Supplementary Information: Novel approach for low CO_2 intensity hydrogen from natural gas

S1 Maximum achievable CO_2 cut

The liquid yield and CO_2 cut achieved in the main separator is highly dependent on the separation temperature and pressure as well as feed CO_2 concentration and overall composition. To illustrate this, Eq. (S1) expresses the estimated CO_2 cut when separating a partially condensed binary H_2/CO_2 mixture:

$$CO_2 cut = \frac{X_{CO_2}\left(f_{CO_2} - Y_{CO_2}\right)}{f_{CO_2}\left(X_{CO_2} - Y_{CO_2}\right)} \tag{S1}$$

In this expression, f_{CO_2} is the overall CO_2 fraction in the incoming feed stream, which varies considerably depending on the tail gas recycle ratio. Y_{CO_2} and X_{CO_2} are the respective equilibrium CO_2 fractions in the vapour and liquid phase separation products for any given temperature and pressure. When combining Eq. (S1) with measurement data for Y_{CO_2} and X_{CO_2} by Fandiño *et al.* [1], the influence of these parameters becomes obvious.

Fig. S1 illustrates the CO_2 cut as a function of the separation pressure and temperature. The chosen feed conditions are the conditions of process configuration 1

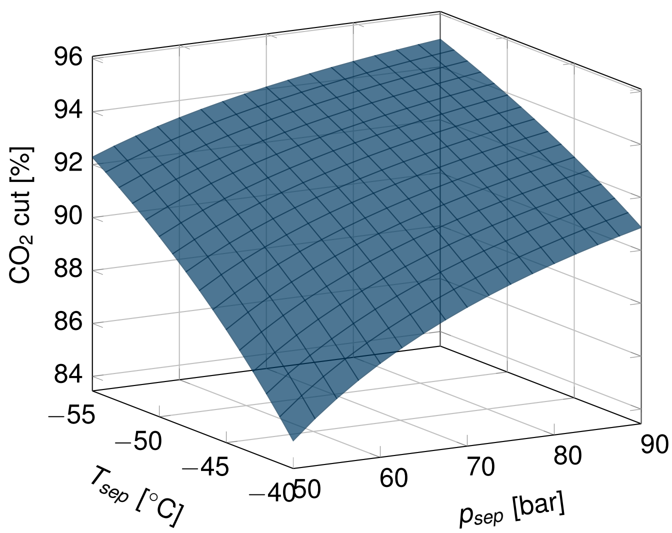

Fig. S1 CO_2 cut as a function of the separation temperature T_{Sep} and pressure p_{Sep} for process configuration 2.

Notes and references

1 O. Fandiño, J. M. Trusler and D. Vega-Maza, *International Journal of Greenhouse Gas Control*, 2015, **36**, 78 – 92.

S2 Figures related to sensitivity analysis in Section 3.2

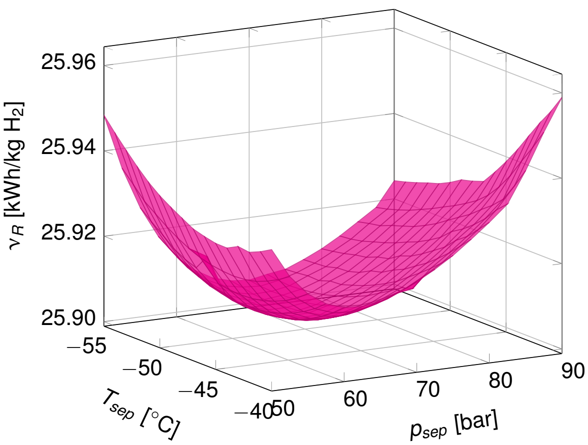

Fig. S2 Specific equivalent power input as a function of the separation temperature T_{Sep} and pressure p_{Sep} for process configuration 1.

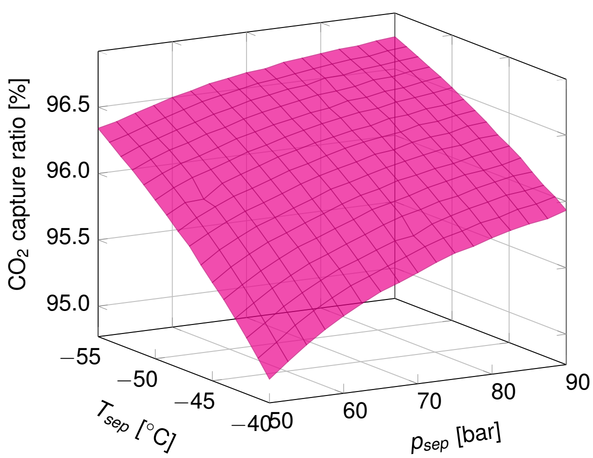

Fig. S3 CO_2 capture ratio as a function of the separation temperature T_{Sep} and pressure p_{Sep} for process configuration 1.

