



# DISPLACE post-combustion carbon capture technology - Integration in a steel plant for mitigation of CO<sub>2</sub> emissions

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## ABSTRACT

The decarbonization of the steel industry, responsible for approximately 7% of global direct energy-related CO<sub>2</sub> emissions, is pivotal in advancing toward a more sustainable future. Carbon capture technologies play a crucial role in achieving this objective. This study presents the description, modelling, and characterization of the DISPLACE carbon capture technology, an isothermal and isobaric adsorption technology using with concentration swing regeneration. The process yields a high-purity CO<sub>2</sub> stream alongside a CO<sub>2</sub>-lean gas stream and its application to the decarbonization of flue gas from oxy-fired hot-stoves in a BF-BOF steel mill is described. Various DISPLACE operating conditions were simulated reaching performances of carbon capture ratios up to 98% and (dry) carbon purities up to 99%. Environmental and economic Key Performance Indicators (KPIs) were assessed, demonstrating the advantage of operating at 400 °C due to the reduced DISPLACE steam-to-carbon ratio. The production of steam for adsorbent regeneration requires additional fuel such as NG or coke oven gas (COG). When operating DISPLACE at optimal conditions and considering COG as fuel, a carbon avoidance greater than 78% can be reached with a SPECCA and a CCA equal to 3.65 GJ/tCO<sub>2</sub> and 91.89 €/tCO<sub>2</sub> respectively, values significantly lower than competitive MEA technology (SPECCA equal to 4.86 GJ/tCO<sub>2</sub> and CCA of 113.33 €/tCO<sub>2</sub>). Additionally, the impact of varying DISPLACE carbon capture ratios (CCR) and carbon purity was evaluated.

## Nomenclature

| Acronyms |                                                       |
|----------|-------------------------------------------------------|
| BF       | Blast Furnace                                         |
| BFG      | Blast Furnace Gas                                     |
| BOF      | Basic Oxygen Furnace                                  |
| BOFG     | Basic Oxygen Furnace Gas                              |
| CCA      | Cost of CO <sub>2</sub> Avoided [€/tCO <sub>2</sub> ] |
| CCR      | CO <sub>2</sub> Capture Ratio                         |
| CCS      | Carbon Capture and Storage                            |
| Co       | Contingencies [€]                                     |
| COG      | Coke Oven Gas                                         |
| EPC      | Engineering, Procurement and Construction [€]         |
| FCF      | Fixed Charge Factor                                   |
| GHG      | Greenhouse Gases                                      |
| HRC      | Hot Rolled Coil                                       |
| LCOHRC   | Levelized Cost Of HRC                                 |
| MEA      | Monoethanolamine                                      |
| NG       | Natural Gas                                           |

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|              |                                                                 |
|--------------|-----------------------------------------------------------------|
| OC           | Owner's cost [€]                                                |
| PEC          | Primary Energy Consumption [GJ/t <sub>product</sub> ]           |
| SEWGS        | Sorption Enhanced Water Gas Shift                               |
| SPECCA       | Specific PEC for CO <sub>2</sub> Avoided [GJ/tCO <sub>2</sub> ] |
| TDPC         | Total Direct Plant Cost [€]                                     |
| TAC          | Total Annualised Cost [M€/y]                                    |
| TEC          | Total Equipment Cost [€]                                        |
| TIC          | Total Installation Cost [€]                                     |
| TPC          | Total Plant Cost [€]                                            |
| Greek        |                                                                 |
| $\epsilon_b$ | Bed porosity [-]                                                |
| $\eta$       | Efficiency [-]                                                  |
| $\rho$       | Gas density [kg/m <sup>3</sup> ]                                |
| $\tau$       | Plant availability [-]                                          |
| $\omega$     | Mass fraction [-]                                               |
| Symbols      |                                                                 |

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|               |                                                               |
|---------------|---------------------------------------------------------------|
| $a_p$         | Particle interfacial area per unit volume [1/m]               |
| $c$           | Molar concentration [mol/m <sup>3</sup> ]                     |
| $C_0$         | Reference cost                                                |
| $C_f$         | Fixed Costs [M€/y]                                            |
| $C_v$         | Variable Costs [M€/y]                                         |
| $d_p$         | Particle diameter [m]                                         |
| $D_z$         | Axial mass dispersion coefficient [m <sup>2</sup> /s]         |
| $e_{CO_2}$    | Specific CO <sub>2</sub> emissions [ $t_{CO_2}/t_{product}$ ] |
| $f$           | Friction factor [-]                                           |
| $k_{LDF}$     | Linear driving force coefficient [1/s]                        |
| $M$           | Molar mass [kg/mol]                                           |
| $\dot{m}$     | Mass flowrate [kg/s]                                          |
| $m_{sorbent}$ | Sorbent mass [kg]                                             |
| $N$           | Molar flux [mol/m <sup>2</sup> s]                             |
| $\dot{n}$     | Molar flowrate [mol/s]                                        |
| $n$           | Plant lifetime [years]                                        |
| $p$           | Pressure [Pa]                                                 |
| $r$           | Interest rate [%]                                             |
| $S_0$         | Reference size                                                |
| $\Delta T$    | Temperature difference [°C]                                   |
| $t$           | Time [s]                                                      |
| $u$           | Superficial gas velocity [m/s]                                |
| $v$           | Interstitial gas velocity [m/s]                               |
| Subscripts    |                                                               |
| $e$           | Electric                                                      |
| $i$           | Species index                                                 |
| $int$         | interphase                                                    |
| $h$           | Hydraulic                                                     |
| $m$           | Mechanical                                                    |
| $p$           | Polytropic                                                    |

## 1. Introduction

In accordance with the Paris Agreement, CO<sub>2</sub> emissions to the atmosphere must be strongly reduced. This is especially difficult for industries that have CO<sub>2</sub> emissions as part of their process streams rather than energy production. In the *Industrial Carbon Management Strategy*, published by EU, the need for carbon capture and storage (CCS) technologies for industry is highlighted (European Commission, 2024).

Gas separation processes based on adsorption are a well-established technology with solid sorbent CO<sub>2</sub> capture processes showing great potential due to their favourable LCA results (Petrescu et al., 2019). Adsorption based separation processes work through selective adsorption of molecules onto the surface of the sorbent under the release of adsorption energy. Sorbent regeneration occurs through either increase of temperature or reduction of the partial pressure and can be enhanced through utilization of a sweeping gas stream or purge. The general kinetics of the adsorption and desorption process are well researched for a large variety of sorbents, each presenting unique adsorption capacities (Helfferich and Ruthven, 1984; Yang, 1997).

Several classes of adsorbent materials are available for the capture of CO<sub>2</sub>, including for example zeolites and metal-organic frameworks for low temperature applications, layered double hydroxides for intermediate temperatures (200–500 °C), and calcium-based adsorbents for high-temperature applications (>400 °C) (Wang et al., 2011). Importantly, layered double hydroxides or hydrotalcite-based adsorbents perform exceptionally well in terms of robustness, regenerability and working capacity (Santamaría et al., 2023). As such, potassium-promoted hydrotalcite has been successfully scaled up for deployment in the sorption-enhanced water-gas shift (SEWGS) process (Sebastiani et al., 2022; Boon, 2023; Manzolini et al., 2020). All industrially relevant applications of CO<sub>2</sub> adsorption are performed in the presence of steam – in general a complicating factor (Kolle et al., 2021). Potassium promoted hydrotalcite, however, is not only robust in the presence of steam (Coenen et al., 2017; Xin et al., 2024), it has been shown to interact with CO<sub>2</sub> and steam which has allowed for the efficient use of steam as a working medium in CO<sub>2</sub> adsorption (Boon et al., 2014, 2015).

In this work, a comprehensive introduction to the novel technology DISPLACE, an isobaric adsorption process for CO<sub>2</sub> capture, is given. The separation is based on the promising behaviour of CO<sub>2</sub> displacement by steam adsorption (Manzolini et al., 2022). Utilizing this unique characteristic of the sorbent, DISPLACE can be operated at an intermediate temperature and high pressure with high pressure products, the CO<sub>2</sub>-lean and CO<sub>2</sub>-rich streams. This technology has been validated on TRL 5 for the steelmaking industry as part of the Horizon 2020 project C<sup>4</sup>U (C<sup>4</sup>U website). In this project a proof-of-concept campaign was successfully performed on a single-column (3000 kg sorbent) pilot with a feed of 400 Nm<sup>3</sup>/h of exhaust gas from oxy-combustion BFG provided by the SSAB blast furnace in Lulea, Sweden. As this was a single-column campaign, the final cyclic performance was not demonstrated, but the potential for CO<sub>2</sub>-rich product purities up to 99% and CO<sub>2</sub> capture rates of up to 95% for a multi-column operation was observed. Additionally, an intensive campaign on bench-scale for the validation of the process model and sorbent isotherms was performed. The results of both these campaigns are the basis for this paper which specifically describes the development of the technology in the context of decarbonising the steelmaking process.

The iron and steel industry poses significant challenges in reducing emissions. This industrial process accounts for approximately 7% of global direct energy-related CO<sub>2</sub> emissions (International Energy Agency, 2020). This is primarily due to its heavy reliance on fossil fuels, particularly coal, in the blast furnace-basic oxygen furnace (BF-BOF) steelmaking route, which currently dominates the steel market with 70% production share (International Energy Agency, 2020). The integration of carbon capture technologies into steel production processes is crucial for advancing towards a net-zero emissions future. Perpiñán et al. (Perpiñán et al., 2023) performed a systematic review of peer-reviewed articles focusing on the integration of carbon capture technologies in the BF-BOF steelmaking route. The analysed carbon capture technologies were categorized into four main groups: i) post-combustion (chemical absorption (Manzolini et al., 2020; Gazzani et al., 2015; Yang et al., 2021), membranes (Yun et al., 2021; Luca and Petrescu, 2021; Baker et al., 2018)), ii) looping processes (calcium looping (Cormos et al., 2020; Tian et al., 2018; Xie et al., 2017), chemical looping (Luo et al., 2018; Katayama et al., 2020; Xiang and Zhao, 2018), other looping processes (Martínez et al., 2018; Sun et al., 2020)), iii) oxygen blast furnaces and top-gas recycling (Tsupari et al., 2015; Arasto et al., 2014; Li et al., 2020; Qie et al., 2020), iv) pre-combustion (chemical absorption (Gazzani et al., 2015; Chung et al., 2018a; Martínez Castilla et al., 2019), adsorption (Jin et al., 2017; Quader et al., 2016; Kim et al., 2015), membranes (Chung et al., 2018b; Jeon et al., 2022; Li et al., 2022; Ramírez-Santos et al., 2018), SEWGS (Petrescu et al., 2019; Manzolini et al., 2020; Gazzani et al., 2015; van Dijk et al., 2018)). The thermal penalty for various carbon capture technologies varies between 1.3 and 6.2 MJ/kgCO<sub>2</sub>. Post-combustion chemical absorption (Chisalita et al., 2019; Biermann et al., 2019; Cormos, 2016), calcium looping (Tian et al., 2018), other looping processes (Fernández et al., 2017, 2020; Martínez et al., 2019), and pre-combustion chemical absorption (Chung et al., 2018b) exhibit different ranges within this spectrum. When it comes to electricity consumption, the differences are more pronounced. Post-combustion chemical absorption, calcium looping, and pre-combustion chemical absorption generally have lower electricity requirements, averaging less than 1 MJ/kgCO<sub>2</sub>. This is because heat consumption is predominant, with most of electricity usage related to CO<sub>2</sub> compression. On the other hand, technologies like membranes (post- and pre-combustion), and adsorption pre-combustion requires a compression step upstream the CO<sub>2</sub> capture process, leading to higher electricity penalties between 1 and 3 MJ/kgCO<sub>2</sub>. From an economic perspective, post-combustion chemical absorption technologies demonstrate a linear relationship between CO<sub>2</sub> capture cost (€/tCO<sub>2</sub>) and CO<sub>2</sub> emission reduction (kgCO<sub>2</sub>/t<sub>steel</sub>) ranging from 38 €/tCO<sub>2</sub> for a CO<sub>2</sub> emission reduction of 400 kgCO<sub>2</sub>/t<sub>steel</sub> to 98 €/tCO<sub>2</sub> in the case of a reduction equal to 1700

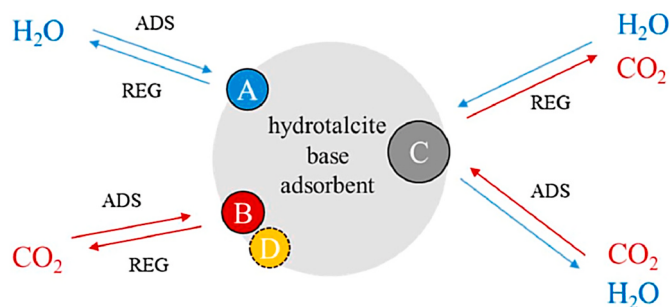


Fig. 1. Adsorption sites on the hydrotalcite based adsorbent for CO<sub>2</sub> and steam. Reprinted from (Coenen et al., 2018a).

kgCO<sub>2</sub>/t<sub>steel</sub> (Perpiñán et al., 2023). Conversely, oxy-blast furnace (Tsupari et al., 2015; Arasto et al., 2014) and calcium looping technologies (Cormos et al., 2020; Cormos, 2016) exhibit varying costs for equivalent levels of CO<sub>2</sub> emissions reduction. In the case of oxy-blast furnace, for a CO<sub>2</sub> reduction of 400 kgCO<sub>2</sub>/t<sub>steel</sub> the cost varies between 58 €/tCO<sub>2</sub> to above 90 €/tCO<sub>2</sub> (Perpiñán et al., 2023). In the instance of SEWGS technology, costs below 40 €/tCO<sub>2</sub> are achievable when the technology is employed for the gas fraction utilized as fuel within the steel mill's power plant (Manzolini et al., 2020).

Interestingly, Perpiñán et al. (Perpiñán et al., 2023) note a lack of literature on carbon capture applied to flue gas from oxy-combustion of steel-making gases (i.e. BFG, BOFG or COG). Therefore, this study aims to bridge this gap by introducing the innovative carbon capture technology named DISPLACE and its application to decarbonize the hot-stoves flue gas from oxy-combustion of blast furnace gas, which represents around 20% of the total CO<sub>2</sub> emissions of a BF-BOF plant. The integration of CCS technologies is recognised as fundamental in mitigating the carbon footprint of a BF-BOF steel mill (Perpiñán et al., 2023). Additionally, the results obtained enable the possibility of better understanding how to optimally run and integrate the DISPLACE technology in an industrial plant and to investigate its application to other CO<sub>2</sub> point sources within a steel mill.

The paper is organised as follows: in Section 2 the DISPLACE technology and the modelling approach are presented along with the methodology used to simulate the oxy-fired hot-stoves, the integration of DISPLACE in a steel plant and the principal KPIs; Section 3 presents and discusses the main results obtained, followed by the conclusion in Section 4.

## 2. Materials and methods

The simulation of the DISPLACE cycle process and its integration into the plant layout of a steel mill are detailed. The decarbonization of flue gas from hot-stoves serves as a specific case study.

