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Supercritical Carbon Dioxide Power Cycle for Stationary Power Generation (WP AC2)

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Supercritical Carbon Dioxide Power Cycle for Stationary Power Generation

- **WP AC2:** s-CO2 cycle with oxy fuel high pressure (HP: 300 bar) combustion for improved efficiency and plant flexibility.
  - **Next Generation Technology: s**-CO2/oxy-combustion strategy can be an effective solution for the full integration of Power-to-Gas, CCUS, and s-CO2 pumping
  - **Technical Challenges:** Availability of detailed reaction schemes (design high pressure combustor), heat transfer mechanism (radical recombination) and impact of trace species on emission and materials.
  - validated chemical reaction schemes at HP is subject to many uncertainties.
  - **Deliverables:**
    1. assessing the capability of the available reaction scheme for NG combustion at HP
    2. evaluating chemical kinetic models for both direct fired oxy-combustion and an indirect fired s-CO2 energy system
    3. developing a reduced reaction scheme and then integrating with CFD for flow field design.
    4. Evaluating and optimising different cycles to determine combustor design parameters, cycle layout and efficiency, including optimal start and enhanced operational flexibility.

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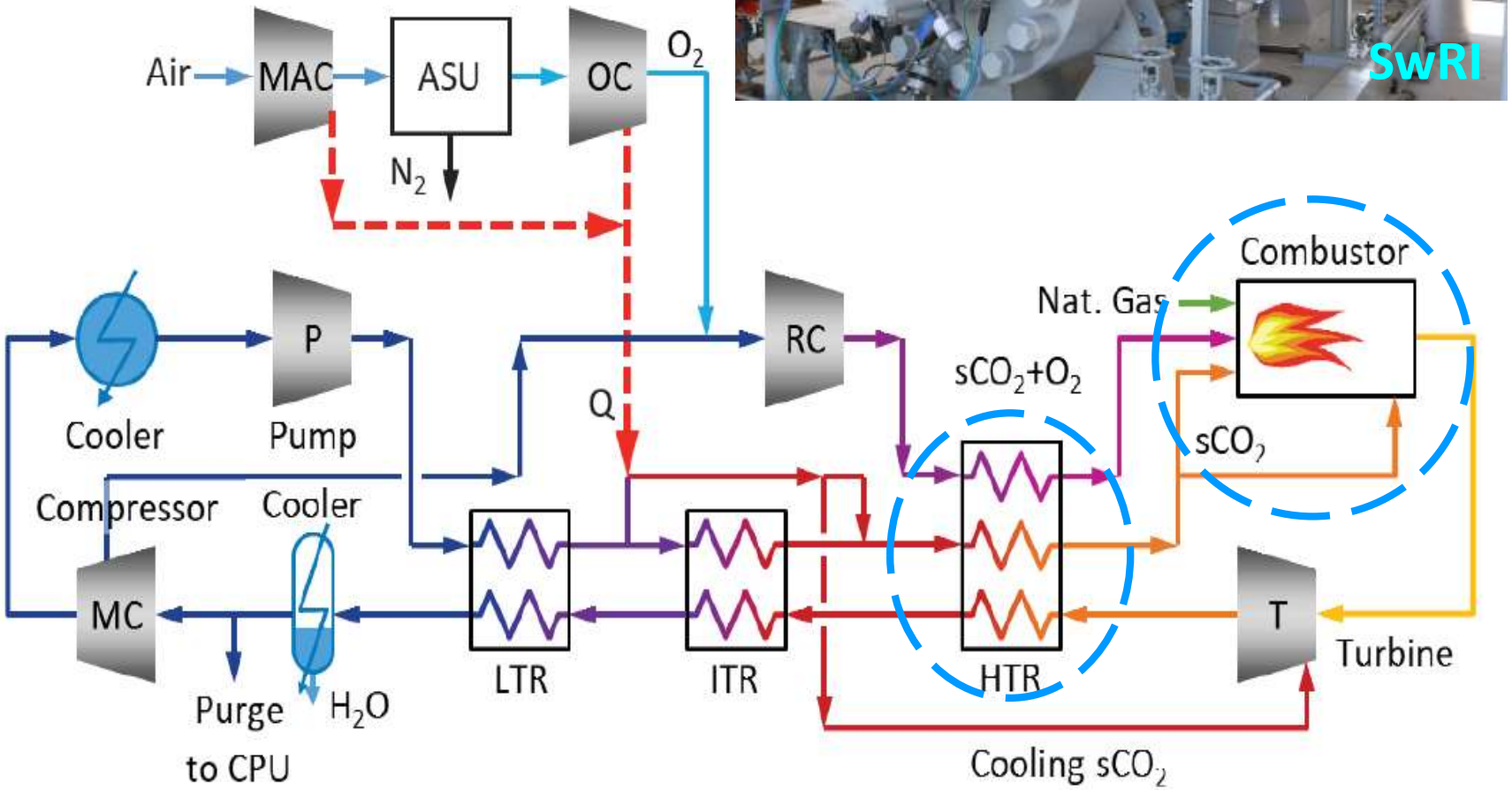
Supercritical Carbon Dioxide Power Cycle for Stationary Power Generation

