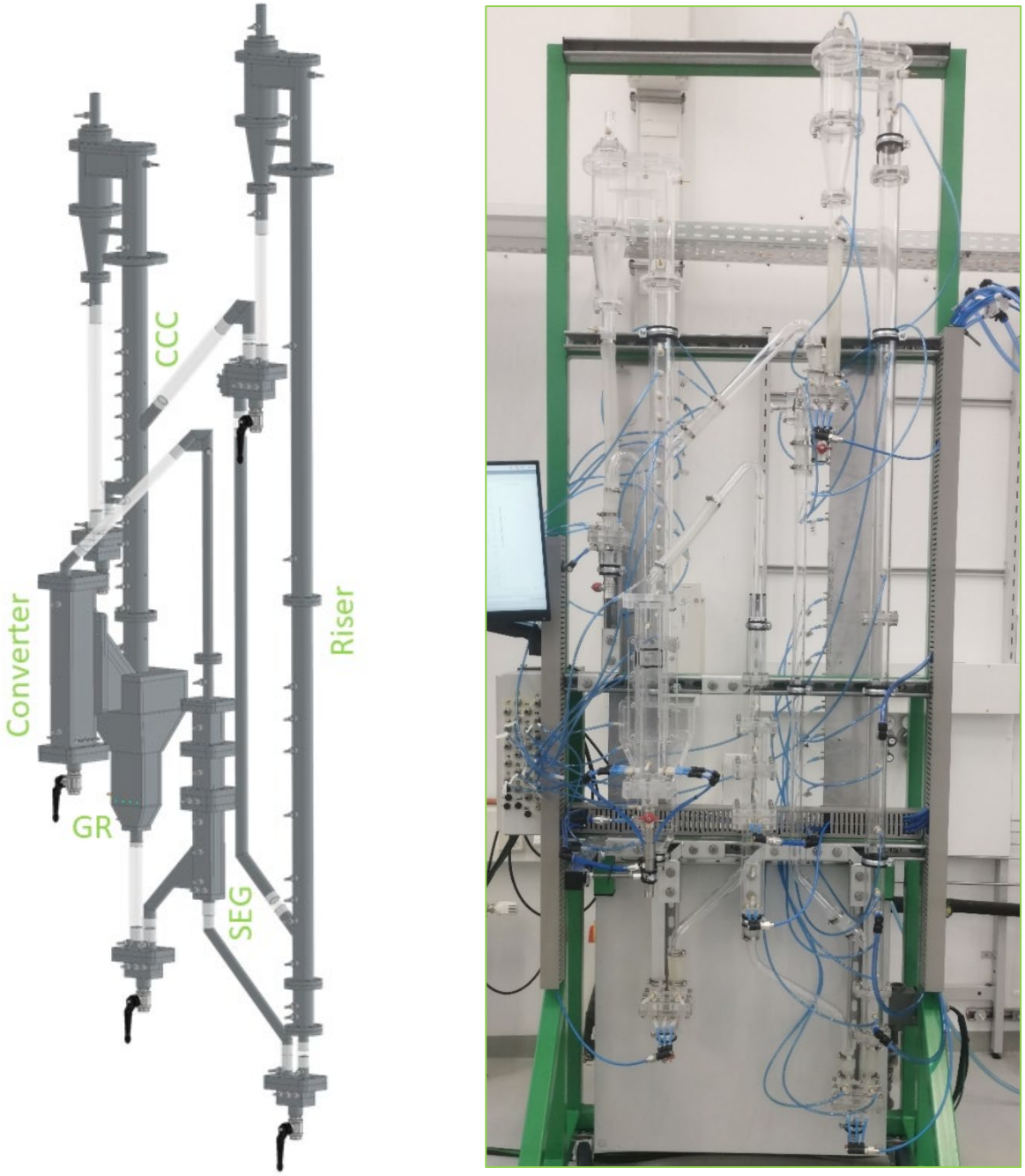


Figure 7 CFM: 3D CAD model and picture.

3.3.1. Geometry

In Table 5 the main reactor geometries of the hot plant and the CFM are listed. Due to the chosen geometric ratio for the scaling, all the geometries of the CFM are the half of those of the hot plant. The geometry of the segregator is a main focus of the CFM investigations and therefore not fixed yet for the hot plant. The diameter of the CCC is the only dimension that does not follow the scaling ratio of 1:2. This is caused by the fact, that in the initial design calculation which was used for the CFM design, a lower steam supply to the converter was considered which led to a lower PG flow rate in the CCC. This minor adjustment

in the scaling dimensions can be easily compensated by installing constrictions with a larger cross section than initially planned.

Table 5 Comparison of the main reactor geometries of the planned hot plant and its CFM.

Geometry	Hot plant	CFM
$\boldsymbol{d_{sv,mean}}$ / µm	~ 350	~ 80
$\boldsymbol{D_{riser}}$ / mm	80	40
$\boldsymbol{H_{riser}}$ / mm	4600	2300
$\boldsymbol{L \times W_{GR,BFB}}$ / mm x mm	150 x 100	75 x 50
$\boldsymbol{D_{GR,CCC}}$ / mm	110	50
$\boldsymbol{H_{GR,total}}$ / mm	3200	1600
$\boldsymbol{L \times W_{CONV}}$ / mm x mm	150 x 80	75 x 40
$\boldsymbol{H_{CONV,bed}}$ / mm	500	250
$\boldsymbol{L \times W_{SEG}}$ / mm x mm	to be determined	currently 35 x 30
$\boldsymbol{D_{SEG,outlet}}$ / mm	to be determined	currently 20
$\boldsymbol{H_{SEG}}$ / mm	to be determined	

3.3.2. Measurement equipment

The volume flow rates of air supplied to the fluidization nozzles of the reactors are measured with analogue variable area flowmeters (Krohne VA40 and DK48) and are adjusted manually via needle valves. The specific measurement ranges of the flowmeters are shown in Table 6.

Table 6 Measurement ranges of the installed flowmeters. If there are more than one fluidization stages for a reactor, they are numbered according to their vertical position (from bottom to top).

Fluidization	Range / Nm^3/h
GR	1.3 – 13
Segregator 1	0.04 – 0.4
Segregator 2	0.5 – 5
Converter	0.8 – 8
Riser 1	0.2 – 16
Riser 2	0.2 – 16
Riser 3	0.2 – 16
Loop seals (4x)	0.14 – 1.4

56 possible pressure measurement nozzles are arranged over the reactors and the loop seals in order to measure the pressure profiles of the reactors and the pressure drops of the tubes transporting bed material. Pressure is measured via electronic pressure transmitters (Kalinsky DS2-420) with different measurement ranges (0-50 mbar, 0-100 mbar, 0-250 mbar and 0-500 mbar) depending on the position of the measurement nozzle. The 4-20 mA signals of the pressure transducers are converted into a voltage signal with 392 Ω precision resistors (0.1 % tolerance), which are placed serially to the transducers. A Raspberry Pi (4B) equipped with voltage measurement DAQ HATs (Digilent MCC118) is used for measuring the voltages (30 % of the maximum 12 bit resolution are used, yielding a step size of 0.08 % of the sensor range) and calculating the corresponding pressure values. The theoretical maximum sample rate for 8 installed DAQ HATs is 5 kS/s for each channel. Because the pressure typically fluctuates at a certain point in a fluidized bed, the measured pressure values must be averaged over time in order to obtain a smooth signal. This is done by calculating a moving average of the sampled pressure measurements.

Furthermore, a stand-alone inductivity-based detection system for ferromagnetic tracer particles can be used for measuring residence time distributions in certain sections of the reactor system [12].

The installation of measurement equipment for measuring solid circulation mass flows (also for selectively measuring mass flows of different particle types) is one of the next steps to improve the versatility of the CFM.

3.3.3. 3D-printed parts

For reasons of flexibility, the constrictions along the CCC are not fixed but can be mounted at fixed heights with screws. This allows investigating different element shapes (3D-printed, example shown in Figure 8) and diameters of constrictions as well as the installation of different numbers of constrictions. Additionally, the model can also be operated without constrictions. This can be useful for reducing the complexity of the system for investigations which are independent of the CCC behavior. For investigations addressing the impact of the constrictions, the non-constricted CCC can be taken as base case.

Figure 8 Example of a 3D-printed constriction, that is mounted in the CCC of the CFM.

Furthermore, the ducts connecting the GR/riser and the corresponding cyclones can be adapted by installing 3D-printed wall attachments. Thereby the inclination and width of the duct can be changed, which for example can be necessary if other bed materials are tested.

3.3.4. Graphical user interface (GUI)

The GUI of the CFM runs directly on the Raspberry Pi which also reads in the signals from the pressure transducers and is displayed by a monitor directly mounted to the iron frame of the CFM. It was created with PyQt, the python implementation of the GUI development framework Qt. As shown in Figure 9, the GUI shows plots of the pressure profiles of the individual reactors (GR, riser, segregator and converter) as well as a plot of the negative gradient of the pressure profile of the CCC, which indicates the bed material hold-up between the constrictions. Additionally, the measured pressure values are also listed numerically. The data can also be logged to a csv-file. In the GUI, the user can adjust the sampling rate, the logging rate as well as the amount of data points used for the moving average. Furthermore, the current fluidization regimes in the different zones of the reactor system can be calculated by entering the set air flow rates.