An optimization process was conducted to determine the optimal

working temperature and pressure for DISPLACE. Elevating the pressure of the feed gas enhances CO<sub>2</sub> capture on the DISPLACE sorbent material, albeit at the cost of increased energy required for feed gas compression. Moreover, the consumption of regeneration steam, expressed as steam-to-carbon ratio, is a crucial parameter influenced by operating conditions. Higher temperatures result in a reduction of this ratio, offering favourable outcomes in terms of overall CO<sub>2</sub> emissions and cost efficiency.

The integration of the DISPLACE technology was executed using Aspen Plus V14, and the results were assessed via environmental Key Performance Indicators (KPIs). Furthermore, the performance of DISPLACE was compared against a conventional post-combustion amine-based carbon capture technology for comprehensive analysis.

### 2.1. The DISPLACE technology

The DISPLACE technology is an isobaric separation technology for the post-combustion capture of CO<sub>2</sub> from flue gases. It is based on a multicolumn concentration swing principle, which delivers the two separated product streams at the operating pressure of the unit. During the feed step, CO<sub>2</sub> is adsorbed onto a sorbent leaving the stream CO<sub>2</sub>-lean, while the sorbent is regenerated by displacing CO<sub>2</sub> on the sorbent with steam leading to the CO<sub>2</sub>-rich product, without the need for a pressure or temperature swing. The basis of the process are the characteristic adsorption sites of the mixed base-metal oxide sorbent derived from hydrotalcites. This sorbent has several sites onto which CO<sub>2</sub> and H<sub>2</sub>O can adsorb (Fig. 1): site B and D are available for CO<sub>2</sub> adsorption and site C is a shared site. Detailed mechanical investigations have identified the presence of distinct sites for the interaction of CO<sub>2</sub> and steam with the adsorbent material (Coenen et al., 2018a). On shared site C, the adsorbed species (CO<sub>2</sub>/H<sub>2</sub>O) is the one with higher partial pressure in the gas phase. When the partial pressure ratio changes, the other species displaces the adsorbed species on the sorbent. The site can be assumed to only be occupied by one species at a time. The DISPLACE process utilises this displacement characteristics of site C to achieve high purity CO<sub>2</sub> product at high capture ratios.

#### 2.1.1. DISPLACE cycle development

The product of a single column separation process without recycles and using gases from BFG oxy-combustion is shown in Fig. 2 (nitrogen is present in BFG and not introduced with the oxidant). The process consists of two steps: adsorption and desorption, both of which can be divided into three sections: 1) void composition, 2) pure product, 3) product tail.

In the case of the adsorption step, the first section (Ads-1) is comprised of a steam-CO<sub>2</sub> mixture which remained in the void fraction after the preceding regeneration (Des-3). The second section is the CO<sub>2</sub>-lean product (Ads-2), which in this case is mostly nitrogen coming with the BFG. The third section is the product once the CO<sub>2</sub> breaks through (Ads-3). Equally, for the desorption step, the first section (Des-1) is the

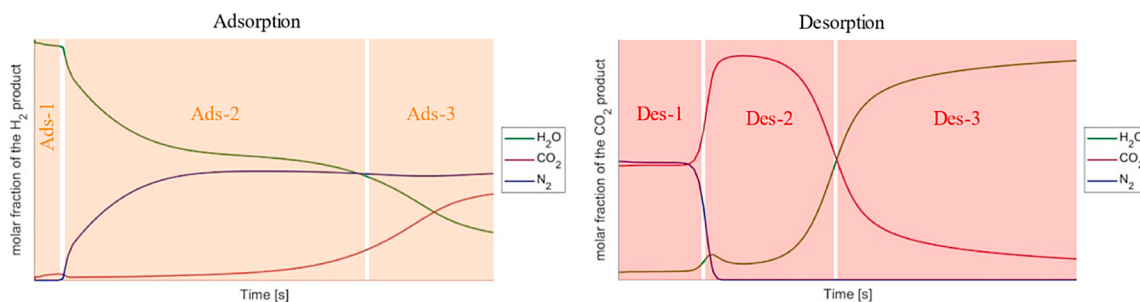
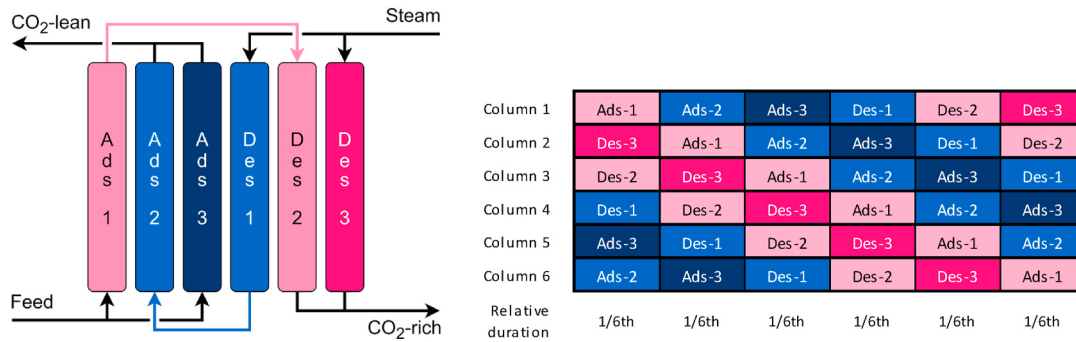


Fig. 2. Product compositions (wet) of a single column DISPLACE process operated at 15 bar and 400 °C without recycles: adsorption (left) and desorption (right). The column was modelled at 2 m height, 0.038 m diameter with a feed flowrate of 15 slpm (2.3% H<sub>2</sub>O, 48% CO<sub>2</sub>, 49.7% N<sub>2</sub>) and a counter current steam flow of 12 slpm (100% H<sub>2</sub>O).



**Fig. 3.** Six column DISPLACE process for a CO<sub>2</sub>-N<sub>2</sub> separation (left) and timing for a 6-column unit (right). The column names indicate which product gas they are producing.

**Table 1**

Mass transfer equations of the 1D heterogeneous column taken from (Boon et al., 2014).

|                            |                                                                                                                                                                                                                                        |     |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| Continuity                 | $\frac{\partial \rho}{\partial t} = -\frac{\partial \rho v}{\partial z} + \frac{1 - \epsilon_b}{\epsilon_b} a_p \sum_i M_i N_i$                                                                                                        | (1) |
| Momentum                   | $0 = -\frac{\partial p}{\partial z} - f \frac{\rho  u  u}{d_p}$                                                                                                                                                                        | (2) |
| Mass balance               | $\frac{\partial(\rho \omega_i)}{\partial t} = -\frac{\partial \rho v \omega_i}{\partial z} + \frac{\partial}{\partial z} \left( D_z \rho \frac{\partial \omega_i}{\partial z} \right) + \frac{1 - \epsilon_b}{\epsilon_b} a_p M_i N_i$ | (3) |
| Intraparticle mass balance | $\frac{\partial \langle c_i \rangle}{\partial t} = k_{LDF,i} (c_{int,i} - \langle c_i \rangle)$                                                                                                                                        | (4) |

remaining feed composition in the void volume of the column. The second section is a high purity and very dry CO<sub>2</sub> stream (Des-2). In the third section still more CO<sub>2</sub> is desorbed, while steam is breaking through (Des-3).

The basic design constraints for the cycle development of the continuous process are.

- one column needs to always receive feed;
- one column needs to always produce CO<sub>2</sub>-lean product;
- one column needs to always produce CO<sub>2</sub>-rich product;
- reduction of the steam consumption by recycling Ads-1 within the cycle;
- increase of the CO<sub>2</sub> purity by recycling Des-1 within the cycle.

These constraints lead to the adoption of at least six columns. Furthermore, to avoid build-up of impurities in the system, there should always be a “flush” after a column received a recycled stream which means that the following step should feed more gas than just replacing the void volume. Taking all the constraints and the process considerations into account while minimizing the number of columns, the six column set-up is identified as the optimal configuration and represented in Fig. 3 together with the corresponding timing.

As the product of Ads-1 is mostly steam with some CO<sub>2</sub>, it is recycled to the desorption step (Des-2) to reduce the steam demand of the process. Any potential impurity build-up in the desorption step due to this recycle is avoided by following the recycle feed with regeneration steam. Likewise, the product from Des-1 which is a similar to feed composition is recycled to the adsorption step to increase the CO<sub>2</sub>-product purity. Any impurities from this recycled stream are flushed out of the system through feed gas in Ads-3.

The adsorption is performed co-currently while desorption is performed counter-currently to keep the end of the bed as clean as possible improving the product purity. A clean sorbent can adsorb CO<sub>2</sub> at very low partial pressures preventing slip.

Alternative processes involving more columns or more complex

mixed recycles are possible and would allow for further optimization. However, this simple set-up fulfils the basic need of the process and allows for the best understanding of the characteristics.

### 2.1.2. DISPLACE modelling

DISPLACE uses an existing model which contains experimentally validated correlations for the interaction, the mass-transfer and the 1D heterogeneous column models (Boon et al., 2014; Coenen et al., 2018b; Sebastiani et al., 2021). The basic equations used within the model are the continuity, momentum and mass balance for a column filled with a sorption bed as well as the specific equation for the intra particle mass transfer using the linear driving force approximation (Table 1).

As the DISPLACE process is operated isobarically with recycles, the column model was built to include and account for column pressure drops for the recycles. The interaction and mass-transfer models have previously been experimentally validated for low to high CO<sub>2</sub> and H<sub>2</sub>O concentrations (0–100%), in a temperature range of 350 °C–450 °C and adsorption and desorption pressure between 10 - 25 bar and 1–4 bar, respectively (Sebastiani et al., 2021). DISPLACE operation is at or just outside these boundaries concerning: i) the operation at temperatures as low as 300 °C and ii) CO<sub>2</sub> desorption with 100% H<sub>2</sub>O at increased pressure as high as 15 bar. The interaction model needed finetuning for both these aspects and experimental results were used for renewed model validation. This will be presented in a future work.

### 2.1.3. DISPLACE cycle optimization

Optimizing the DISPLACE process for a specific process integration is a multivariable process. The most impactful parameters are: (i) system pressure, (ii) column size (diameter and height), (iii) number of trains, (iv) cycle step lengths and (v) steam-to-carbon (S/C) ratio of the desorption steam feed relative to the flue gas adsorption feed. Specific performance in terms of CO<sub>2</sub>-purity at dry conditions (CP, equation (5)) and carbon capture ratio (CCR, equation (6)) are defined by the process integration and downstream unit requirements (Section 2.2). As a result of the column size, the cycle time and the captured CO<sub>2</sub>, a process productivity is derived. The productivity (equation (7)) is a measure on how effectively the sorbent material has been used. A higher productivity indicates less sorbent needed for the same amount of CO<sub>2</sub> captured. A sensitivity study on the process parameters is conducted where above-mentioned parameters are varied to identify the most suitable performance.

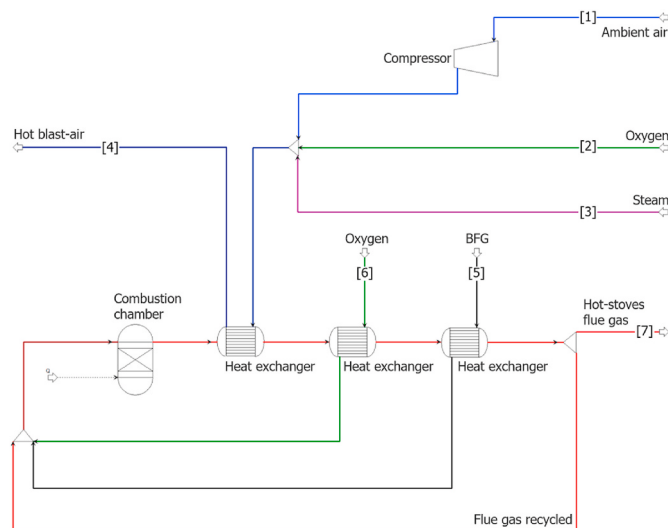
$$CP[\%] = \frac{(\dot{n}_{CO_2})_{CO_2-product,dry}}{\sum_i (\dot{n}_i)_{CO_2-product,dry}} \cdot 100 \quad (5)$$

$$CCR[\%] = \frac{(\dot{m}_{CO_2})_{CO_2-product}}{(\dot{m}_{CO_2})_{feed}} \cdot 100 \quad (6)$$

**Table 2**

Oxy-fired hot-stoves streams with corresponding thermodynamic conditions.

| Stream                            | $\dot{m}$<br>[kg/s] | T<br>[°C] | P<br>[bar] | Composition [%vol] |                 |       |                |                |      |                  |
|-----------------------------------|---------------------|-----------|------------|--------------------|-----------------|-------|----------------|----------------|------|------------------|
|                                   |                     |           |            | H <sub>2</sub>     | CO <sub>2</sub> | CO    | O <sub>2</sub> | N <sub>2</sub> | Ar   | H <sub>2</sub> O |
| Ambient air [1]                   | 135.43              | 12        | 1.013      | –                  | 0.04            | –     | 20.72          | 77.22          | 0.92 | 1.10             |
| Oxygen [2]                        | 7.26                | 60        | 1.1        | –                  | –               | –     | 99.9           | 0.01           | 0.09 | –                |
| Steam [3]                         | 0.84                | 175       | 9          | –                  | –               | –     | –              | –              | –    | 100.0            |
| Hot blast air [4]                 | 144.09              | 1118      | 4          | –                  | 0.04            | –     | 24.13          | 72.98          | 0.87 | 1.98             |
| BFG [5]                           | 77.21               | 30        | 1.11       | 2.3                | 20.54           | 21.79 | –              | 51.36          | –    | 4.01             |
| O <sub>2</sub> for combustion [6] | 10.66               | 60        | 11         | –                  | –               | –     | 99.9           | 0.01           | 0.09 | –                |
| Hot-stoves flue gas [7]           | 87.88               | 140       | 1.01       | –                  | 41.90           | –     | 1.00           | 50.81          | 0.04 | 6.25             |

**Fig. 4.** Aspen Plus simulation of oxy-fired hot-stoves.

$$\text{Productivity} \left[ \frac{\text{mol}_{\text{CO}_2}}{\text{kg}_{\text{sorbent}} \text{h}} \right] = \frac{(\dot{n}_{\text{CO}_2})_{\text{CO}_2\text{-product}}}{m_{\text{sorbent}}} \quad (7)$$

## 2.2. DISPLACE technology applied to gas from a steel plant

The integration of the DISPLACE technology into a blast furnace-basic oxygen furnace steel mill has been examined. In this section, the innovative decarbonization process applied to the hot-stoves flue gases is presented. Since this is the first time that the DISPLACE process is evaluated, several operating temperatures and pressure were explored to identify the optimal region.

### 2.2.1. Flue gas from the hot-stoves

In a conventional steel mill, the reduction of iron-bearing materials, such as iron ore lump, sinter and/or pellets, takes place in the blast furnace. These materials, along with additives (i.e. limestone) and reducing agents (i.e. coke) are fed from the top of the furnace. Additionally, hot blast air, enriched with oxygen, is injected in the lower part of the furnace guaranteeing the production of carbon monoxide from coke and therefore, the reduction of iron ores into metallic iron (Remus et al., 2013).

