CFD and kinetic modelling of post-combustion CO_2 absorber

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CONTENTS

1 THE PURPOSE OF THE WORK

The purpose of this CFD work is to study gas flow field in a post-combustion CO_2 absorber in order to provide guidelines to design such absorbers. The design of these units is challenged by their huge size: the column diameter typically ranges around 10-20 m. Commercial full-scale applications of such systems are not yet operational, just a handful of demonstration projects have been / are running in the world.

The findings of the CFD study will also be incorporated here in a steady-state process simulation using ASPEN Plus simulation software, in an effort to establish the impact of gas flow maldistribution on CO_2 capture efficiency.

2 BACKGROUND

2.1 Literature review

Before the modelling work was started, a literature review on CFD modelling in post combustion CO_2 capture absorbers was carried out. It was figured out that relatively scarce information is available directly about this matter. The best sources found were:

- *D. Mewes et al. (Leibniz University of Hannover, publications 1999-2010)* developed an elementary cell model for 2-phase flow in structured packings. The porous bed was subdivided into elementary cells to provide a macroscopic flow field at the scale of the entire porous structure. In packed beds an elementary cell is the smallest structure recurring periodically in all three dimensions. Model includes three continuous Eulerian phases: gas and two liquid phases (one along each channel layer or preferential flow direction).

- *L. Raynal et al. (Institut Francais du Pétrole, publications 2001-2010)* developed a multi-scale approach for simulating the 2-phase flow in structured packings using information from smaller scale as an input data for the next level:
  (A) Corrugation scale: 2D gas-liquid VOF --> liquid hold-up and velocity at gas-liquid interface
  (B) Smallest periodic element of real packing geometry: 3D liquid flow --> relationship between pressure drop and gas superficial velocity
  (C) Column scale: packed bed as porous media --> optimum design

Some studies found were not applicable in the current work, because the 2-phase flow in the absorber was studied in very small scale (cm-dm scale instead of say 10-20 m).

Another more common literature review about multiphase flow in structured packings was carried out. As a result, some studies mainly in the field of trickle beds were found, but they were not found useful for the current project.

2.2 Modelling strategy

The modelling was decided to be carried out as follows:

1. 1-phase flow of flue gases in the bottom part of the absorber including the bottom bed --> velocity field at the bed inlet in different cases
2. Comparison of different cases in Aspen plus to determine the influence on CO_2 capture

3 MODEL DESCRIPTION

Figure 1 illustrates the modelled geometry consisting of the flue gas inlet pipe(s), the bottom bed and the vapour flow space below the bed. The bottom bed is in charge of bringing gas (travelling upwards) and liquid (falling down) in contact and enabling CO_2 absorption from gas to the liquid solvent.

The geometry was created in ANSYS Workbench 13, from which it was imported in STP-format to Salome. In Salome the boundaries of the geometry were named and exported to STL-format. The STL-files were then used in the open-source computational mesh generator SnappyHexMesh. The 1-phase gas flow field was solved using the porousSimpleFoam solver of openFOAM 2.0.1. The column diameter was assumed to be 18 m.

