WP AC2: Advanced, high-efficient cycles using GTs with sCO_2 or direct oxy-fired CCGT-CCS (Modelling combustion in supercritical CO_2 for power cycles)

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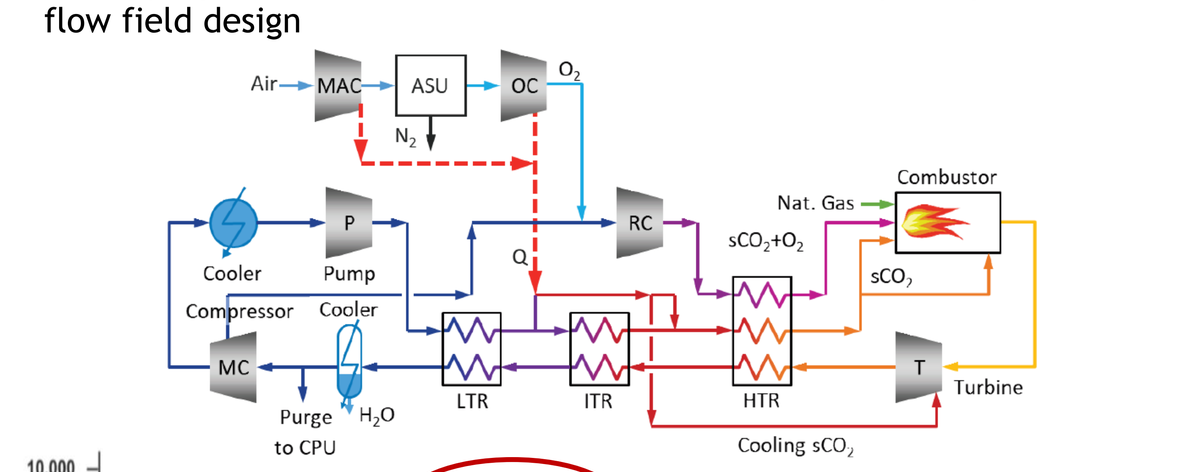
Funded by the UKCCSRC as part of its Core Research Programme, in partnership with the **University of Sheffield** and **Cardiff University**
Dates: **1st April 2017 – ongoing**

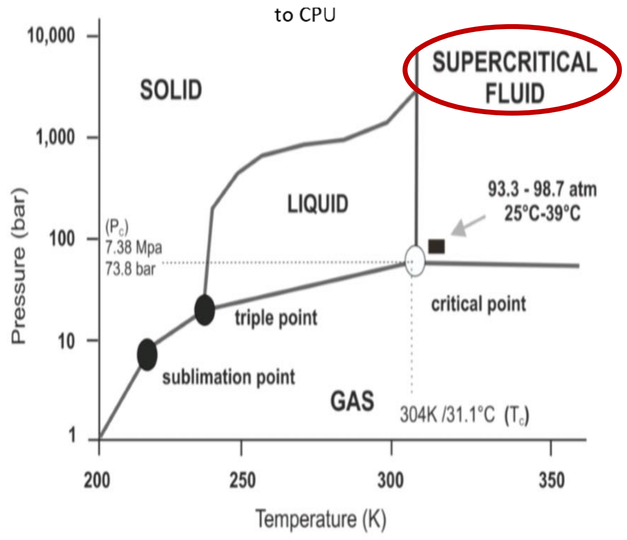
Project overview and objectives

Exhaust gas recycling/selective CO_2 recycling are used to enhance exhaust gas CO_2 levels, reduce volumetric flowrates and decrease the size/costs of the capture plant. However, there are significant changes to combustion and hot gas path environments that impact on operability, materials and component lives. CCGT plants with CO_2-rich strategies can be 'recoded' for supercritical CO_2 (sCO_2) for improved plant efficiency and flexibility.