- Direct-fired s-CO2 cycles: high efficiency and integral ability to capture CO2 at HP.
- Reduced inefficiency associated with phase change heat transfer throughout the cycle
- CO2 (working fluid) is non-toxic, and less corrosive than steam
- high cycle pressures, turbomachinery sizes are compact



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Available validated Chemical Kinetics Reaction Schemes

- ***Deliverable: assessing the capability of the available reaction scheme for NG combustion at HP***
  - **Aramco Mech V2:** newly developed detailed chemical kinetic mechanism that characterises the kinetic and thermochemical properties of a large number of C1-C4 based hydrocarbon and oxygenated fuels over a wide range of experimental conditions (NUI Galway)
  - **GRI Mech V3.0:**optimized mechanism designed to model natural gas combustion, including NO formation and reburn chemistry
  - **USC-Mech II:** High-Temperature Combustion Reaction Model of H2/CO/C1-C4 Compounds (Southern California)
  - **FFCM Mech:** Foundational Fuel Chemistry Model (Stanford)

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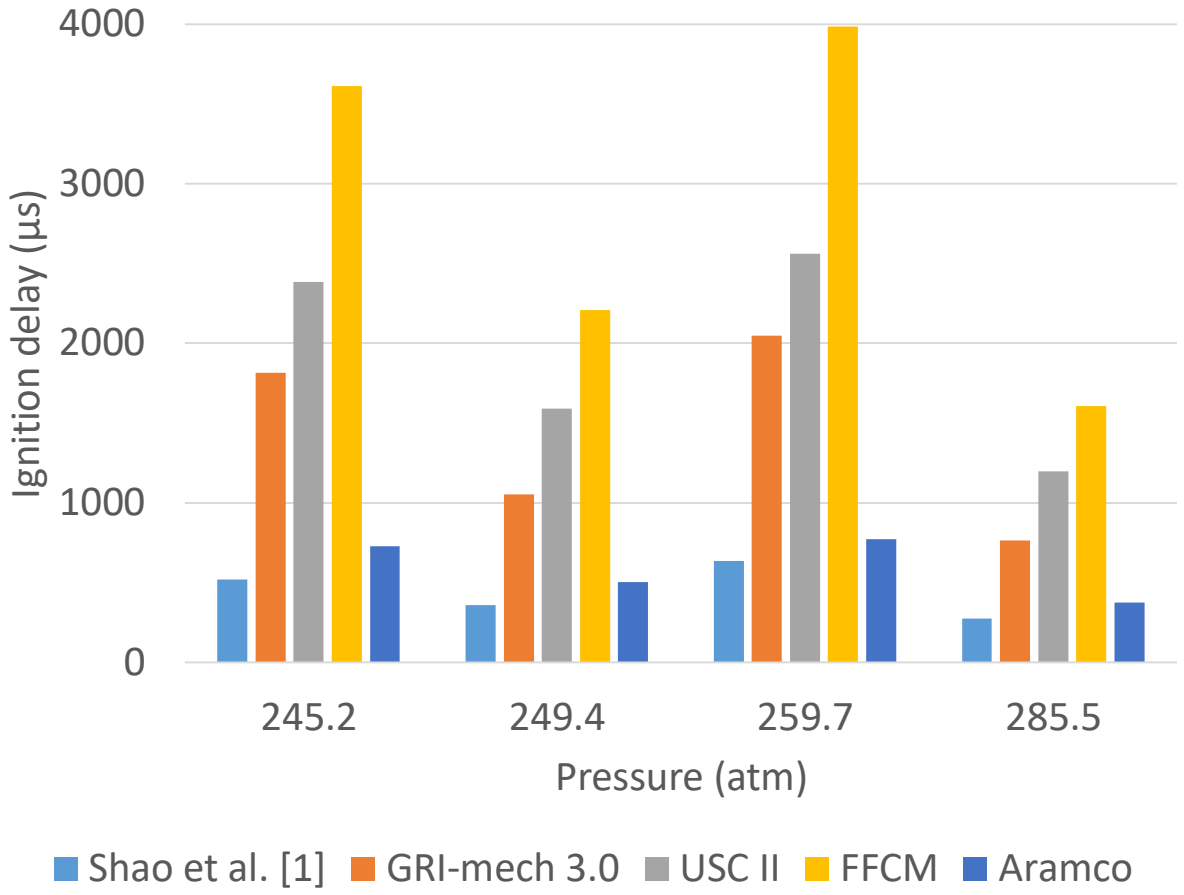
Ignition delay times