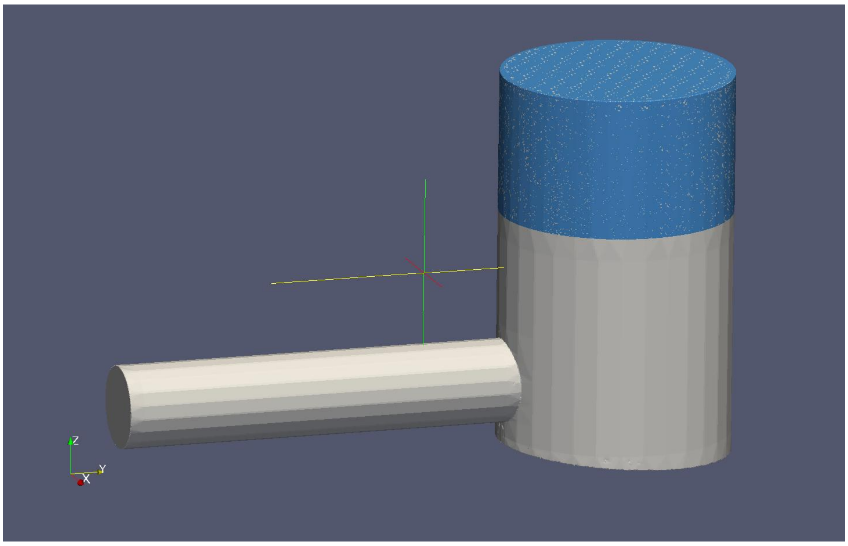
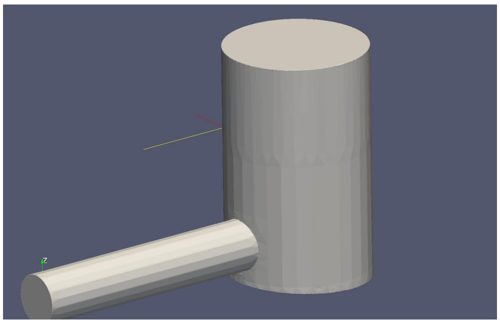
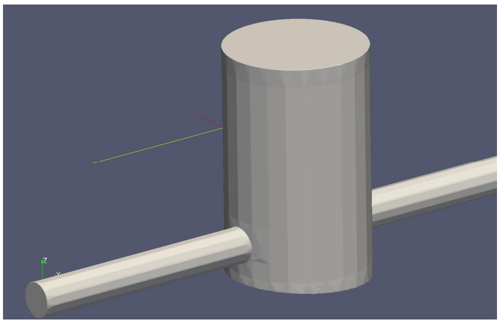


Figure 1 Left: modelled reactor. Right: front face culled to show the impingement plate.

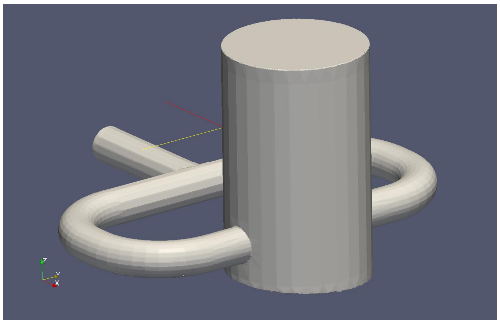
Six different cases shown in Figure 2 were simulated.

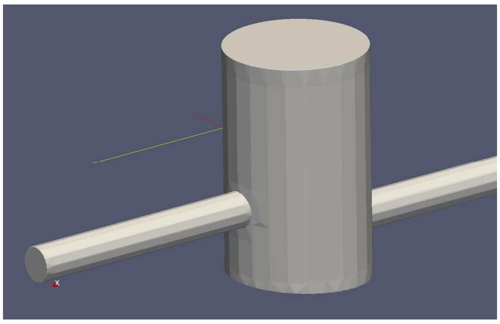
1-sided inlet 2-sided inlet



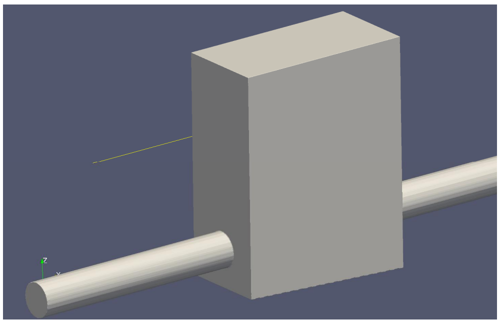


2-sided real inlet 2-sided staggered





2-sided inlet, rectangular column 1-sided tangential inlet



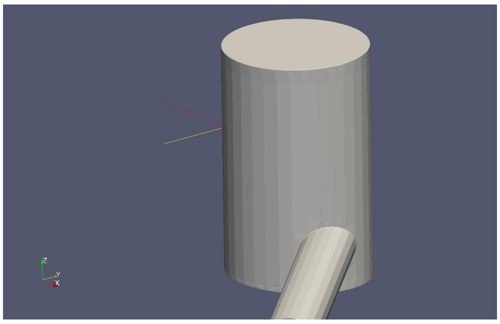


Figure 2 Simulated cases.

The computational mesh shown in Figure 3 had about 1 000 000 computational cells depending on the case. It consisted mainly of hexahedral cells, but some prism, tet-wedge and polyhedral elements were used where needed. The used mesh was relatively coarse, as the CPU times in these preliminary simulations were kept short. A short mesh dependency study showed, however, that the results could be considered representative.

