Development of an open-source toolkit to design and evaluate the performance of low carbon infrastructure for industrial clusters

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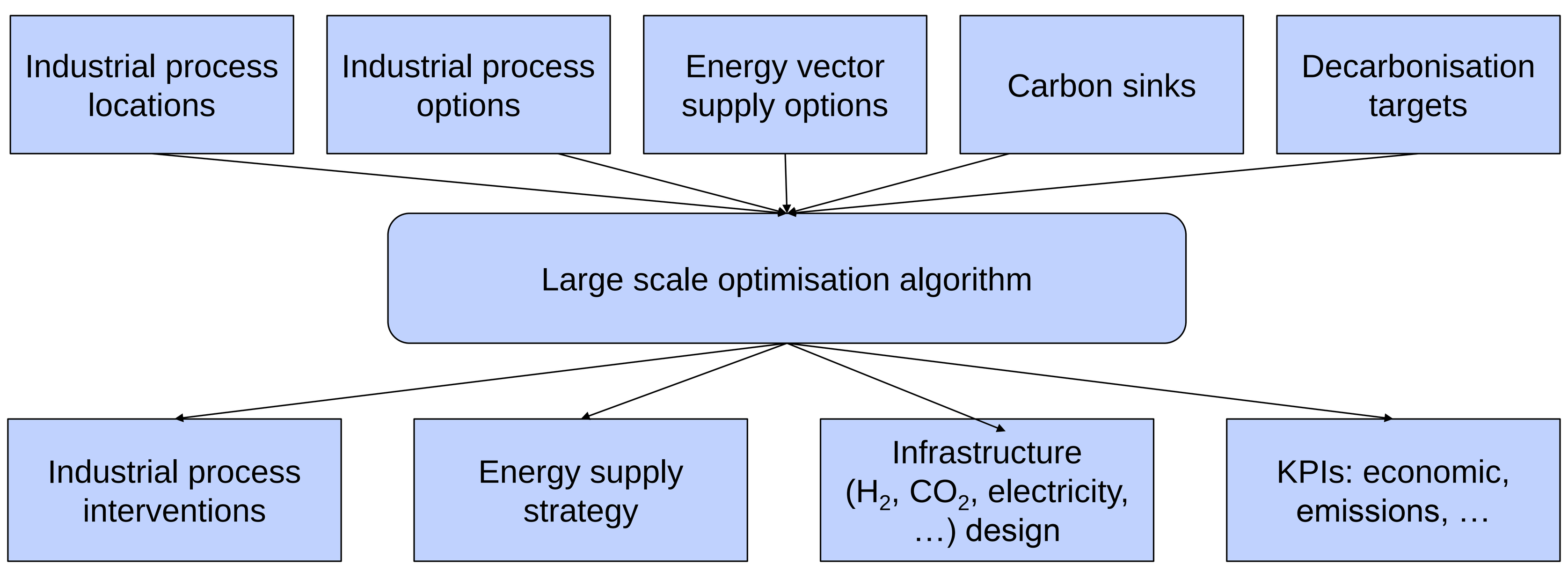
Objective

Development of a toolkit to design low carbon infrastructure for industrial clusters. This project is building on our experience of process and system level modelling as well as life cycle analysis to develop a model-based toolkit which can be used to analyse and design supporting infrastructure and key investments for low carbon industrial clusters. Issues such as what is the right balance of electricity, CCS, hydrogen and heat cascading for a particular cluster can be explored, quantifying the solutions with a range of energetic, economic and environmental metrics.

Academically, this requires four key tasks: [1] Framework development; [2] Model and tool development [3] Cluster case studies and model refinement [4] Model finalisation.

Industrially, the objective is to engage at least two clusters in the case studies and evaluation and use the toolkit to support them in their roadmap development. Tools of this nature are also useful to technology developers who can gain insights into the potential roles for their technologies in industrial decarbonisation.

