SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

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

Action number: CM1404-43837
STSM title: Reduction of chemical kinetics mechanisms suitable for solid fuel combustion simulations
STSM start and end date: 10/03/2019 to 31/03/2019
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PURPOSE OF THE STSM:

The purpose of the STSM was to build a workflow aimed at reducing reaction mechanisms suitable for improved combustion description of a renewable solid fuel, more precisely sewage sludge. The need for such mechanisms arose from the use of detailed reaction mechanisms in sludge combustion simulations, where combustion in our laboratory furnace was considered. These simulations show that application of detailed mechanisms significantly increases accuracy of gas phase combustion modeling. In regards with this it was also found that the ability of simulations to provide a valid combustion description in cases of small to medium scale furnaces is especially dependent on chemical kinetics due to there present dimensional constraints and to them connected importance of valid combustion description from fuel bed onwards. However, as the use of detailed reaction mechanisms also drastically increases computational demands, it becomes apparent that reduced mechanisms, derived from suitable detailed reaction mechanisms, are required in order to arrive at computationally less demanding simulations with desired level of accuracy. In order to build a workflow for construction of such mechanisms, CKL ELTE mechanism reduction tools were used in connection with available validated 3D CFD results from our laboratory.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSM

The work during the STSM was performed with SEM (simulation error minimization) package, which enables one, for certain considered conditions, to identify and eliminate redundant species in a detailed reaction mechanism. Additionally, this can be then complemented by identification and elimination of reactions which have a low impact in the observed conditions. The work done with this package during the STSM can be described with the following steps:

1.) Introduction to the use of SEM package for reduction of reaction mechanisms
The workflow in which SEM package proceeds was explained together with the role of available specific settings, which allow the user to build reduced mechanisms according to the main characteristics and conditions of an observed combustion case.

2.) Performing initial reduction attempts to define best possible approaches for our needs
First reduction attempts were focused on trying various settings with the aim of finding those allowing for creation of much reduced mechanisms, where the accuracy is not the top priority. In the next step, settings which lead to improved overall accuracy were determined. The reason for such an approach is the tool's workflow, which is built on gradual addition of species to the initially proposed group of most important ones in order to arrive at a reduced mechanism with desired accuracy.

3.) Preparation and conduction of reduction runs in order to obtain suitable reduced mechanisms
Conclusions from previous step were combined in order to perform reduction attempts with the goal of obtaining reduced mechanism candidates, exhibiting desired accuracy across variety of conditions.
4.) Preparation of tools for initial assessment of reduced mechanisms' suitability
Conducting reduction attempts where a larger group of combustion conditions is considered was found to heavily increase computational times. Instead, it was decided that reduction should be done considering a small group of conditions. In order to quickly confirm if so obtained reduced mechanism is accurate across a larger group of combustion conditions, a Matlab code for its application in these was developed. This tool allows one to compare reduced mechanism with the reference one and identify its accuracy as well as potentially troublesome areas. In such manner, it can be quickly confirmed if a certain reduced mechanism, based on a smaller group of observed conditions, already meets the overall demands without computationally expensive reduction attempts combining various conditions at once.
5.) Additional elimination of low impact reactions in the reduced mechanisms
Elimination of low impact reactions was done only after a certain reduced mechanism was found to meet all requirements in the previous step.
6.) Application of reduced mechanisms to 3D CFD simulations
The final step was application of reduced mechanisms to combustion simulations, which were already conducted before with the reference mechanism. Final and thorough validation of a certain reduced mechanism was thus performed, where it was identified if the mechanism is a suitable candidate for use in 3D CFD simulations.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The described work was done with the use of ethanol reaction mechanism featuring 47 species as the reference mechanism. Reduction was performed for isobaric combustion conditions in adiabatic system, where the initial gas temperature was set at 800 K. Initial gas composition was varied according to its effect on combustion propagation results observed in 3D CFD simulations where fast, gradual and unstable combustion propagation were identified. Representative compositions leading to first two were used to propose different combustion conditions considered in reduction attempts.
Various reduced mechanism candidates were obtained, where those most promising include from 29 to 45 species. In order to determine if the candidates are suitable for use in 3D CFD simulations, their performance with different gas compositions was assessed with the specifically developed tool. This performs combustion calculations for various conditions and enables direct comparison of results obtained with reference and reduced mechanism. The most appropriate were found to be reduced mechanism candidates with 33 and 42 species. Their comparison with the reference mechanism for the case of 12 different initial gas compositions is given on Figures 1 and 2 in form of temperature increase during transfer from ignition to complete combustion.

