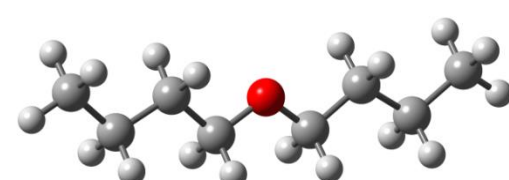


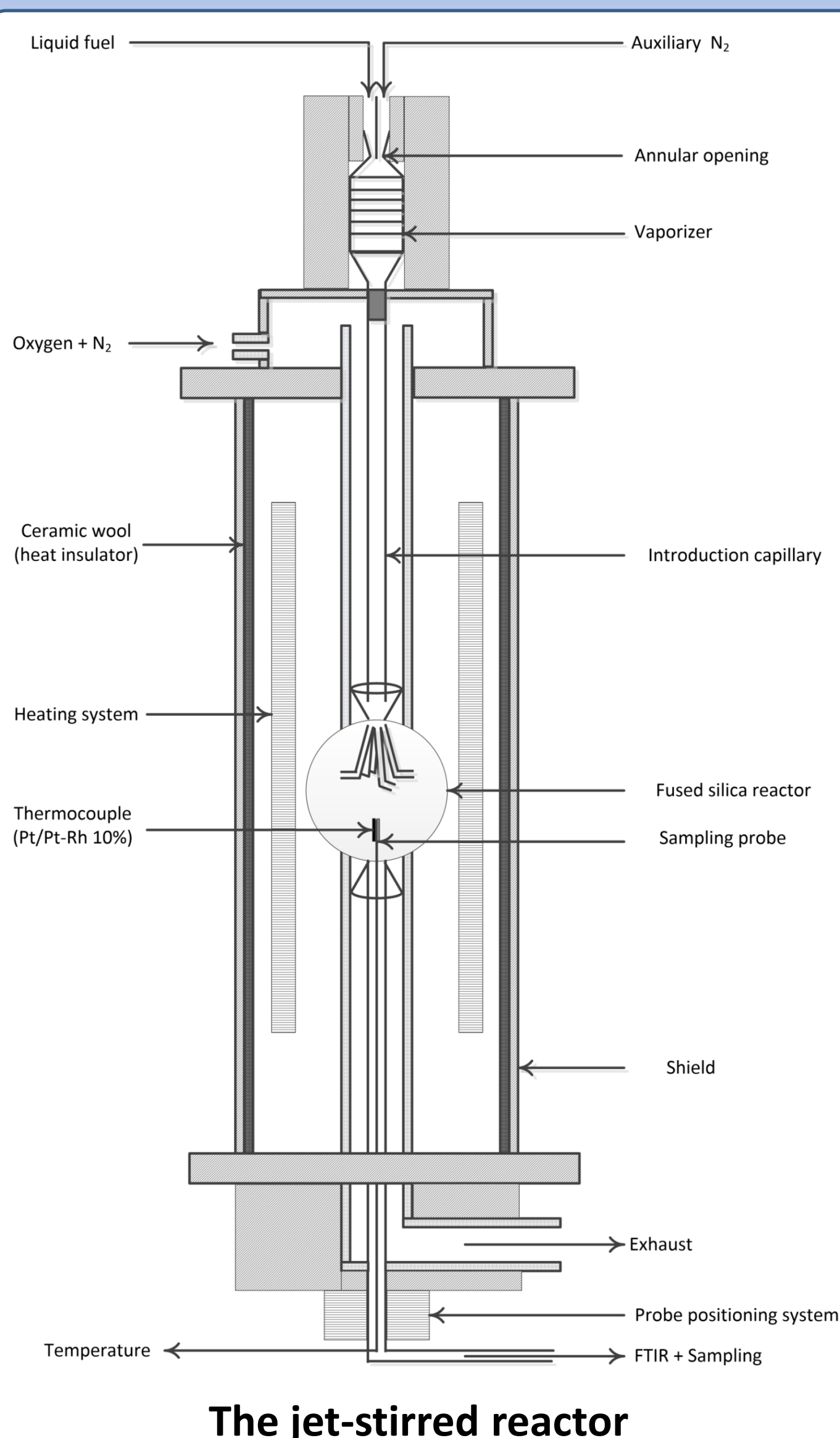
## 1. Introduction

- Dibutyl-ether (DBE) is an interesting alternative fuel: it has a high energy content, a high cetane number and it is also liquid in normal conditions.
- Few studies on this compound were carried out so far, and only one mechanism describing its oxidation is available[1]. This mechanism was validated for flame speed and ignition delay times but the authors underlined that more data are needed to verify it.