The hot-stoves are high-temperature heat exchangers in which cold ambient air is heated up to the desired temperature (900–1350 °C). They are operated on a cyclical basis. A mix of BFG and COG is usually used as fuel to generate hot combustion gases that are circulated through a network of pipes and chambers made of heat-resistant refractory materials until these materials reach the correct temperature (1100–1500 °C). Then the combustion gases are cut off and the cold ambient air is introduced in the opposite direction. The hot bricks release the heat to the cold air in contact with them. The cycle lasts until the blast air can reach the desired temperature. Subsequently a new

cycle is started (Remus et al., 2013).

Within the C<sup>4</sup>U project, the adoption of oxy-fired hot-stoves has been proposed. In this case, only BFG is used as fuel, and it is burnt with oxygen instead of air. This has the double effect of lowering the amount of BFG used in the hot-stoves and increasing the concentration of CO<sub>2</sub> in the flue gases effectively favouring the carbon capture process. It must be pointed out that the CO<sub>2</sub> will still be diluted in the exhaust gases as BFG contains relevant amount of N<sub>2</sub> (around 51% as reported in Table 2).

The optimal incorporation of the DISPLACE technology into the steel mill layout has been carried out considering diverse operating conditions in terms of temperature and pressure. The focus has been specifically on cases where carbon capture exceeds 90%, ensuring a minimum carbon purity of 95% on dry basis. Through comprehensive simulations of the DISPLACE cycles, key parameters, including the number of columns, size dimensions, and steam consumption, have been accurately computed.

To assess the integration of DISPLACE technology, Aspen Plus V14 has been employed, utilizing the cycle performances determined in the preceding step.

### 2.2.2. Thermodynamic assessment – hot-stoves simulation

The oxy-fired hot stove have been simulated in Aspen Plus V14 using the RKS-BM property model (Fig. 4). The mass flow rate of cold air, oxygen and steam has been adapted from (IEAGHG Technical Report, 2013) considering the same specific mass flow (kg/t<sub>HRC</sub>) and the same thermodynamic conditions. Therefore, the composition, temperature and pressure of hot blast air are the same as reported in (IEAGHG Technical Report, 2013). The Aspen Plus model thus has been used to compute the mass flow rates of the BFG and the oxygen used for combustion as well as the composition of the flue gas.

In this study a conventional steel mill producing 3.16 Mt<sub>HRC</sub>/y is considered. The mass flow rate of BFG used as fuel in the hot-stoves is equal to 77.21 kg/s corresponding to 1.60 GJ/t<sub>HRC</sub>. The CO<sub>2</sub> emissions associated to the hot-stoves flue gas are 47.47 kg<sub>CO2</sub>/s equal to 0.443 t<sub>CO2</sub>/t<sub>HRC</sub>. The resulting gas conditions are shown in Table 2 and refer to the streams of Fig. 4.

### 2.2.3. Thermodynamic assessment – DISPLACE integration

The plant scheme of the integration of the DISPLACE technology for decarbonization of flue gas from hot-stoves is shown in Fig. 5. The flue gas from hot-stoves (red stream) is at 140 °C and slightly above the atmospheric pressure. Before being compressed, it is cooled to 35 °C to minimize compression work and contributing to the pre-heating up to 102 °C of a portion of the water used for generating steam, utilized in the DISPLACE columns. Similarly, the outlet gas streams from the DISPLACE process, i.e. the CO<sub>2</sub>-rich stream (grey stream) and the CO<sub>2</sub>-lean gas stream (green stream), are cooled generating steam. A furnace is adopted to supply the heat to the gas stream exiting the compressor and for superheating of the steam to the DISPLACE working temperature. This furnace alternately uses NG and COG as fuels. Prior to entering the furnace, the fuel and combustion air are preheated by the furnace flue gases (black stream). To prevent the presence of non-condensable

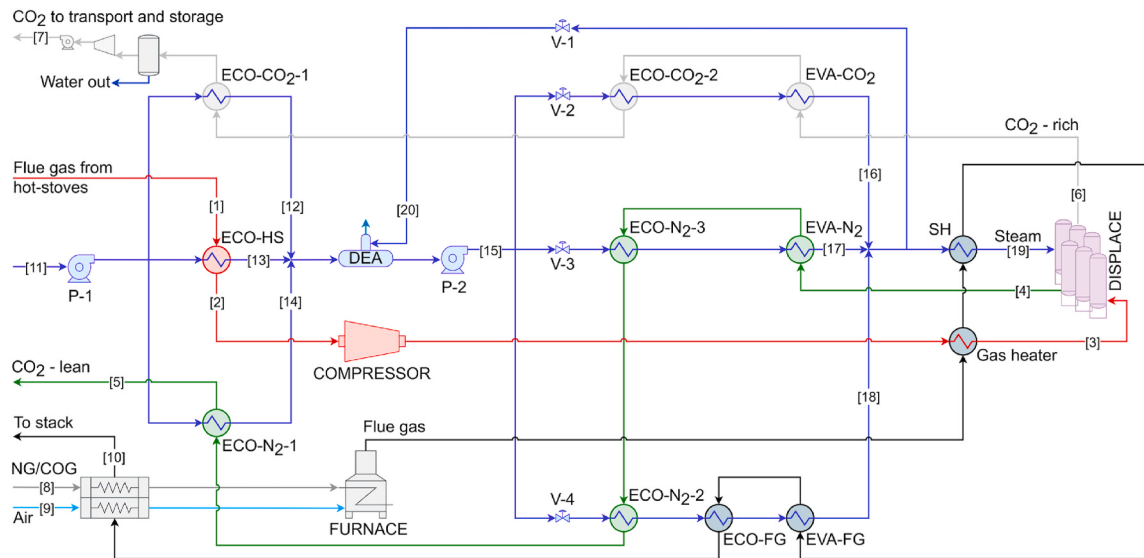


Fig. 5. Plant scheme of the integration of DISPLACE technology for decarbonization of flue gas from hot-stoves.

Table 3

Assumptions for the thermodynamic assessment.

| Parameter                                    | Unit                   | Value |
|----------------------------------------------|------------------------|-------|
| NG LHV                                       | MJ/kg                  | 46.87 |
| COG LHV                                      | MJ/kg                  | 40.21 |
| Electricity CO <sub>2</sub> emissions        | kgCO <sub>2</sub> /MWh | 250   |
| Water recovery from CO <sub>2</sub> stream   | %                      | 90    |
| Plant availability                           | h/y                    | 8200  |
| Steel plant capacity                         | Mt <sub>HRC</sub> /y   | 3.16  |
| Heat Exchangers                              |                        |       |
| - Minimum ΔT gas-gas heat exchanger          | °C                     | 15    |
| - Minimum ΔT gas-liquid heat exchanger       | °C                     | 10    |
| - ΔT subcooling in the economizers           | °C                     | 5     |
| - Economizer hot-side pressure drops         | bar                    | 0.2   |
| - Economizer cold-side pressure drops        | bar                    | 0.7   |
| - Evaporator hot-side pressure drops         | bar                    | 0.2   |
| Turbomachines                                |                        |       |
| - Pumps hydraulic efficiency                 | %                      | 75    |
| - Pumps mechanical efficiency                | %                      | 95    |
| - Compressor polytropic efficiency           | %                      | 85    |
| - Compressor mechanical efficiency           | %                      | 95    |
| CO <sub>2</sub> compression train            |                        |       |
| - Compressor number of stages                | –                      | 3     |
| - Compressor discharge pressure              | bar                    | 80    |
| - Compressor polytropic efficiency stage 1,2 | %                      | 80    |
| - Compressor polytropic efficiency stage 3   | %                      | 75    |
| - Compressor mechanical efficiency           | %                      | 95    |
| - Pump discharge pressure                    | bar                    | 110   |
| - Pump hydraulic efficiency                  | %                      | 75    |
| - Pump mechanical efficiency                 | %                      | 95    |

Table 4

Assumptions adopted in the Aspen model of the MEA carbon capture sections.

| Unit                        | Aspen Plus model                                                                                                                               |
|-----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------|
| Absorber                    | RadFrac Rate-Based; 25 stages; MELLAPAK 250Y; Condenser: None; Reboiler: None                                                                  |
| Stripper                    | RadFrac Rate-Based; 20 stages; MELLAPAK 250Y; Condenser: Partial-Vapor-Liquid; Reboiler: Kettle                                                |
| Heat exchanger              | HeatX Pinch point ΔT = 10 °C                                                                                                                   |
| Pump                        | Discharge pressure = 2.5 bar; $\eta_h = 0.75$ ; $\eta_m = 0.95$                                                                                |
| CO <sub>2</sub> compression | Mcompr 3 stages; Discharge pressure = 80 bar; $\eta_{p,1,2} = 0.8$ ; $\eta_{p,3} = 0.75$ ; $\eta_m = 0.95$ ; T <sub>intercooling</sub> = 28 °C |
|                             | Pump Discharge pressure = 110 bar; $\eta_h = 0.75$ ; $\eta_m = 0.95$                                                                           |

Table 5

Assumptions for the economic assessment.

| Parameter                              | Unit             | Value |
|----------------------------------------|------------------|-------|
| NG/COG price                           | €/MWh            | 50    |
| Electricity price                      | €/MWh            | 125   |
| Discount rate                          | %                | 8.00  |
| Lifetime                               | years            | 25    |
| Fixed Charge Factor                    | %                | 9.37  |
| Water cost                             | €/m <sup>3</sup> | 1     |
| N° additional employees per CC section | –                | 15    |
| Annual salary                          | €/y              | 60000 |
| O&M costs                              | % TPC•FCF        | 5     |

species in the steam, a deaerator was included (Fig. 5). The CO<sub>2</sub>-rich stream is taken to the conditions for transport and storage (110 bar) through a multistage compressor, reaching pressures of up to 78 bar, liquefaction to 25 °C and subsequently pumped to a pressure of 110 bar as described in (Wright et al., 2011; Zecca et al., 2023). The specifications of the streams indicated in Fig. 5 are given in Appendix 5.1. Since many different operating conditions of DISPLACE were analysed in this work, as detailed in the following chapters, only the results regarding the case 5 bar–400 °C are shown.

Simulations of DISPLACE integration were performed using Aspen Plus 14, incorporating the assumptions detailed in Table 3. The composition of natural gas (NG) and coke oven gas (COG) were taken from (IEAGHG Technical Report, 2013).

#### 2.2.4. Reference technology – MEA post-combustion carbon capture

The reference technology adopted in this study to assess DISPLACE performance is the widely used post-combustion technology based on MEA scrubbing. According to the authors' knowledge there is no commercially available large scale CO<sub>2</sub> capture system based on physical adsorption, therefore MEA which is a well proven and commercially ready technology was selected for comparison.

A detailed description of the process can be found in (Zecca et al., 2023). The MEA post-combustion CO<sub>2</sub> capture process has been simulated in Aspen Plus V14 using the unsymmetric electrolyte NRTL property method (ENRTL-RK). The model includes the following key features: (i) true species including ions, (ii) activity-based reaction kinetics, (iii) rate-based models for columns with structured packing.

The electrolyte solution chemistry has been modelled with a CHEMISTRY model as the global electrolyte calculation option in the simulation. Chemical equilibrium is assumed with all the ionic

**Table 6**

PEC of electricity generation.

| Parameter                  | Unit                                    | RES | NGCC | USC  |
|----------------------------|-----------------------------------------|-----|------|------|
| Electricity C.I.           | [kg <sub>CO2</sub> /MWh <sub>e</sub> ]  | 0   | 350  | 850  |
| Plant efficiency           | [MW <sub>e</sub> /MW <sub>LHV</sub> ]   | –   | 0.60 | 0.42 |
| PEC electricity generation | [MWh <sub>LHV</sub> /MWh <sub>e</sub> ] | 0   | 1.67 | 2.38 |

reactions. In addition, a REACTION model has been created and used to model the reactions occurring in the absorber and in the stripper. All reactions are assumed to be in chemical equilibrium except those of CO<sub>2</sub> with OH<sup>−</sup> and CO<sub>2</sub> with MEA. The assumptions used to model the carbon capture section in Aspen Plus are shown in Table 4 while more details are provided in section 5.2.

### 2.2.5. Economic assessment

In this section, the methodology adopted to perform the economic assessment is described. General assumptions are summarized in Table 5. The electricity and NG prices were computed using the data reported in (International industrial energy prices). For both of them, average values in EU have been calculated considering the prices of 2019 and 2022. In the case of electricity, annual industrial electricity prices including environmental taxes and levies for very large consumers were considered. Similarly, for NG, annual industrial prices including taxes for large consumers were used. The price of COG is assumed to be the same of NG on energy basis.

The total plant cost (TPC) was computed starting from equipment costs according to the bottom-up methodology described in (Manzolini et al., 2020).

Focusing on the DISPLACE technology, the TEC is calculated using equations (8)–(11).

$$TEC_{DISPLACE}[\text{€}] = C_{\text{columns}} + C_{\text{bulk material and freight}} + C_{\text{valves}} \quad (8)$$

$$C_{\text{valves}}[\text{€}] = \sum_{i=1}^n (C_{\text{valve},i} \cdot n_{\text{valves per column},i} \cdot n_{\text{columns per train}} \cdot n_{\text{train}}) \quad (9)$$

$$C_{\text{columns}}[\text{€}] = C_{\text{steel}}[\text{€/kg}] \cdot m_{\text{column}} \cdot n_{\text{columns per train}} \cdot n_{\text{train}} \quad (10)$$

$$C_{\text{bulk material and freight}}[\text{€}] = 0.77 \cdot C_{\text{columns}} \quad (11)$$

The DISPLACE total plant cost (TPC) is calculated from TEC using equations (12) and (13) and the values shown in Table 13.

$$TDC_{DISPLACE}[\text{€}] = TEC_{DISPLACE} + C_{\text{construction}} + C_{\text{other}} \quad (12)$$

$$TPC_{DISPLACE}[\text{€}] = TDC_{DISPLACE} + EPCM_{\text{services}} + C_{\text{contingency}} \quad (13)$$

The total plant cost (TPC) of the auxiliary equipment (i.e. compressors, furnaces, heat exchangers, etc.) and of the MEA carbon capture section were computed through equations (35)–(39) and using the values reported in Table 14.

Finally, the total annualised cost (TAC) is computed considering: i) the total plant cost (TPC) annualised through the fixed charge factor (FCF); ii) the variable costs as the cost of electricity ( $C_{\text{el}}$ ), the cost of natural gas ( $C_{\text{NG}}$ ), the cost of water ( $C_{\text{H}_2\text{O}}$ ); iii) the fixed costs ( $C_{\text{f}}$ ); and iv) the operation and maintenance costs ( $C_{\text{O\&M}}$ ).

$$TAC \left[ \frac{\text{M€}}{\text{y}} \right] = TPC \cdot FCF + C_{\text{el}} + C_{\text{NG}} + C_{\text{H}_2\text{O}} + C_{\text{f}} + C_{\text{O\&M}} \quad (14)$$

More details on the procedure adopted to perform the economic assessment of the MEA and DISPLACE technologies are given in the appendix (section 5.4).

