

SHORT TERM SCIENTIFIC MISSION (STSM) SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: **CM1404-Chemistry Of Smart Energy Carriers And Technologies (SMARTCATS)**

STSM title: Computational Singular Perturbation (CSP) analysis on the LES of non-conventional combustion regime

STSM start and end date: 03/11/2018 to 17/11/2018

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PURPOSE OF THE STSM:

Because of the strong interactions between the chemistry and turbulence in MILD [1, 2] combustion, combustion models that consider finite rate chemistry is supposed to be included in the model. The model we chose for MILD combustion is Partially Stirred Reactor (PaSR) [3] model with Large Eddy Simulation (LES). In PaSR model, the proper choice of chemical time scale and mixing time scale is involved and the definition of chemical time scale need to be carefully defined. At the same time, there are also some research work on the use of Implicit LES (ILES) [4, 5] combustion model on this kind of flame, indicating that the use of combustion model is not necessary because the distributed flame structure can be resolved using the fine LES grid. In the present research, the Tangential Stretch Rate (TSR) [6, 7] of the ILES combustion model simulation results is obtained with the Computational Singular Perturbation (CSP) analysis tool. Furthermore, the participation indexes of different processes are discussed and the fast and slow modes of the system based on each species are presented, in order to understand the interactions between chemical reaction and turbulence in MILD combustion.

(max.200 words)

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

The ILES combustion model simulation results of a simplified burner (axis-symmetric free round jet burner) with hot co-flow of low oxygen contents (3%, 6% and 9% by mass) are available before the short scientific mission and from the work of last year. The grantee has already learned about how to use the code of CSPTk, which is an in-house code from the host institution. Therefore, the focus of the current work is to discuss the results already obtained from the CSP analysis and explore the differences between the three cases with different co-flow oxygen contents: because the case with 3% oxygen by mass in the co-flow is a fully MILD condition, the 9% is close to conventional combustion condition and the 6% is the transitional condition.

After having the output from the CSP solver, post-processing is necessary for checking the results. The CSP analysis is done on the 2D axis-symmetric plane of the cylinder CFD mesh. The CFD post-processing tool tecplot is used here. The 2D TSR results from the three cases are first compared with the extended TSR results, to show the influence from the fluid dynamics process, like diffusion and convection. The locations of interest are then identified from the TSR and extended TSR profiles. In order to check theses locations in detail, the slices across the radial direction on different axial locations are analyzed separately. The participation indexes for difference forward and backward reactions as well as convection and diffusion terms are plotted with 1D line. Only participation indexes which are more than 0.05 is plotted, showing the most important processes. Finally, the fast-slow modes of the system on 2D plane are presented after modifying the CSPTk code slightly, showing the leading scales for chemical reaction.

(max.500 words)

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The TSR analysis on the 3% case is first presented in Figure 1:

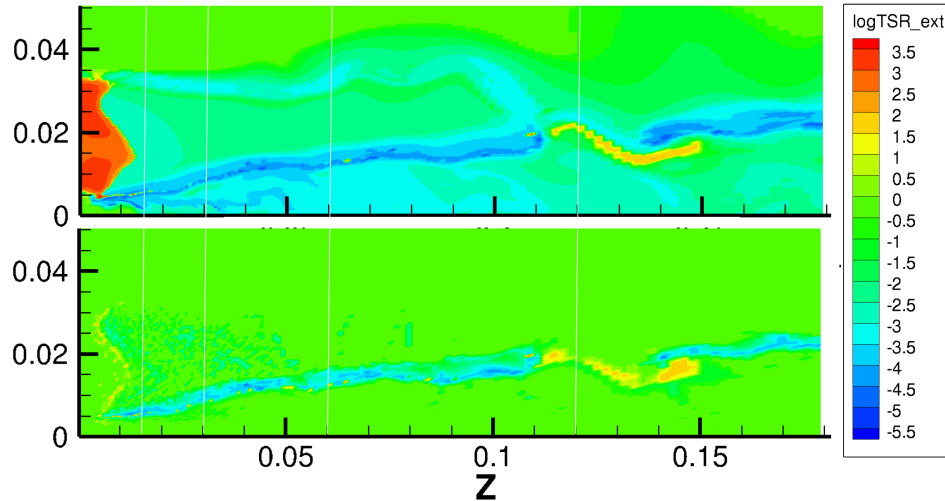
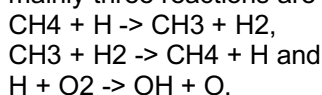


Figure 1: logTSR and extended logTSR from the 3% co-flow oxygen level case (the legend on the right hand side show both the logTSR and extended logTSR).

