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:development of a novel chemical time scale estination tool for non-conventional combustion
STSM start and end date: 08/10/2017 to 20/10/2017
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PURPOSE OF THE STSM:

Because of the strong interaction between the chemistry and turbulence in MILD[1, 2] combustion, using combustion model based on the mixing is not valid anymore. Detailed chemistry is supposed to be included in the model. The model we chose for MILD combustion is Partially Stirred Reactor (PaSR)[3] combustion model with Large Eddy Simulation (LES). On one hand, in PaSR model, the chemical time scale in involved, making it possible to consider the importance of chemistry in the combustion model. However, the definition of chemical time scale need to be carefully defined. On the other hand, there are also some research work on the use of Implicit LES (ILES)[4] on this kind of flame, proving that the use of combustion model is not necessary.
Therefore, the purpose of the current work is to first, analyze the Tangential Stretch Rate (TSR)[5, 6] of the ILES simulation results with the Computational Singular Perturbation (CSP) tool from the Department of Mechanical and Aerospace Engineering in Sapienza University of Rome and try to understand the interaction between chemical reaction and turbulence in MILD combustion. Second, the definition chemical time scale in PaSR model need to be discussed and implemented.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

The work carried our during the STSM can be mainly separated into two parts.

1. TSR analysis on the ILES data

The ILES simulation results are already valid before the arrival of the grantee, but the TSR analysis tool called CSPtk is an in-house confidential code from the host institute. Therefore, the first step is to install this Fortran based code on the grantee's computer. The next step is to learn how to use the CSP tool (data arrangement, running the solver and code update) and to understand the theory behind it from some publications available regarding the TSR analysis from the host institute. After having the output from the CSP solver, post-processing is necessary for checking the results. A CFD post-processing tool called tecplot is used here. The grantee also acquired the skills of using tecplot visualization function.
One difficulty the grantee has met is the data required for the extended TSR analysis. They are the diffusive term and connvective term in the CFD simulation, especially for the temperature field. The energy equation of enthalpy is used in the CFD simulation, while the convective and diffusive term of temperature is needed. Therefore, extra time was spent on the study of the different froms of energy equations and trying to find out the connections between them.
The TSR analysis is first conducted on the interpolated data written out from the sample function in OpenFOAM. Data interpolation gives smooth profiles, whereas losing some details of the flame. As a result, the non-interpolated data is written out for the later analysis. The TSR result compared with the extended TSR results are available with non-interpolated data. The sampling surface are along the centerline and on three different radial locations close to

the chemical TSR explosive region. For the extended TSR, currently only the diffusive term is included in the analysis. Because the convective term is giving some fluctuative results, which is not meaningful. The reason for the fluctuative results is that, there is pressure wave in the simulation domain. Right now the pressure wave problem has been solved by adjusting the pressure boundary condition.

2. Finding a proper definition for the chemical time scale in PaSR model

The current definition of chemical time scale in PaSR model is based on the species and only one controlling scale is chosed as the chemical time scale in a specific cell. In order to consider the differences of chemical time in some slow processes, for example, soot formation and NOx production, the chemical time scale for every species is proposed. But this will result in im-balance for the over-all reaction rate and species mass fraction. A new definition of chemical time scale for every reaction is further presented. But the definition of "chemical time scale for every reaction" is still controversial. The original definition of the chemical time scale for every reactions is based on some simplification assumptions by Lam [7], whereas might not apply in MILD combustion.

In summary, the first part of the work has been successfully conducted, leaving some issues which are relatively easy to solve. The results are also expected to be included in the recent publication. The second part of the work still need more discussion and it will be included in the future collaborations.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The results obtained will be mainly presented with figures.

The CSP analysis on the chemical TSR will be first presented in Figure 1:

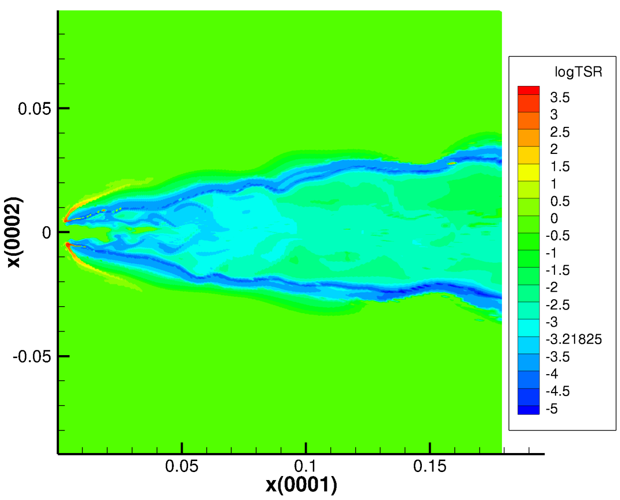

Figure 1 Logrithmic expression of the chemical TSR

We can see from Figure 1 that, there are explosive chearacteristic (positive value of the logTSR) of the flame in the area close to the jet exit. This indicates the trend of the chemical composition to ignite and react. For the further downstream, the logTSR value are mostly smaller than 0, this represents the contractive, dissipative process of the flame. According to the profile in Figure 1, the regions with higher temperature are mostly contractive.