- Comparison to shock tube data
- IDT = peak OH from Cantera PSR
- Sensitivity analysis on OH formation
  - Both atmospheric and supercritical
- Significant variation in model results



[1] Shao, J.; Choudhary, R.; Davidson, D. F.; Hanson, R. K.; Barak, S. & Vasu, S. Ignition delay times of methane and hydrogen highly diluted in carbon dioxide at high pressures up to 300 atm *Proceedings of the Combustion Institute*, **2019**, *37*, 4555 - 4562

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Sensitivity analysis

- Sensitivity analysis on ignition based on OH
- Calculated reaction sensitivity as $$S_k = \max\left(\frac{k_r}{y_{OH}}\frac{\delta y_{OH}}{\delta k_r}\right)$$
- Sensitivity calculated for:
  - T_0 = 1100 K, P=1 atm, CH_4: 7.5%, O_2: 15%, CO_2: 77.5%
  - T_0 = 1100 K, 285 atm , CH_4: 7.5%, O_2: 15%, CO_2: 77.5%

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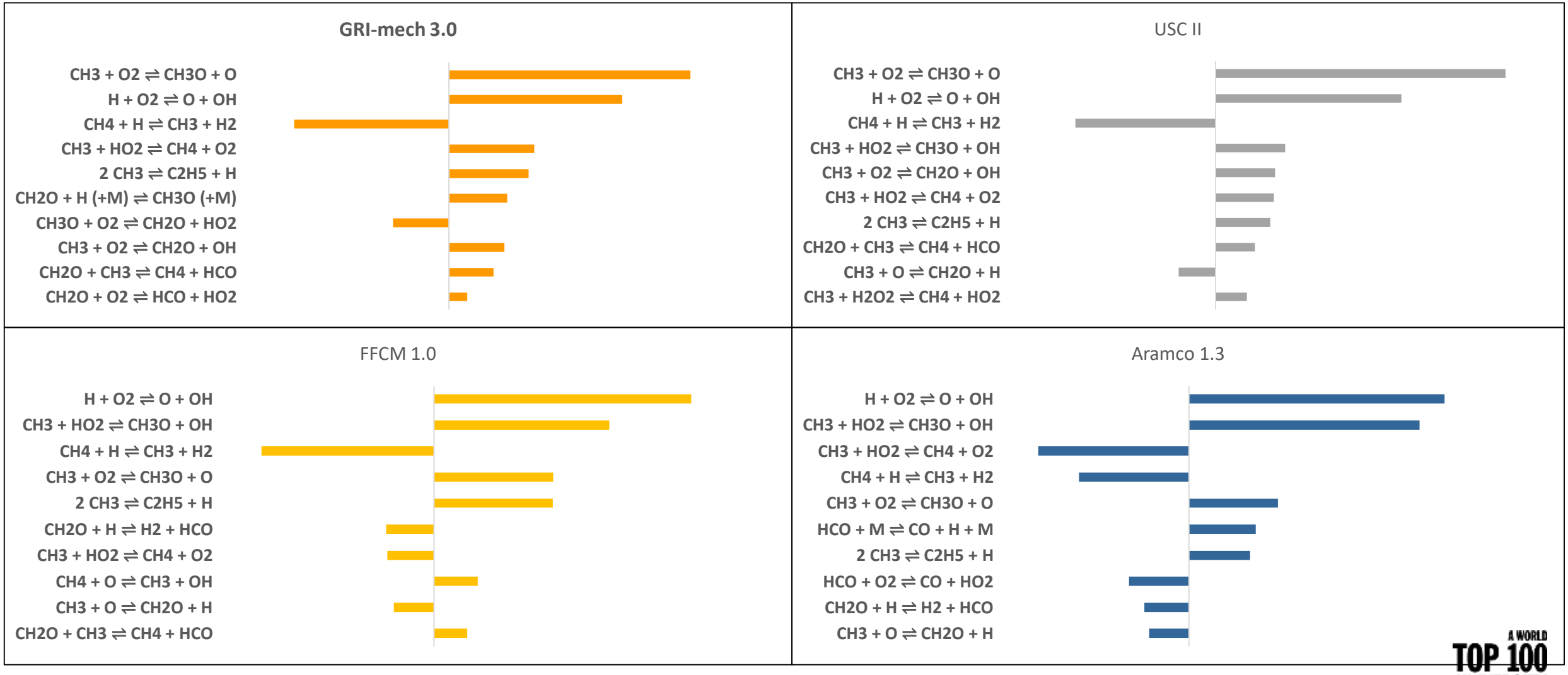
Sensitivity at atmospheric pressure