Both logTSR and extended logTSR (TSR with diffusive and convective terms) show that the flame is slightly explosive close to the jet exit location and mainly contractive further downstream. The location of the upstream hot co-flow (location from around $Z = 0$ to $Z = 10$ mm) area is strongly explosive in the chemical TSR profile. This is because that the co-flow condition provided from the Boundary Condition (BC) is not at equilibrium state, therefore the species in the hot co-flow react for a short distance and reach equilibrium condition further downstream. Obvious difference on the values of logTSR and logTSR_ext can be captured across the 2D domain, indicating the influences from the diffusion and convection in the current flame. In order to discuss the contribution of each process in detail, the axial locations of $Z = 15/30/60/120$ mm are chosen and plot with lines, as indicated in Figure 2.

The participation indexes of chemical reactions for the 3% and 9% cases are compared. After comparing the chemical reactions on all the interested locations from the 3% and 9% cases, one can find out that mainly three reactions are important for all the locations and cases:



For the first two reactions, they are chain propagation reactions and the last one is chain branching, which is important to activate the reactions of the whole system. If we compare the participation indexes of the reactions on $Z = 15$ mm of the 3% and 9% case, the backward reaction of 36 becomes more important for the 9% case: $\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$. The location such reaction is becoming important is at $R < 10$ mm, which is the interactive location between the fuel stream and the co-flow stream. But the index for such reaction is still very small, therefore it is not the main focus of the current discussion. What's more obvious is that the forward reaction of 43: $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$ becomes much more important for the location close to the centerline when the co-flow oxygen level is increased to 9%. Because the 9% case has more oxygen in the co-flow, higher O_2 concentration in the co-flow promotes the reaction from left hand side to right hand side.

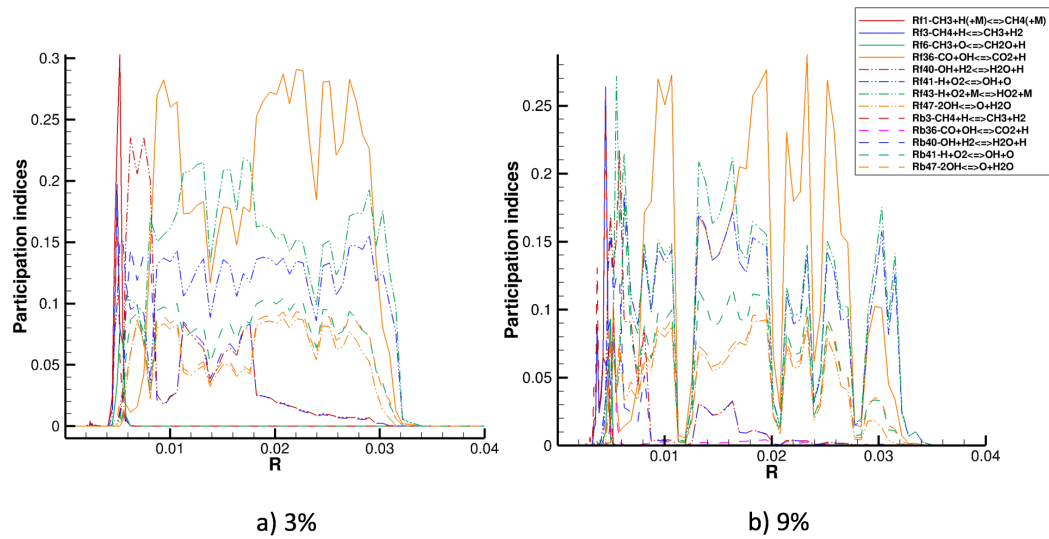


Figure 2: Participation indexes of the reactions on $Z = 15$ mm of the 3% and 9% cases.