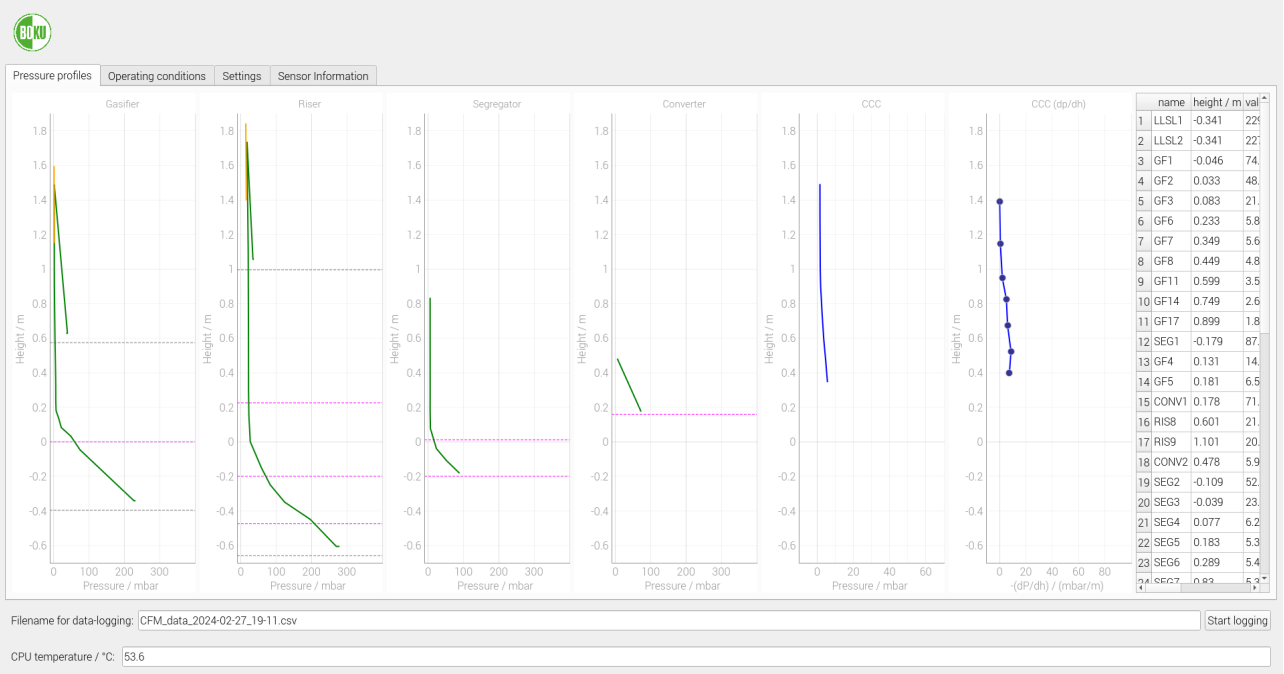


Figure 9 Screenshot of the GUI of the CFM. The green curves indicate the measured pressure profiles of each reactor. The blue profiles indicate the pressure profile of the CCC (necessary to determine the bed material hold-up of the CCC). Dotted horizontal lines indicate the heights of fluidization nozzles.

3.4 First insights

So far, first test runs were conducted to verify the general operability of the reactor system. It was shown that, as intended, two solid circulation loops (main loop: GR-segregator-riser, internal loop: GR-segregator-converter) can be established. Via the fluidization settings, the solid mass flow in each loop can be adjusted.

A first set of 3D-printed constrictions (shown in Figure 8) was successfully installed in the CCC. Visually and in the pressure profile of the CCC, their expected impact was observed. Zones with increased bed material hold-up between the constrictions caused an increased pressure drop over the CCC. Exemplarily, the pressure profiles for two operating points with different flow rates passing the CCC, are depicted in Figure 10.

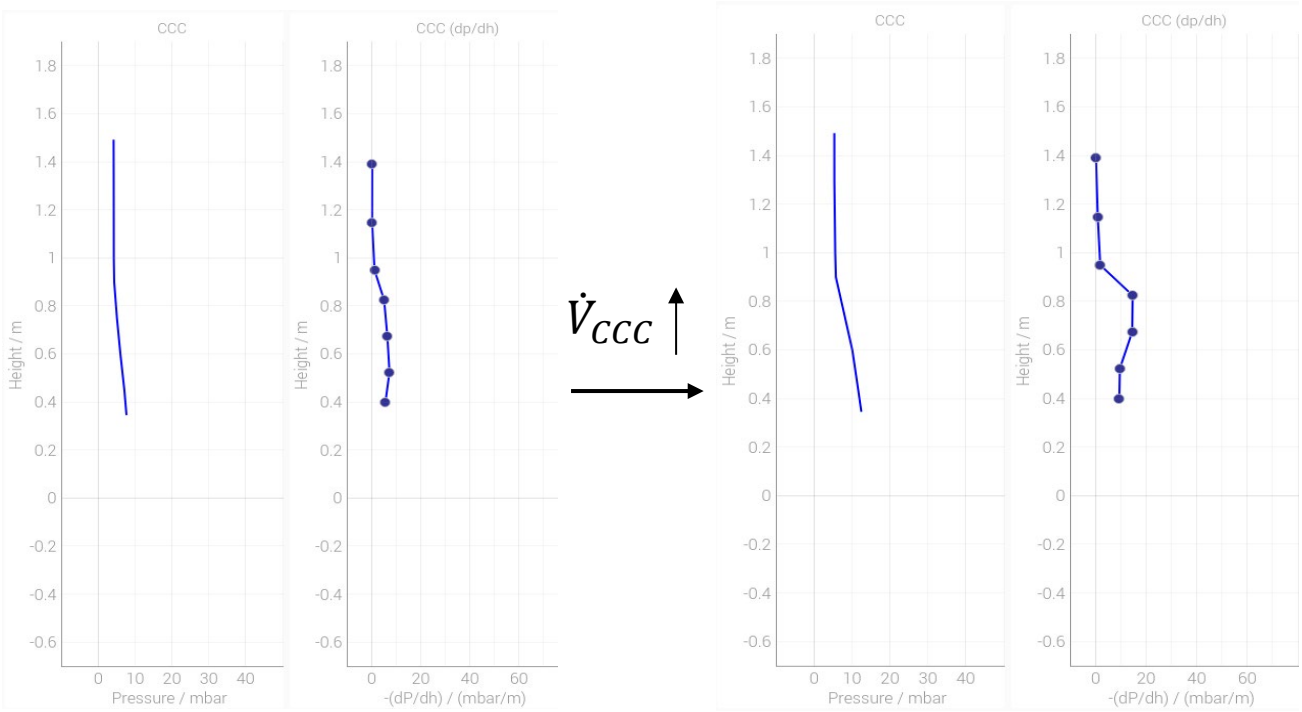


Figure 10 Illustration of the effect of the constrictions in the CCC. Increasing the gas flow rate in the CCC causes a higher bed material hold-up in the CCC and a correspondingly higher pressure drop. The pressure drop becomes clearly evident in the plot of the negative pressure gradient of the CCC. The higher the pressure gradient at a certain height, the higher the hold-up in this zone.

A first attempt to insert dummy char particles (polypropylene particles (PPP)) has shown difficulties to accomplish uniform mixing of bed material and PPP in the GR and therefore also the segregation phenomena could not be studied. The reason for this is most probably, that too much bed material and too much PPP were inserted into the system. Therefore, the bed surface level in the GR was at the middle of the height of the expansion between the smaller reactor cross section and the freeboard, which caused a corresponding lower U/U_{mf} at the top of the BFB and hence less mixing. Another possible challenge that was encountered so far, is the pneumatic transport of the PPP from the segregator to the converter after successful segregation. Because even though the lower-density PPP tend to float in a slightly fluidized bed, their terminal velocity U_t, the minimal velocity needed to realize pneumatic transport of an individual particle, is higher, than the terminal velocity of the bed material. In the upcoming months systematic investigations will be conducted to study the behavior of the segregator. Based on the conclusions drawn throughout these studies, the CFM will be further adapted and optimized.

4. Conclusion and outlook

This report details the advancements in work package 1 of the "CarbonNeutralLNG" project, which focuses on the development and construction of a 50 kW_{th} e-gasifier. The main take-away from this report is the development of an innovative multi-fluidized bed gasification reactor, which shows significant potential for improving key performance indicators such as cold gas efficiency and carbon conversion, while also enhancing the process flexibility. Steady state process simulation was employed to explore the novel process and to determine the process parameters relevant for designing the reactors (volume flow rates and electric power demand). Due to the innovative nature of the additional reactors required for this process, as opposed to traditional dual fluidized bed (DFB) reactors, cold flow model (CFM) studies have been initiated to refine the process design. A CFM has been constructed to examine the fluid dynamics within the system and to optimize reactor geometries. This necessary step has resulted in an adaptation of the original timeline outlined for this work package. The development of this novel reactor concept is inherently iterative, introducing uncertainties into the timeline for the process development and eventual realization of the hot lab-scale plant. Efforts are being made to ensure that alternative data sources, from process simulations and literature reviews, are available for collaborative tasks. In the upcoming months, CFM studies will be conducted to determine the optimal process design, reactor geometries, and operating conditions. Additionally, investigations into electric heating concepts will be conducted using a 20 kW_{th} bubbling fluidized bed reactor. The findings from these studies are critical for designing larger-scale reactor systems based on this new concept and will also aim at future objectives for integrating electrical energy sources into existing or new fluidized bed systems. These results will guide the detailed engineering of the 50 kW_{th} test plant.