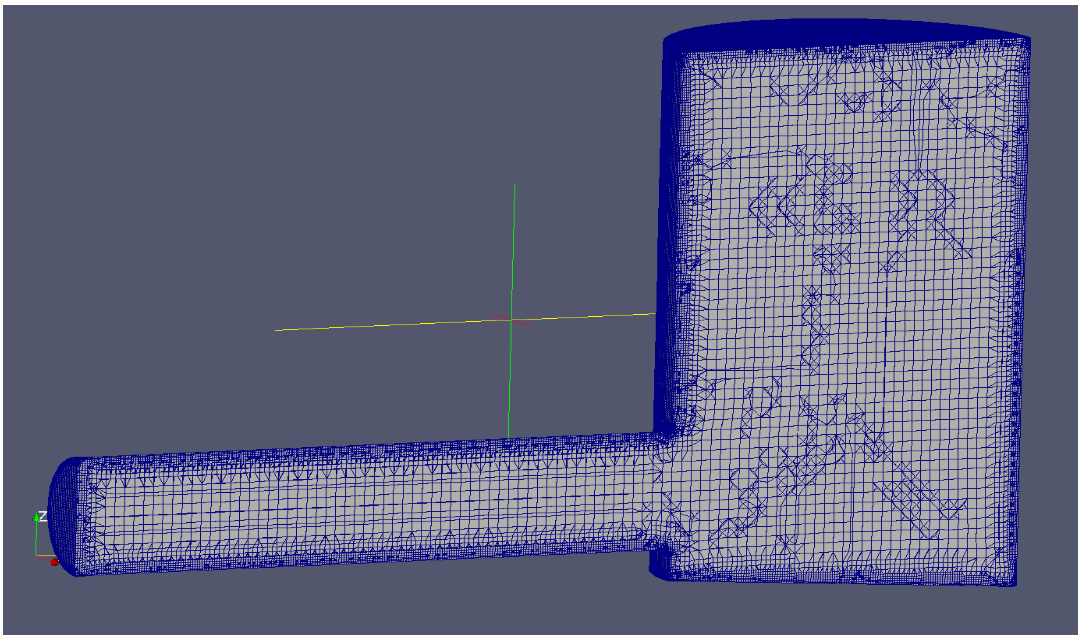


Figure 3 The computational mesh of Case1.

3.1 Used models and boundary conditions: 1-phase flow

The used material properties are listed in Table 1 and the boundary conditions in Table 2. Transport equations were solved for continuity, momentum in x-, y- and z-directions, energy, turbulence kinetic energy and its dissipation. Gas was assumed incompressible and a steady state (static) solution was calculated. The size of the inlet pipe was selected so that inlet velocity equalled about 16 m/s.

Table 1 Material properties.

Name	ρ ***[kg/m³]***	ν [m²/s]
Gas	1.2	1.5e-05

Table 2 Boundary conditions.

Boundary	***Variable***	***Value***	Unit
Inlet	Mass flow	2 400 000	kg/h
Outlet	Relative pressure	0	Pa

3.2 Modelling the fixed bed

The fixed bed was modelled as homogeneous porous media. In this approach the bed structure is not modelled in detail but as a lump. The bed resistance is described by source terms added to the momentum transport equations. The source term S_i reads:

$$S_i = -\left(\mu D + \frac{1}{2}\rho \left|u_{jj}\right| F\right) u_i \qquad (2.2.1)$$

Here the first term corresponds to viscous loss term and the second term to inertial loss term. It can be noted that the first term creates a pressure drop proportional to the velocity and the second term proportional to velocity squared. Here the isotropic loss coefficient values (D = 4 m^{-2} and F = 40 m^{-1}) were iteratively selected to obtain a pressure loss of about 1200 Pa over the bed. More information on modelling porous media in openFOAM can be found for example in /1/.

4 CFD SIMULATION RESULTS

4.1 Velocity field at bed inlet

Figure ***4*** shows the velocity magnitude field at the horizontal bed inlet cross section. Based on the figures, the following conclusions can be made:

- 2-sided feed pipe arrangement leads to a smoother bed inlet velocity profile than 1-sided arrangement.
- Staggering gas inlet pipes i.e. placing them on different levels leads to unnecessary velocity peaks appearing mainly on top of the uppermost inlet pipe.
- Rectangular column with 2-sided inlet provides similar results to equivalent cylindrical case.
- Tangential 1-sided inlet leads to a strongly swirling velocity field below the bed, hence the red colour in Figure ***4*** is caused by the high x- and y-velocity components in this case.