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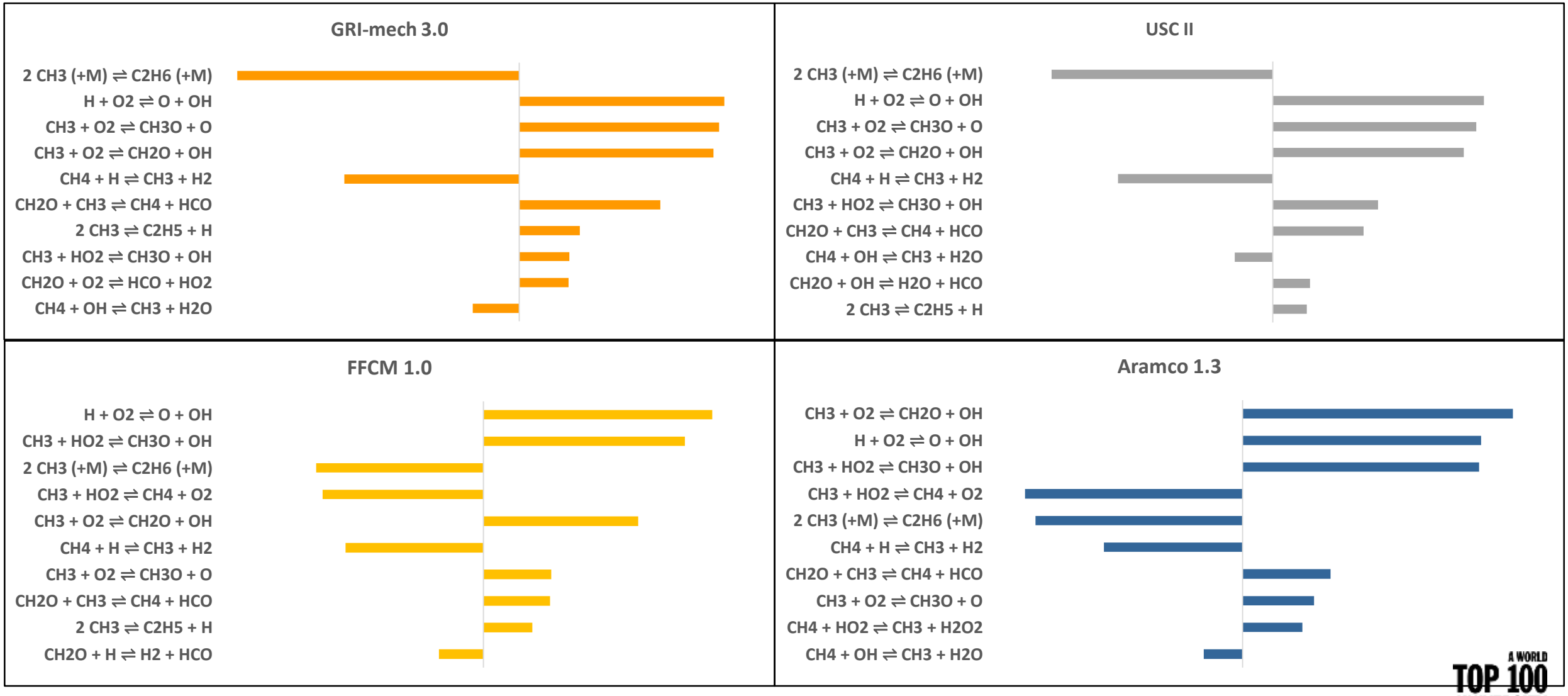
Sensitivity at supercritical pressures