Nomenclature

Latin

d_{sv}	m	Particle Sauter diameter
D	m	Reactor diameter
H	m	Reactor height
L	m	Length
m	kg	Mass
P_{el}	kW	Electrical power
P_{th}	kW	Thermal feedstock power
$\dot{Q}$	kW	Heat flow rate
T	°C	Temperature
U	m/s	Superficial gas velocity
U_{mf}	m/s	Minimum fluidization velocity
U_{se}	m/s	Significant entrainment velocity
U_t	m/s	Terminal particle velocity
$\dot{V}$	Nm^3/h	Volume flow rate
W	m	Width
w	-	Weight fraction
y	-	Volume fraction of gas mixture

Greek

β	g/Nm^3	Mass concentration
η	-	Efficiency
λ	kg/kg	Air-to-fuel ratio
μ	Pa·s	Dynamic viscosity
$\varphi_{S/F}$	-	Steam to fuel ratio
ρ	kg/m^3	Density

Dimensionless numbers

Ar	Archimedes number
Fr	Froude number
Re_p	Reynolds particle number

Subscripts

Bed	Bed material
CONV	Converter
f	Fluid
GR	Gasification reactor
p	Particle
PG	Product gas
RIS	Riser
SEG	Segregator
wf	Water free basis

Abbreviations

BFB	Bubbling fluidized bed
CCC	Counter-current column
CFB	Circulating fluidized bed
CFM	Cold flow model
DFB	Dual fluidized bed
GR	Gasification reactor
GUI	Graphical user interface
LHV	Lower heating value
MFB	Multi fluidized bed
P&I	Piping and instrumentation
PG	Product gas
PPP	Polypropylene particles
SER	Sorption enhanced reforming

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Appendix

Detailed model description for process simulation in IPSEpro

Institute of Chemical and Energy Engineering (IVET)

Model description for E-Gasifier

April 11, 2024

by

Gregor Karte

Contents

1 Unit models

1.1 Gasification reactor (GR)

1.1.1 Gasification

Gasification of biomass is modelled using a combination of a kinetic model for calculating the degree of fuel conversion and a pseudo-equilibrium model for determining the resulting gas composition. Drying and devolatilization are assumed to occur instantaneously. Depending on the gasification temperature, the remaining char yield is estimated via correlation 1 published by Pitkäoja and Ritvanen [1].

$$\dot{m}_{char,devol.} = \max[-1.72 \cdot 10^{-4}\, T + 0.3037,\ 0.17] \cdot \dot{m}_{biomass,wf} \tag{1}$$

Subsequent conversion of biomass char $\dot{m}_{char,pyr}$ through steam gasification is modelled with an n^{th}-order uniform reaction model:

$$\frac{\mathrm{d}X(t)}{\mathrm{d}t} = k_0 \cdot \mathrm{e}^{\frac{-E_A}{RT}} \cdot p_{H2O}^{n} \cdot (1 - X(t)) \tag{2}$$

The model parameters are taken from Barrio et al. [2] (determined from char from beech wood):

Table 1: Parameters of the kinetic model for steam gasification of biomass char.

E_A	$\frac{\text{kJ}}{\text{mol}}$	211
k_0	$\text{s}^{-1}\text{bar}^{-0.51}$	$1.71 \cdot 10^7$
n	-	0.51

Integration and rearranging of equation (2) yields the mass flow of residual char exiting the reactor after a mean residence time τ:

$$\dot{m}_{char,t=\tau} = \exp\left(-k_0 \cdot \text{e}^{\frac{-E_A}{RT}} \cdot p_{H2O}^n \cdot \tau\right) \cdot \dot{m}_{char,t=0} \tag{3}$$

The mean residence time of the char is assumed to equal the mean residence time of the bed material which can be concluded from the inventory of the reactor and the mass flow rate of circulating bed material. The composition of the char exiting the GR is estimated depending on the pyrolysis temperature (equals the temperature of the BFB in the GR) with empirically determined correlations by Neves et al. [3]:

$$w_{C,char} = 0.93 - 0.92 \cdot \text{e}^{-0.0042\,T} \tag{4}$$

$$w_{H,char} = -0.0041 + 0.1 \cdot \text{e}^{-0.0024\,T} \tag{5}$$

The mass fraction of oxygen results from closing the elemental balance (other elements are neglected).

The product gas (PG) is modelled to consist of H_2O, H_2, CO, CO_2, CH_4, C_2H_4, C_2H_6, N_2, HCl, H_2S, fly char, dust (originating from bed material and fuel ash) and tar. The feedstock fractions of N, Cl and S are directly converted to N_2, HCl and H_2S. The amounts of fly char, dust must be estimated. The remaining PG components are concluded from empirical data depending on the SER gasification temperature. The volume fractions of CH_4, C_2H_4, C_2H_6 and tars are computed via polynomial fits of data from [4]. For the remaining compounds H_2O, H_2, CO and CO_2 the logarithmic deviation from the equilibrium of the water-gas shift (WGS) reaction $p\delta_{eq,wgs}$

$$p\delta_{eq,wgs} = \log_{10}\left(\frac{\frac{p_{H2} \cdot p_{CO2}}{p_{H2O} \cdot p_{CO}}}{K_{wgs}(T)}\right) \tag{6}$$

is computed according to a correlation published by Fuchs et al. [5]. The gasification temperature inserted to these correlations is the bed temperature of the GR (not the temperature of the exiting PG). Due to the counter-current flow of hot bed material and PG in

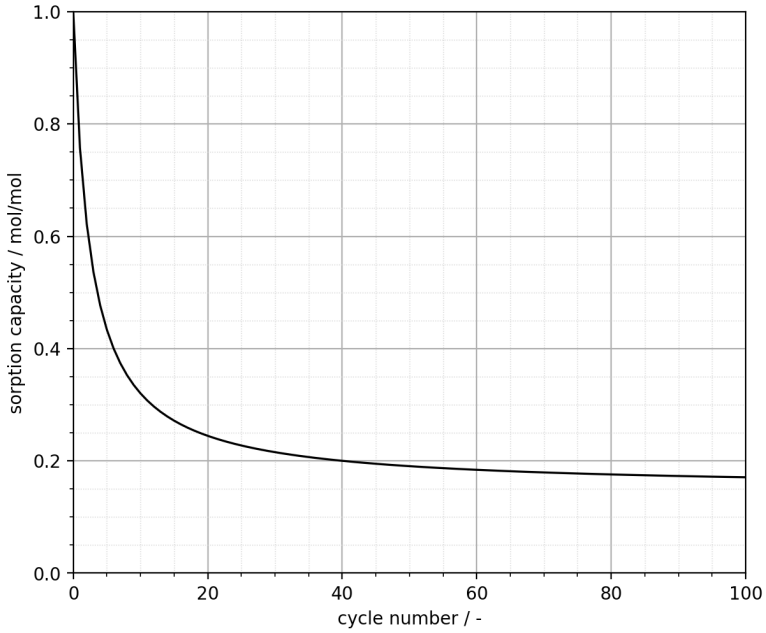

Figure 1: Sorption capacity of CaO depending on the number of calcination/carbonation cycles.

counter-current column, the PG exits the GR with a temperature $T_{PG,GR} > T_{GR}$, which must be defined. The ash input as part of the fuel feed becomes part of the bed material in the GR.

1.1.2 Carbonation

The amount of CO_2 captured via carbonation of CaO affects the PG composition and the composition of exiting bed material. It is either limited by the flow rate and sorption capacity (maximum degree of carbonation conversion) of the entering bed material or thermodynamically (equilibrium of CO_2 and $CaO/CaCO_3$). The entering CaO is not fully carbonated in the GR. The sorption capacity decreases with an increasing carbonation/calcination cycle number as described by the correlation shown in Figure 1 published by Fuchs et al [6]. Due to the continuous bed material make-up stream, CaO particles in the system have different numbers of calcination/carbonation cycles, hence different sorption capacities. Consequently, an average sorption capacity X_{ave} must be used (the higher the make-up, the higher X_{ave}). For this GR-model, X_{ave} is set to 0.2.

The thermodynamic state of the carbonation reaction is assessed via the logarithmic deviation from equilibrium $p\delta_{eq,Ca}$.

$$p\delta_{eq,Ca} = \log_{10}\left(\frac{\frac{1}{p_{CO2}}}{K_{Ca}(T)}\right) \tag{7}$$

Fuchs et al. published a correlation for $p\delta_{eq,Ca}$ depending on the SER gasification temperature, which was found based on empirical data from SER experiments in different scientific lab-scale plants [5]. As a conservative assumption, this correlation is taken as thermodynamic limit $p\delta_{eq,Ca,max}(T)$, e.g. the CO_2 concentration of the PG leaving the GR can not take on values lower than given by the correlation. The result from this setup is, that as long as $p\delta_{eq,Ca}$ is calculated to be lower than $p\delta_{eq,Ca,max}(T)$, the actual carbonation conversion X_{Ca} equals X_{ave} (amount of captured CO_2 is fixed). Otherwise $p\delta_{eq,Ca}$ is set to $p\delta_{eq,Ca,max}(T)$ (volume fraction of CO_2 in PG is fixed) and X_{Ca} (now $< X_{ave}$) is calculated accordingly.

1.2 Segregator

Due to the lack of substantial data and models of the dynamical behaviour of the segregation process in a fluidized binary mixture, the separation process is merely modelled with two efficiency values, which describe the degree of separation for both components (char and bed material):

$$\eta_{char,SEG} = \frac{\dot{m}_{char,conv,in}}{\dot{m}_{char,seg,in}} \tag{8}$$

$$\eta_{bed,SEG} = \frac{\dot{m}_{bed,ris,in}}{\dot{m}_{bed,seg,in}} \tag{9}$$

In case of imperfect separation ($\eta_{char/bed,SEG} < 1$), there is a char stream from the segregator to the riser and/or a bed material stream to the converter.