4.2 Velocity field at vertical cross section (x = 0 m)

Velocity fields at vertical x = 0 m plane are shown in Figure ***5***. Only the 1-sided inlet cases, in particular with the tangential inlet arrangement, differ from the other cases. The velocity levels are higher below the bed in these cases.

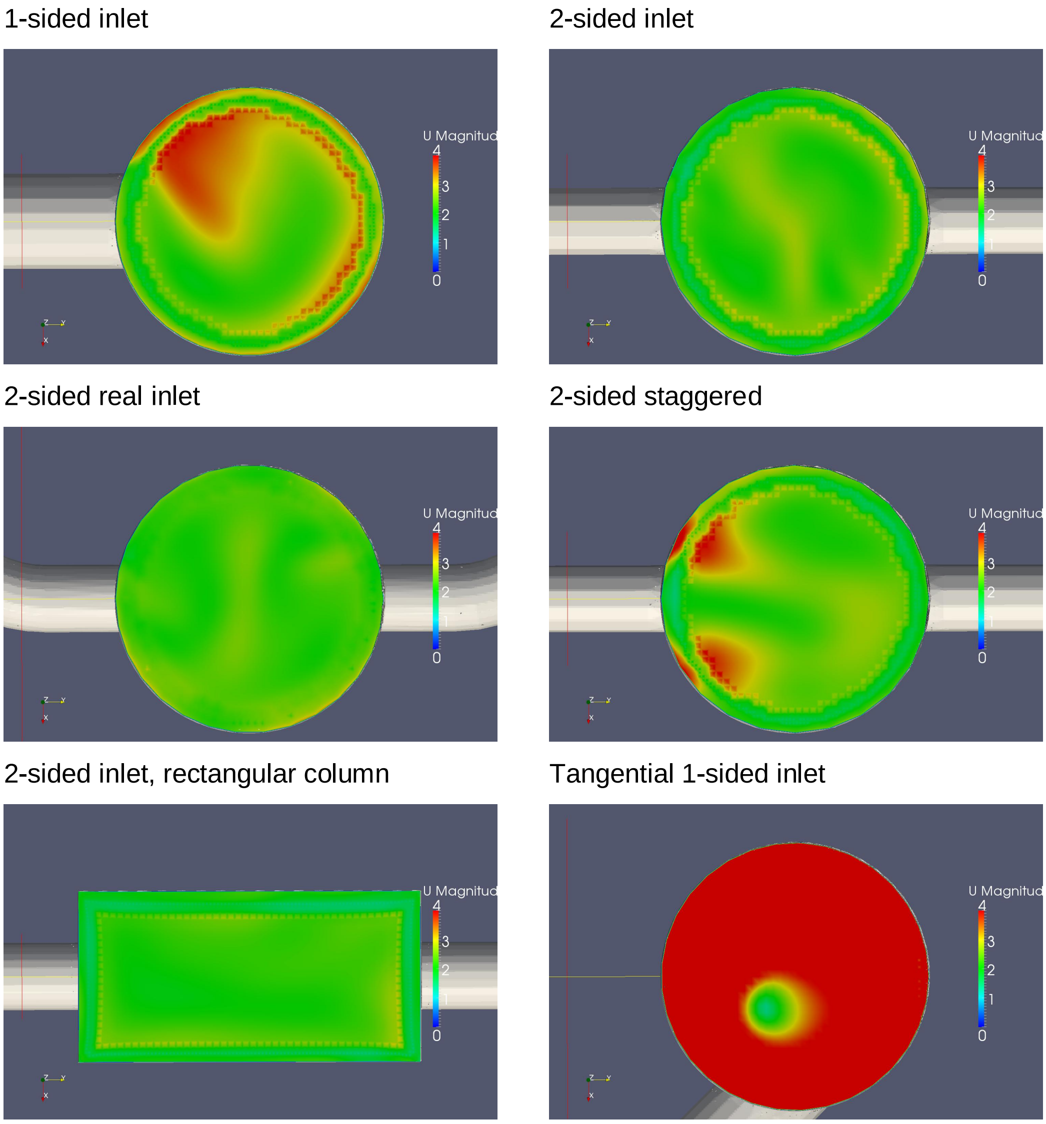


Figure 4 Velocity (magnitude) field at bed inlet at scale 0-4 m/s.