In a system of chemical reaction, there are slow modes which control the direction of reaction for the whole system, and there are also fast modes which follow the slow modes. Identifying the slow and fast modes and how many slow modes in the combustion system is able to help us understand the flame in a chemical reaction point of view. For example, in Figure 3, the number of slow modes plus 1 is presented in the 2D plane. One should know that the location with temperature less than 300 K is blanked out. The red color represents higher number of slow modes and blue indicates lower number. In this specific case, if $M+1 = 14$, it means that the location is dormant. For other number of $M+1$, like in the co-flow area, the orange color which indicates $M+1 = 12$ is shown. This might implies an equilibrium state. As discussed above, the co-flow provided by the BC reacts for a short distance and reaches equilibrium at around $Z = 15$ mm. After $Z = 100$ mm, the orange color disappears, that's because that the air stream starts to entrench and reacts with the fuel stream. With the blue color, which means there are more fast modes than the slow ones, in the 2D contour plot, we are also able to identify the area with high heat release.

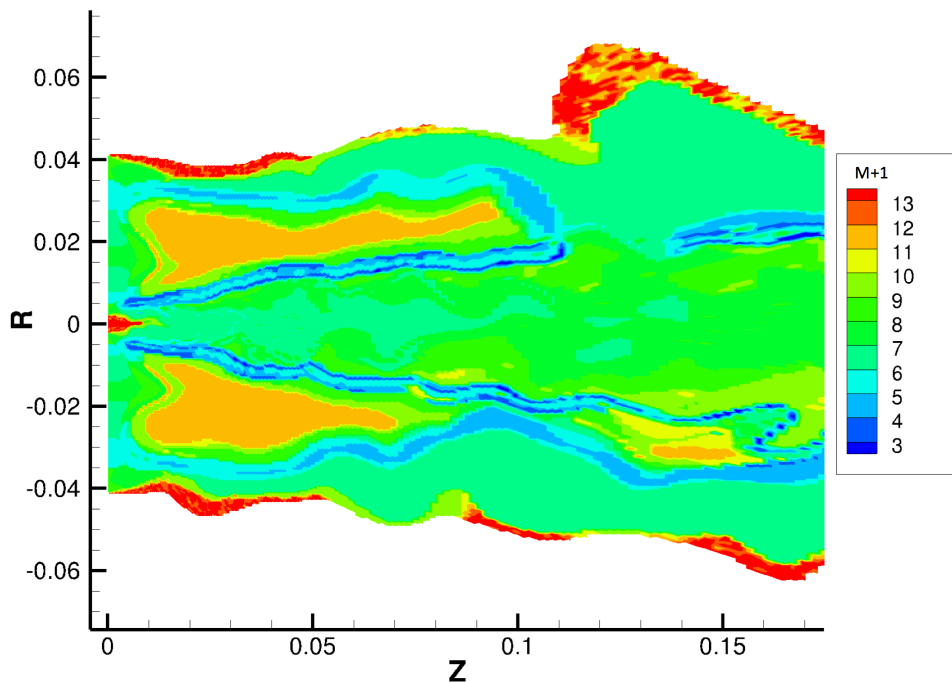


Figure 3: Number of slow modes from the 3% case.

Finally, in Figure 4, the location with HCO as fast mode is colored with the total number of slow modes. The location with temperature more than 350 K is blanked out. Compared to species like H_2 , CH_4 , O_2 as well as CO_2 , H_2O and CO , the species of HCO, H_2O_2 , H and O are most time the fast modes which follows the major species. The location with HCO as slow mode is not inside the reaction region with most

of the heat release, but in the co-flow area. However, for H₂O₂ (not shown here), it is mainly inside the fuel stream and the reactive location with more heat release. H₂O₂ is fast almost inside the whole domain of the co-flow stream. For H₂, as expected, most area is marked with slow, except the equilibrium region inside the co-flow stream.