1.3 Converter

In the converter, steam gasification of the entering char takes place. The char is assumed to be dry, fully devolatized and free of ash. The kinetics of the char conversion via steam gasification is modelled likewise to the GR via equation 3. The composition of the entering and exiting char is assumed to be equal. For gasification of biomass char, low C_2H_4, C_2H_6 and tar concentrations are reported [7]. Therefore, the PG exiting the converter is modelled to only contain CH_4, H_2O, H_2, CO and CO_2. Because of the high gasification temperature, the water gas shift reaction is set to be in equilibrium ($p\delta_{eq,wgs} = 0$). The required energy of the endothermic reaction is supplied electrically ($P_{el,CONV}$).

1.4 Riser (Calcination reactor)

In the riser, the bed material is heated and $CaCO_3$ is completely calcined. Thermal energy is solely electrically supplied ($P_{el,RIS}$). The required steam flow rate for the fluidization of the riser is set to meet a superficial gas velocity typical for fast fluidized bed reactors independently of the required mass flow rate of bed material (4-8 $\frac{m}{s}$ according to [8]). This means, the higher the amount of released CO_2, the lower the required steam supply. It is assumed, that the solid mass flow rate can be adjusted via staged steam fluidization. The separation efficiency of the cyclone determines the required make-up stream of fresh bed material. The flue gas only contains H_2O and CO_2.

2 Material streams

2.1 Organic feedstock

The biomass feedstock is modelled to consist of the elements C, H, O, N, S and Cl. Its heating value is determined based on the composition via the correlation of Boie. The water content of the feedstock must be set.

2.2 Ash

Ash is modelled to consist of CaO (contributing to the carbonation-calcination cycle) and SiO_2, which represents the chemically invariant part of the ash.

2.3 Fresh bed material

Fresh limestone is assumed to be 100 % $CaCO_3$.

2.4 Char

The composition of char is calculated via equations (4) and (5) at $T = T_{GR}$.

2.5 Tar

Tar is modelled as pure Naphthalene, as it is a main component of tars from biomass gasification ($w_{C,tar} = 0.94,\ w_{H,tar} = 0.06$).

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[3] Daniel Neves et al. “Characterization and prediction of biomass pyrolysis products”. In: *Progress in Energy and Combustion Science* 37 (5 2011), pp. 611–630. ISSN: 03601285. DOI: 10.1016/j.pecs.2011.01.001.

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Technical CAD drawings of CFM

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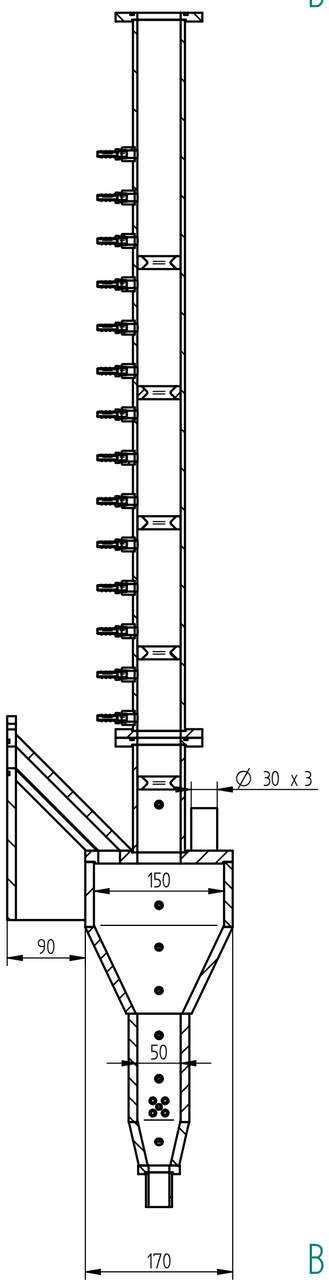

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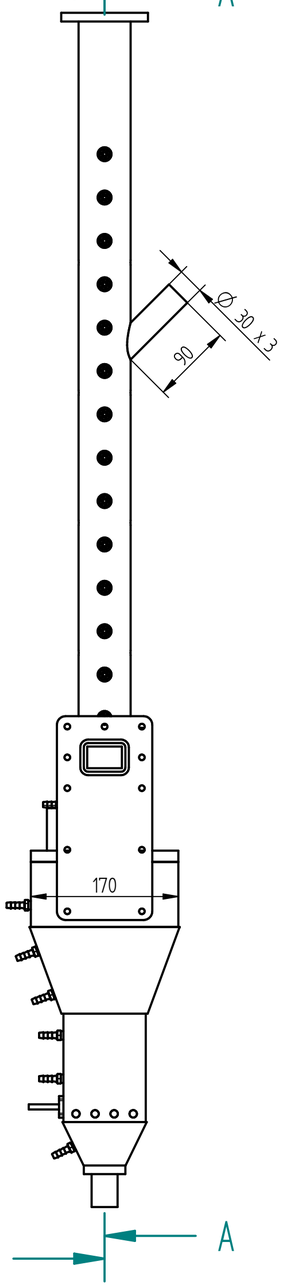

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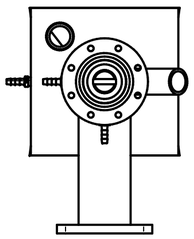

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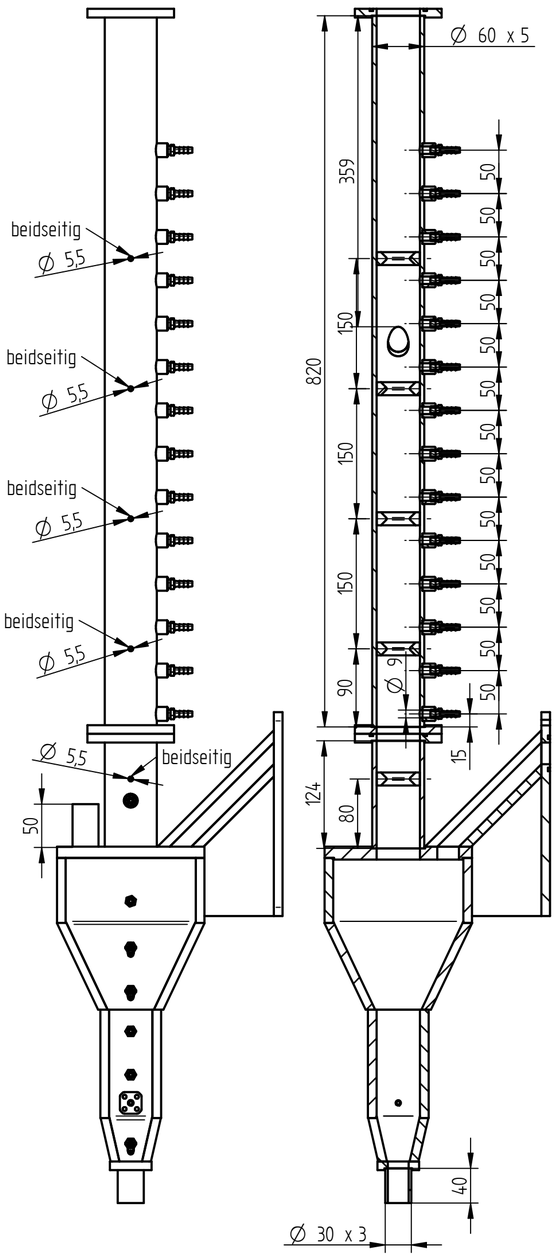

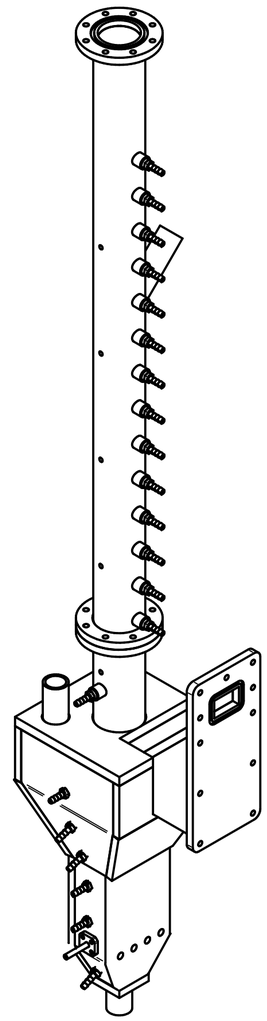

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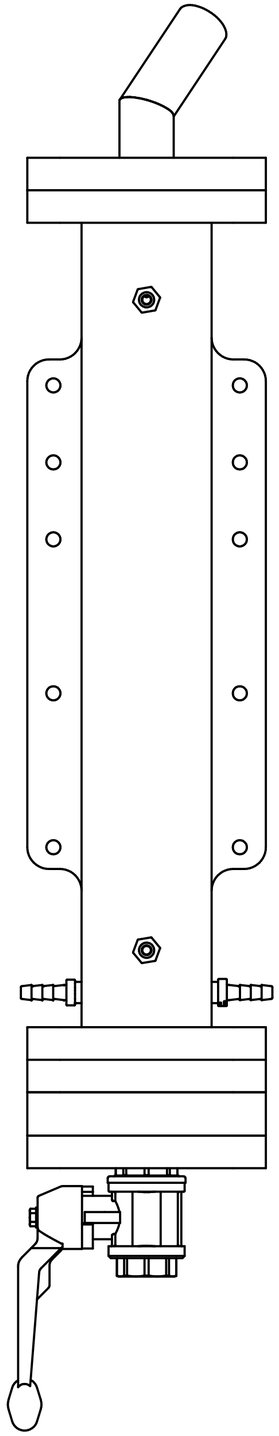