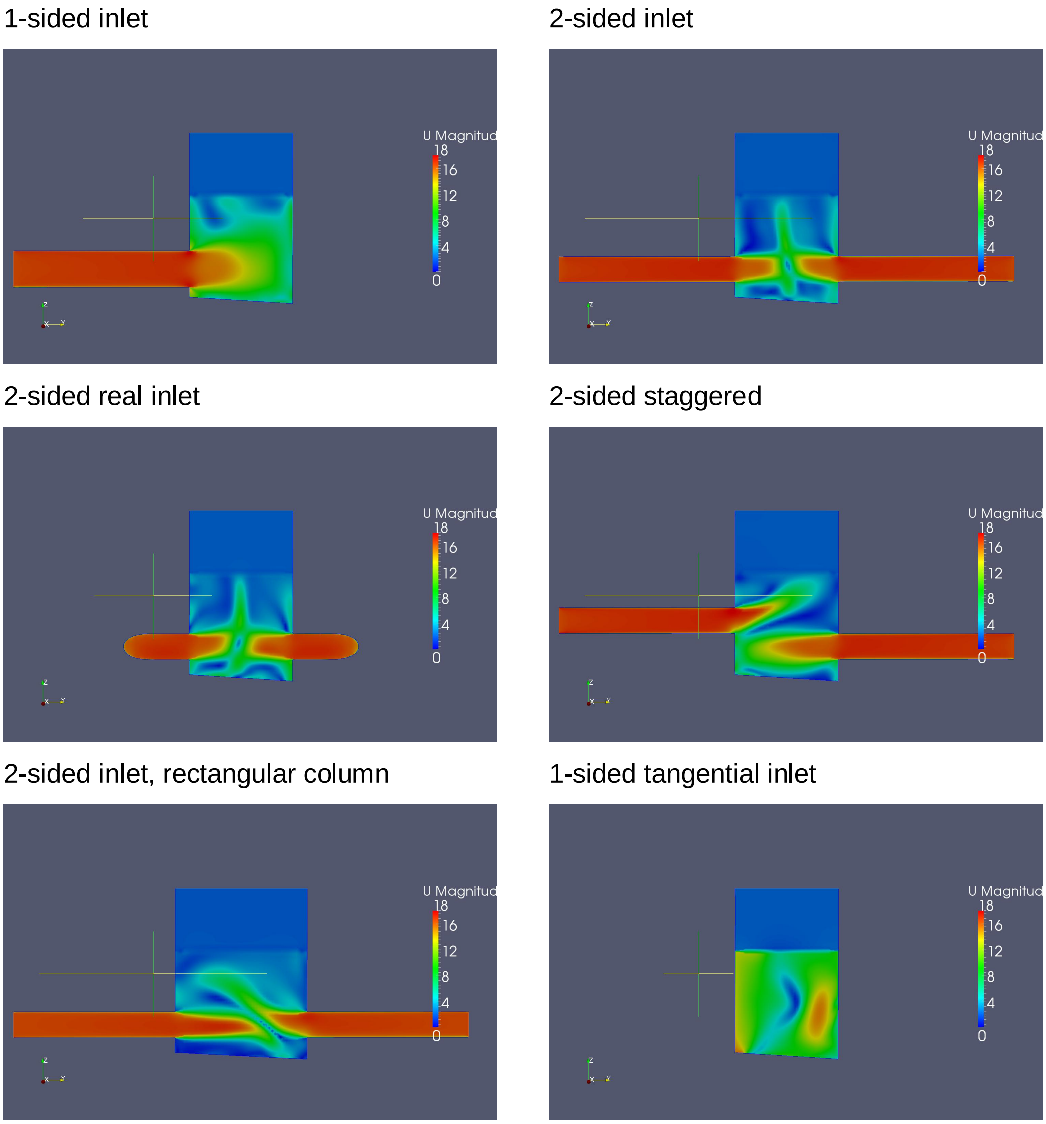


Figure 5 Velocity (magnitude) field at plane x = 0 m, scale 0-18 m/s.