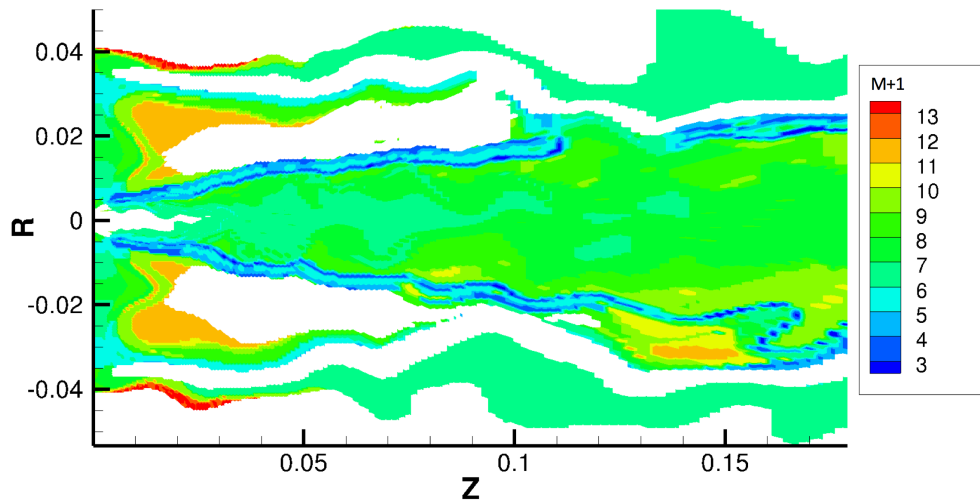


Figure 4: Number of slow modes from the 3% case with HCO slow mode location blanking out.

In summary, by doing analysis on the LES data of the MILD combustion with different co-flow oxygen levels using the CSPTk tool, we are able to see the importance of each processes which feature the source from chemical reaction or fluid dynamics process. The differences between the MILD condition and conventional condition can also be captured, though not obvious. This helps us to understand the interactions between turbulence and chemistry better. The next step is to run LES on a case with 21% of oxygen in the co-flow, which is a fully conventional flame. The TSR of this case will be compared to that of the 3% case. More obvious differences regarding the TSR value, participation indexes and the slow-fast modes are expected to be observed.

FUTURE COLLABORATIONS (if applicable)

Further collaboration will be mainly focused on two aspects:

Firstly, the research of the current scientific mission is aiming at scientific publication, further collaboration on the paper writing will definitely be important.

Secondly, during the process of analyzing the LES results of MILD combustion, the proper definition of chemical time scale and Damköhler number drew attention from both sides of the collaborator. Therefore, further work on finding out or defining a chemical time scale which is representative for a wide range of combustion conditions, or at least, suitable for MILD condition will be discussed.

- [1] J. A. Wüning, J. G. Wüning, Flameless oxidation to reduce thermal NO-formation, Progress in Energy and Combustion Science 23 (1997) 81-94.
- [2] A. Cavaliere, M. de Joannon, MILD combustion, Progress in Energy and Combustion Science 30 (2004) 329-366.
- [3] V. I. Golovitchev, J. Chomiak, Numerical modelling of high temperature air "flameless" combustion, Chalmers University of Technology, Göteborg, 41296 Sweden.
- [4] A. Wawrzak, A. Tyliczszak, Implicit LES study of hydrogen forced ignition in a temporally evolving mixing layer, 10th Mediterranean Combustion Symposium, Naples, Italy, 2017.
- [5] Zhiyi Li, Alberto Cuoci, Alessandro Parente, Large Eddy Simulation of MILD combustion using finite rate chemistry: Effect of combustion sub-grid closure, Proceedings of the Combustion Institute 000 (2018) 1-11.
- [6] Valorani, M., Paolucci, S., Martelli, E., Grenga, T., & Ciottoli, P. P. (2015). Dynamical system analysis of ignition phenomena using the Tangential Stretching Rate concept. Combustion and Flame, 162(8), 2963–2990.
- [7] Valorani, M., Ciottoli, P. P., & Galassi, R. M. (2017). Tangential stretching rate (TSR) analysis of non-premixed reactive flows. Proceedings of the Combustion Institute, 36(1), 1357–1367.