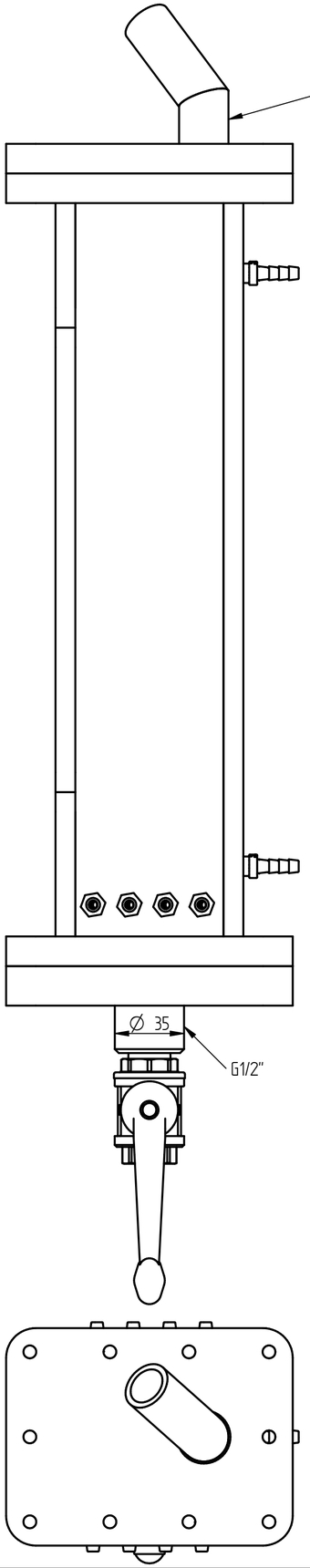

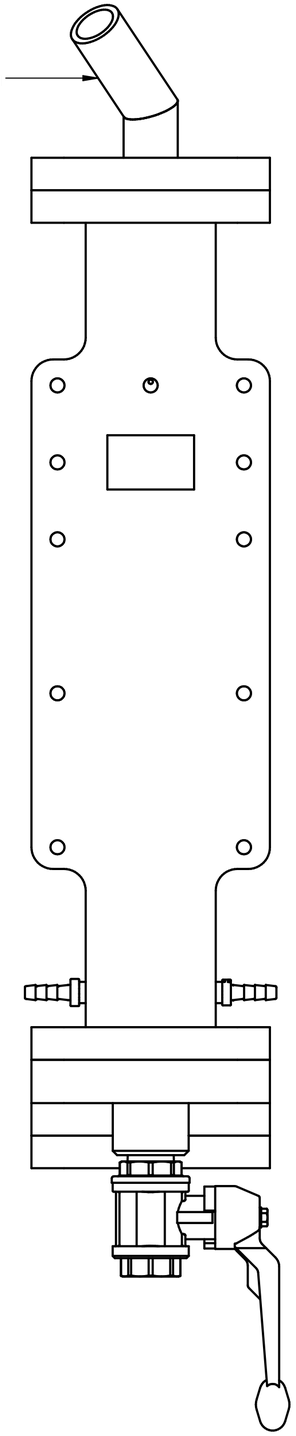

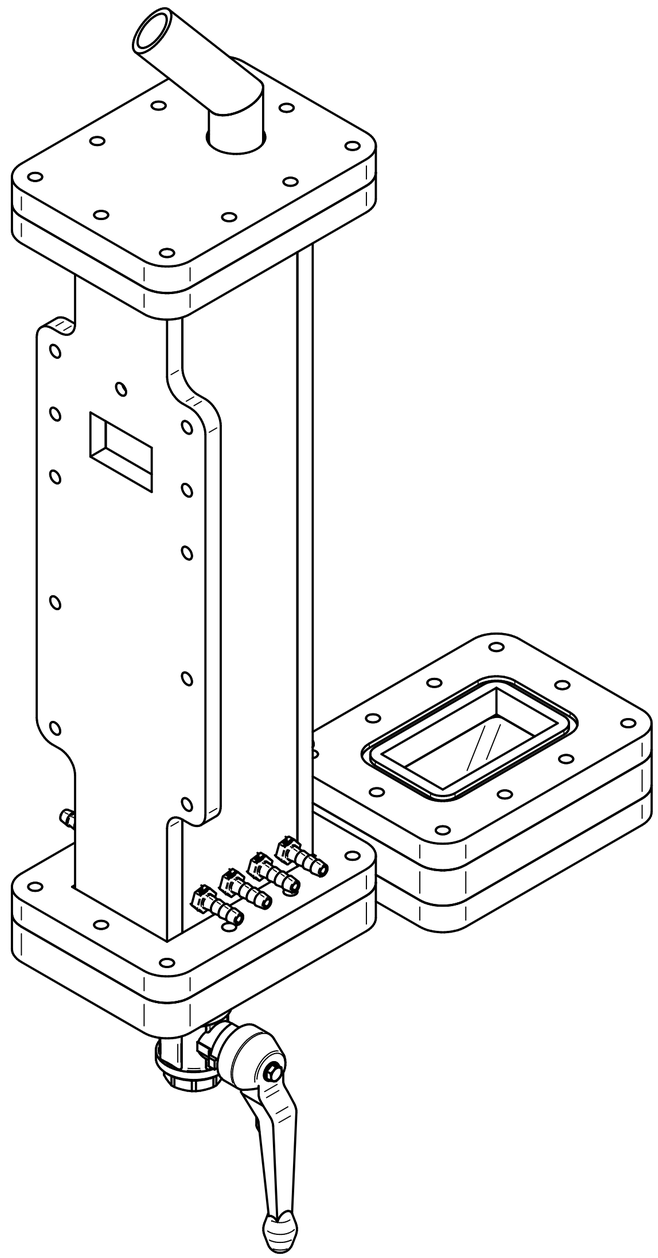

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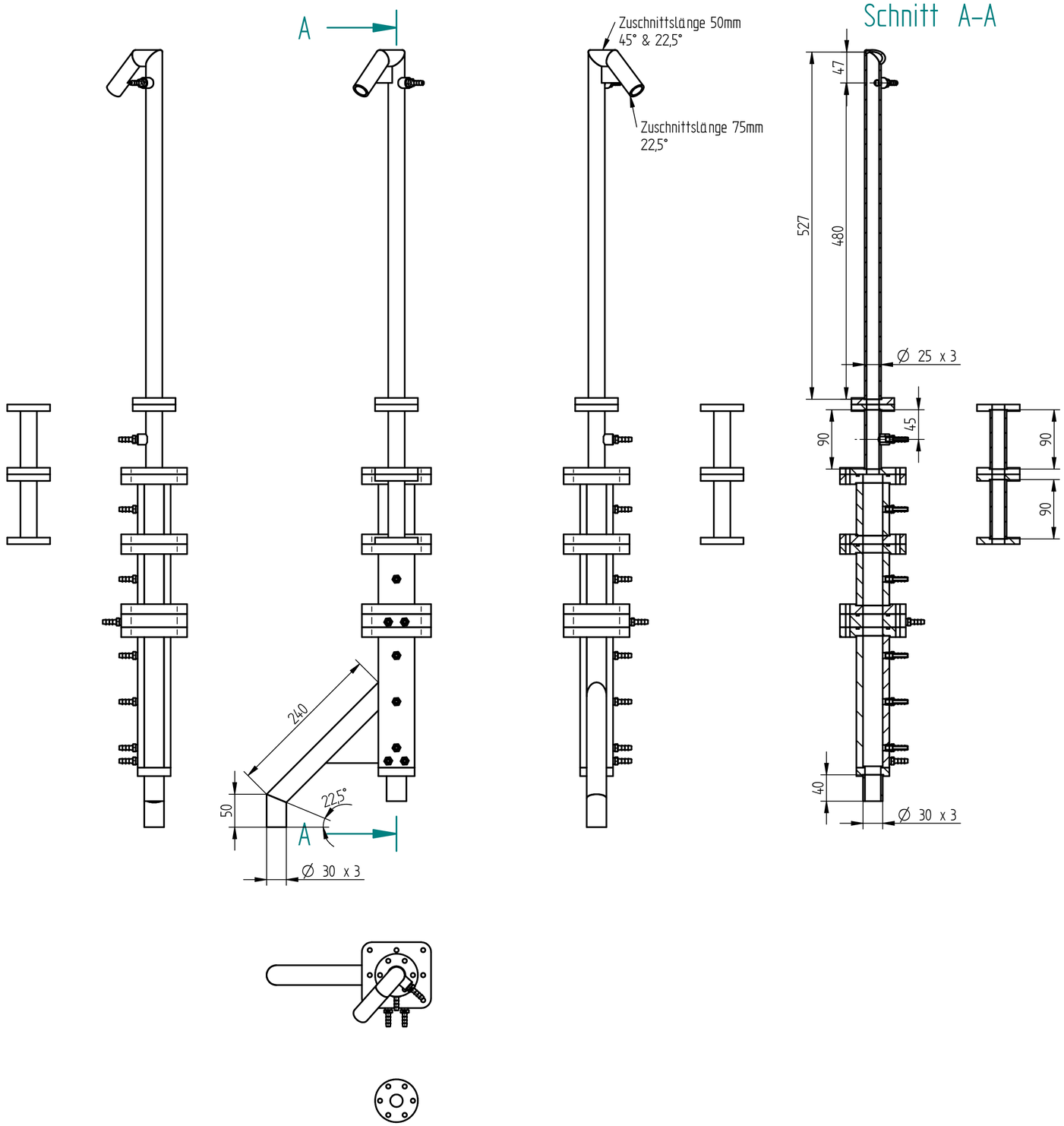

