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Le Minh Dinh, Olivier Herbinet, Frederique Battin-Leclerc

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Experimental and Modeling Study of the Oxidation of Methane in a Jet-Stirred Reactor with CO₂ dilution: Comparison between Literature Models

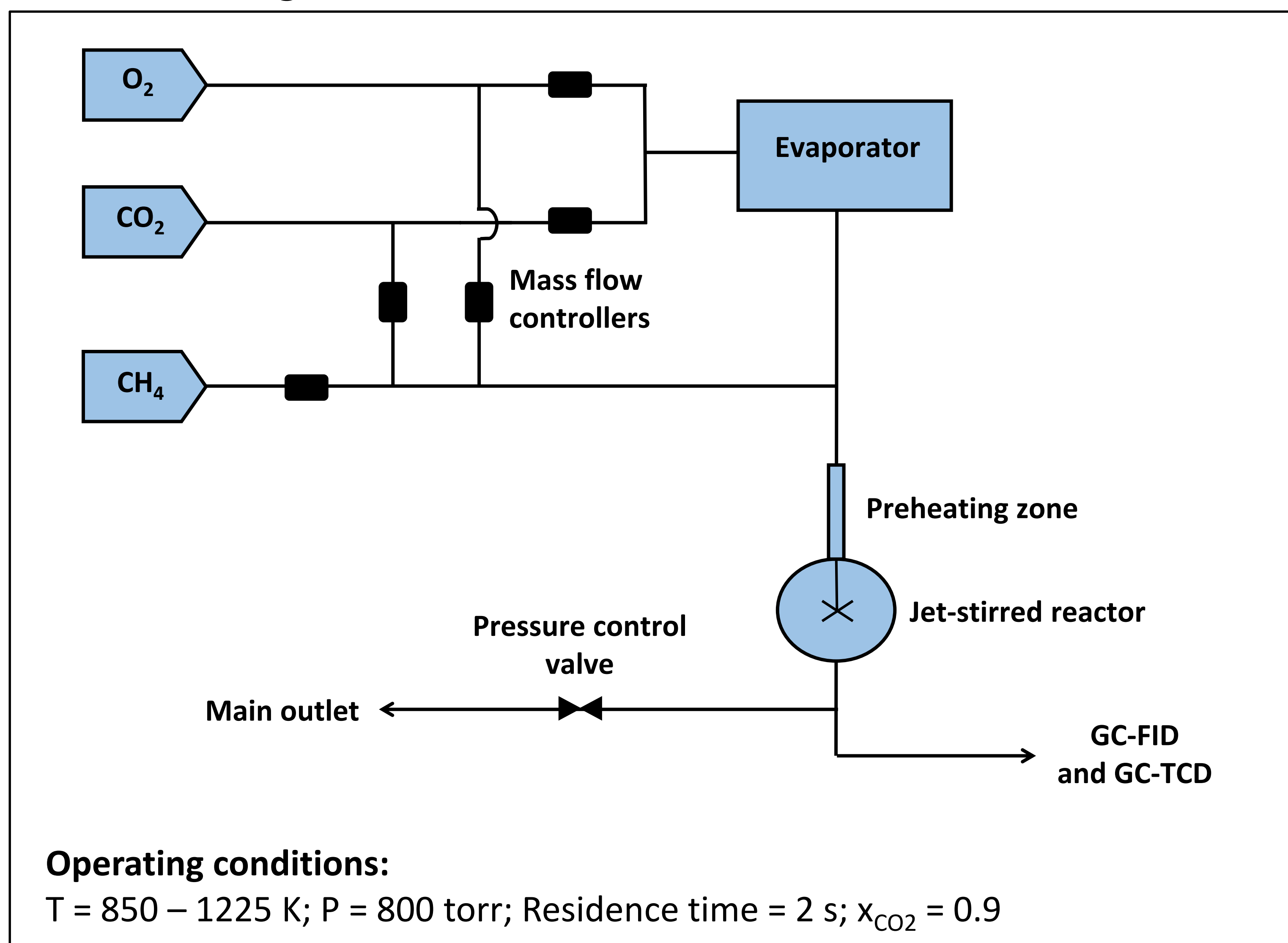
Le Minh Dinh, Olivier Herbinet, and Frédérique Battin-Leclerc

Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France

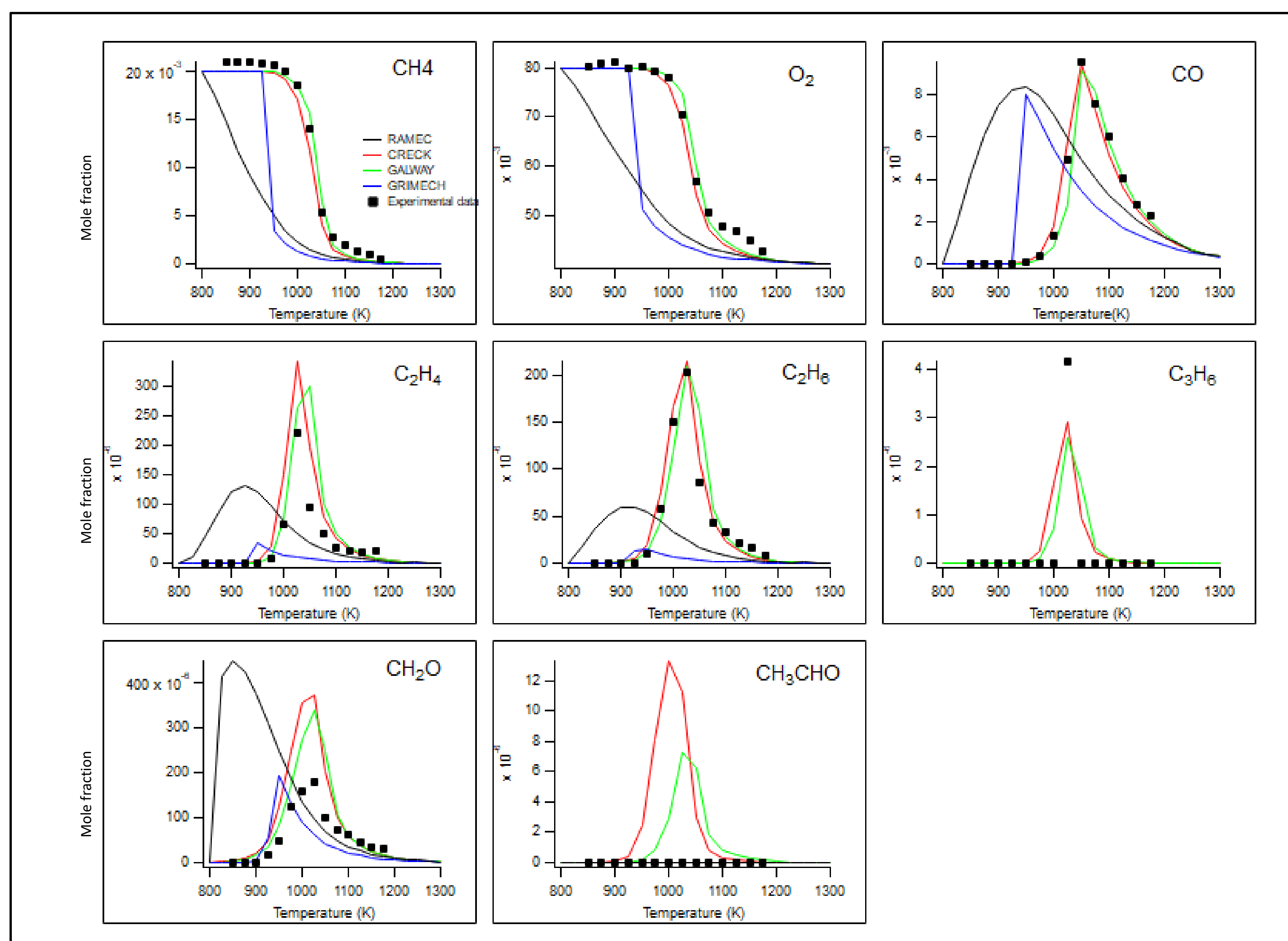
Context:

The combustion of methane (CH₄), which is a highly exothermic reaction, plays a fundamental role to many industrial applications. In this work, the experimental investigations of CH₄ oxidation were performed in a jet-stirred reactor, from fuel-lean to fuel-rich mixtures. The mole fraction profile of outlet products was acquired through gas chromatography quantification of the species in the gas phase¹. Four literature models were considered for the comparisons, with among them three detailed kinetic models built by research teams that are recognized for their contributions in kinetics (Politecnico di Milano – CRECK, University of Ireland in Galway – GALWAY, and Berkeley University – GRIMECH), and one reduced model (RAMEC). All of them were validated against a large number of experimental data with methane abundant environment, but rarely under the CO₂ dilution condition. Simulations based on detailed kinetic schemes were conducted to assess the performances of four models in oxyfuel combustion, with an emphasis on overall reactivity and also for some specific reaction products. Oscillating behavior of the CH₄ combustion can also be observed as the steady state of the combustion is hardly reached under some specific conditions^{1,2}.