4.3 Velocity field at horizontal cross sections

Velocity fields at horizontal z = 0 m to z = 1.5 m planes are shown in Figure 6. Only the 1-sided inlet case is studied here. Figure 6 shows that the in the gas distribution levels out during the first meter of the column, after which the loading is constant over the whole cross section.

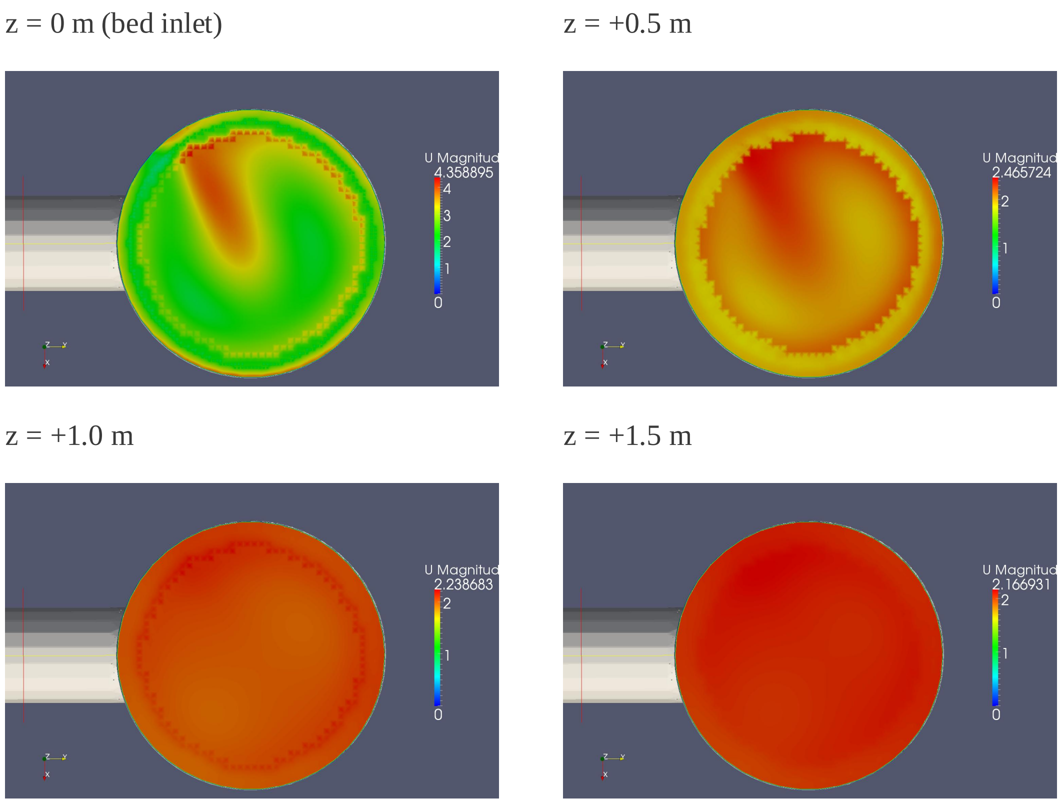


Figure 6 Velocity distribution at various elevations from the bed inlet.

5 STEADY-STATE PROCESS SIMULATION

5.1 Simulation model

This study deals with the absorption of CO_2 using 30 % MEA solution. The two main components of a CO_2-MEA capture process are the absorber and a stripping column. The stripper is omitted from this first simulation, but the composition of the MEA feed has is such that it represents the steady state conditions of a complete CO_2-MEA process. Chapter 5.4 describes the case with the stripping column included. The absorption column is an 18 m diameter 11 m high counter current column.

The simulations are performed using Aspen Plus V7.3, and are based on physical data and kinetic models from Aspen's Rate Based MEA model. The chemistry includes kinetic expressions for the reactions considered to be rate limiting (e.g. between MEA and CO_2). The electrolyte-NRTL model with Redlich-Kwong equation of state is used to calculate the vapour and liquid properties.