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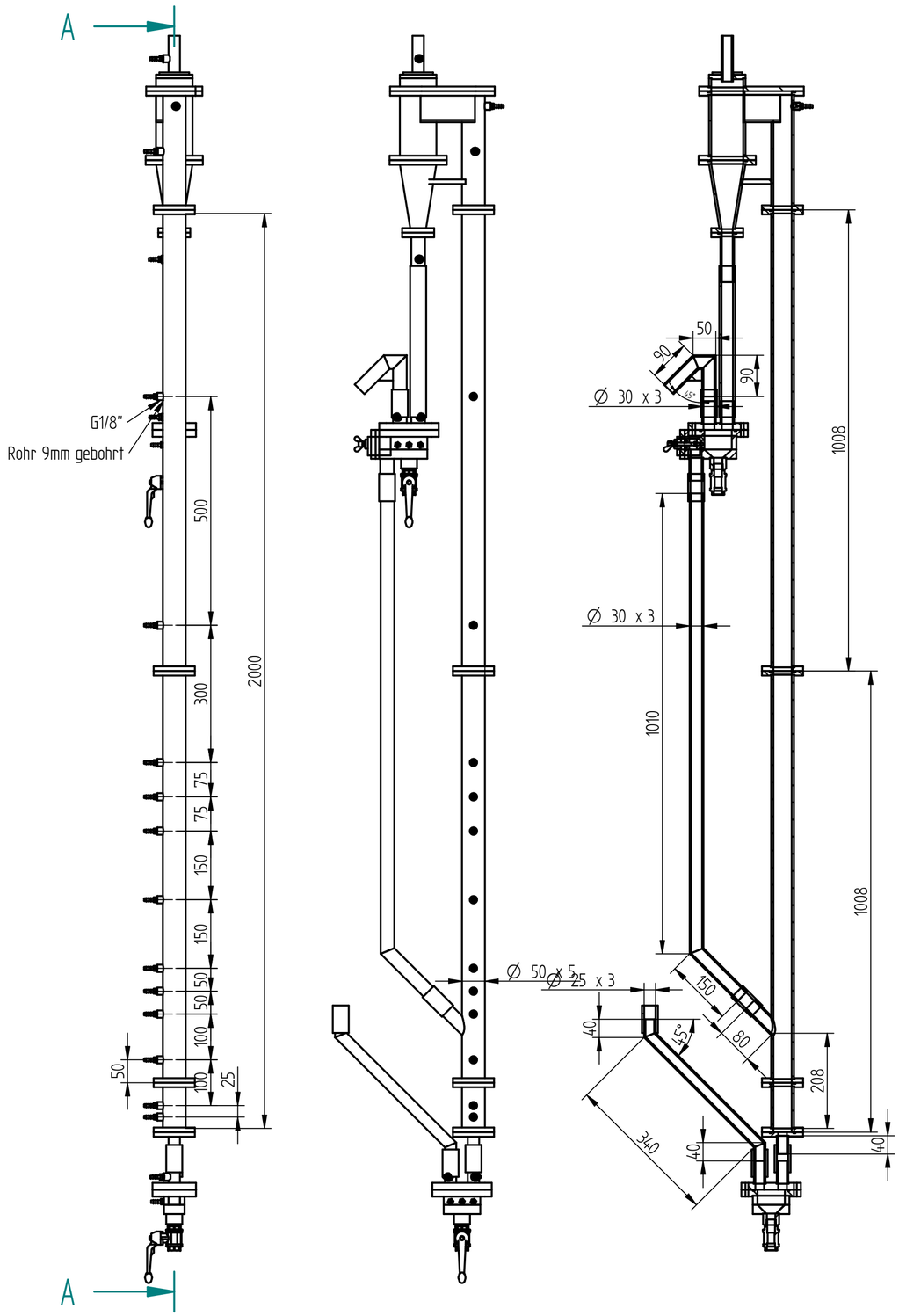

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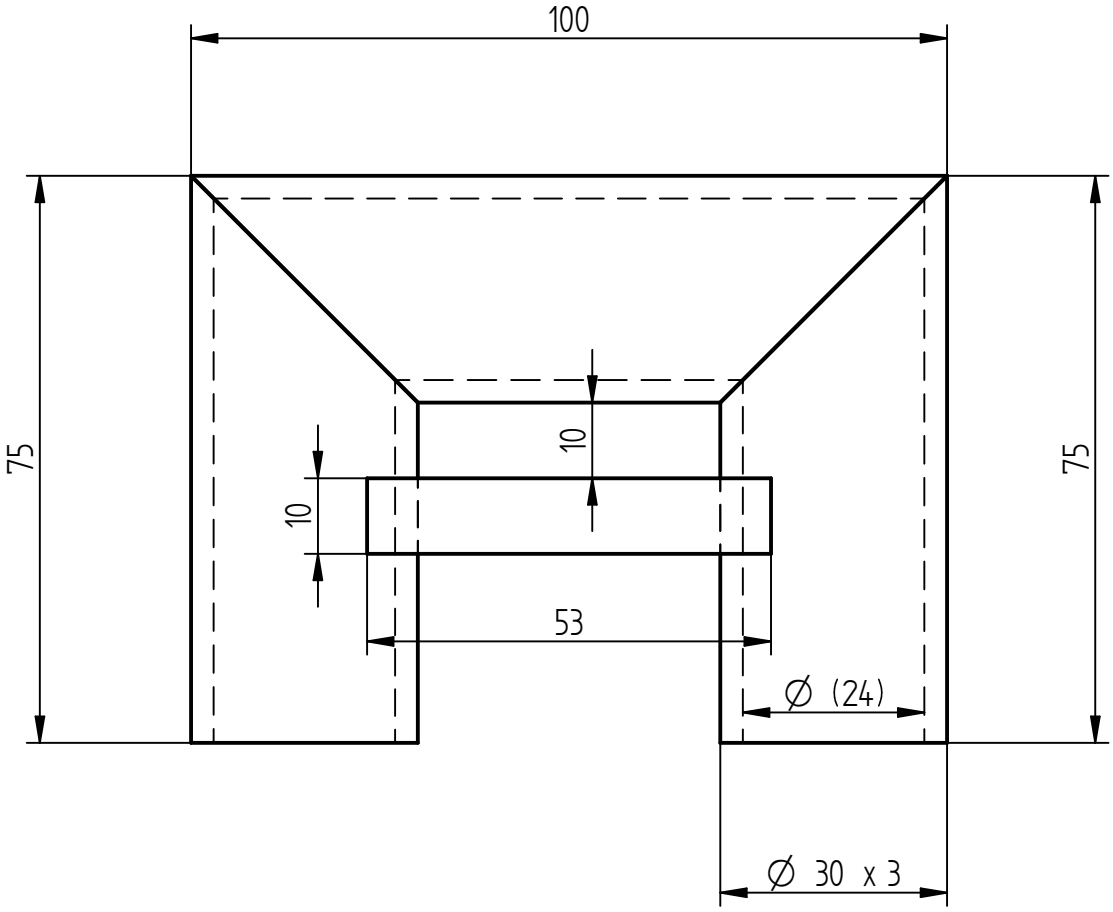

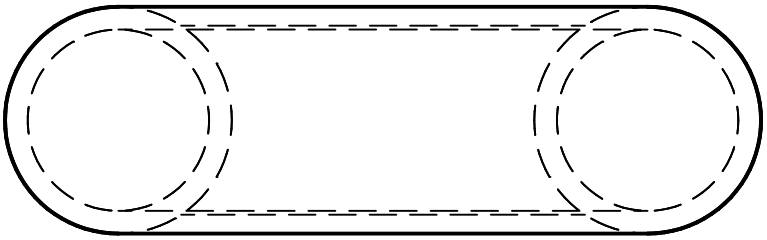

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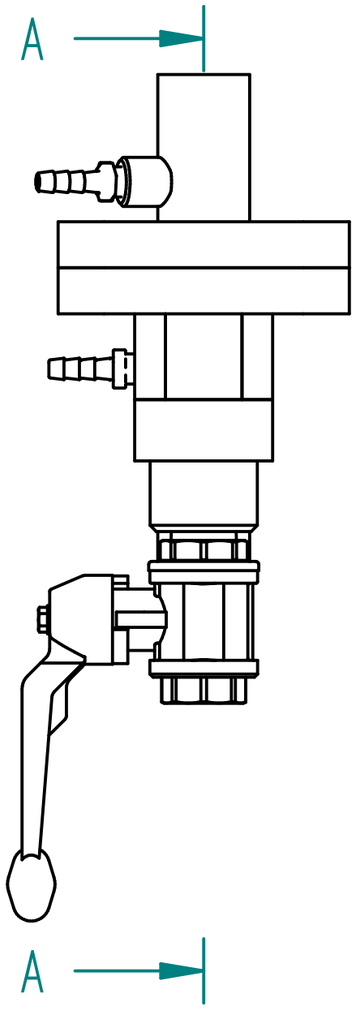