Methodology: cluster design toolkit

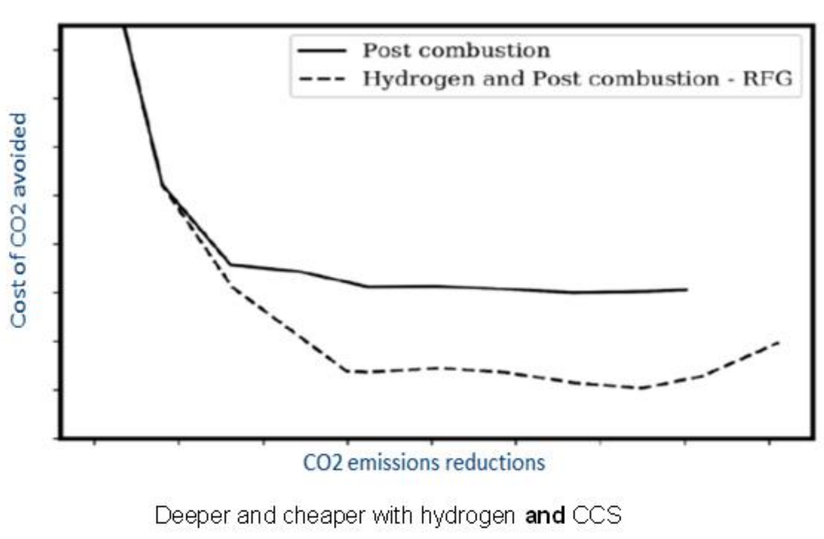


Input parameters:

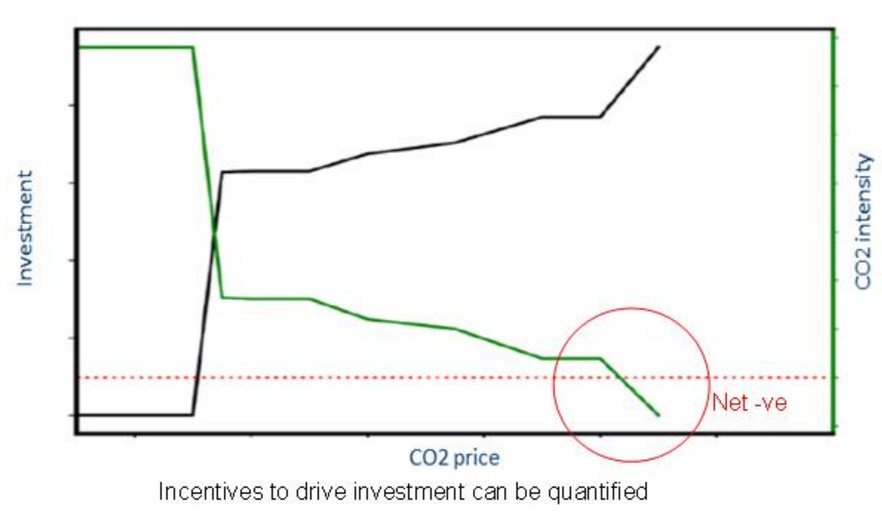
- Geographical locations of the existing industrial assets and options for their decarbonisation (e.g. new technology, fuel switching, CCS)
- Location and capacity of carbon sinks
- Potential locations of supporting technologies (e.g. H2 production)
- Availability of other energy supplies (e.g. electricity, biofuels)
- Decarbonisation targets

Investment and operational decisions:

- Binary variables to determine which interventions take place in each asset
- Binary variables defining investment in new energy supply technologies
- Binary variables for investment in new infrastructure
- Continuous variables for process operations and flows (H2, CO2, electricity, …) through networks.



Deeper and cheaper with hydrogen and CCS



Incentives to drive investment can be quantified

Scope: considered industries and technologies

The optimisation model contains (a) an accurate representation of the industrial processes and mapping of options for modification (portfolio, e.g., fuel switch or carbon capture, or other), (b) spatial configuration and representation of the temporal evolution of the system, (c) representation of the wider hinterland and possible interactions (e.g. access to CO_2 transport backbones), and (d) key performance indicators that reflect a range of parameters addressing the techno-economic performance for individual companies as well as for the total cluster, regional economic benefits, and environmental impacts. Following this framework, the toolkit is able to optimise for alternative cluster-level system designs. It explores the role of different technologies and interventions and evaluates the effects of different business models that regional and central governments may wish to employ to achieve net-zero clusters.

In a first development round, the model focuses on UK's major carbon dioxide emitting industry sectors. These include:

- Refineries
- Iron & Steel mills
- Cement and Lime
- Power plants
- Chemicals

The toolkit incorporates models, i.e. component models, to describe the baseline processes within these industries, as well as intervened process. Such interventions entail various technological alteration like carbon capture technologies, fuel switch to hydrogen or ammonia, or alternative process layout or integration with other industries. Each process modification is described in a separate process simulation model.