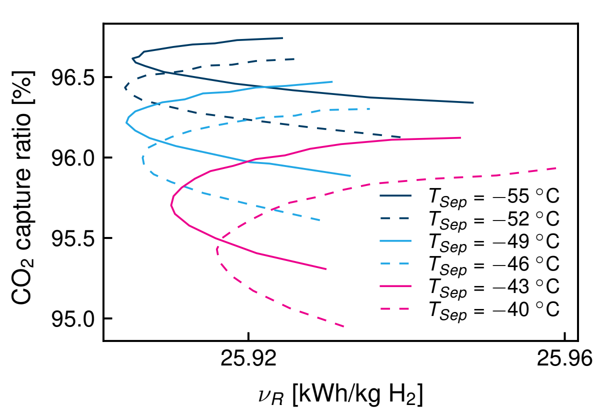

Fig. S4 CO_2 capture ratio as a function of the specific equivalent power input at constant temperatures T_{Sep} for process configuration 1. The reader is referred to the web version for colour coding.

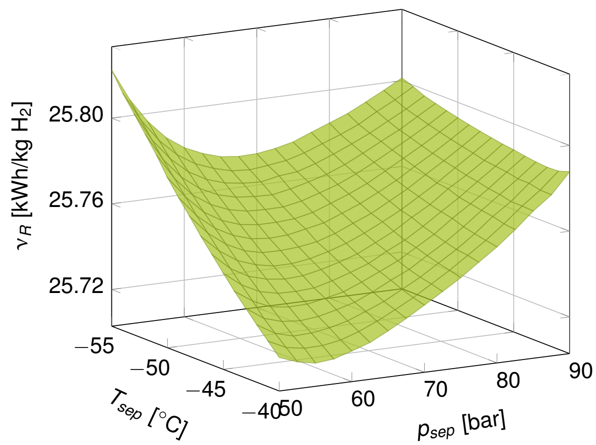

Fig. S5 Specific equivalent power input as a function of the separation temperature T_{Sep} and pressure p_{Sep} for process configuration 3.

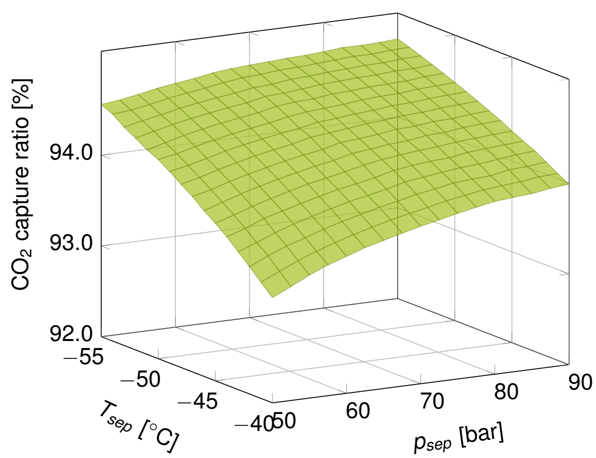

Fig. S6 CO_2 capture ratio as a function of the separation temperature T_{Sep} and pressure p_{Sep} for process configuration 1.

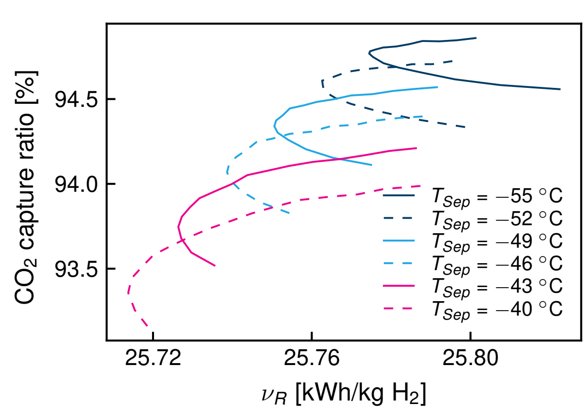

Fig. S7 CO_2 capture ratio as a function of the specific equivalent power input at constant temperatures T_{Sep} for process configuration 3. The reader is referred to the web version for colour coding.

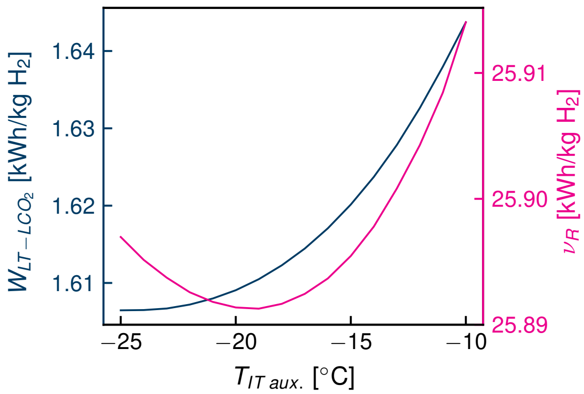

Fig. S8 Specific energy demand of liquefaction section (left axis) and the specific equivalent power requirement (right axis) as a function of the outlet temperature of the IT refrigeration loop for process configuration 1. The reader is referred to the web version for colour coding.