### 2.3. Key performance indicators

The evaluation of the performance of the DISPLACE carbon capture technology is made through environmental and economic key per-

mance indicators, typical of this research field and available in (Manzolini et al., 2020; Zecca et al., 2023; Khallaghi et al., 2022). The environmental indexes considered in this study are the primary energy consumption (PEC), the specific CO<sub>2</sub> emissions ( $e_{\text{CO}_2}$ ), the CO<sub>2</sub> capture ratio (CCR), the specific primary energy consumption for CO<sub>2</sub> avoided (SPECCA) and CO<sub>2</sub> avoidance (CA). The SPECCA indicator is defined as the additional primary energy required (in GJ) to avoid the emission of 1 ton of CO<sub>2</sub> producing the same amount of product.

$$PEC \left[ \frac{\text{GJ}_{\text{LHV}}}{\text{t}_{\text{HRC}}} \right] = \frac{\dot{m}_{\text{fuel}} \text{LHV}_{\text{fuel}} + PEC_{\text{el}} + \dot{Q}_{\text{req}}/\eta_{\text{th}}}{\dot{m}_{\text{HRC}}} \quad (15)$$

$$e_{\text{CO}_2} \left[ \frac{\text{t}_{\text{CO}_2}}{\text{t}_{\text{HRC}}} \right] = \frac{\dot{m}_{\text{CO}_2}}{\dot{m}_{\text{HRC}}} \quad (16)$$

$$\text{SPECCA} \left[ \frac{\text{GJ}_{\text{LHV}}}{\text{t}_{\text{CO}_2}} \right] = \frac{PEC_{\text{capture}} - PEC_{\text{no capture}}}{e_{\text{CO}_2, \text{no capture}} - e_{\text{CO}_2, \text{capture}}} \quad (17)$$

$$CA[\%] = \frac{e_{\text{CO}_2, \text{no capture}} - e_{\text{CO}_2, \text{capture}}}{e_{\text{CO}_2, \text{no capture}}} \cdot 100 \quad (18)$$

The PEC associated to the electricity generation varies in relation to its carbon footprint. In this study, the values provided in Table 6 are taken as reference and linear interpolation is employed for intermediate scenarios. In the renewable energy scenario, where the carbon intensity of imported electricity from the grid is 0 kg<sub>CO2</sub>/MWh<sub>e</sub>, implying no fossil fuel consumption during operation, hence ignoring the carbon footprint of green electricity production, the PEC related to electricity generation is deemed as 0 MWh<sub>LHV</sub>/MWh<sub>e</sub>. When the electricity carbon intensity reaches 350 kg<sub>CO2</sub>/MWh<sub>e</sub>, it is assumed that the electricity is generated in a natural gas combined cycle (NGCC) plant with an efficiency of 60%. Another scenario considered involves a coal ultra-supercritical cycle (USC), having an efficiency of 42% and a carbon footprint of 850 kg<sub>CO2</sub>/MWh<sub>e</sub>.

The economic performance is assessed in terms of levelized cost of hot rolled coil (LCOHRC) and cost of CO<sub>2</sub> avoidance (CCA). In equation (19),  $\tau$  indicates the plant availability.

$$\text{LCOHRC} \left[ \frac{\text{€}}{\text{t}_{\text{HRC}}} \right] = \frac{\text{TAC}}{\dot{m}_{\text{HRC}} \cdot 8760 \cdot \tau} \cdot 10^6 \quad (19)$$

$$\text{CCA} \left[ \frac{\text{€}}{\text{t}_{\text{CO}_2}} \right] = \frac{\text{LCOHRC}_{\text{capture}} - \text{LCOHRC}_{\text{no capture}}}{e_{\text{CO}_2, \text{no capture}} - e_{\text{CO}_2, \text{capture}}} \quad (20)$$

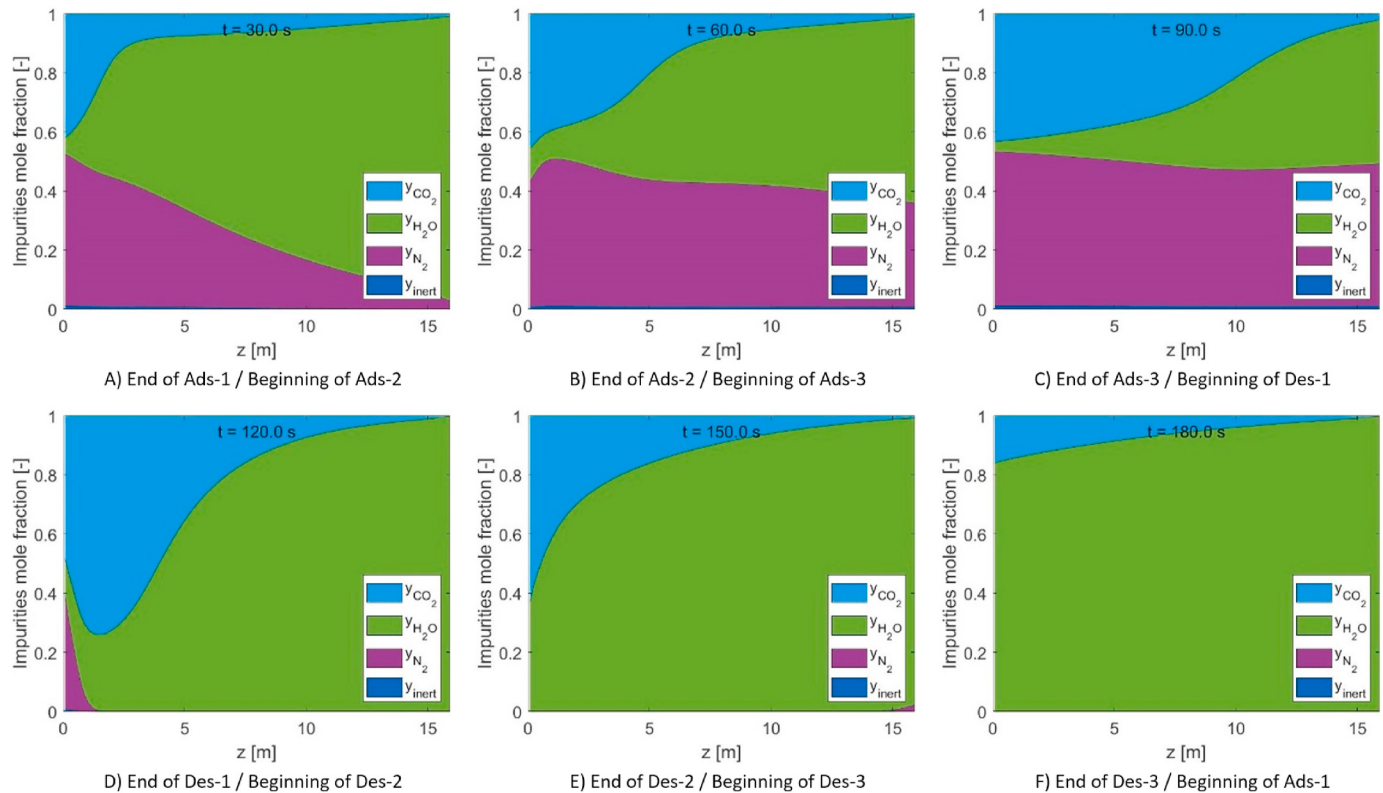
## 3. Results and evaluation

### 3.1. DISPLACE performance at different operating conditions

The DISPLACE performance is modelled using hot-stoves off gases as reported in Table 2 and assuming operating temperatures ranging from 300 °C to 400 °C. The process comprises four trains, each consisting of six columns. The height of each column is fixed at 16 m, with varying diameters: 3, 3, 2.75, and 2.5 m, corresponding to operating pressures of 5, 6, 7, and 10 bar, respectively. The diameter is mainly influenced by the volumetric flowrate and allowable linear gas velocity as well as the amount of sorbent required (based on the working capacity). Generally, in adsorption based separation systems a high system pressure and thus a high partial pressure of the adsorbing components leads to an increase of the sorbent capacity. However, for DISPLACE most of the capacity results from the displacement site, on which the adsorption of CO<sub>2</sub> and steam are independent of system pressure. High gas velocity creates an adsorption process limited by the mass transfer to the sorbent (equation (4)) while a low velocity leads to a process driven by axial dispersion rather than convection. The optimal velocity lies in between, leading to a sharp mass transfer zone resulting in high purity products and the best utilization of the adsorbent in the column. A higher utilization leads to a higher productivity as defined in equation (7). In order to model the

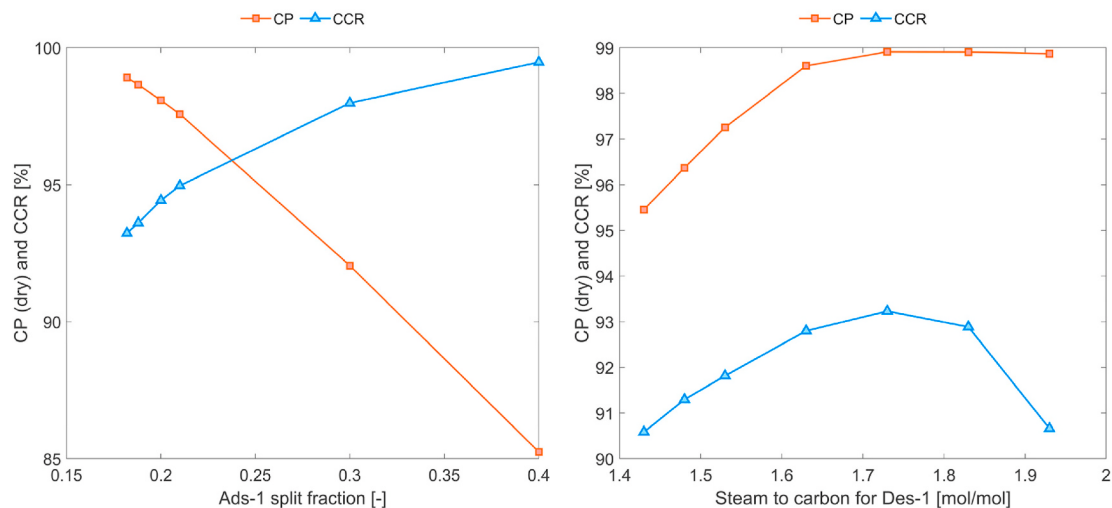
**Table 7**Linear driving force parameter [ $s^{-1}$ ] range for each step of the DISPLACE process.

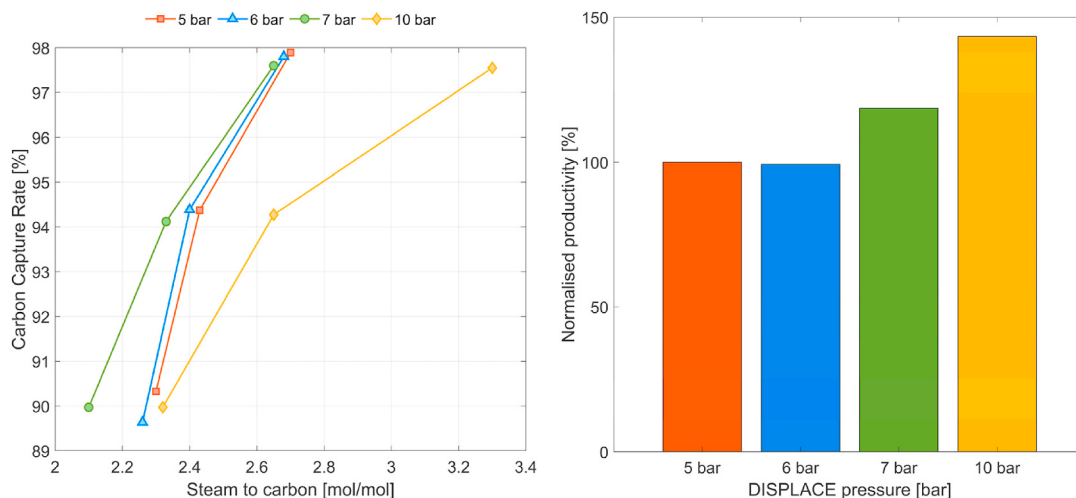
| Pressure | Parameter                  | Ads-1     | Ads-2     | Ads-3     | Des-1     | Des-2     | Des-3     |
|----------|----------------------------|-----------|-----------|-----------|-----------|-----------|-----------|
| 5 bar    | CO <sub>2</sub> $k_{LDF}$  | 0.02–0.22 | 0.02–0.20 | 0.02–0.22 | 0.02–0.27 | 0.03–0.3  | 0.03–0.22 |
|          | H <sub>2</sub> O $k_{LDF}$ | 0.04–0.35 | 0.04–0.25 | 0.02–0.16 | 0.02–0.35 | 0.05–0.35 | 0.1–0.35  |
| 10 bar   | CO <sub>2</sub> $k_{LDF}$  | 0.02–0.8  | 0.05–0.4  | 0.1–0.36  | 0.03–0.7  | 0.05–0.75 | 0.03–0.7  |
|          | H <sub>2</sub> O $k_{LDF}$ | 0.02–0.2  | 0.02–0.18 | 0.02–0.15 | 0.02–0.2  | 0.02–0.2  | 0.02–0.18 |

**Fig. 6.** Composition of the gas phase in the void fraction of the column for each step for a cycle operated at 10 bar with a CCR of 99.4% and a CP of 98.6%. The top three steps are after being fed co-currently (left-to-right) the bottom three steps are after being fed counter currently (right-to-left).

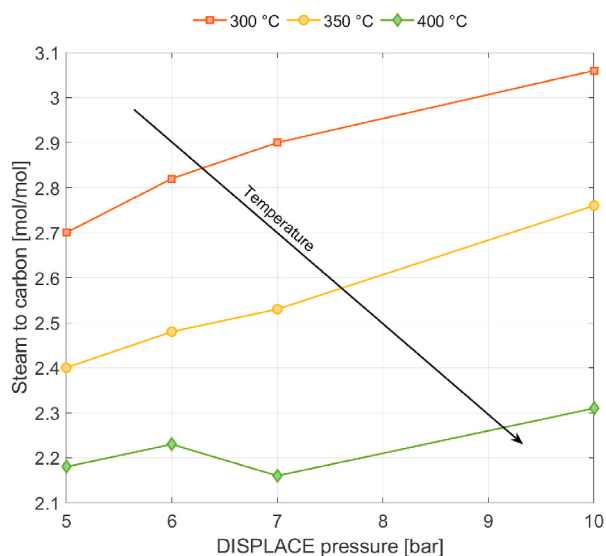
mass transfer from the bulk gas phase and the adsorption site, a linearised correlation for intraparticle resistance to mass transfer is introduced. Characteristic values for the linear driving force to the sorbent,

$k_{LDF}$ , are listed for each step in Table 7. These values are a function of intraparticle diffusion, sorbent pellet diameter and slope of the isotherm. Due to the Langmuir-like shape of the isotherm, the slope of

**Fig. 7.** Behaviour of the system at 6 bar and 400 °C for different feed split ratio for Ads-1/Ads-3 (left) and different S/C ratios fed to the first desorption step (right) while keeping all other design parameters constant.