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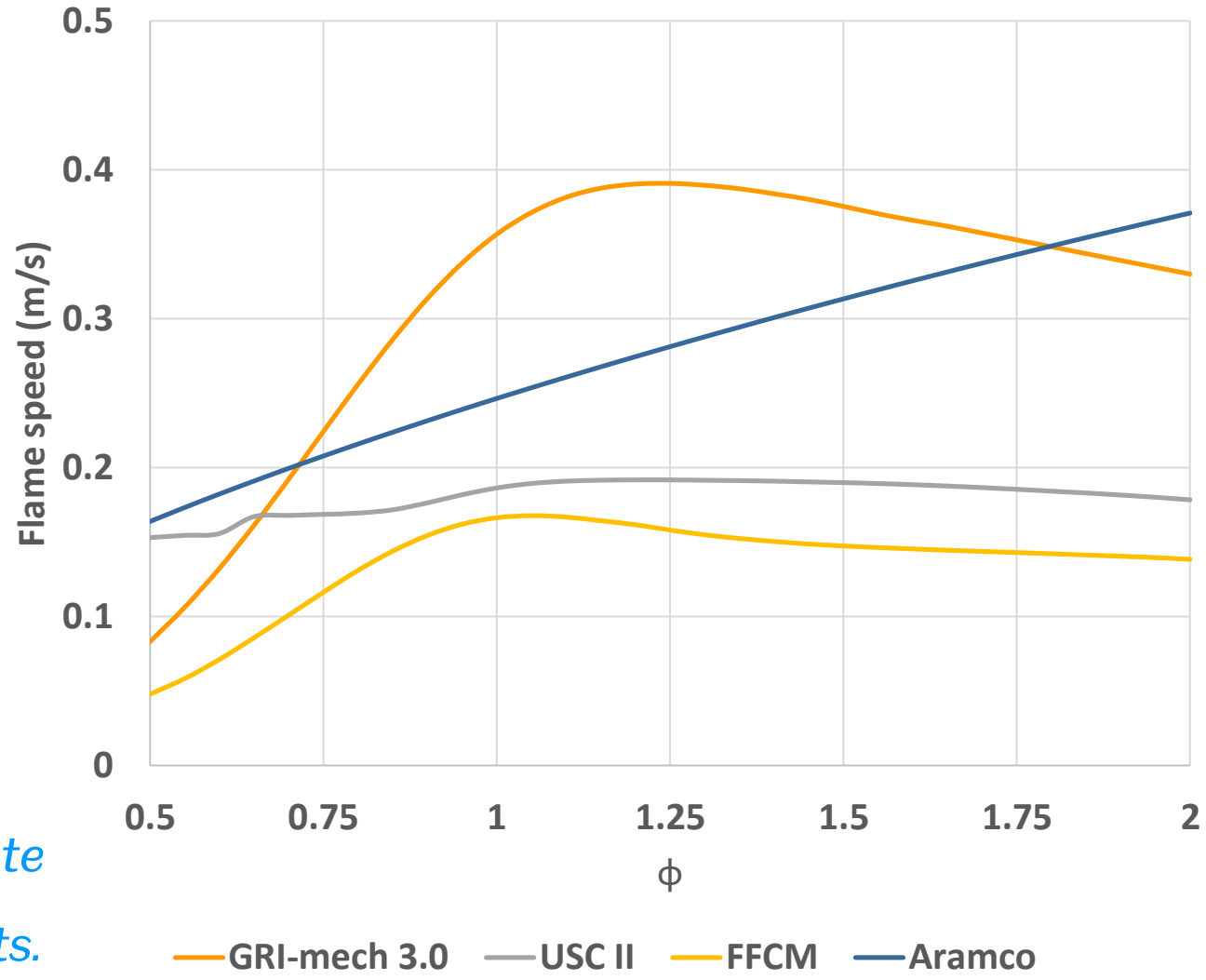
Laminar flame speed