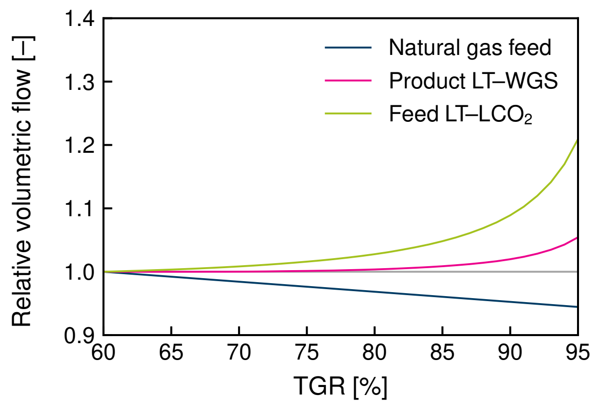

Fig. S9 Relative volumetric flows for process configuration 1 and a feed temperature to the LT–WGS reactor of $200\,°C$. The grey line corresponds to a constant value of 1.0. They grey line corresponds to a constant value of 1.0. The reader is referred to the web version for colour coding.

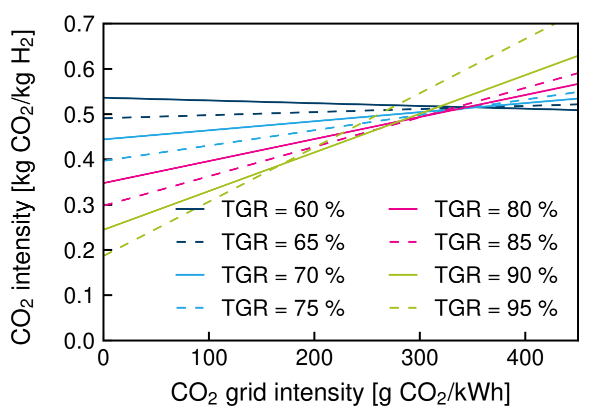

Fig. S10 CO_2 intensity of hydrogen as a function of the CO_2 grid intensity for process configuration 1 and a feed temperature to the LT–WGS reactor of $200\ °C$. The reader is referred to the web version for colour coding.

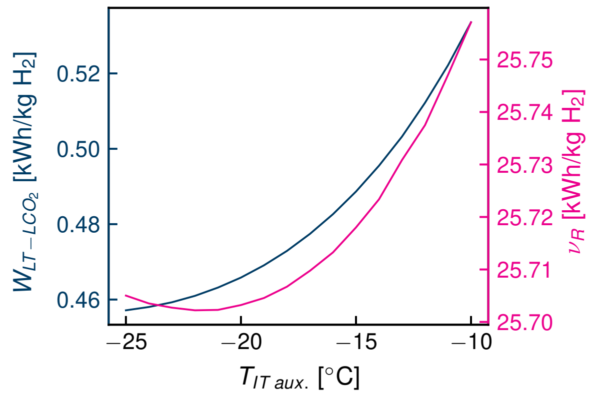

Fig. S11 Specific energy demand of liquefaction section (left axis) and the specific equivalent power requirement (right axis) as a function of the outlet temperature of the IT refrigeration loop for process configuration 3. The reader is referred to the web version for colour coding.

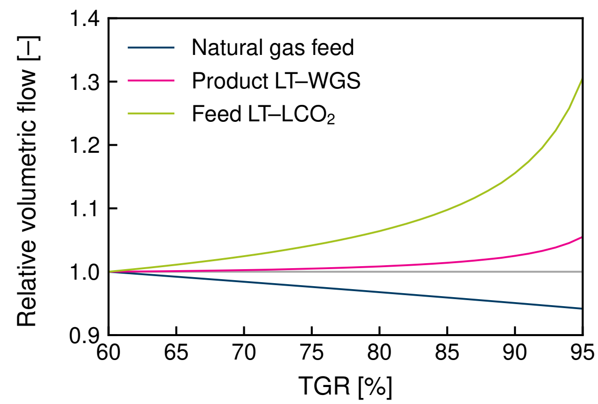

Fig. S12 Relative volumetric flows for process configuration 3 and a feed temperature to the LT–WGS reactor of $225\,°C$. The grey line corresponds to a constant value of 1.0. They grey line corresponds to a constant value of 1.0. The reader is referred to the web version for colour coding.

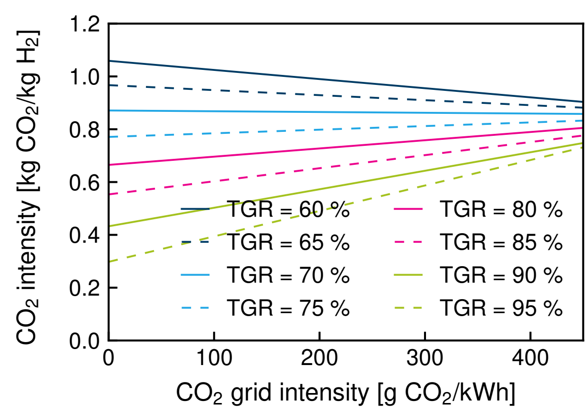

Fig. S13 CO_2 intensity of hydrogen as a function of the CO_2 grid intensity for process configuration 3 and a feed temperature to the LT–WGS reactor of $225\ °C$. The reader is referred to the web version for colour coding.