5.2 Modelling strategy

For this study, the CFD case with a once sided inlet was chosen. Based on the CFD simulation results it is assumed the flow maldistribution can be characterized by dividing the absorber cross-section into three parts, based on the different gas flow velocities. Part 1 is considered to have a "normal" velocity determined by total flow rate and cross-sectional area. This part covers 55 % of the absorber cross-section. 25 % of the area is considered to have a flow velocity which exceeds the normal flow by 67 %, whereas the remaining 20 % of the cross-section has a velocity of 76 % below the normal. This is simulated in Aspen Plus by three parallel absorbers with the above mentioned cross-sectional areas, and flows which correspond to the respective fluid velocities.

Three such simulations cases are considered:

1. Even loading throughout the height of the absorber, as a base case.
2. Uneven loading throughout the height of the absorber.
3. Uneven loading which levels out after the inlet section.

Case 3 is modelled with three parallel absorbers to describe the bottom section with uneven loading up to 1 m and a singe absorber to describe the upper 10 m of the column with uniform loading.

5.3 Aspen results for the absorber

The base case scenario (1) where even loading is assumed calculates a CO_2 capture of 95 % of the incoming CO_2. The pressure drop over the column is 1.63 kPa. Case 2 with uneven loading throughout the column gives a significant drop in the efficiency with less than 80 % capture. The part of the cross-section with increased flow velocity, which accounts for 41 % of the flow, suffers a dramatic decrease in capture efficiency to 57 %. The part with reduced flow velocity captures nearly all of the incoming CO_2, but that part accounts for only 4 % of the total flow. Table 3 presents the results of case 1 and 2.

Table 3 Case 1 and 2 results and input parameters.

	Base case	Non-constant Flow			
		Normal	Increased	Reduced	
Design		ABSO1	ABSO2	ABSO3	Overall
Area	260,16	143,09	65,04	52,03	260,16
Fraction of total area		0,55	0,25	0,20	1,00
Diameter	18,20	13,50	9,10	8,14	
Flow/area relative to normal		1,00	1,67	0,24	
Flow split fraction		0,55	0,41	0,04	1,00
Results					
Section pressure drop (kPa)	1,63	1,63	4,17	0,09	
Loading (kmol/hr/m2)	314,40	314,40	515,61	62,88	
CO2 in (kmol/hr)	3296,00	1812,80	1351,36	131,84	3296,00
CO2 out (kmol/hr)	166,73	103,56	572,69	0,02	676,27
Capture %	94,94	94,29	57,62	99,98	**79,48**

Case 3, where the loading levels out after one meter, shows little distinction from the base case. The increased velocity part of bottom section has a capture efficiency of 3.32 %, compared to the benchmark of the normal velocity part which has an efficiency of 5.31 %. In total, the calculated CO_2 capture in this case is just below 95 %, or practically the same as for the base case. Table 4 presents these results in more detail.

Table 4 Case 3 results and input parameters. Case 1 base case is included for comparison.

	Base Case	Non-uniform flow section (bottom)				Uniform section (top)	Total
		Normal	Increased	Reduced			
Design		ABSO1	ABSO2	ABSO3	Overall		
Area (m2)	260,16	143,09	65,04	52,03	260,16	260,16	260,16
Fraction of total area		0,55	0,25	0,20	1,00		
Diameter (m)	18,20	13,50	9,10	8,14		18,20	
Height (m)		1,00	1,00	1,00		10,00	11,00
Flow/area relative to normal		1,00	1,67	0,24			
Flow split fraction		0,55	0,41	0,04	1,00		
Results							
Section pressure drop (kPa)	1,63	0,13	0,38	0,01		1,53	
Loading (kmol/hr/m2)	314,40	309,82	515,61	75,46		316,89	
CO2 in (kmol/hr)	3296,00	1786,43	1351,36	158,21	3296,00	3127,93	3296,00
CO2 out (kmol/hr)	166,73	1691,49	1306,46	129,98	3127,92	168,45	168,45
Capture %	94,94	5,31	3,32	17,84	5,10	94,61	**94,89**

5.4 Simulations including stripping column

Given the similarities between the absorber and the stripping column, it may be assumed that the latter also suffers from uneven gas loading. Since this is a closed loop process, inefficiencies in the stripping column will adversely affect the absorption column performance. Assuming a similar gas distribution for the stripper as for the absorber, the modelling of the column can be done in a similar fashion to the above model. The bottom section is represented by three parts with different cross sectional areas and different loading, with the top section again considered uniform. The areas and velocities are the same as for the absorber. The stripping column used here is 11 m tall and 10 m in diameter.