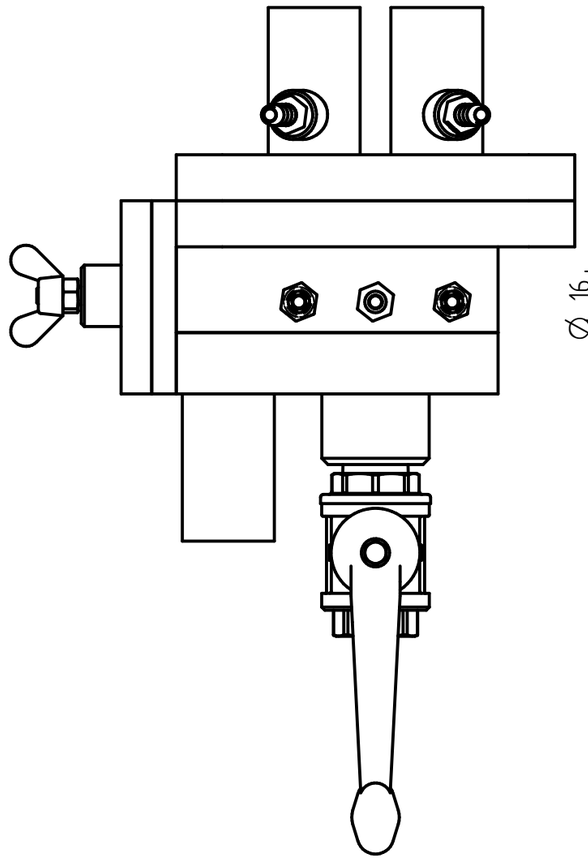

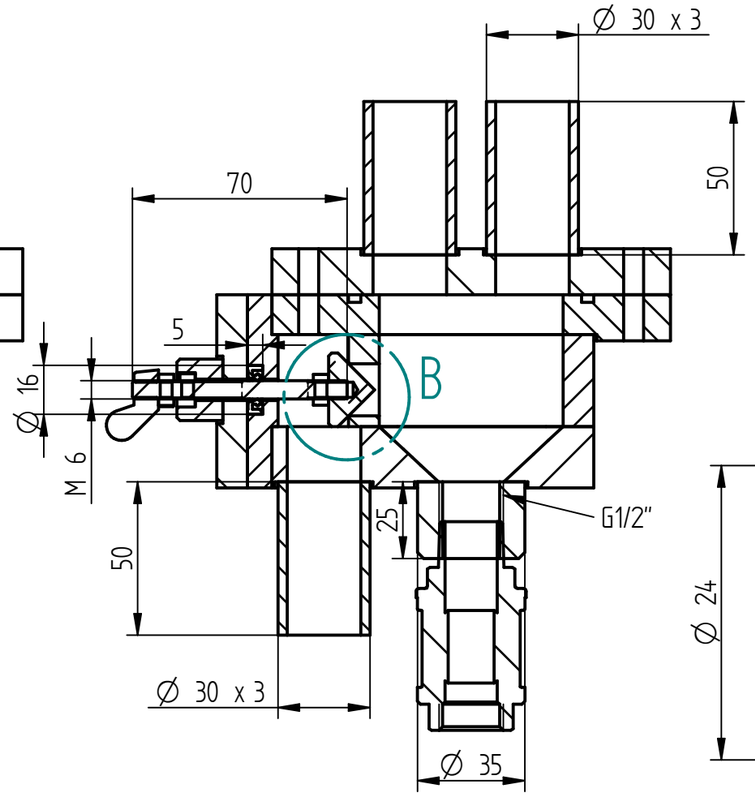

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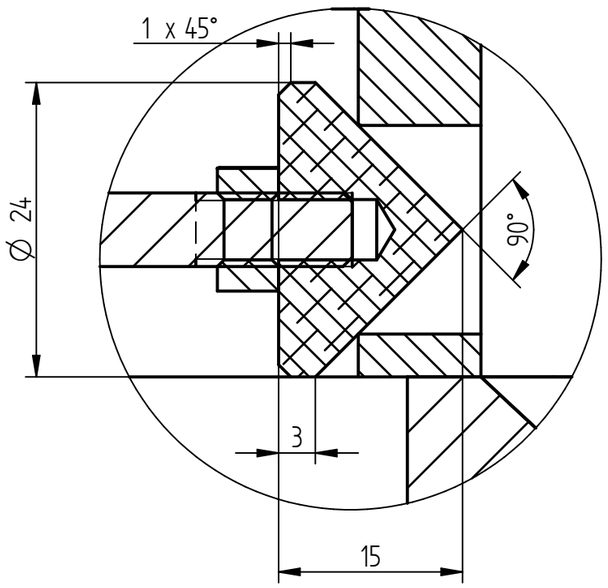

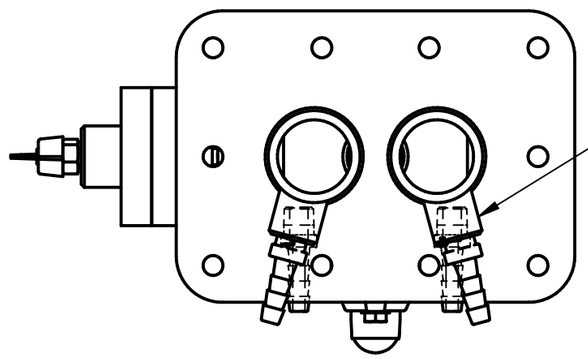

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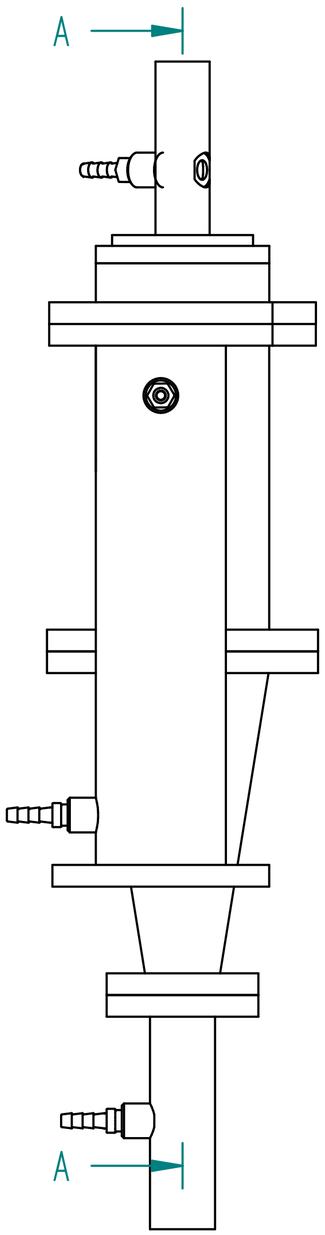