Acknowledgements

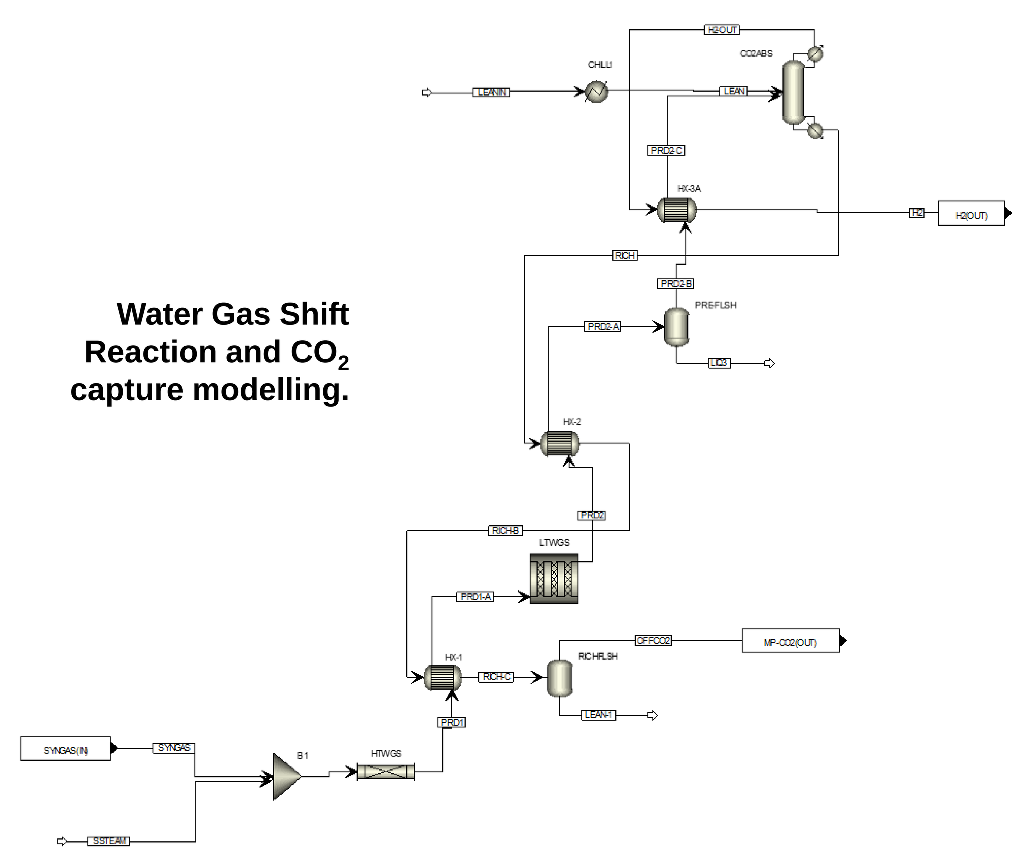
This research is carried out as part of the UKRI (EPSRC) funded
"Industrial Decarbonisation and innovation Centre (IDRIC)" project, Grant Reference: EP/V027050/1.

Process simulation toolkit for industrial decarbonisation

Aiming at accurately representing industrial process options for decarbonisation, component process simulation models (such as fuel switch, carbon capture, H_2 and NH_3 production, CO_2 storage and utilisation) are developed. The tools being developed quantify flows of materials, natural resources, energy, intermediate products or emissions at component unit process level, based on fundamental physical/chemical principles or process simulations which, to a greater extent, account for the technological, spatial and temporal characteristics of decarbonisation options under consideration. The tool elements are implemented in Python, Matlab or Aspen Plus.