**Fig. 8.** Trade-off between steam demand and carbon capture rate (left) and between system pressure and productivity (right) with the productivity normalised to the 5 bar case. Unless otherwise stated the CCR is 90%, the CP 95% and the temperature is 400 °C.



**Fig. 9.** Steam-to-carbon as function of DISPLACE working temperatures and pressures (CCR = 90%, CP = 95%).

the isotherm is very steep for low partial pressures leading to low  $k_{LDF}$  values which in turn results in lower mass transfer towards the sorbent.

Fig. 6 shows an example of the gas composition of the void fraction gas phase in the column after each step. This in turn means it is the starting composition for the following step.

- At the end of Ads-1, the column has been fed with feed gas to the point that a small amount of  $N_2$  has broken through. The outlet of this column is fed to Des-2 where we can see this  $N_2$  in the gas phase of the column.
- Ads-2 has been fed with the gas of the void volume from Des-2 which is what is left in the column after the adsorption step. This recycle stream is similar in composition to the feed stream.
- Finally in Ads-3 the column is fed with feed gas until a specific amount of  $CO_2$  breaks through.
- The near-feed composition in the column is then flushed out with steam in Des-1 and recycled to Ads-2. The remainder of the column shows the block plug of  $CO_2$  which has been formed by displacing  $CO_2$  from the sorbent with steam.

- The column state at the end of Des-2 is the result from recycling the steam from Ads-1 with a small amount of  $N_2$  breakthrough
- In Des-3 the column is fully flushed with steam to achieve a high degree of regeneration.

The results from the parametric analysis show a high dependency of the process performance on the flowrates towards Ads-1 and Des-1. As these steps determine the amount and composition of the recycled gas, they directly influence the purity of the  $CO_2$  product and the preloading of the sorbent. If Ads-1 is fed too much or Des-1 is fed too little, then large amount of impurities go towards the  $CO_2$  product, thus reducing the  $CO_2$  purity (Fig. 7, left). Additionally, if Des-1 is fed with too much steam, then the  $CO_2$  plug is recycled to Ads-2 and will occupy adsorption sites effectively reducing the working capacity of the system, leading to a reduced CCR (Fig. 7, right).

Next to the flowrates to Ads-1 and Des-1 the temperature of the system impacts the working capacity of both steam and  $CO_2$ , as shown in Fig. 9. At lower temperature, the capacity to adsorb  $CO_2$  increases, reducing the amount of required sorbent. However, the capacity to adsorb steam increases even further leading to larger steam demands per mol of  $CO_2$  fed. So, while the system is operated at a lower temperature and thus will require less heating of the feed stream, the steam demand increases.

Overall, the sensitivity studies show a trade-off between CCR and CP vs. steam demand (Fig. 7, right), productivity vs. system pressure (Fig. 8) and steam demand vs. temperature (Fig. 9), thus allowing several operating points and system designs to achieve the same performance. In Fig. 8, cases at 400 °C with a carbon purity of 95% and, unless otherwise mentioned, a carbon capture ratio of 90% are shown. The figures clearly show the thermodynamic advantage of DISPLACE to operate at pressure below 7 bar, but from an economic point of view, the higher the pressure the higher the productivity is with advantages on the process costs.

In Table 8, the molar flow rate as well as the composition of the  $CO_2$ -rich stream leaving the DISPLACE column is indicated. As can be observed in Fig. 9, increasing the working temperature has the beneficial effect of diminishing the steam-to-carbon ratio.

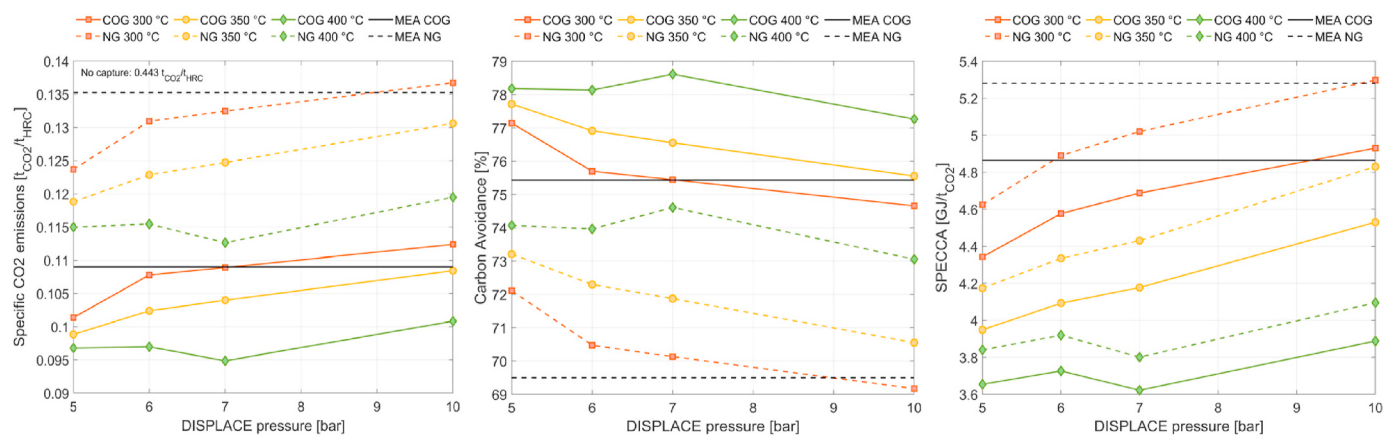
After analysing the simulations corresponding to the cases outlined in Table 8, as depicted in Figs. 10 and 13, it was observed that the best results were achieved at 400 °C. This confirms the advantageous impact of elevating the operating temperature of DISPLACE, which in turn diminishes the steam-to-carbon ratio, thereby reducing the amount of steam required for  $CO_2$  capture, as illustrated in Fig. 9. Consequently, additional simulations were conducted at 400 °C, exploring various values of carbon purity (CP) – 95%, 97%, and 99% – and carbon capture

**Table 8**DISPLACE performance at different operating conditions with corresponding CO<sub>2</sub> rich stream thermodynamic conditions.

| Case                   | Unit    | 1     | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     | 10    | 11    | 12    |
|------------------------|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| P                      | bar     | 5     | 5     | 5     | 6     | 6     | 6     | 7     | 7     | 7     | 10    | 10    | 10    |
| T                      | °C      | 300   | 350   | 400   | 300   | 350   | 400   | 300   | 350   | 400   | 300   | 350   | 400   |
| D                      | m       | 3     | 3     | 3     | 3     | 3     | 3     | 2.75  | 2.75  | 2.75  | 2.5   | 2.5   | 2.5   |
| CP                     | %       | 95.41 | 95.27 | 95.41 | 95.26 | 95.22 | 95.45 | 95.22 | 95.24 | 95.64 | 95.16 | 95.30 | 95.32 |
| CCR                    | %       | 91.20 | 90.71 | 90.38 | 90.20 | 90.25 | 90.58 | 90.27 | 90.11 | 90.85 | 90.12 | 90.05 | 90.19 |
| S/C                    | mol/mol | 2.70  | 2.40  | 2.18  | 2.82  | 2.48  | 2.26  | 2.90  | 2.53  | 2.16  | 3.06  | 2.76  | 2.31  |
| CO <sub>2</sub> stream | kmol/s  | 1.56  | 1.45  | 1.38  | 1.38  | 1.32  | 1.28  | 1.62  | 1.48  | 1.32  | 1.51  | 1.50  | 1.36  |

| CO <sub>2</sub> -rich stream composition at reactor outlet |      |       |       |       |       |       |       |       |       |       |       |       |       |
|------------------------------------------------------------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| - Ar                                                       | %vol | 0.06  | 0.07  | 0.07  | 0.07  | 0.07  | 0.07  | 0.06  | 0.06  | 0.07  | 0.06  | 0.06  | 0.07  |
| - H <sub>2</sub> O                                         | %vol | 33.89 | 29.15 | 26.00 | 26.07 | 22.28 | 20.09 | 36.85 | 30.81 | 22.25 | 32.26 | 31.93 | 24.73 |
| - H <sub>2</sub>                                           | %vol | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO                                                       | %vol | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO <sub>2</sub>                                          | %vol | 63.08 | 67.50 | 70.61 | 70.43 | 74.01 | 76.27 | 60.13 | 65.89 | 74.37 | 64.46 | 64.87 | 71.75 |
| - N <sub>2</sub>                                           | %vol | 2.97  | 3.29  | 3.33  | 3.43  | 3.64  | 3.56  | 2.96  | 3.23  | 3.32  | 3.22  | 3.13  | 3.46  |
| - O <sub>2</sub>                                           | %vol | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |

**Fig. 10.** Specific CO<sub>2</sub> emissions, Carbon Avoidance and SPECCA considering both NG and COG as fuels.

rate (CCR) – 90%, 94%, and 98%, as detailed in Table 9. While certain data points in the matrix are absent, specifically all cases where CCR equals 98% and CP equals 97%, along with the case where CCR equals

**Table 9**

Steam-to-carbon ratio at 400 °C for different working pressures, CP and CCR.

| CCR    | 90%  | 90%  | 90%  | 94%  | 94%  | 94%  | 98%  | 98%  |
|--------|------|------|------|------|------|------|------|------|
| CP     | 95%  | 97%  | 99%  | 95%  | 97%  | 99%  | 95%  | 99%  |
| 5 bar  | 2.30 | 2.35 | 2.50 | 2.43 | NA   | 2.75 | 2.70 | 3.37 |
| 6 bar  | 2.26 | 2.32 | 2.47 | 2.40 | 2.44 | 2.58 | 2.68 | 2.95 |
| 7 bar  | 2.10 | 2.15 | 2.42 | 2.33 | 2.65 | 2.71 | 2.65 | 3.46 |
| 10 bar | 2.32 | 2.40 | 2.48 | 2.65 | 2.73 | 2.74 | 3.30 | 3.25 |

**Table 10**

Results obtained considering the cases of Table 8 and the MEA reference case.

| Case | P [bar] | T [°C] | Flue gas compression [MW <sub>e</sub> ] | CO <sub>2</sub> Compression [MW <sub>e</sub> ] | Total Electricity [MW <sub>e</sub> ] | Fuel consumption [MW <sub>th</sub> ] |
|------|---------|--------|-----------------------------------------|------------------------------------------------|--------------------------------------|--------------------------------------|
| 1    | 5       | 300    | 16.01                                   | 11.38                                          | 27.39                                | 125.71                               |
| 2    | 5       | 350    | 16.01                                   | 11.33                                          | 27.34                                | 112.49                               |
| 3    | 5       | 400    | 16.00                                   | 11.28                                          | 27.28                                | 102.55                               |
| 4    | 6       | 300    | 17.81                                   | 10.30                                          | 28.11                                | 130.15                               |
| 5    | 6       | 350    | 17.81                                   | 10.31                                          | 28.11                                | 115.31                               |
| 6    | 6       | 400    | 17.81                                   | 10.34                                          | 28.15                                | 104.11                               |
| 7    | 7       | 300    | 19.37                                   | 9.53                                           | 28.90                                | 132.74                               |
| 8    | 7       | 350    | 19.37                                   | 9.51                                           | 28.88                                | 116.80                               |
| 9    | 7       | 400    | 19.36                                   | 9.57                                           | 28.93                                | 100.17                               |
| 10   | 10      | 300    | 23.13                                   | 7.80                                           | 30.93                                | 137.16                               |
| 11   | 10      | 350    | 23.13                                   | 7.79                                           | 30.93                                | 124.97                               |
| 12   | 10      | 400    | 23.14                                   | 7.80                                           | 30.94                                | 105.19                               |
| MEA  | –       | –      | 2.99                                    | 16.21                                          | 19.20                                | 154.76                               |

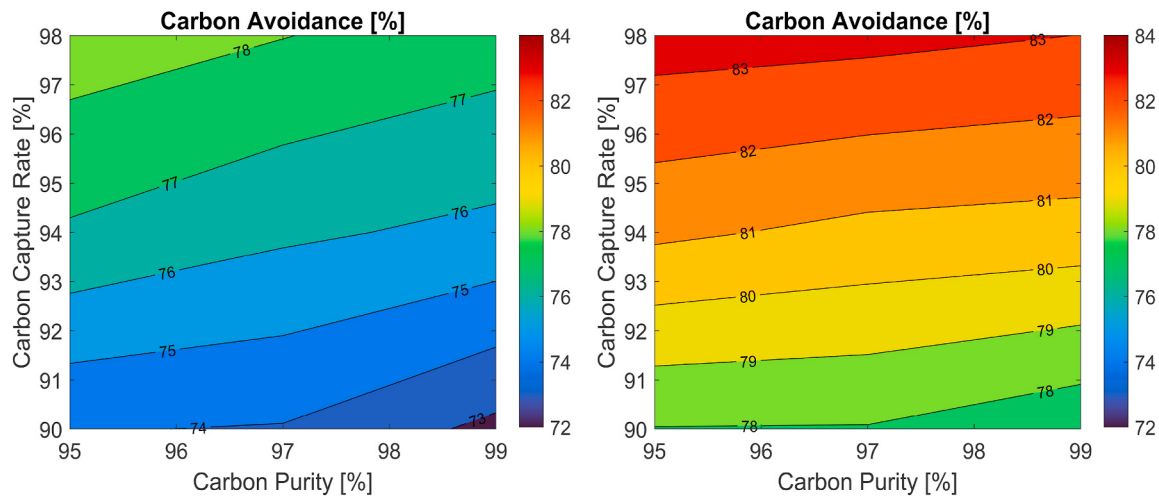
94% and CP equals 97% at 5 bar, the remaining cases provide sufficient coverage to generate comprehensive results across different CP and CCR values. The general trends are a higher S/C need for higher purity and/or capture rates for each pressure level. The trends between the various pressure levels show a local minimum for 7 bar. This is a consequence of the shape of the isotherm for CO<sub>2</sub> and H<sub>2</sub>O respectively. At 7 bar the combination of the CO<sub>2</sub> and steam capacities is the most favourable leading to a low S/C.

To maintain conciseness, Table 9 exclusively presents the steam-to-carbon ratio. Supplementary details pertinent to the simulations are provided in appendix, Table 16, Section 5.3.

**Table 11**

Economic results obtained considering the cases of Table 8, the MEA reference case and NG or COG as fuel.