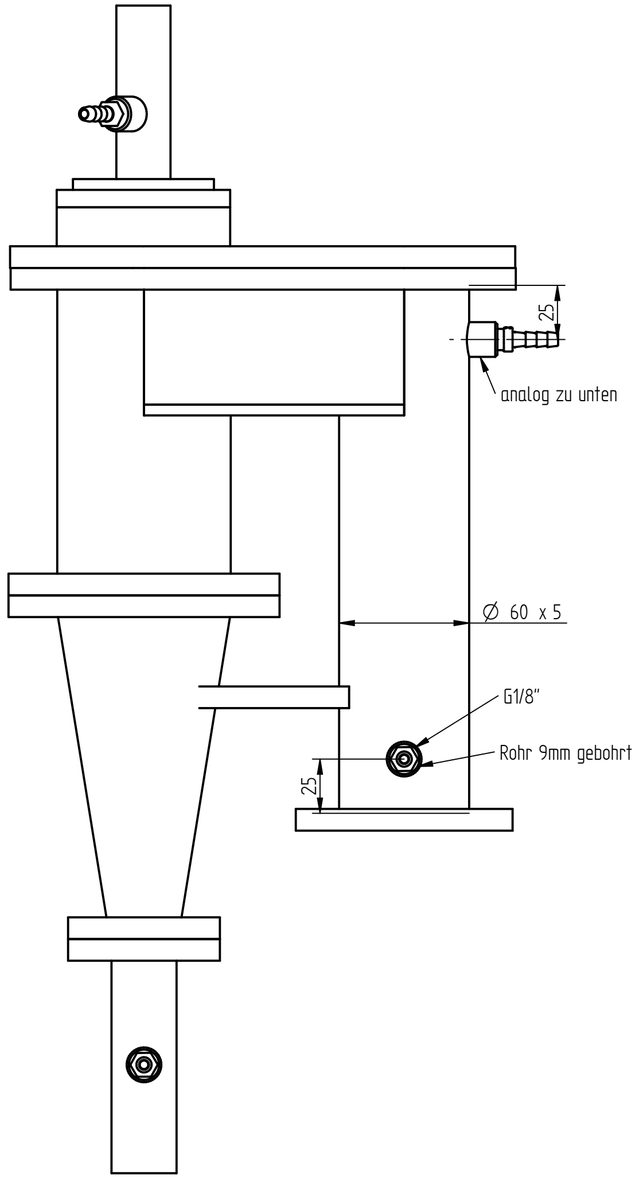

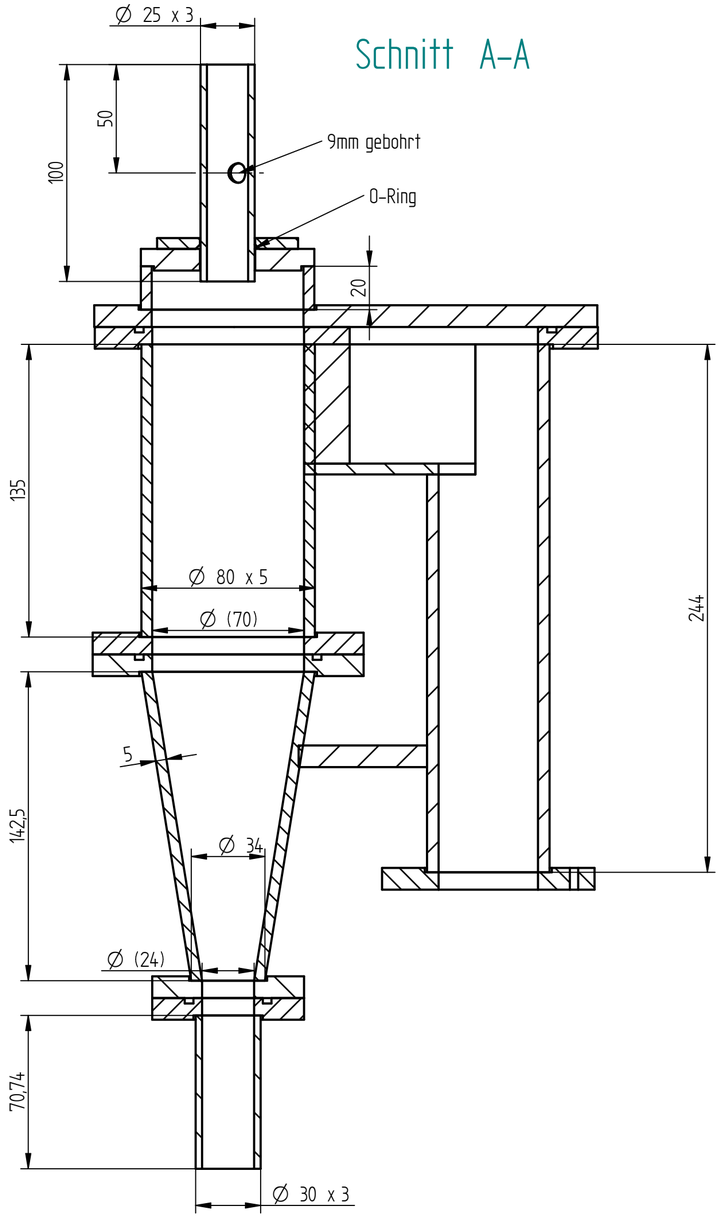

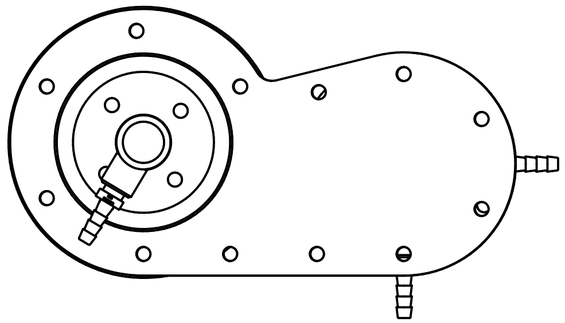

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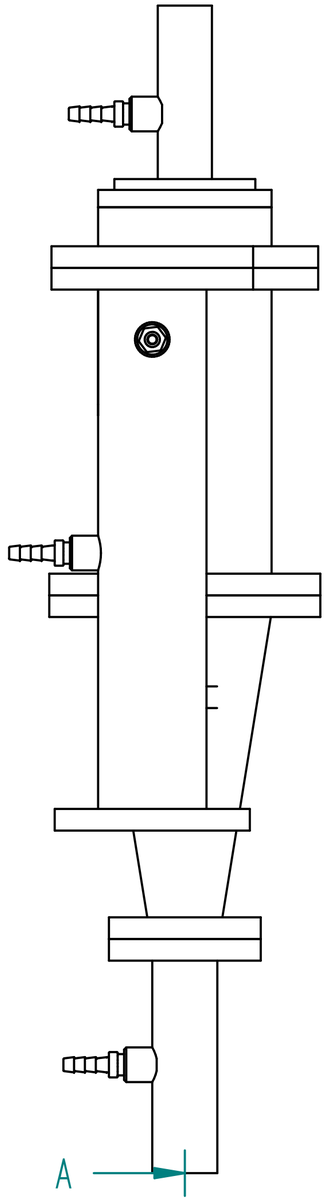

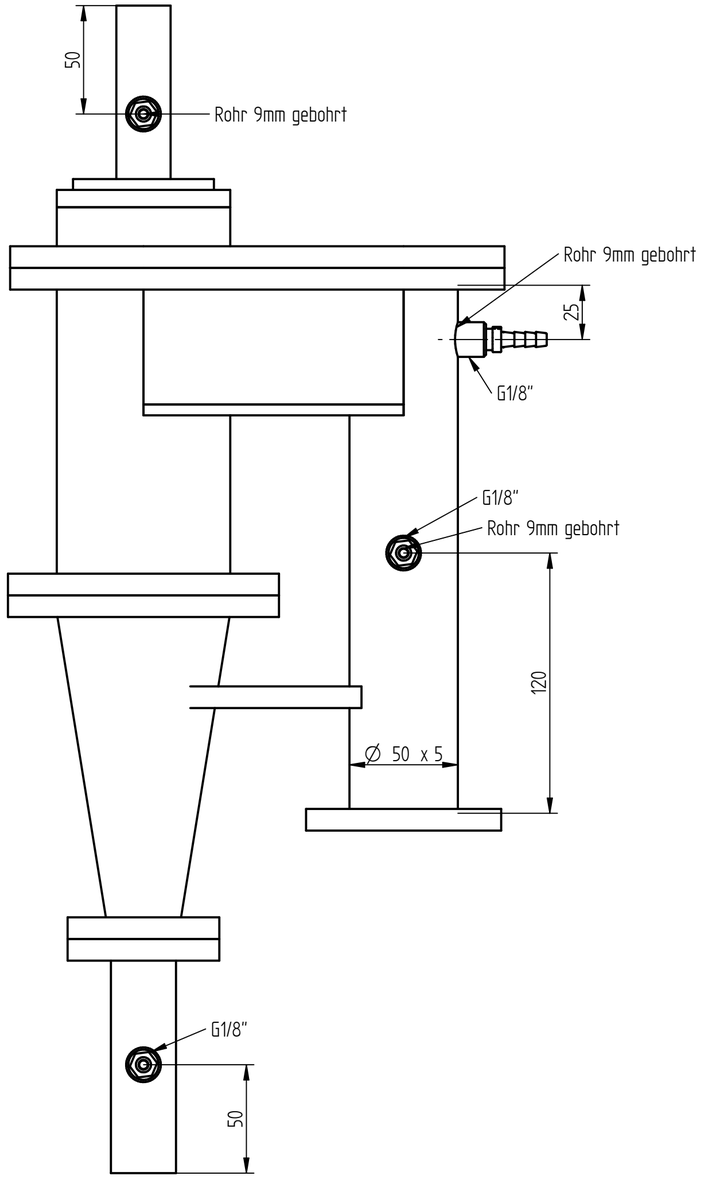

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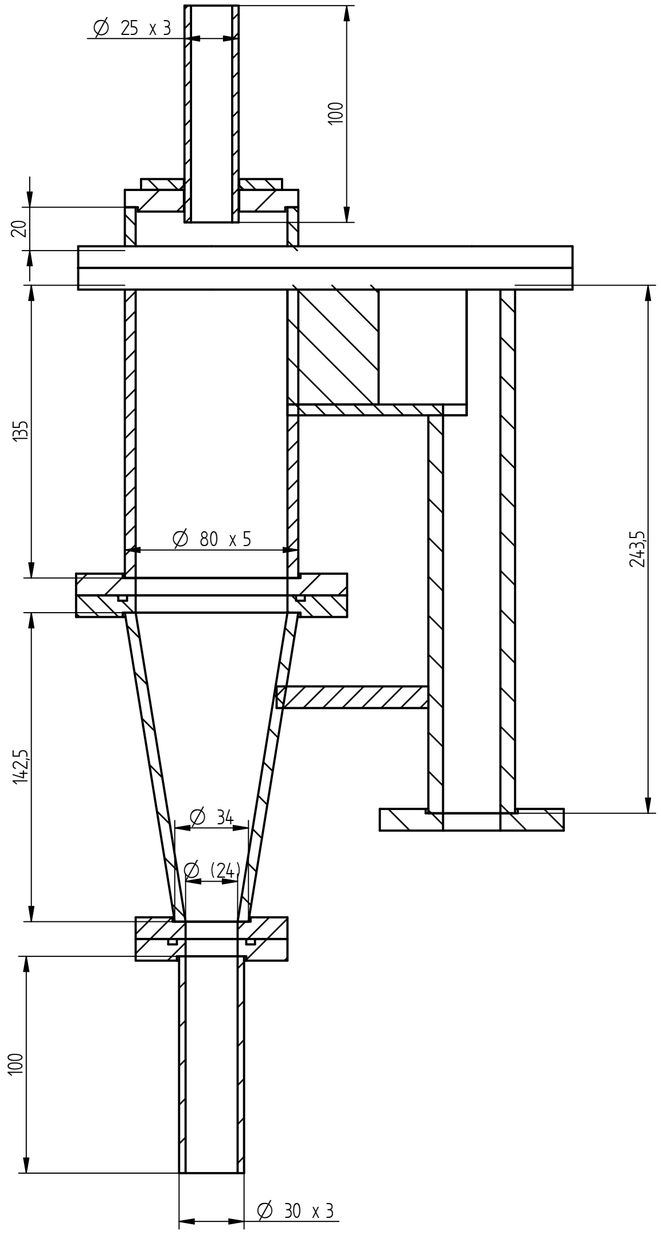

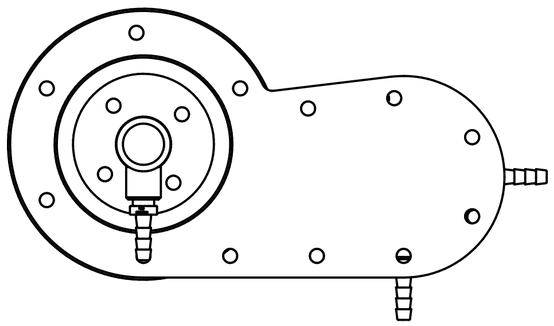

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DRAWN	Fahrngruber	03/10/2023
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J.Fuchs GmbH
3800 Schwarzenau - Austria
www.jfuchs.at

UNLESS OTHERWISE SPECIFIED
DIMENSIONS ARE IN MILLIMETERS
GENERAL TOLERANCES: ISO 2768 mK
ALL EDGES DEBURRED
RA 6,3

Project/Kunde: BOKU

TITLE: Zyklon_Plexi2

SIZE: A2 | DWG NO | REV: 00

SCALE: 1:2 | SHEET 1 OF 1