The aim of this study is to compare computations obtained from the model proposed by Cai et al.[1] and experimental data obtained in JSR. Modifications to improve the mechanism are also proposed.



## 2. Experimental



The jet-stirred reactor

### Conditions investigated

- Constant pressure and residence time (0,07s and 1atm).
- 1000 ppm of DBE diluted in N<sub>2</sub>.
- Equivalence ratios: 0.5, 1, 2.

### Analyses

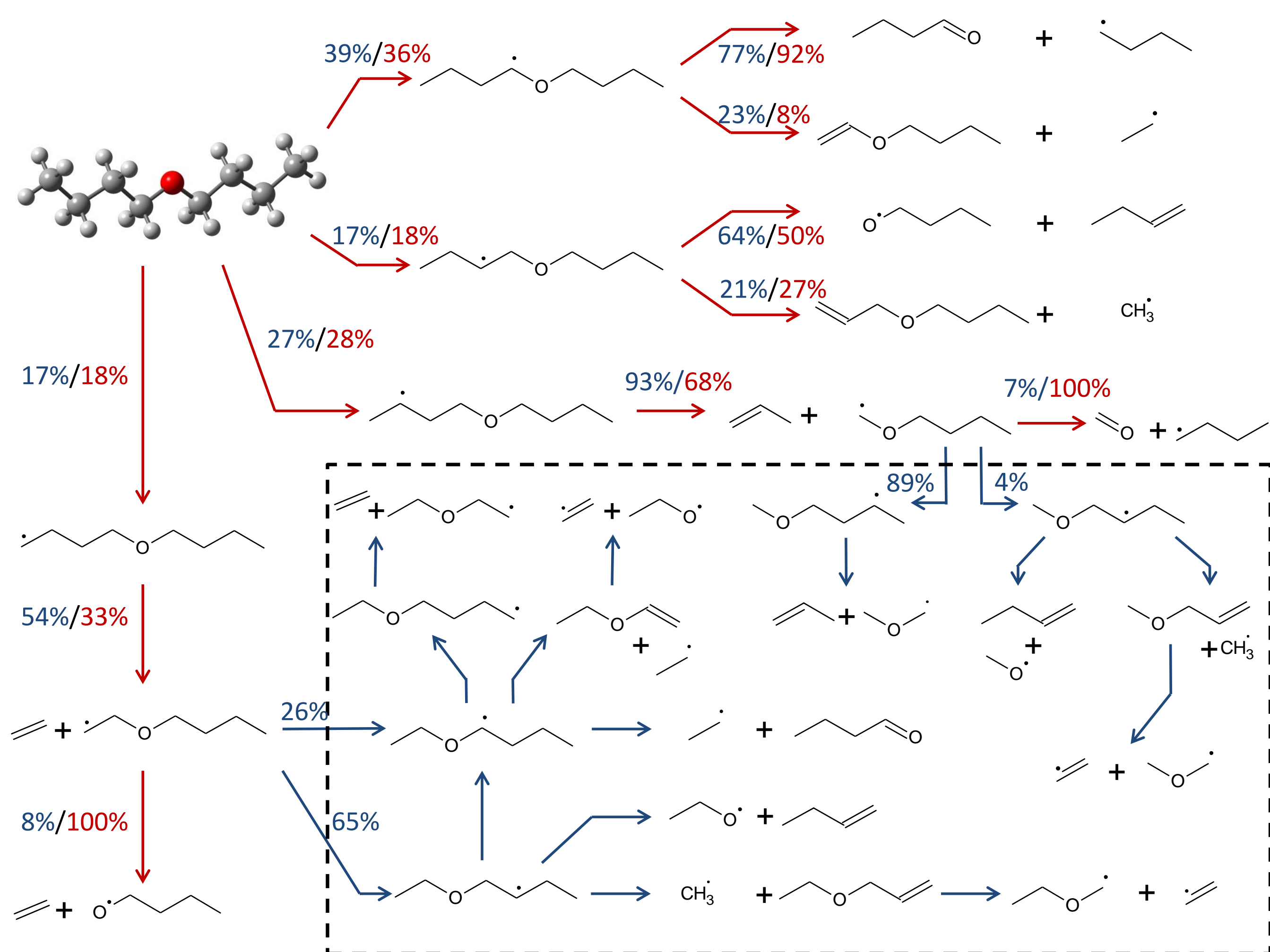
- Online FTIR for CO, CO<sub>2</sub>, CH<sub>2</sub>O, and H<sub>2</sub>O.
- Offline GC/FID, MS for other products.