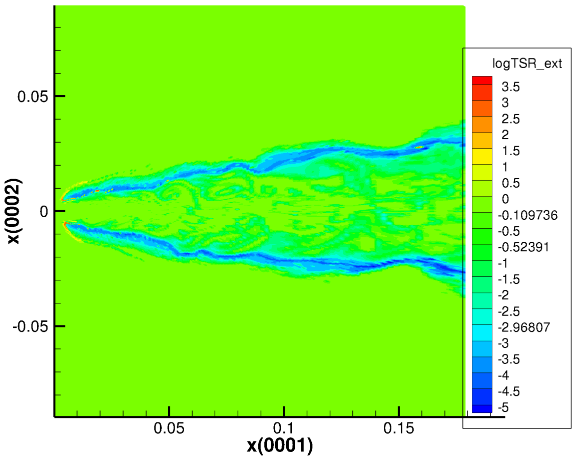

Figure 2 Logrithmic expression of the extended TSR (chemical + diffusive term)

The extended TSR shows the effect of both chemistry and fluid dynamics. Currently we are having some problems with the convective term of the energy equation and scalar transport equation, which will be addressed in the later part of the report. Therefore, only the diffusive term is considered here in the extended TSR profile. With the inclusion of fluid dynamic effect, we can see that the explosive nature of the flame near the jet outlet is suppressed by the diffusion and the contractive area is also reduced further downstream.
Regarding the problem of the convective term term, similar pattern of fluctuation was found for the velocity and vorticity profiles. There is also a pressure fluctuation inside the whole domain, this can be seen in the left figure of Figure 3:

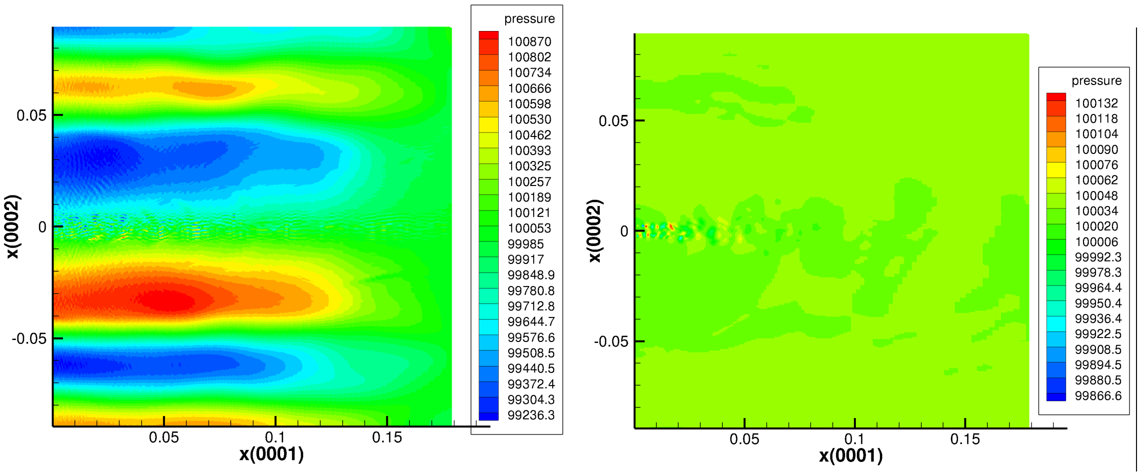

Figure 3 Pressure variation in the field with small lInf factor (left) and large lInf factor (right)

The problem of this pressure variantion comes from the boundary condition parameter used. Theoretically, the outlet condition should not have any influence on the fluid in the domain, whereas in numerical simulations, it cab be the case that the outlet boundary condition reflects the wave. Using wavetransimissive boundary condition helps to avoid the reflection of the wave. In the former simulations, the lInf which measures how far away the far-field condition should be is 0.5. This value is not enough to alleviate the waves. As a result, in the later simulation, the lInf = 4 is used. This helps to decrease the pressure variations. As one can see in the right side of Figure 3. Right now the case with the adjusted lInf value is running and the convective term is expected to be added in to the extended TSR analysis.
The radial profiles on 10mm, 20mm and 30mm locations are also shown here to examine the explosive region close to the jet outlet further:

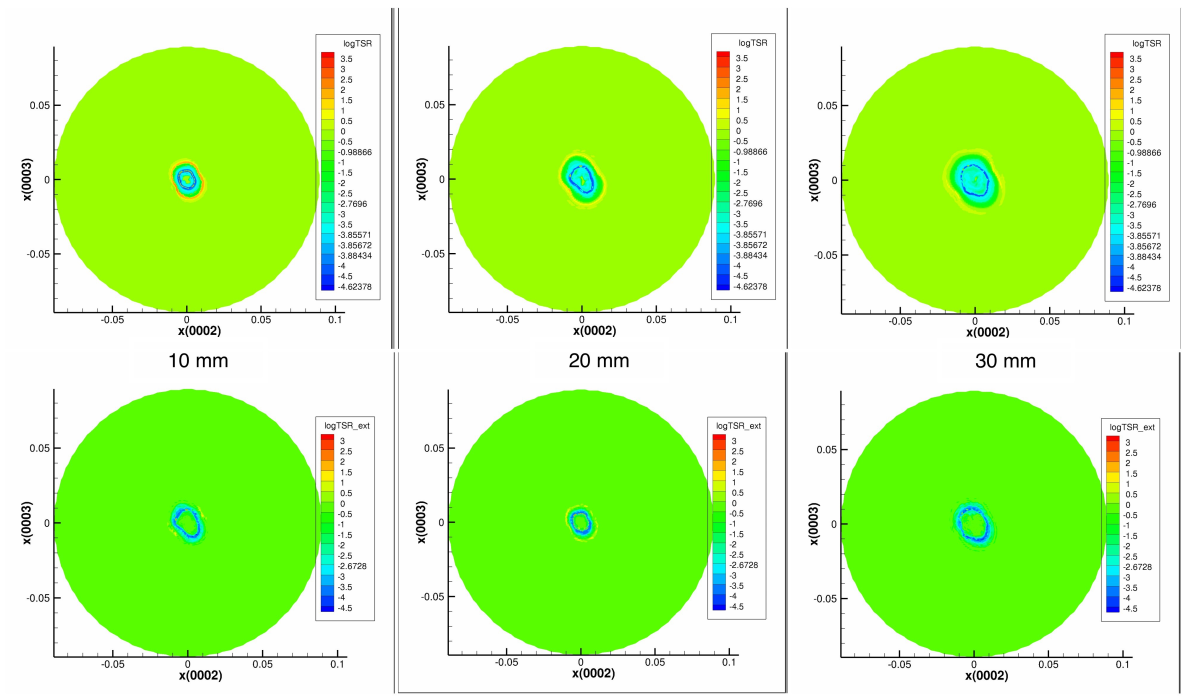

Figure 4 Radial locations of logTSR and logTSR_extended value

Several plots across the radial direction are presented in Figure 5:

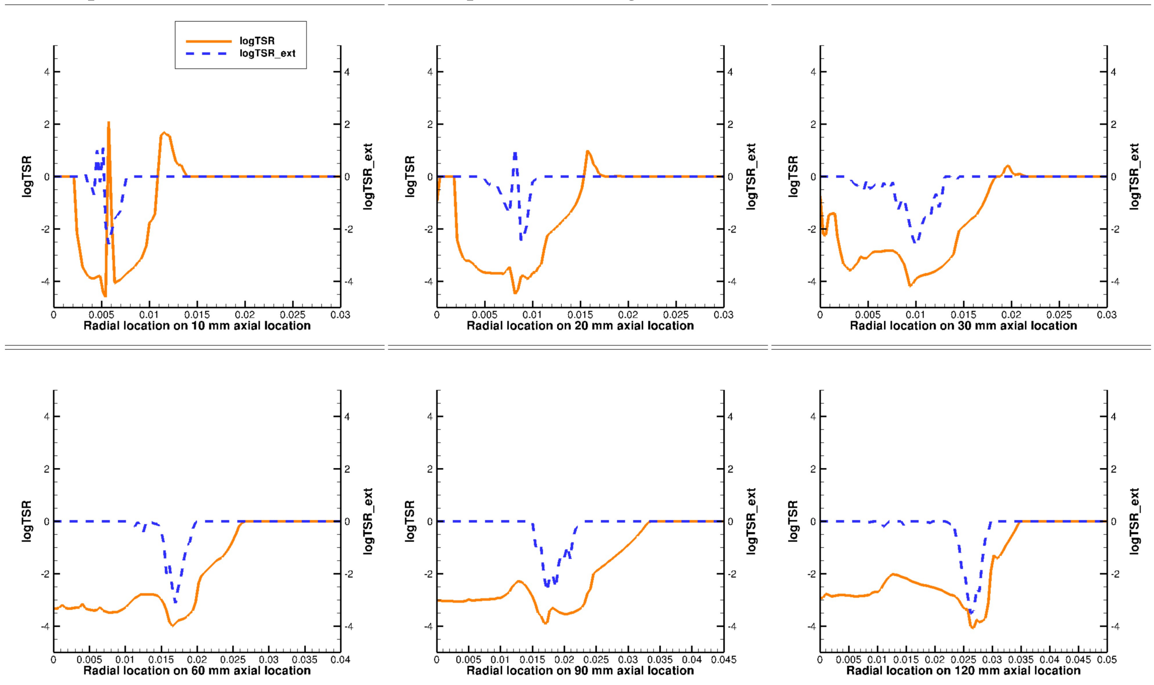

Figure 5 Radial locations of logTSR and logTSR_extended value – line plot

From Figure 4 and Figure 5, it is not hard to find out that the absoluted logarithmic value of extended TSR is lower than that with TSR, especially after 10 mm axial location. The diffisuion part in fluid dynamics effect is trying to “suppress” the explosive or contractive nature of the flame. On the 10 mm axial location, more complicated interaction between the chemistry and fluid dynamics can be captured. The addition of diffusive term has changed the flame from contractive to explosive before 5 mm radial position and it does the opposite after 5 mm. Therefore, the turbulence is playing more important role upstream of the flame, especially on the locations where the chemical logTSR is positive.

In TSR analysis, the participation of every reactions is also available, helping us to see the importance of one single reaction in a certain region:

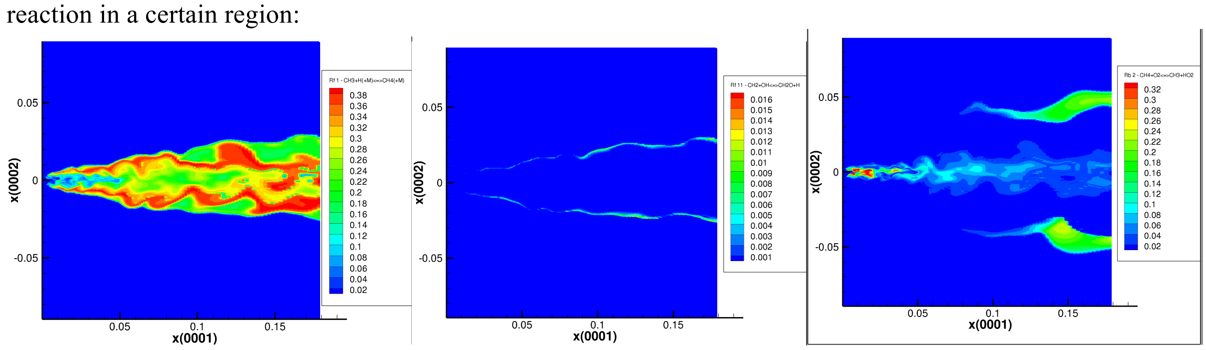

Figure 6 Participations of different reactions in chemical TSR

For example, in Figure 6, the first forward reaction is dominant in the whole flame domain, whereas the eleventh forward reaction only plays a role in the region with higher temperature. The second backward reaction is more important in the jet core region.

In summary, the TSR results help us to understand the explosive and contractive nature of the flame. The interaction between chemical reaction and turbulence is captured. Further more, the participation of every reaction can be clearly identified, providing the possibility to analyse flame phenomenon in combustion process, especially non-conventional flame that are not yet fully studied.

FUTURE COLLABORATIONS (if applicable)

Currently, the grantee has learned how to conduct TSR and extended TSR analysis with the CSP tool from the host institute. Further analysis with the convection term need to be carried out. The pressure wave problem in the field that

leads to the fluctuations of the convection term is expected to be solved. Moreover, the discussion on whether chemical time scale can be applied on every reaction is still going on.
Skype meetings will be arranged for the results discussion from TSR analysis and solution for the chemical time scale in PaSR model.

References:

[1] J. A. Wünning, J. G. Wünning, Flameless oxidation to reduce thermal NO-formation, Progress in Energy and Combustion Science 23 (1997) 81-94.
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[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. Tyliszczak, Implicit LES study of hydrogen forced ignition in a temporally evolving mixing layer, 10th Mediterreanian Combustion Symposium, Naples, Italy, 2017.
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[6] 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.
[7] S. H. Lam, Model reductions with special CSP data, Combustion and Flame 160 (2013) 2707-2711.