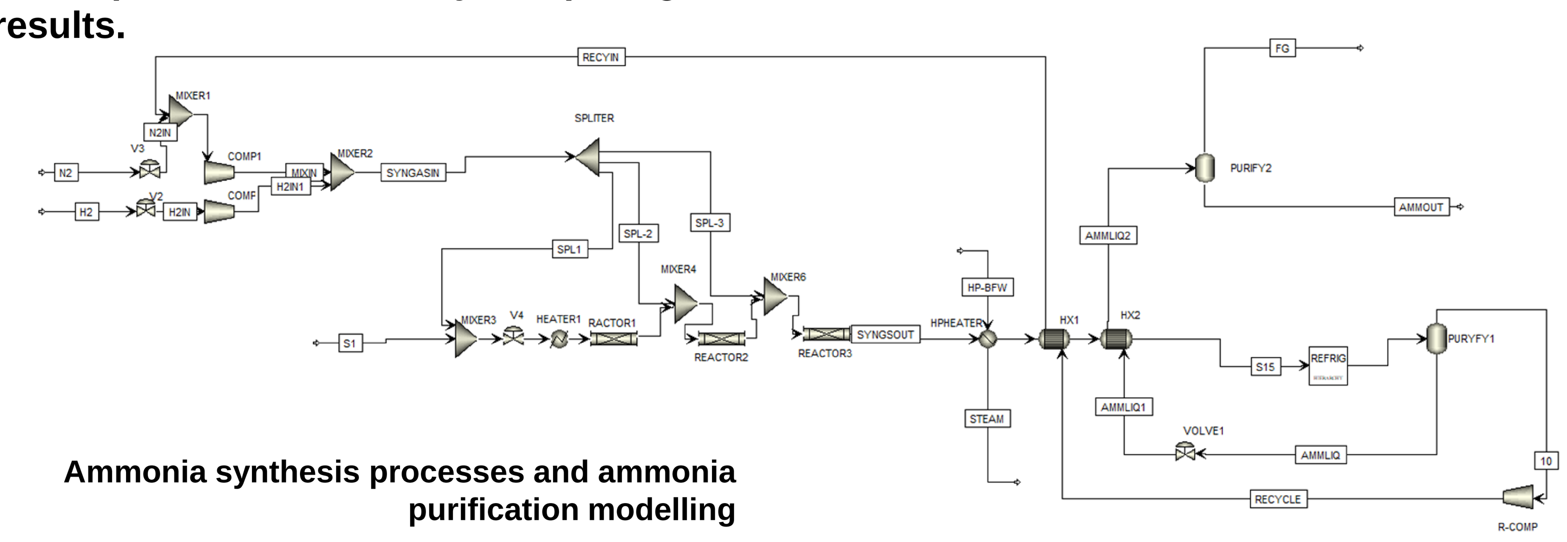
The aim is to provide asset owners/operating companies the ability to evaluate optimal technology and infrastructure options; understanding of interdependencies with other operators; optimal integration with neighbouring industries. In addition, the toolkit facilitates to develop a comprehensive and quantitative LCI database, which models inputs/outputs of processes at high level of detail, allowing to account for technical and geographic differences for alternative cluster-level system designs.

Hydrogen production and ammonia production are key technological solutions for industrial cluster decarbonisation. The Water Gas Shift Reaction (WGS) and CO_2 capture model (part of hydrogen production processes) and the ammonia synthesis and purification model developed in Aspen Plus are illustrated as examples. The high temperature WGS reactor and low temperature WGS reactor are modelled as Aspen Plus plug flow reactors based on Langmuir-Hinshelwood - Hougen - Watson (LHHW) kinetics models. Rectisol® processes based CO_2 capture are modelled, which use methanol atsub-zero temperatures to purify synthesis gas and remove CO_2.

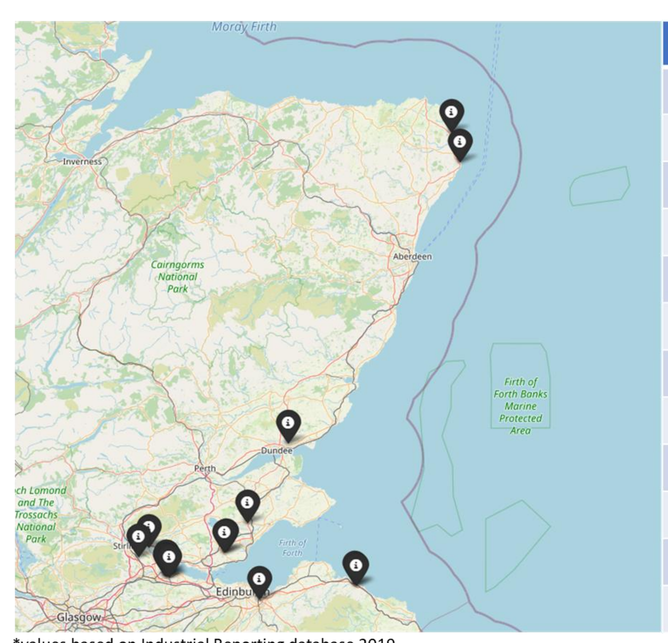


Water Gas Shift Reaction and CO_2 capture modelling.