### Numerical

- The PSR subroutine of Chemkin II[2] used to model the experimental data.
- Modeling focused on the high temperature region (no low temperature chemistry considered yet).
- Bond dissociation energies of DBE and butanol were calculated using the G3B3 compound method implemented in the Gaussian 09 software[3].

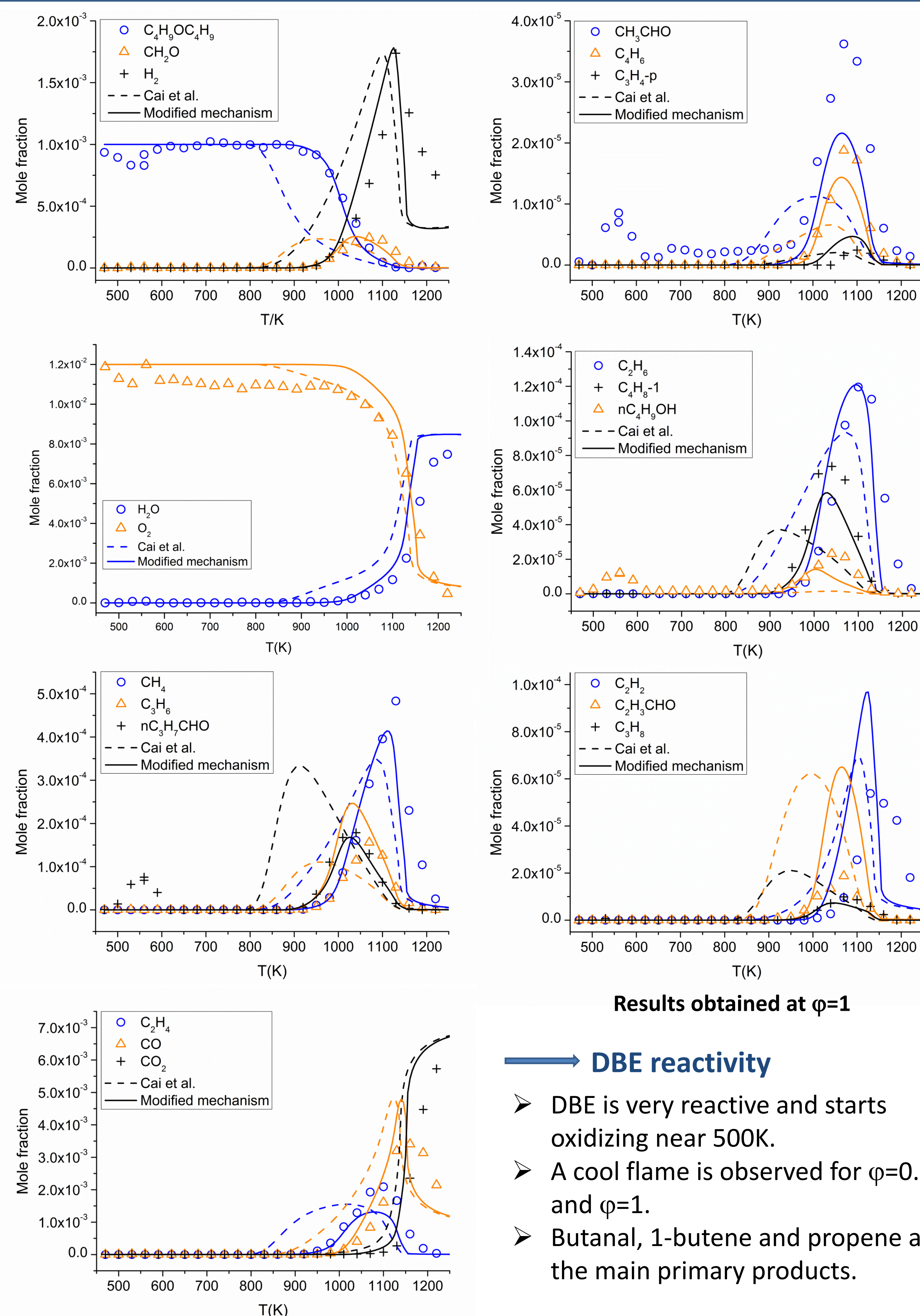
## 3. Mechanism modifications

- The isomerization of the radicals CH<sub>2</sub>OC<sub>4</sub>H<sub>9</sub> and C<sub>2</sub>H<sub>4</sub>OC<sub>4</sub>H<sub>9</sub> were added as well as the decomposition and isomerization of the subsequent products.
- These modifications changed the repartition of the different pathways.