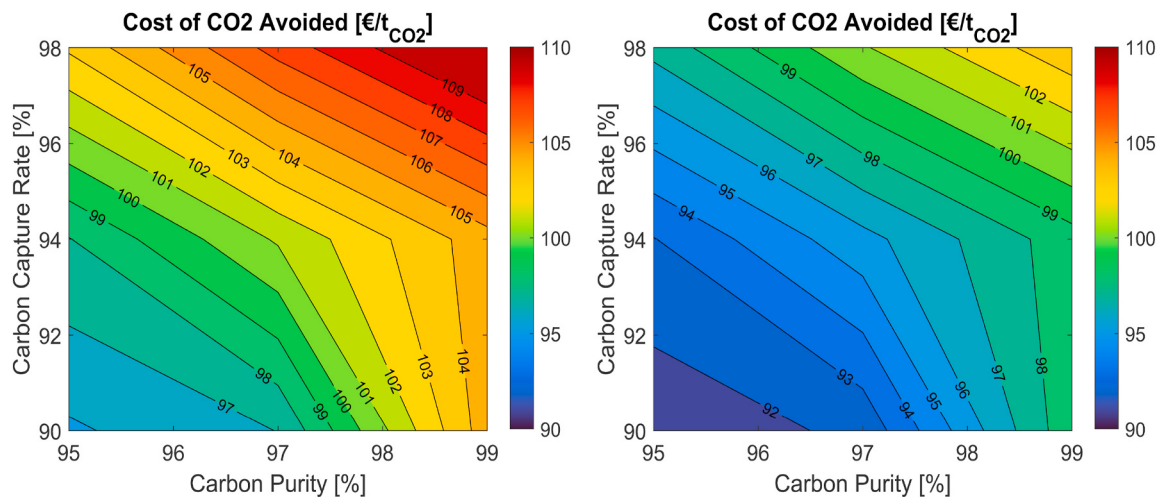
| Case | P<br>[bar] | T<br>[°C] | DISPLACE Capex<br>[M€/y] | Other Capex<br>[M€/y] | Total Capex<br>[M€/y] | Electricity<br>[M€/y] | Fuel<br>[M€/y] | Other costs<br>[M€/y] | LCOHRC<br>[€/t <sub>HRC</sub> ] | CCA NG<br>[€/t <sub>CO2</sub> ] | CCA COG<br>[€/t <sub>CO2</sub> ] |
|------|------------|-----------|--------------------------|-----------------------|-----------------------|-----------------------|----------------|-----------------------|---------------------------------|---------------------------------|----------------------------------|
| 1    | 5          | 300       | 6.07                     | 21.96                 | 28.03                 | 28.08                 | 51.54          | 3.60                  | 35.20                           | 110.09                          | 103.17                           |
| 2    | 5          | 350       | 6.35                     | 21.07                 | 27.43                 | 28.02                 | 46.12          | 3.45                  | 33.23                           | 102.36                          | 96.66                            |
| 3    | 5          | 400       | 6.59                     | 20.45                 | 27.04                 | 27.96                 | 42.05          | 3.33                  | 31.77                           | 96.70                           | 91.84                            |
| 4    | 6          | 300       | 6.60                     | 22.28                 | 28.88                 | 28.81                 | 53.36          | 3.79                  | 36.34                           | 116.29                          | 108.59                           |
| 5    | 6          | 350       | 6.98                     | 21.28                 | 28.26                 | 28.82                 | 47.28          | 3.60                  | 34.16                           | 106.55                          | 100.40                           |
| 6    | 6          | 400       | 7.25                     | 20.56                 | 27.81                 | 28.85                 | 42.69          | 3.45                  | 32.53                           | 99.18                           | 94.10                            |
| 7    | 7          | 300       | 6.20                     | 22.54                 | 28.74                 | 29.62                 | 54.42          | 3.71                  | 36.87                           | 118.54                          | 110.48                           |
| 8    | 7          | 350       | 6.50                     | 21.42                 | 27.93                 | 29.61                 | 47.89          | 3.53                  | 34.48                           | 108.17                          | 101.79                           |
| 9    | 7          | 400       | 6.76                     | 20.18                 | 26.94                 | 29.65                 | 41.07          | 3.35                  | 31.96                           | 96.62                           | 91.89                            |
| 10   | 10         | 300       | 6.51                     | 22.92                 | 29.44                 | 31.70                 | 56.24          | 3.89                  | 38.38                           | 125.10                          | 116.20                           |
| 11   | 10         | 350       | 6.84                     | 22.20                 | 29.04                 | 31.70                 | 51.24          | 3.71                  | 36.61                           | 117.00                          | 109.52                           |
| 12   | 10         | 400       | 7.10                     | 20.63                 | 27.72                 | 31.71                 | 43.13          | 3.45                  | 33.55                           | 103.55                          | 98.13                            |
| MEA  | –          | –         | –                        | –                     | 35.29                 | 19.68                 | 62.05          | 2.79                  | 37.91                           | 123.00                          | 113.33                           |

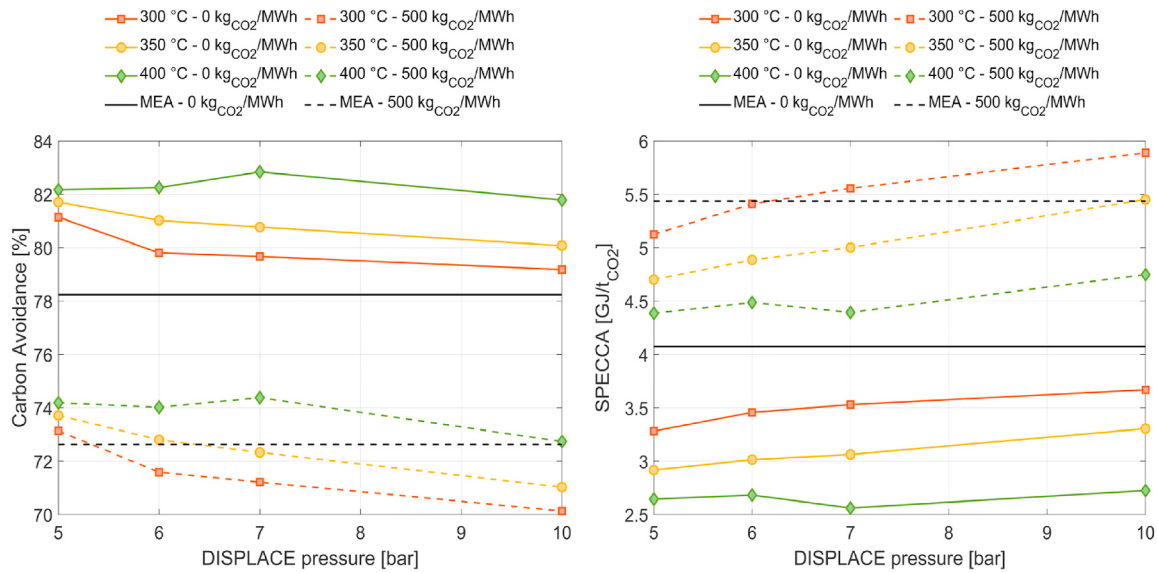
**Fig. 11.** Carbon avoidance as a function of CP and CCR for cases in Table 9, NG case (left) and COG case (right).

### 3.2. DISPLACE integration performance

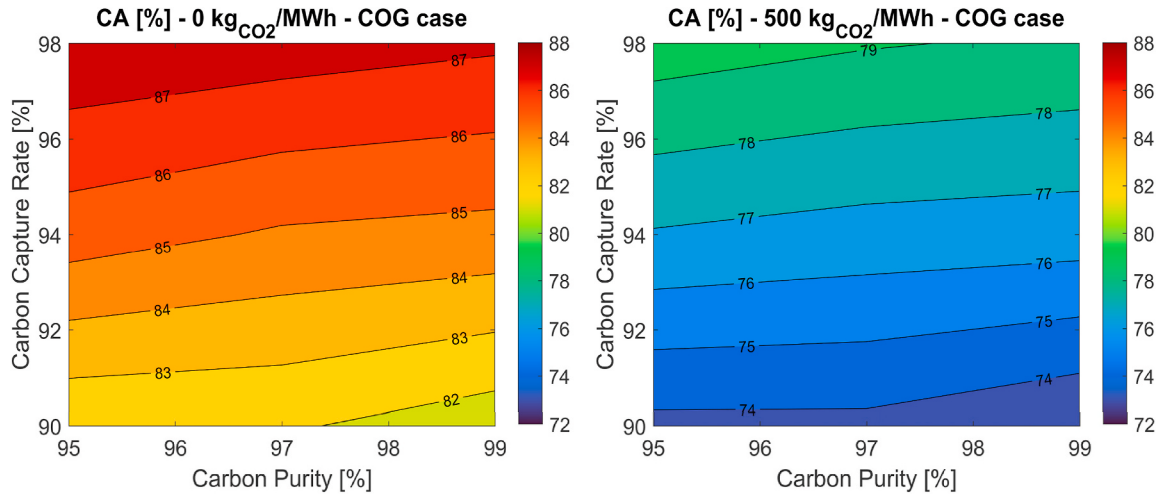
In this section, the main results of the techno-economic assessment for the DISPLACE integration with steel gases are presented and assessed through the KPIs. Table 10 and Table 11 display the comprehensive results obtained for various DISPLACE working pressures and

temperatures, encompassing both NG and COG scenarios. These results are also visually depicted in Fig. 10. Table 10 shows that elevating the DISPLACE operating pressure results in a higher total electricity consumption due to increased power demand by the flue gas compressor. However, the presence of a CO<sub>2</sub>-rich stream at the same pressure level as DISPLACE reduces the energy needed for compression to the levels

**Fig. 12.** Cost of CO<sub>2</sub> avoided as a function of CP and CCR for cases in Table 9 for NG (left) and COG (right) case. For each combination of CP and CCR the case with the minimum CCA is selected.



**Fig. 13.** Carbon Avoidance (left) and SPECCA (right) considering COG as fuel and assuming different carbon footprint of imported electricity (0 kg<sub>CO2</sub>/MWh and 500 kg<sub>CO2</sub>/MWh).



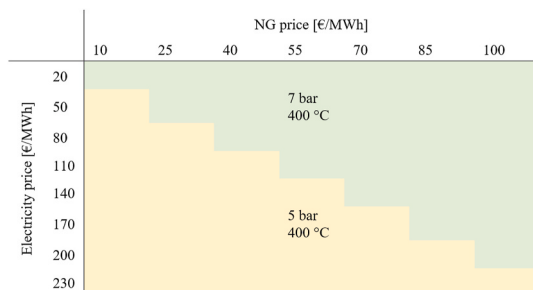
**Fig. 14.** Carbon avoidance as a function of CP and CCR for cases in Table 9 assuming COG as fuel, for different carbon footprint of imported electricity (0 kg<sub>CO2</sub>/MWh and 500 kg<sub>CO2</sub>/MWh).

required for transport and storage. This dynamic counteracts the escalating energy demand of the flue gas compressor, thus limiting the overall increase in electricity consumption. Fuel consumption is driven

by the steam demand, so it increases at lower operating temperature. When utilizing NG as the fuel source to supply the additional heat required for the CO<sub>2</sub> capture process, a carbon avoidance up to 74.6% is achievable (7 bar and 400 °C). Generally, elevating the DISPLACE

**Table 12**

Optimal working conditions of DISPLACE for different NG and electricity prices considering both NG and COG as fuel.



**Table 13**

Equipment reference cost.

| Component                                | Scaling parameter                    | C <sub>0</sub> [M€] | S <sub>0</sub> | f    | Ref.                    |
|------------------------------------------|--------------------------------------|---------------------|----------------|------|-------------------------|
| CO <sub>2</sub> compressor and condenser | Power, MW                            | 55.24               | 50.5           | 0.67 | Manzolini et al. (2020) |
| CO <sub>2</sub> capture unit (MEA)       | CO <sub>2</sub> mass flow rate, kg/s | 85.25               | 53.7           | 0.8  | Manzolini et al. (2020) |
| Compressor                               | Power, MW                            | 10.17               | 15.3           | 0.67 | Manzolini et al. (2020) |
| NG Boiler                                | Heat duty, MW                        | 2.95                | 10             | 1    | Khallaghi et al. (2022) |
| Heat exchanger                           | Heat transfer, MW                    | 16.25               | 138            | 0.6  | Guo et al. (2014)       |
| Pump                                     | Volumetric flow [m <sup>3</sup> /h]  | 0.28                | 250            | 0.14 | Huijgen et al. (2007)   |

**Table 14**

Methodology used to compute the total plant cost of the additional equipment (Manzolini et al., 2020).

| Cost                          |        | Value |
|-------------------------------|--------|-------|
| Total Installation Cost (TIC) | % TEC  | 104   |
| Indirect Costs (IC)           | % TDPC | 14    |
| Contingency (Co)              | % EPC  | 10    |
| Owner's Costs (OC)            | % EPC  | 5     |

working temperature proves advantageous due to the reduced steam-to-carbon ratio, subsequently minimizing the amount of fuel needed to supply the extra heat. The use of COG offers additional benefits in terms of CO<sub>2</sub> avoidance due to its hydrogen-rich composition. The layout of the C<sup>4</sup>U steel mill facilitates the utilization of COG, as the absence of a dedicated power plant allows for the utilization of blast furnace gas in certain processes instead of COG, such as slab reheating, thereby enhancing the availability of COG within the steel plant. For this reason, the possibility of using COG was also evaluated.

Comparative analysis with the reference post-combustion MEA process is also presented, with energy consumption of 3.30 GJ/tCO<sub>2</sub> at the reboiler and a carbon purity of 99.31%. The reboiler heat requirement was assumed to be met through steam generated in a NG/COG fired steam generator. Notably, operating at 400 °C demonstrates a clear advantage for DISPLACE over the MEA process in terms of carbon avoidance. In relation to SPECCA, the DISPLACE exhibits a lower value compared to the MEA case particularly when operating between 350 °C and 400 °C. When considering coke oven gas (COG), the SPECCA is further reduced with respect to the NG case because of the higher carbon avoidance that can be reached.

Focusing on the scenarios operating at 400 °C as detailed in section 5.3, Fig. 11 illustrates the carbon avoidance as a function of carbon purity and DISPLACE carbon capture rate, for both the NG and COG cases. An increase in the carbon capture rate (CCR) allows for higher carbon avoidance levels, while a shift towards elevated carbon purity values amplifies the DISPLACE steam-to-carbon ratio, thereby reducing the overall carbon avoidance as the additional steam has to be produced through a NG/COG fired steam generator.

Table 11 shows the economic outcomes: at the same operating temperature, an increase in operating pressure leads to a rise in DISPLACE capital expenditure. However, higher pressure allows for a reduction in column radius, thereby partially mitigating this effect. Consequently, transitioning from 6 to 7 bar, the DISPLACE capital cost decreases. When maintaining the same operating pressure, DISPLACE capital expenditure increases with temperature, while additional equipment costs exhibit the opposite trend. This results in a trend with

**Table 15**

Number of valves per column.

| Valve                         | N° valves |
|-------------------------------|-----------|
| Feed valve                    | 1         |
| Recycle valve                 | 2         |
| CO <sub>2</sub> product valve | 1         |
| Lean product valve            | 1         |
| Steam valve                   | 1         |

minor fluctuations in capital costs. Conversely, operating costs are more influenced by DISPLACE operating conditions, aligning with trends in electricity and fuel consumption. The adoption of DISPLACE proves advantageous compared to the reference MEA scrubbing, particularly in cases operating at 350 and 400 °C. It is important to emphasize the difference in TRL between the two technologies, which leads to greater uncertainty regarding the performance and cost of DISPLACE technology when evaluating its potential at an industrial scale. As mentioned earlier, MEA scrubbing is a mature technology that has already been proven on an industrial scale. Nevertheless, the estimation of the MEA carbon capture section's CAPEX was derived from literature sources and, as such, carries inherent uncertainties. The adoption of COG reduces the cost of CO<sub>2</sub> avoided because of the higher carbon avoidance. For scenarios operating at 400 °C (Table 9), the cost of CO<sub>2</sub> avoided is computed while varying CP and DISPLACE CCR (see Fig. 12). The increase of CCA is the consequence of the higher steam-to-carbon ratio demanded by DISPLACE when shifting towards higher values of CP and CCR. For the same reason described before, the COG case shows lower values of CCA.