Ammonia synthesis process based on reactors with Ru-based catalyst is modelled, as the Ru-based catalyst become a promising candidate for a more efficient, much safer, and less energy intensive ammonia synthesis in the future. A feed-quench-type process configuration with 3 ammonia synthesis reactors is applied. Ammonia synthesis reactors are modelled as Aspen Plus plug flow reactors based on LHHW kinetics model. The inlet N_2 to H_2 ratio, reactors length and flow rate among 3 reactors can be optimised to match the ammonia purity target. The ammonia gas in the synthesis loop is liquefied by ammonia evaporation in the ammonia chiller and discharged to ammonia storage. The models developed are validated by comparing with literature data. The results match well literature results.

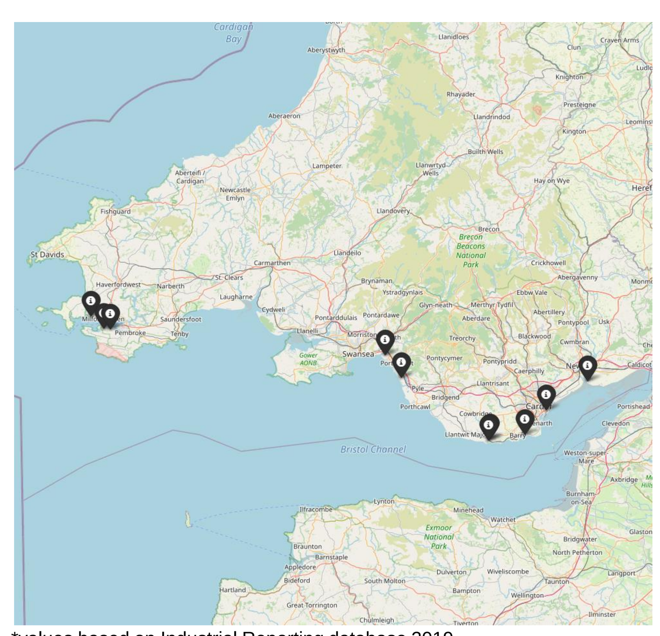


Ammonia synthesis processes and ammonia purification modelling



Sites (operator)	CO2* [kt]
Dunbar Works (Tarmac Cement and Lime)	559
Dunbar Energy Recovery Facility (Viridor)	274
Grangemouth Refinery	1340
Grangemouth CHP plant	641
INEOS Infrastructure Grangemouth	429
INEOS Chemicals Grangemouth	522
Kinneil Terminal (INEOS)	345
Fife Ethylene Plant (Exxonmobil)	680
Fife NGL Plant (Shell UK)	250
Markinch Biomass CHP (RWE)	487
Peterhead Power Station (APACHE)	1579
St Fergus North Sea Gas Terminal (Shell UK)	303

*values based on Industrial Reporting database 2019



Sites (operator)	CO2* [kt]
Pembroke Refinery (Valero)	2,160
Pembroke Power Station (RWE)	4,280
South Kook LNG Terminal	237
Port Talbot Steelworks (Tata Steel)	6,430
Aberthaw (Lafarge Tarmac Cement and Lime)	371
Aberthaw Power Station (RWE)	660
Barry CHP (Dow Silicones)	131
Cardiff Energy Recovery Facility (Viridor)	364
? Severn Power Station ?	716

*values based on Industrial Reporting database 2019

Case studies

The toolkit is developed and tested with the engagement of two industrial clusters: the Scottish and the South Wales clusters. Both clusters have unique characteristics, cover a wide array of industrial processes and are not currently funded (in the first wave) by BEIS. The Scottish cluster is centred around the Grangemouth refinery with its surrounding chemical processes (including Mossmoran sites). The Feeder 10 pipeline connects those sites to St.Fergus, from where the CO_2 can be injected into the Miller oil field. In contrast, the South Wales cluster does not have direct access to a CO_2 sink, which requires CO_2 transport by ships. Given that dependency on sea routes, the Pembroke refinery and adjacent regasification terminal are attractive to consider a blue hydrogen infrastructure to supply the wider hinterland.