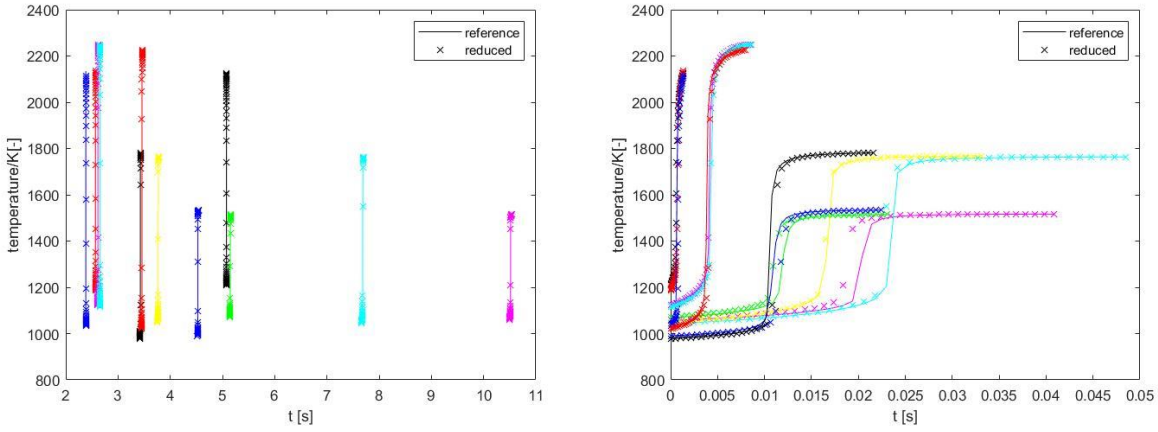

Figure 1. Comparison of temperature increase profiles obtained with the reference and reduced mechanism with 33 species. Graphs present same data with strarting points joined in the right one for a more detailed presentation.

The reduced mechanism with 33 species shows to be in good overall correspondence with the reference mechanism. The errors can be seen to occur due to the shift in the ignition time, which becomes most apparent in cases with slower ignition. There, the reduced mechanism preceeds the reference one for approximately 0,002 s at most, which is more than sufficient accuracy for our utilization in 3D CFD of

stationary combustion. In case of reduced mechanism with 42 species, these errors are much decreased and the mechanism shows practically identical results with the reference one.