Pathways considered by Cai et al[1] (red) and added pathways (blue). Flux are also presented at T=1070K and for φ=1.

## 4. Results and discussion



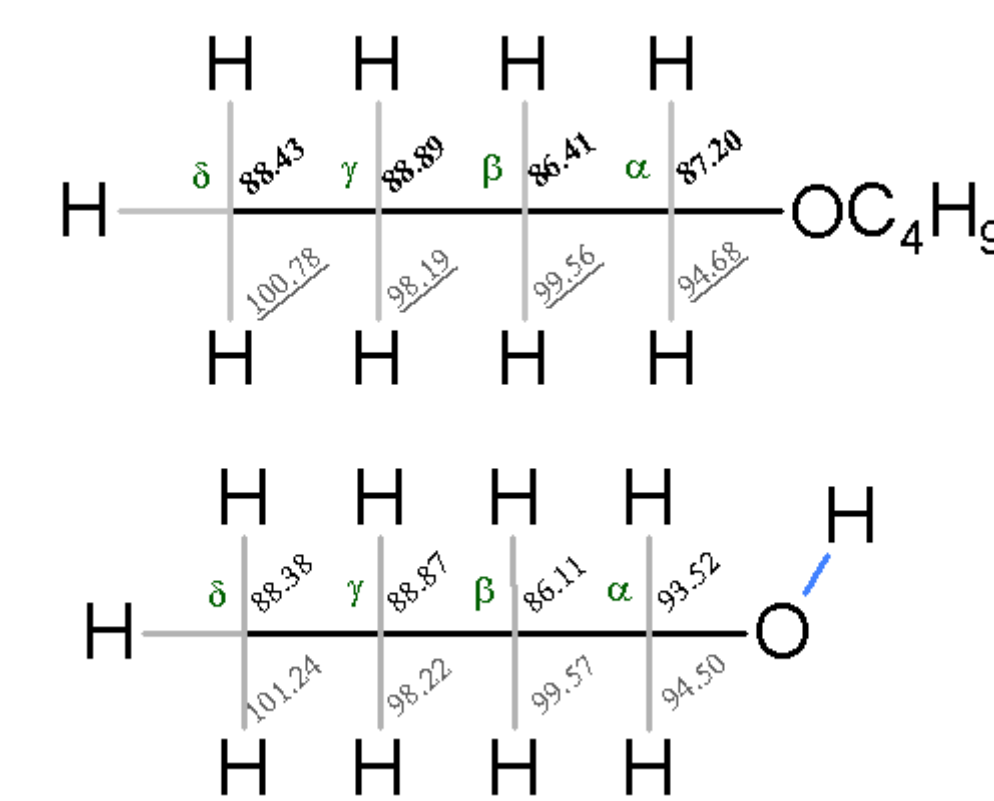
Results obtained at φ=1

### DBE reactivity

- DBE is very reactive and starts oxidizing near 500K.
- A cool flame is observed for φ=0.5 and φ=1.
- Butanal, 1-butene and propene are the main primary products.

### Bond dissociation energies

- Bond dissociation energies of DBE close to those of butanol.
- The CO bond as well as the C<sub>α</sub>-C<sub>β</sub> bond are the weakest and the C<sub>α</sub>-H bond is much weaker than the others
- β-scissions producing butanal, propene and 1-butene favored.



Bond dissociation energies of DBE and butanol (kcal/mol)

### Mechanisms vs experiments

- The mechanism proposed by Cai et al. is too reactive.
- It also failed in accurately predicting the species profiles obtained by experiments.
- The modified mechanism produces better predictions but some adjustments are still needed.

## 4. Conclusion and perspectives

- DBE is very reactive and the model proposed by Cai et al. was not able to accurately predict the results obtained by experiments. Modifications brought through this work improved a lot the predictions.
- Next step: experiments at 10 atm, modeling of the low temperature region and adjustments on the high temperature region.

## Acknowledgements

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- [3] Frisch, M.J. et al. Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, (2009)