- Cantera Free Flame with ideal gas
- Very significant variation for models
- Similar at atmospheric conditions
- No experimental comparison

Laminar flame speed: *intrinsic characteristic of premixed combustible mixtures. It is the speed at which an un-stretched laminar flame will propagate through a quiescent mixture of unburned reactants.*



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Summary of WP-AC2 : D1

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- At P>60bar many of the fundamental assumptions underlying present combustion modelling (Chemical Kinetics & CFD) become invalid
- Basic research is needed to characterize the physical properties and chemical oxidation mechanisms of O2/CH4/CO2 at high pressures in order to understand reaction initiation, branching, propagation and termination under these conditions.
- Fundamental understanding of the chemistry and physics of O2/CH4/CO2 in high-pressure regimes will require new developments in experimental, and numerical techniques. The ability to predict fuel/species properties (fuel flexibility), reaction rates, and ignition behaviour is crucial for developing combustor for Supercritical Carbon Dioxide Power Cycle for Stationary Power Generation

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High Pressure Shock Tube Studies of O2/CH4/CO2 Combustion

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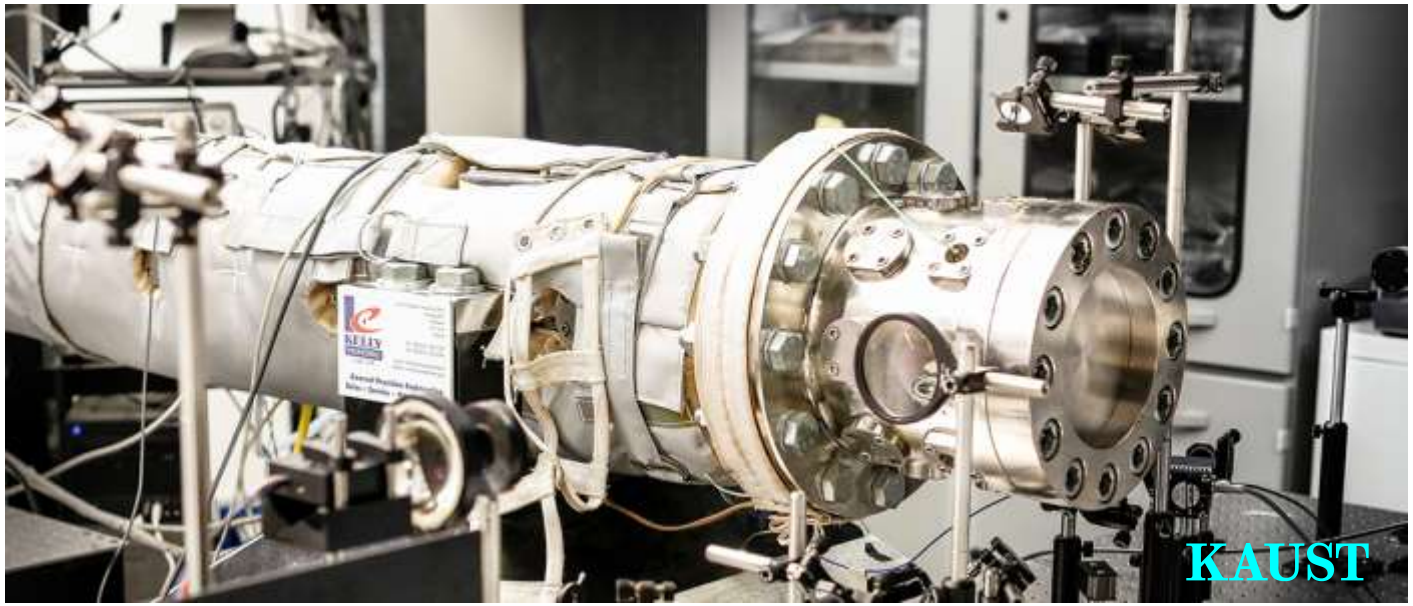
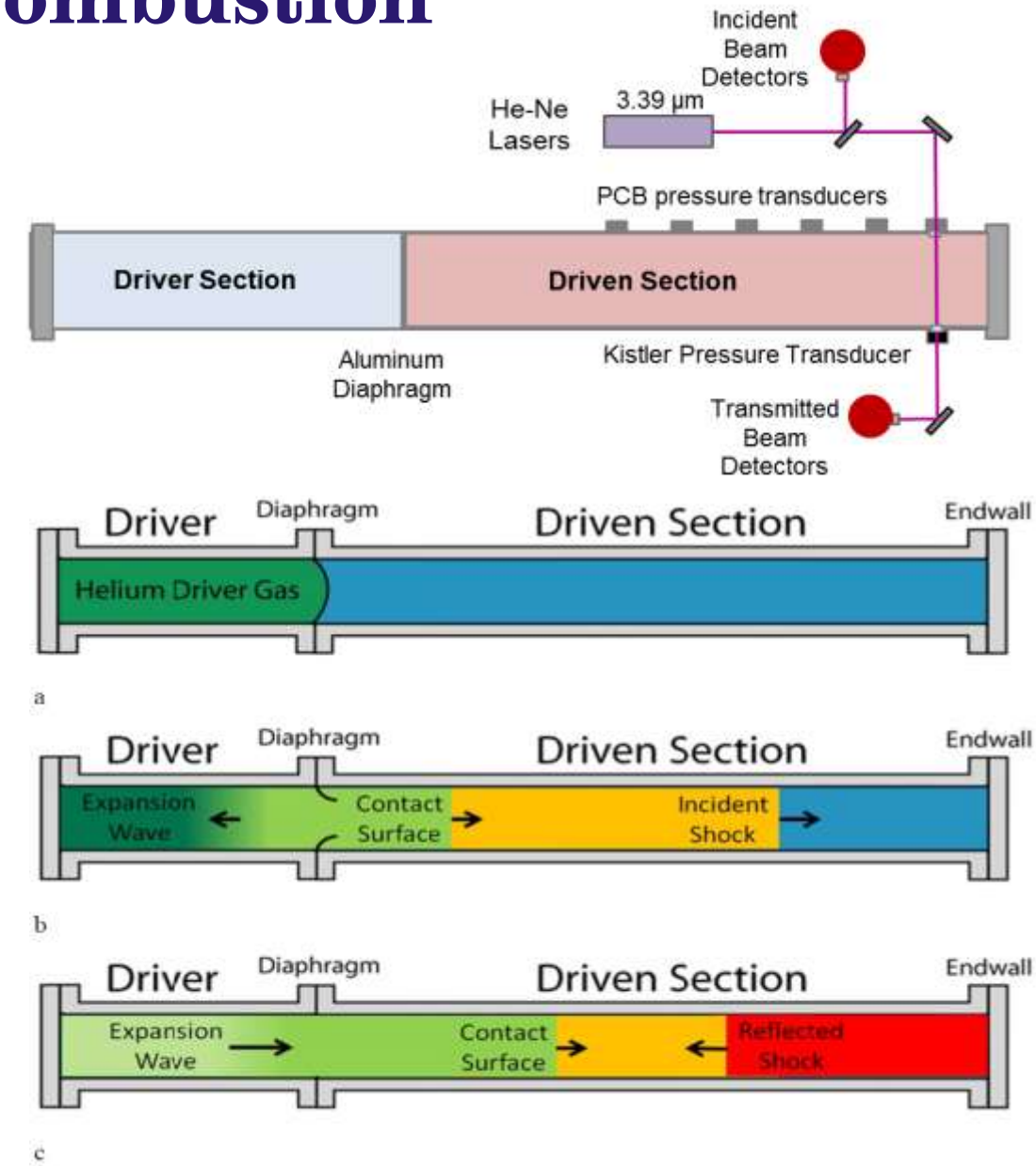
- Shock tube/laser absorption are well-suited kinetics studies and ignition delay process.
- Shock Tube measurements can be used to make new chemical kinetic models and evaluate the accuracy of existing chemical kinetic models





S-CO2 Combustion: Technology Challenges

- We are building a heated high-pressure shock tube capable of operating at pressures of up to 300 atm. to study:
  - Ignition behaviour of a large range of fuels at high pressure (fuel flexibility)
  - Chemical kinetics of various fuels under homogeneous conditions of temperature and pressure
  - Measurements of stable intermediates during fuel pyrolysis
  - Ignition delay times will be measured at high pressure in the gas-phase for several fuels in various oxidizers behind reflected shock waves
  - Available from 01/2021, 2 RAs + DTC PhD (James Harman) starting 09/2019 + 2 RAs
- **PACT Welcomes Contribution/collaboration/partnership on developing sCO2 Carbon Dioxide Power Cycle for Stationary Power Generation**

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