This (non-optimized) case gives a CO_2 capture efficiency for the whole process of 80.36 %, when the gas is distributed evenly throughout both columns. With uneven gas distribution in the bottom section (1m) of both columns, the CO_2 capture efficiency decreases only nominally to 80.20 %. This relatively insignificant reduction in efficiency, due to gas flow maldistribution, is seen with various pressures in the stripping column (a factor which greatly influences the performance of the stripper).

6 SUMMARY

In this report, gas flow field in a post-combustion CO_2 absorber has been studied by CFD modelling. The computational domain included the inlet piping, the bottom part of the absorber and the lowest bed. Six different geometries were simulated as shown in Figure 2. Based on the modelling results it can be concluded that:

- 2-sided feed pipe arrangement leads to a smoother bed inlet velocity profile than 1-sided arrangement.
- Rectangular column with 2-sided inlet provides similar results to equivalent cylindrical case.
- Staggering gas inlet pipes i.e. placing them on different levels leads to unnecessary velocity peaks appearing mainly on top of the uppermost inlet pipe.
- Tangential 1-sided inlet leads to a strongly swirling velocity field below the bed, which is not desired.

The process simulations based on the above CFD simulations indicate that the parts of the absorption column with an uneven gas flow distribution suffer from a significantly reduced CO_2 capture efficiency. However, since the gas flow evens out quickly in a packed bed column, the impact of the initial irregularities is negligible. When the liquid distribution is taken into account, the capture efficiency is certain to be affected. This was however not considered in this study.

Results from simulations with the stripping column included, and assuming similar gas distribution as for the absorber, also points to a negligible effect of the gas maldistribution on the CO_2 capture.

7 RECOMMENDATION FOR FURTHER WORK

1-phase gaseous flow field was here studied. However, in reality liquid droplets fall down from the bottom of the lowest bed creating some degree of resistance to the gas flow. The influence this has on the predicted gas inlet profiles should be studied.

In any further work it must also be taken care of that the gas inlet piping is designed so that the flow distribution is fully developed and totally even at the boundary of the CFD model mesh.

A detailed modelling of the 2-phase flow field in the bed is not reasonable at this stage. At a macroscopic level, the porous zone model is capable of representing the pressure resistance the gas flow encounters. Looking at the flow field in a smaller scale, say packing channel scale or smaller, the isotropic porous model cannot describe the influence of these structures on the flow field. Flow field in the modelled packed bed is therefore strongly simplified. On the other hand, including a detailed geometrical packing model in the absorption column model is not sensible with today's computational resources and therefore compromises have to be made.

Markus Duss has explained in his paper : “A new method to predict the susceptibility to form maldistribution in packed columns based on pressure drop correlations” a novel method for predicting the effects of maldistribution on packing efficiency. He introduces three new terms: the potentially available force to shift liquid, the vapour maldistribution susceptibility factor and the driving force to induce maldistribution. J. F. Billingham and M. J. Lockett explain in their paper "A simple method to assess the sensitivity of packed distillation columns to maldistribution" how the for distillation a method of dividing a column cross-section to parallel columns is sensitive to designer choices and ill-suited for design work. There is no reason to expect the results much differ for absorption.

A XX step development program was thus designed:

1. Applying the Duss equations for Aspen+ rate based model.

   Note: the vapour maldistribution susceptibility factor should be also considered as the liquid maldistribution is more probable and expected to cause serious problems more easily.

2. Defining the column for Aspen+ rate based model in such a manner that sections of minimum and maximum liquid/vapor ratio are considered and Duss findings can be verified by detecting the disappearance of any of the reacting components at the balance limit.
3. If vicinity of potentially available force to shift liquid or driving force to induce maldistribution is detected a new porous model will be developed to study the effect of the laterally different apparent porosity of the packing for the gas flow. This porosity would be introduced to the model by pressure loss correlations.

As long as a CFD model with full process simulator and detailed mechanical features is elusive the final workhorse for these applications could be Neste Jacobs oy in-house process simulator Flowbat equipped with section model that could model individual packing blocks with their interactions with adjoining blocks. This combined with CFD based initial gas distribution models would be a very powerful tool.

Sources

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3. J.F. Billingham and M.J. Lockett, *Chem. Eng. Res. Des.*, 80(2002) 373-382