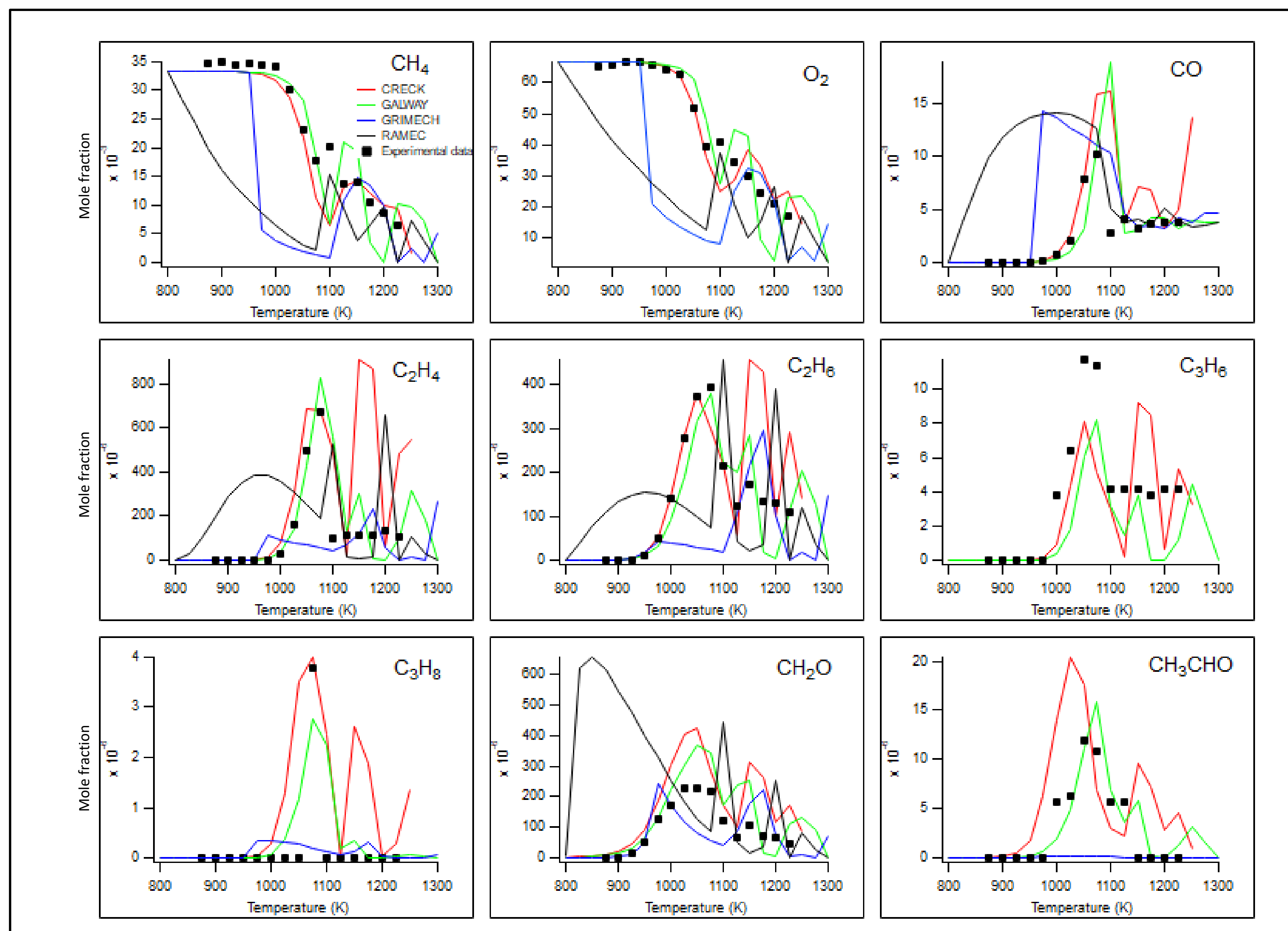
Schematic diagram of the instrument:



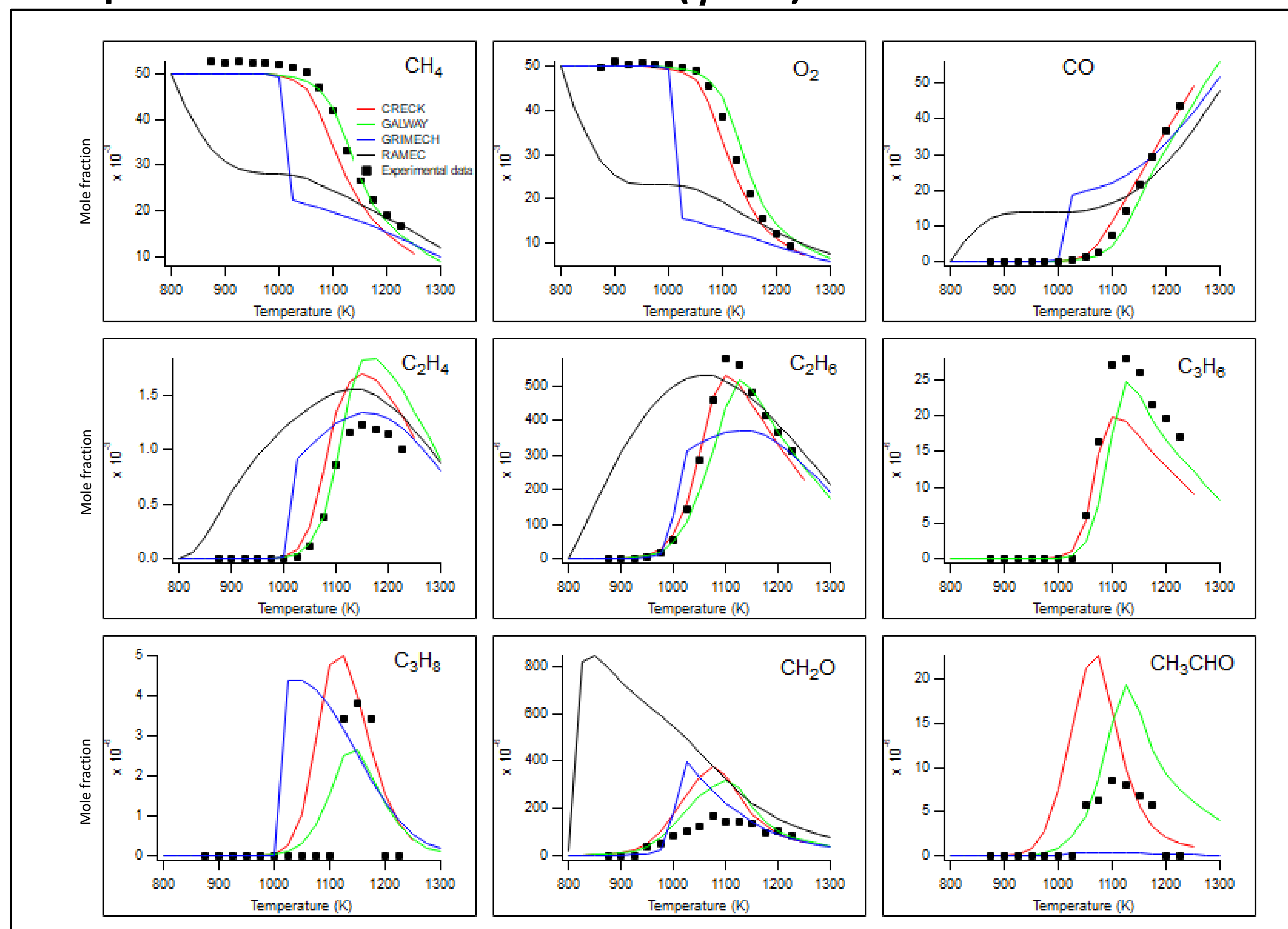
Comparisons for the lean condition ($\phi = 0.5$):



Comparisons for the stoichiometric condition ($\phi = 1$):



Comparisons for the rich condition ($\phi = 2$):



Conclusions:

- The CRECK and GALWAY models provide the best agreement under the CO₂ diluted conditions, and product mole fractions are overall well reproduced. The main difference between 2 models may come from the number of species and reactions which is larger in the GALWAY model compared to the CRECK one.
- Strong oscillating behavior is obtained for temperature above 1100 K, especially in the stoichiometric condition. No oscillations were detected in the rich condition.
- A further kinetic analysis can be conducted to better understand the prediction performances and to explain the model failure.

[1] M. Lubrano Lavadera et al. / Energy & Fuels **2018**, 32(10), 10088–10099

[2] A. Stagni et al. / Chemical Engineering Journal **2020**, 385, 123401