### 3.2.1. Sensitivity on carbon footprint of imported electricity

The carbon footprint of imported electricity significantly impacts the overall CA together with SPECCA. The impact of carbon footprint of imported electricity set at 0 kgCO<sub>2</sub>/MWh, and 500 kgCO<sub>2</sub>/MWh are depicted in Fig. 13, alongside the reference MEA case for comparison. Under the renewable energy scenario (0 kgCO<sub>2</sub>/MWh) and utilizing COG, it is possible to reach a carbon avoidance above 82% and a SPECCA close

**Table 16**

Assumptions for the DISPLACE economic assessment.

| Cost               |                                   | Value |
|--------------------|-----------------------------------|-------|
| Construction works | % C <sub>columns</sub>            | 170   |
| Other costs        | % TEC + C <sub>construction</sub> | 3.5   |
| EPCM services      | % TDC <sub>DISPLACE</sub>         | 17.5  |
| Contingency        | %TDC <sub>DISPLACE</sub> + EPCM   | 15    |

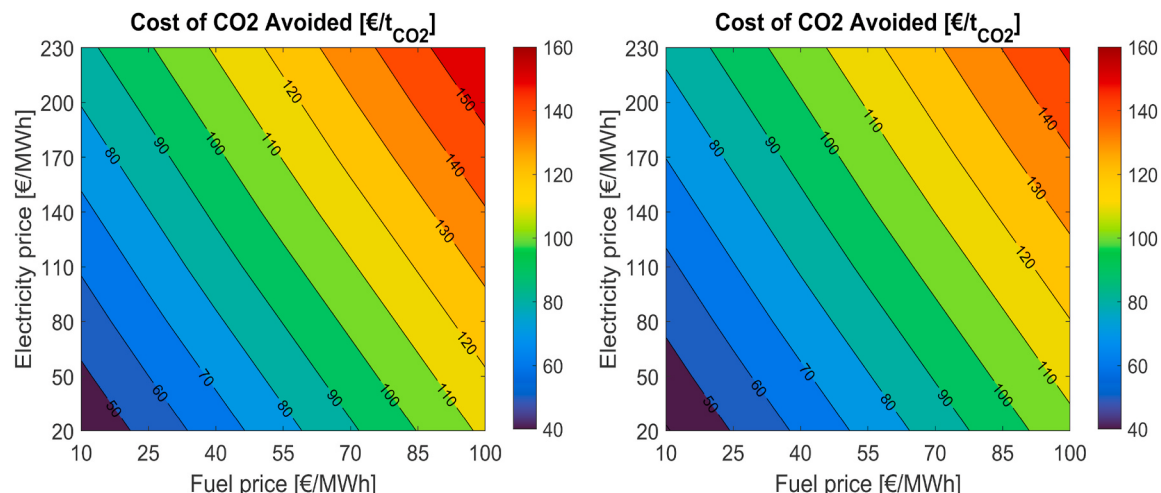


Fig. 15. Cost of CO<sub>2</sub> avoided as function of fuel and electricity prices for the NG case (left) and for COG case (right).

to 2.5 GJ/t<sub>CO2</sub>, which is significantly lower than the MEA case. These trends can be extended to the NG case with a reduction of CA by around 4–6% points and an increase in SPECCA by 0.2–0.5 MJ/kg<sub>CO2</sub>. Fig. 14 illustrates carbon avoidance as a function of CP and DISPLACE CCR for cases operating at 400 °C (Table 9): the highest value of carbon avoidance (higher than 87%) is reached for CCR = 98%, CP = 95% in the renewable energy scenario using COG as additional fuel.

### 3.2.2. Sensitivity on natural gas and electricity price

The economic outcomes are significantly influenced by the prices of electricity and NG. Given the considerable uncertainty associated with these factors, a sensitivity analysis is conducted. The results shown in this section are referred to the cases listed in Table 8. For each combination of NG and electricity prices outlined in Table 12, the corresponding DISPLACE working temperature and pressure that minimize the CCA are identified. At low NG prices and escalating electricity costs, the 5 bar pressure – 400 °C temperature combination becomes the most cost-effective option because of the lower overall power consumption at 5 bar pressure, resulting in savings in electricity procurement. Conversely at higher NG prices the best combination results to be 7 bar–400 °C due to the reduced DISPLACE steam-to-carbon ratio.

Fig. 15 illustrate the cost of CO<sub>2</sub> avoidance against fuel and electricity prices. The utilization of COG allows for reduced CCA values, owing to the enhanced carbon avoidance achievable with COG.

## 4. Conclusion

This article introduces the innovative DISPLACE carbon-capture technology, which is based on adsorption of CO<sub>2</sub> and steam on solid materials. In particular, the feasibility of utilizing DISPLACE for decarbonizing exhaust gases emitted from the hot-stoves in a BF-BOF steel plant is thoroughly analysed.

The DISPLACE technology is a multi-column, cyclic, concentration swing process operated isobarically for the capture of CO<sub>2</sub>. Carbon capture rates (CCR) of up to 98% and (dry) CO<sub>2</sub> purities (CP) of up to 99% can be achieved. The benefits of the system are the low temperature variation due to similar heat of adsorption between the two adsorbing species and the low fatigue of the unit due to the isobaric operation. The major trade-offs of the system were identified as the performance (CP and CCR) vs steam demand, system temperature vs steam demand and system pressure vs productivity/system size. As the system pressure requires feed pressurisation but also produces higher pressure CO<sub>2</sub>, the choice of the final design is not only a technical one but also impacted by the integration option based on available heat sources and downstream units and unit size vs energy consumption decision.

The integration of DISPLACE technology into a steel mill layout was performed using Aspen Plus V14. An optimization process was conducted on two crucial DISPLACE design parameters: operating temperature and pressure. These parameters significantly influence the steam required for the DISPLACE carbon capture system. Results demonstrated a distinct advantage in operating at 400 °C due to reduced steam consumption for the DISPLACE technology, leading to lower energy penalties associated with steam generation. Two different fuels, NG and

COG, were evaluated to fulfil the process heat requirement. Additionally, a benchmark post-combustion carbon capture technology based on MEA scrubbing was modelled and compared to DISPLACE. Key performance indicators (KPIs) revealed the superiority of DISPLACE over MEA especially when operating at 400 °C.

In the renewable energy scenario, the best case resulted in achieving over 82% carbon avoidance and a SPECCA close to 2.5 GJ/t<sub>CO2</sub>. From an economic perspective, the cost of avoided CO<sub>2</sub> was found to be 91.89 €/t<sub>CO2</sub> for 7 bar–400 °C using COG, or 96.62 €/t<sub>CO2</sub> when using imported NG. In both cases, the cost associated with DISPLACE process was significantly lower compared to the MEA case (equal to 113.33.42 €/t<sub>CO2</sub> and 123.00 €/t<sub>CO2</sub> respectively).

In conclusion, DISPLACE technology emerges as a promising solution for decarbonizing processes within BF-BOF steel mills, with the potential for significant emissions reduction in this industrial sector.

Future works will investigate the optimal integration of DISPLACE within integrated steelworks considering different exhaust gases as the ones from sinter plant or reheating ovens, including the optimal integration to minimize the additional impact will be identified. Separately, experimental results and model validation will be detailed.

### CRedit authorship contribution statement

**Nicola Zecca:** Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization. **Leonie Lücking:** Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **Dora-Andreea Chisăliță:** Investigation, Formal analysis. **Jurriaan Boon:** Writing – review & editing, Validation, Methodology. **H.A.J. van Dijk:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **J.A.Z. Pieterse:** Project administration, Funding acquisition. **Antonio Giuffrida:** Project administration, Funding acquisition. **Giampaolo Manzolini:** Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization.

### Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Jurriaan Boon has patent #WO2022053676A1 issued to TNO. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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The work reflects only the authors' views, and the European Union is not liable for any use that may be made of the information contained therein.

## Appendix

### Streams specifications of DISPLACE plant integration

In Table 13 the specifications of the streams indicated in Fig. 5 are given. Since many cases were analysed, for sake of brevity results referring to the 5 bar–400 °C case are presented.

**Table 13**

Main streams specifications of DISPLACE plant integration. Case 5 bar–400 °C.s

| Stream | Temperature<br>[°C] | Pressure<br>[bar] | Mass flow rate<br>[kg/s] | Composition [%mol] |                |     |                 |                |                |                 |                               |                               |                                |
|--------|---------------------|-------------------|--------------------------|--------------------|----------------|-----|-----------------|----------------|----------------|-----------------|-------------------------------|-------------------------------|--------------------------------|
|        |                     |                   |                          | H <sub>2</sub> O   | H <sub>2</sub> | CO  | CO <sub>2</sub> | N <sub>2</sub> | O <sub>2</sub> | CH <sub>4</sub> | C <sub>2</sub> H <sub>6</sub> | C <sub>3</sub> H <sub>8</sub> | C <sub>5</sub> H <sub>12</sub> |
| 1      | 140.0               | 1.1               | 87.9                     | 6.2                | –              | –   | 41.9            | 50.8           | 1.0            | –               | –                             | –                             | –                              |
| 2      | 35.0                | 0.9               | 87.9                     | 6.2                | –              | –   | 41.9            | 50.8           | 1.0            | –               | –                             | –                             | –                              |
| 3      | 400.0               | 5.0               | 87.1                     | 4.7                | –              | –   | 42.6            | 51.6           | 1.0            | –               | –                             | –                             | –                              |
| 4      | 399.1               | 4.8               | 78.8                     | 60.3               | –              | –   | 3.0             | 36.0           | 0.7            | –               | –                             | –                             | –                              |
| 5      | 126.9               | 4.0               | 78.8                     | 60.3               | –              | –   | 3.0             | 36.0           | 0.7            | –               | –                             | –                             | –                              |
| 6      | 400.0               | 4.8               | 50.7                     | 26.0               | –              | –   | 70.6            | 3.3            | –              | –               | –                             | –                             | –                              |
| 7      | 34.9                | 110.0             | 43.0                     | 0.3                | –              | –   | 95.3            | 4.4            | –              | –               | –                             | –                             | –                              |
| 8      | 20.0                | 1.2               | 2.2                      | –                  | –              | –   | 1.8             | 0.4            | –              | 83.9            | 9.2                           | 3.3                           | 1.2                            |
| 9      | 15.0                | 1.0               | 41.6                     | –                  | –              | –   | –               | 79.0           | 21.0           | –               | –                             | –                             | –                              |
| 10     | 99.9                | 1.0               | 43.8                     | 15.4               | 0.1            | 0.1 | 8.5             | 72.5           | 3.0            | –               | –                             | –                             | –                              |
| 11     | 15.0                | 1.0               | 42.9                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 12     | 102.0               | 1.3               | 2.2                      | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 13     | 102.0               | 1.3               | 30.1                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 14     | 102.0               | 1.3               | 10.6                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 15     | 107.2               | 7.2               | 43.3                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 16     | 157.5               | 5.8               | 6.6                      | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 17     | 157.5               | 5.8               | 13.2                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 18     | 157.5               | 5.8               | 23.2                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 19     | 400.0               | 5.4               | 42.4                     | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |
| 20     | 152.9               | 4.5               | 0.5                      | 100.0              | –              | –   | –               | –              | –              | –               | –                             | –                             | –                              |

*MEA post-combustion carbon capture modelling*

Details about the CHEMISTRY and the REACTION Aspen Plus models used to simulate the MEA carbon capture system are presented in this section.

CHEMISTRY model:

|             |                                                                                                  |      |
|-------------|--------------------------------------------------------------------------------------------------|------|
| Equilibrium | $\text{MEA}^+ + \text{H}_2\text{O} \rightleftharpoons \text{MEA} + \text{H}_3\text{O}^+$         | (21) |
| Equilibrium | $\text{MEACCO}^- + \text{H}_2\text{O} \rightleftharpoons \text{MEA} + \text{HCO}_3^-$            | (22) |
| Equilibrium | $\text{CO}_2 + 2\text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{HCO}_3^-$     | (23) |
| Equilibrium | $\text{HCO}_3^- + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{CO}_3^{2-}$ | (24) |
| Equilibrium | $2\text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{OH}^-$                      | (25) |

The equilibrium constant of the reactions (21)–(25) is calculated adopting equation (26) with the constants listed in Table 14.

$$\ln(K_{eq}) = A + B/T + C \cdot \ln(T) + D \cdot T + E \cdot ((P - P_{ref})/P_{ref}) \quad (26)$$

**Table 14**

Constants used in equation (26).

| Reaction                                                                                         | A         | B        | C        | D           | E |
|--------------------------------------------------------------------------------------------------|-----------|----------|----------|-------------|---|
| $\text{MEA}^+ + \text{H}_2\text{O} \rightleftharpoons \text{MEA} + \text{H}_3\text{O}^+$         | –3.038325 | –7008.36 | 0        | –0.00313489 | 0 |
| $\text{MEACCO}^- + \text{H}_2\text{O} \rightleftharpoons \text{MEA} + \text{HCO}_3^-$            | –0.52135  | –2545.53 | 0        | 0           | 0 |
| $\text{CO}_2 + 2\text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{HCO}_3^-$     | 231.465   | –12092.1 | –36.7816 | 0           | 0 |
| $\text{HCO}_3^- + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{CO}_3^{2-}$ | 216.049   | –12431.7 | –35.4819 | 0           | 0 |
| $2\text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{OH}^-$                      | 132.899   | –13445.9 | –22.4773 | 0           | 0 |

REACTION model:

|             |                                                                                                           |      |
|-------------|-----------------------------------------------------------------------------------------------------------|------|
| Equilibrium | $\text{MEA}^+ + \text{H}_2\text{O} \rightleftharpoons \text{MEA} + \text{H}_3\text{O}^+$                  | (27) |
| Equilibrium | $2\text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{OH}^-$                               | (28) |
| Equilibrium | $\text{HCO}_3^- + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{CO}_3^{2-}$          | (29) |
| Kinetic     | $\text{CO}_2 + \text{OH}^- \rightleftharpoons \text{HCO}_3^-$                                             | (30) |
| Kinetic     | $\text{HCO}_3^- \rightleftharpoons \text{CO}_2 + \text{OH}^-$                                             | (31) |
| Kinetic     | $\text{MEA} + \text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{MEACCO}^- + \text{H}_3\text{O}^+$ | (32) |
| Kinetic     | $\text{MEACCO}^- + \text{H}_3\text{O}^+ \rightleftharpoons \text{MEA} + \text{CO}_2 + \text{H}_2\text{O}$ | (33) |

The power law expressions are used for the rate-controlled reactions:

$$r = kT^n \exp\left(-\frac{E}{RT}\right) \prod_{i=1}^N (x_i \gamma_i)^{a_i} \quad (34)$$

Where:  $r$  = rate of reaction;  $k$  = pre-exponential factor;  $T$  = absolute temperature;  $n$  = temperature exponent;  $E$  = activation energy;  $R$  = universal gas constant;  $N$  = number of components in the reaction;  $x_i$  = mole fraction of component  $i$ ;  $\gamma_i$  = activity coefficient of component  $i$ ;  $a_i$  = stoichiometric coefficient of component  $i$  in the reaction equation.