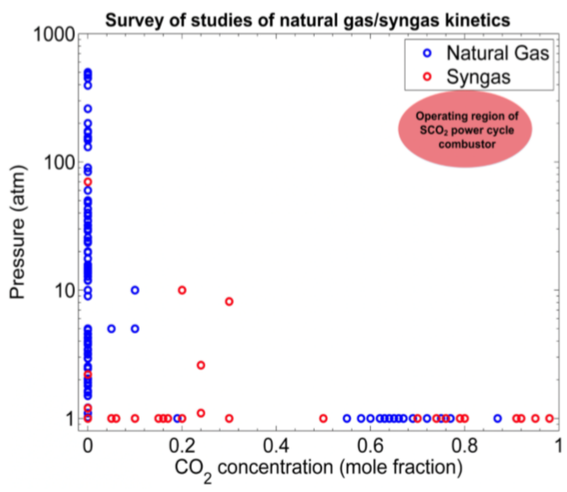
Main objectives: to evaluate and optimise different cycles and determine combustor design parameters, cycle layout and efficiency, including optimal start and enhanced operational flexibility, by:

- assessing the capability of available reaction schemes for natural gas at pressures of ≤200 bar by collecting available data generated using Quantum Mechanic simulation and Boxed Molecular Dynamic simulation
- evaluating the kinetic models for both direct fired oxy-combustion and an indirect fired sCO_2 energy systems
- developing a reduced reaction scheme and then integrating with CFD for flow field design





Phase diagram of CO_2, highlighting the supercritical fluid region.



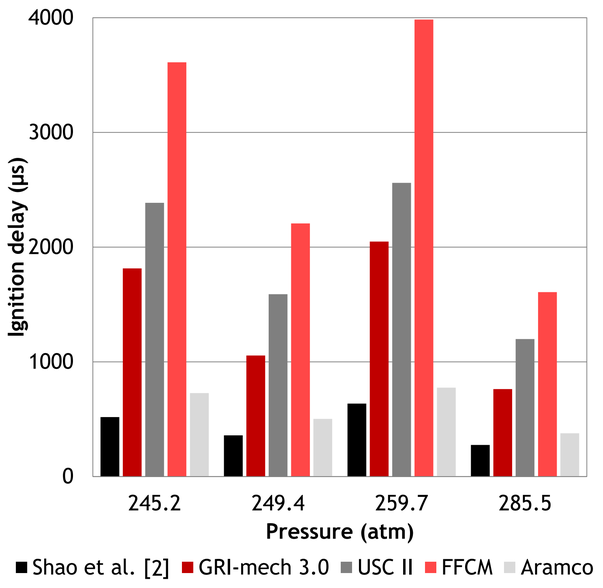
Survey of studies of natural gas/syngas kinetics compared to the target operating range for cycles using sCO_2 [1].

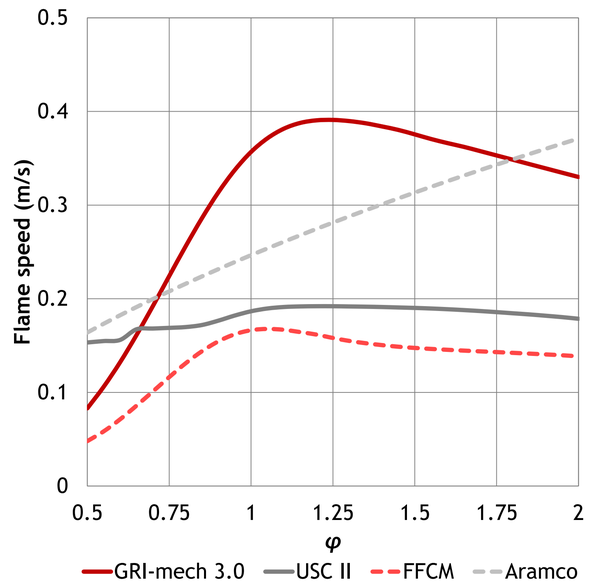
Available validated reaction schemes

Assessing the capability of available chemical kinetic reaction schemes for natural gas combustion at high pressure, comparing four models (**GRI Mech V3.0**; **USC-Mech II**; **FFCM Mech**; and **Aramco Mech V2**) found that:

- ignition delay for the high pressure cases by Shao et al. [2] used a range of reaction mechanisms
- laminar flame speed could be calculated for methane at 300 bars in an oxidiser containing 30-70 vol% O_2-CO_2, with an inlet temperature of 800 K
- the validated reaction mechanisms in both instances give significantly different results between models, not true of similar cases at 1 bar

[1] Sun, W., Ranjan, D., Lieuwen, T., Menon, S. (2018) Investigation of Autoignition and Combustion Stability of High Pressure Supercritical Carbon Dioxide Oxy-combustion, UTSRProjectDEFE0025174, Available: netl.doe.gov/sites/default/files/eventproceedings/2015/utsr/Wednesday/Sun.pdf
[2] Shao, J., Choudhary, R., Davidson, D. F., Hanson, R.K., Barak, S., Vasu, S. (2019) Ignition delay times of methane and hydrogen highly diluted in carbon dioxide at high pressures up to 300 atm, *Proceedings of the Combustion Institute 37*, 4555-4562





Effect of supercritical CO_2 as a diluent

A clear issue is the lack of laboratory data. Ongoing research using shock tubes and kinetic modelling shows that the thermochemical effects of a CO_2 diluent in oxyfuel combustion at the proposed operating conditions are encouraging. Initial literature surveys show a focus should be made on measuring the relative effects of:

- supercritical fluid, where transport properties are more like a liquid
- diluent CO_2 where heat transfer is significantly higher than O_2 and CH_4

The subsequent effect on ignition delay time, emissions and operability compared to standard methane-air combustion especially at higher pressures is in evidence but requires more proof to select the most appropriate mechanism.

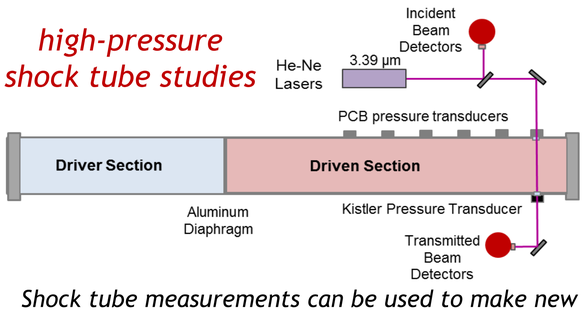
Emerging findings

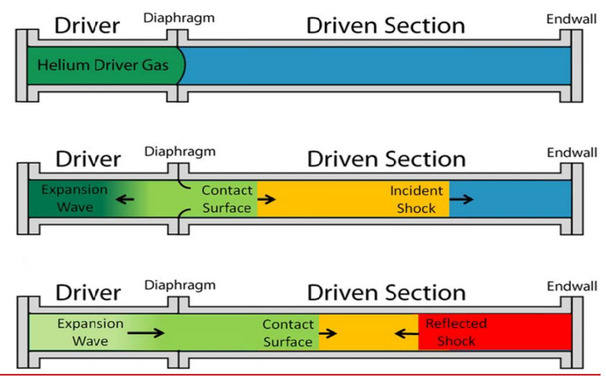
- Sensitivity analysis varies significantly between models and between atmospheric and supercritical pressures
- Whilst kinetic modelling and EoS models using existing reaction mechanisms are available and likely to be close enough to real operating conditions, validation will be needed to add confidence to field

Next steps

- Focus on implementing EoS model with a CH_4 mechanism and identifying the underlying reasons why discrepancies exist
- Heat transfer will require significant analysis, as convective heating to combustor walls will be challenging to predict, and radiative heat transfer also needs to be taken into consideration
- The nature of the underlying chemistry will also require significant validation; a new and unique 200 bar shock-tube and heat transfer test bed facilities at the BEIS/ERDF Translational Energy Research Centre will provide opportunities to investigate chemical kinetics and heat transfer mechanisms required for design of the sCO_2 combustion system

high-pressure shock tube studies





Shock tube measurements can be used to make new chemical kinetic models and evaluate the accuracy of existing chemical kinetic models

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The UKCCSRC is supported by the EPSRC as part of the UKRI Energy Programme.

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