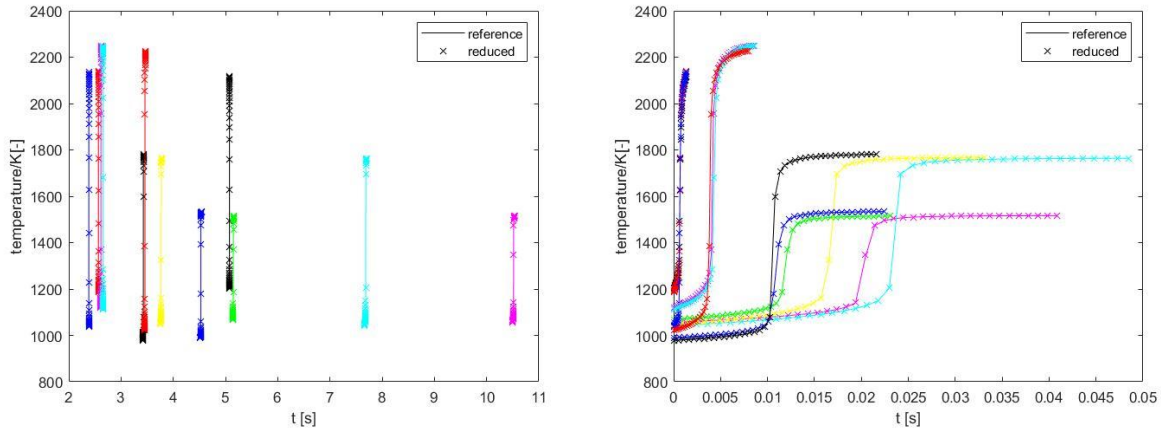

Figure 2. Comparison of temperature increase profiles obtained with the reference and reduced mechanism with 42 species. Graphs present same data with strarting points joined in the right one for a more detailed presentation.

The two mechanisms were, due to positive results in initial comparison, applied to 3D CFD simulations, in which their validity can be confirmed. Figures 3 and 4 present the temperature fields obtained with the reference and two reduced mechanisms in simulations of sludge combustion in our laboratory furnace for cases of gradual and fast combustion propagation. Figure 5 additionally presents same results for the case of combustion where temperature close to the inlet (fuel bed top) exhibits values between fast and gradual combustion. Table 1 completes this comparison with temperature and CO mass fraction data at the position where these values were also measured in experiments (0,3 m from the inlet to the freeboard).

Figure 3. Comparison of temperature field obtained with three mechanisms for case of gradual combustion.

Figure 4. Comparison of temperature field obtained with three mechanisms for case of fast combustion.

Figure 5. Comparison of temperature field obtained with three mechanisms for transition case between gradual and fast combustion.

Table 1. Comparison of T and CO mass fraction at measuring height between three used mechanisms.

	Gradual combustion prop.		Fast combustion prop.		Transition combustion	
	T [K]	CO m.fr. [-]	T [K]	CO m.fr. [-]	T [K]	CO m.fr. [-]
Reference mech.	915	0,03	1173	3,0e-05	1057	0,018
42 species red.mech.	896	0,03	1172	2,5e-05	966	0,024
33 species red.mech.	872	0,03	1171	3,4e-05	993	0,022

Results show that both reduced mechanisms capture the effects of gas composition on combustion propagation. Figures 3-5 reveal only minor differences between obtained temperature fields in all three cases. Results given in Table 1. show some differences in the average temperature at the observed position when gradual and intermediate combustion propagation cases are considered. Observing the correspondence of CO mass fractions and the fact that reporting position is located close to the inlet in the zone of high temperature gradients, it can be concluded that both reduced mechanisms not only capture correct combustion trends but also offer suitable accuracy for their application in considered combustion simulations. Finally, comparison of computational times showed that these decrease linearly with the decrese in the number of species.

FUTURE COLLABORATIONS (if applicable)

Future collaboration is in first step based on reduction of other mechanisms. After the successful reduction of ethanol mechanism the work on reducing the n-heptane combustion mechanism has started and is to be followed by reduction of the propene mechanism, as these two mechanisms were also used in our combustion simulations. Since the two mechanisms feature a larger number of species compared to ethanol, the further collaboration will aim to identification of additional approaches to perform such mechanism reduction in an efficient manner.

The common point of the three mentioned reference mechanisms is that 3D CFD simulations were performed with all of them. There exist also other mechanisms, which include even larger amount of species and their direct application to 3D CFD simulations is at the moment impractical, although they appear as suitable candidates from the chemical kinetics point of view. Therefore a chance for future collaboration is also in the development of validation methods which do not require 3D CFD results with the reference mechanism in order to confirm suitability of a certain reduced mechanism.

Finally, a future collaboration is also possible in the field of applying other tools developed at CKL ELTE to increase the performance of 3D CFD combustion simulations.