In equation (34), the factor  $n$  is zero,  $k$  and  $E$  are given in Table 15.

**Table 15**  
Parameters used in equation (34).

| Reaction                                                                                                  | k        | E [cal/mol] |
|-----------------------------------------------------------------------------------------------------------|----------|-------------|
| $\text{CO}_2 + \text{OH}^- \rightleftharpoons \text{HCO}_3^-$                                             | 1.33e+17 | 13249       |
| $\text{HCO}_3^- \rightleftharpoons \text{CO}_2 + \text{OH}^-$                                             | 6.63e+16 | 25656       |
| $\text{MEA} + \text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{MEACCO}^- + \text{H}_3\text{O}^+$ | 3.02e+14 | 9855.8      |
| $\text{MEACCO}^- + \text{H}_3\text{O}^+ \rightleftharpoons \text{MEA} + \text{CO}_2 + \text{H}_2\text{O}$ | 5.52e+23 | 16518       |

### DISPLACE performances at 400 °C

Table 16 shows the performances of DISPLACE when operating at 400 °C and for different values of CP and CCR.

**Table 16**  
DISPLACE performances for the cases at 400 °C.

| Case                                                       | Unit    | 1     | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     | 10    | 11    | 12    |
|------------------------------------------------------------|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| P                                                          | bar     | 5     | 5     | 5     | 5     | 5     | 5     | 5     | 6     | 6     | 6     | 6     | 6     |
| T                                                          | °C      | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   |
| D                                                          | m       | 3     | 3     | 3     | 3     | 3     | 3     | 3     | 3     | 3     | 3     | 3     | 3     |
| CP                                                         | %       | 95.69 | 97.06 | 98.69 | 95.40 | 98.57 | 94.83 | 99.22 | 95.44 | 97.33 | 98.63 | 94.79 | 97.27 |
| CCR                                                        | %       | 90.33 | 90.22 | 89.94 | 94.37 | 94.03 | 97.89 | 97.64 | 89.64 | 90.28 | 90.01 | 94.38 | 93.97 |
| S/C                                                        | mol/mol | 2.30  | 2.35  | 2.50  | 2.43  | 2.75  | 2.70  | 3.37  | 2.26  | 2.32  | 2.47  | 2.40  | 2.44  |
| CO <sub>2</sub> stream                                     | kmol/s  | 1.54  | 1.53  | 1.54  | 1.74  | 1.91  | 2.14  | 2.61  | 1.31  | 1.34  | 1.41  | 1.61  | 1.58  |
| CO <sub>2</sub> -rich stream composition at reactor outlet |         |       |       |       |       |       |       |       |       |       |       |       |       |
| - Ar                                                       | %vol    | 0.06  | 0.04  | 0.02  | 0.06  | 0.02  | 0.05  | 0.01  | 0.07  | 0.04  | 0.02  | 0.07  | 0.04  |
| - H <sub>2</sub> O                                         | %vol    | 33.71 | 34.41 | 36.27 | 38.75 | 46.02 | 48.04 | 59.31 | 22.80 | 25.13 | 30.21 | 33.20 | 33.90 |
| - H <sub>2</sub>                                           | %vol    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO                                                       | %vol    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO <sub>2</sub>                                          | %vol    | 63.43 | 63.67 | 62.89 | 58.44 | 53.21 | 49.27 | 40.38 | 73.67 | 72.87 | 68.84 | 63.32 | 64.29 |
| - N <sub>2</sub>                                           | %vol    | 2.80  | 1.89  | 0.82  | 2.76  | 0.76  | 2.63  | 0.31  | 3.45  | 1.96  | 0.94  | 3.41  | 1.77  |
| - O <sub>2</sub>                                           | %vol    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| Case                                                       | Unit    | 13    | 14    | 15    | 16    | 17    | 18    | 19    | 20    | 21    | 22    | 23    | 24    |
| P                                                          | bar     | 6     | 6     | 6     | 7     | 7     | 7     | 7     | 7     | 7     | 7     | 7     | 10    |
| T                                                          | °C      | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   | 400   |
| D                                                          | m       | 3     | 3     | 3     | 2.75  | 2.75  | 2.75  | 2.75  | 2.75  | 2.75  | 2.75  | 2.75  | 2.5   |
| CP                                                         | %       | 98.96 | 95.29 | 98.70 | 95.32 | 96.94 | 98.55 | 95.31 | 96.86 | 98.74 | 95.43 | 98.85 | 95.31 |
| CCR                                                        | %       | 94.29 | 97.80 | 98.13 | 89.97 | 90.12 | 90.37 | 94.12 | 94.23 | 93.63 | 97.60 | 97.72 | 89.97 |
| S/C                                                        | mol/mol | 2.58  | 2.68  | 2.95  | 2.10  | 2.15  | 2.42  | 2.33  | 2.65  | 2.71  | 2.65  | 3.46  | 2.32  |
| CO <sub>2</sub> stream                                     | kmol/s  | 1.61  | 1.97  | 2.04  | 1.35  | 1.36  | 1.50  | 1.65  | 1.89  | 1.83  | 2.07  | 2.72  | 1.44  |
| CO <sub>2</sub> -rich stream composition at reactor outlet |         |       |       |       |       |       |       |       |       |       |       |       |       |
| - Ar                                                       | %vol    | 0.01  | 0.05  | 0.01  | 0.07  | 0.05  | 0.02  | 0.06  | 0.04  | 0.01  | 0.05  | 0.02  | 0.07  |
| - H <sub>2</sub> O                                         | %vol    | 36.03 | 43.76 | 47.40 | 24.72 | 26.28 | 34.06 | 35.58 | 44.37 | 44.19 | 46.60 | 60.73 | 29.06 |
| - H <sub>2</sub>                                           | %vol    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO                                                       | %vol    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO <sub>2</sub>                                          | %vol    | 63.31 | 53.58 | 51.92 | 71.75 | 71.47 | 64.98 | 61.40 | 53.88 | 55.11 | 50.95 | 38.82 | 67.61 |
| - N <sub>2</sub>                                           | %vol    | 0.65  | 2.60  | 0.67  | 3.46  | 2.21  | 0.94  | 2.96  | 1.71  | 0.69  | 2.39  | 0.43  | 3.26  |
| - O <sub>2</sub>                                           | %vol    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| Case                                                       | Unit    | 25    | 26    | 27    | 28    | 29    | 30    | 31    |       |       |       |       |       |
| P                                                          | bar     | 10    | 10    | 10    | 10    | 10    | 10    | 10    |       |       |       |       |       |
| T                                                          | °C      | 400   | 400   | 400   | 400   | 400   | 400   | 400   |       |       |       |       |       |
| D                                                          | m       | 2.5   | 2.5   | 2.5   | 2.5   | 2.5   | 2.5   | 2.5   |       |       |       |       |       |
| CP                                                         | %       | 97.12 | 98.73 | 95.37 | 97.28 | 98.79 | 95.07 | 98.91 |       |       |       |       |       |
| CCR                                                        | %       | 90.41 | 90.39 | 94.27 | 93.86 | 93.98 | 97.55 | 98.11 |       |       |       |       |       |
| S/C                                                        | mol/mol | 2.40  | 2.48  | 2.65  | 2.73  | 2.74  | 3.30  | 3.25  |       |       |       |       |       |
| CO <sub>2</sub> stream                                     | kmol/s  | 1.48  | 1.37  | 1.91  | 1.87  | 1.66  | 2.65  | 2.26  |       |       |       |       |       |
| CO <sub>2</sub> -rich stream composition at reactor outlet |         |       |       |       |       |       |       |       |       |       |       |       |       |
| - Ar                                                       | %vol    | 0.04  | 0.02  | 0.05  | 0.03  | 0.02  | 0.04  | 0.01  |       |       |       |       |       |

(continued on next page)

**Table 16** (continued)

| Case               | Unit | 25    | 26    | 27    | 28    | 29    | 30    | 31    |
|--------------------|------|-------|-------|-------|-------|-------|-------|-------|
| - H <sub>2</sub> O | %vol | 32.19 | 27.70 | 44.14 | 44.42 | 38.07 | 58.19 | 52.59 |
| - H <sub>2</sub>   | %vol | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO               | %vol | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| - CO <sub>2</sub>  | %vol | 65.86 | 71.38 | 53.27 | 54.07 | 61.19 | 39.75 | 46.90 |
| - N <sub>2</sub>   | %vol | 1.91  | 0.90  | 2.53  | 1.48  | 0.73  | 2.02  | 0.50  |
| - O <sub>2</sub>   | %vol | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |

### Capital cost estimation procedure

In the case of the MEA post-combustion carbon capture section the methodology described in Section 2.2.5 has been adopted using the values listed in Table 15 and in Table 13 along with equations (35)–(41). The reference values found in literature and used to carry out the economic assessment have been updated through the CEPCI index computed as the average between the years 2019 and 2022. Therefore the CEPCI index used in this work is equal to 712.47 and the resulting values are shown in Table 14 (in column “C<sub>0</sub>”).

$$C_{e,i} = n \cdot C_{0,i} \left( \frac{S_{e,i}}{n \cdot S_{0,i}} \right)^f \quad (35)$$

$$TEC = \sum_{i=1}^n C_{e,i} \quad (36)$$

$$TDPC = TEC + TIC \quad (37)$$

$$EPC = TDPC + IC \quad (38)$$

$$TPC = EPC + Co + OC \quad (39)$$

$$FCF = \frac{r(1+r)^n}{(1+r)^n - 1} \quad (40)$$

$$TAC \left[ \frac{M€}{y} \right] = TPC \cdot FCF + C_{el} + C_{NG} + C_{H_2O} + C_f + C_{O\&M} \quad (41)$$

In the case of the DISPLACE technology, the following methodology was adopted. The steel selected to manufacture the DISPLACE is carbon steel P355GH. Regarding the economic assessment of the additional equipment necessary to be installed for the carbon capture process through the DISPLACE technology (i.e. compressors, pumps, etc.) the methodology described for the MEA carbon capture section was used with the values listed in Table 14. Equations (42)–(70) were used to compute the DISPLACE total plant cost.

$$T_{design} [^{\circ}C] = T_{working} + 30 \quad (42)$$

$$P_{design} [bar] = P_{working} + 2.2 \quad (43)$$

$$f_d [MPa] = \min \left( \frac{R_{p0.2/T}}{1.5}; \frac{R_{m/20}}{2.4} \right) \quad (44)$$

$$R_{p0.2/T} [MPa] = 0.0007 \cdot T_{design}^2 - 0.7794 \cdot T_{design} + 403.69 \quad (45)$$

$$R_{m/20} [MPa] = 510 \quad (46)$$

$$z [mm] = 0.85 \quad (47)$$

$$CA [mm] = 3.00 \quad (48)$$

$$t_{wall} [mm] = \frac{P_{design}/10 \cdot D_e \cdot 1000}{2 \cdot f_d \cdot z + P_{design}/10} \quad (49)$$

$$t_{hemispherical\ head} [mm] = \frac{P_{design}/10 \cdot D_{column} \cdot 1000}{4 \cdot f_d \cdot z + P_{design}/10} \quad (50)$$

$$SF = 1.50 \quad (51)$$

$$t_{vessel\ wall} [mm] = t_{wall} \cdot SF + CA \quad (52)$$

$$t_{vessel\ head} [mm] = t_{hemispherical\ head} \cdot SF + CA \quad (53)$$

$$D_i [m] = D_e - 2 \cdot t_{vessel\ wall} \quad (54)$$

$$V_{vessel} [m^3] = \pi/4 \cdot (D_e^2 - D_i^2) \cdot H \quad (55)$$

$$V_{\text{hemispherical head}} [\text{m}^3] = 4/3\pi \cdot \left( (D_e/2)^3 - (D_e/2 - t_{\text{vessel head}}/1000)^3 \right) \quad (56)$$

$$m_{\text{column}} [\text{kg}] = 7850 [\text{kg}/\text{m}^3] \cdot (V_{\text{vessel}} + V_{\text{hemispherical head}}) \quad (57)$$

$$c_{\text{columns}} [\text{€}] = c_{\text{steel}} [\text{€/kg}] \cdot m_{\text{column}} \cdot n_{\text{columns per train}} \cdot n_{\text{train}} \quad (58)$$

In addition the costs of the valves and of the sorbent have been taken into consideration.

$$v_{\text{max}} [\text{m/s}] = \sqrt{122/\rho_{\text{gas}}} \quad (59)$$

$$v [\text{m/s}] = 5 \quad (60)$$

$$v [\text{m/s}] = v_{\text{max}} - v_A \quad (61)$$

$$\dot{V}_{\text{gas}} [\text{m}^3/\text{s}] = \frac{\dot{m}_{\text{in}}}{2 \cdot \rho_{\text{gas}} \cdot n_{\text{train}}} \quad (62)$$

$$A_{\text{valve}} [\text{m}^2] = \dot{V}_{\text{gas}} / v \quad (63)$$

$$D_{\text{valve}} [\text{m}] = 2\sqrt{A_{\text{valve}}/\pi} \quad (64)$$

$$c_{\text{valve}} [\text{€}] = 10000 + 2500 \cdot (2 \cdot \text{round\_up}(D_{\text{valve}}/0.025/2)) \quad (65)$$

$$c_{\text{valves}} [\text{€}] = \sum_{i=1}^n (c_{\text{valve},i} \cdot n_{\text{valves per column},i} \cdot n_{\text{columns per train}} \cdot n_{\text{train}}) \quad (66)$$

The quantity of valves per each vessel is shown in Table 16.

The total plant cost of the DISPLACE columns and valves is computed with the following equations and the assumptions listed in Table 16.

$$\text{TEC}_{\text{DISPLACE}} [\text{€}] = c_{\text{columns}} + c_{\text{bulk material and freight}} + c_{\text{valves}} \quad (67)$$

$$c_{\text{bulk material and freight}} [\text{€}] = 0.77 \cdot c_{\text{columns}} \quad (68)$$

$$\text{TDC}_{\text{DISPLACE}} [\text{€}] = \text{TEC}_{\text{DISPLACE}} + c_{\text{construction}} + c_{\text{other}} \quad (69)$$

$$\text{TPC}_{\text{DISPLACE}} [\text{€}] = \text{TDC}_{\text{DISPLACE}} + \text{EPCM}_{\text{services}} + c_{\text{contingency}} \quad (70)$$

## Data availability

The data that has been used is confidential.

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