COST Action CM1404 STSM report: Modelling of Biomass Gasification and Pyrolysis

Cathleen Perlman

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1 Introduction

LOGEsoft is a software product for analysis and simulation of chemical conversion processes for engineering applications, including a module for modelling and simulation of gasification of small biomass particles.

LOGEsoft uses a CPU efficient stochastic reactor approach for biomass gasification modelling and can therefore be used more economically than CFD applications. Prior to the SRSM, char oxidation reactions have been considered in a very primitive and limited fashion in the software whereas at NTNU much work has been done on model development of these heterogeneous conversion reactions. During the STSM the char gasification know-how at NTNU has been incorporated into LOGEsoft through a user subroutine, feeding back source terms for char gasification to the LOGEsoft chemistry solver. Implementation of any user subroutine requires good cooperation between user and software developer as new problems and questions frequently occur that can best and most efficiently be addressed and solved during personal collaboration. Validation is performed based on experimental data and CFD.

Furthermore, the heat and mass transfer model in LOGEsoft neglects temperature gradients within the biomass particles. While this assumption may be true for very small particles (for example in entrained flow reactors), typical carbonisation processes use large particles, where intra-particle transport phenomena can no longer be neglected. To include said phenomena in the software, a considerable amount of preparation and implementation is needed, which has been addressed during this STSM.

2 Work Carried out During the STSM

At the start of the STSM there was a primary concern from NTNU regarding the validity of the LOGEsoft gasification model as it was observed that heat was released during the pyrolysis even though this is an endothermic process.

The first step of the STSM thus consisted of validation of the LOGEsoft gasification model and implementation of necessary modifications to the equations solved.

During this investigation it became evident that the heat of pyrolysis was treated incorrectly as the energy required to convert solids to gas was not considered. This was rectified through the addition of the term

$$\frac{dT_{s,\text{pyr}}}{dt} = \frac{\Delta H_{\text{pyr}}}{C_{p,s}\rho_s}\left(\frac{1}{V}\frac{dm}{dt} - \frac{m}{V^2}n_{par}\frac{\pi}{6}3d^2\frac{dd}{dt}\right)$$

to the solids temperature equation. The previous heat of reaction term which, in a standard fashion for gas-surface interaction systems, was calculated as

$$\frac{dT_s}{dt} = \frac{-1}{C_{p,s}\rho_s}\left(\sum_{i=1}^{n_g}\omega_{i,p}h_{i,p} + \sum_{i=1}^{n_s}\omega_{i,s}h_{i,s}\right)$$

was removed since there is no additional energy exchange between the solids and the pore gas, which are considered to have the same temperature. By using a static value for the heat of pyrolysis it can also be assured that uncertainties in the polynomial coefficients which are normally used to calculate enthalpy for individual species can be avoided. Since it is difficult to find reliable coefficients for solid species, this is a a great advantage.

Validation of the updated temperature equation was performed against experimentally available data as well as CFD data available from simulations carried out at NTNU. Preliminary results for a few select cases are shown in Figure 1.

It was concluded that the LOGEsoft gasification model with the updated temperature equation produces reasonable results with trends matching those produced by CFD simulations.

Prior to the STSM, the foundation of a char gasification user subroutine had been developed at NTNU with support from LOGE. While the routine did indeed gasify the char, gasification rates were found to be lower than expected. During the STSM it transpired that the rates have been calculated based on a single solid particle's size and volume rather than on all the solid particles in the reactor. To correct this and simplify the usage of the user routine, the subroutine interface was updated so that solids size properties are passed through the subroutine interface, guaranteeing the integrity between the calculations performed directly by LOGEsoft and those performed in the user subroutine. It was also ascertained that heat of reaction for the char gasification user subroutine was accounted for through an additional update of the solids temperature equation:

$$\frac{dT_{s,\text{char}}}{dt} = \frac{\Delta H_{\text{char}}}{C_{p,s}\rho_s} = \frac{1}{C_{p,s}\rho_s}\left(\sum_{i=1}^{n_g}h_{i,p}\Delta\omega_{i,p} + \sum_{i=1}^{n_s}h_{i,s}\Delta\omega_{i,s}\right)$$

Validation of the effects of the char gasification user subroutine is currently in progress.

Since the LOGEsoft gasification model does not consider thermal gradients within the solids, it was discussed how to incorporate a particle conversion model, such as the one in [1], into the software. NTNU are currently working on implementing the model presented in [1] and results are to be presented at the 2016 European Biomass Conference and Exhibition [2].

To maximise usability, it was decided that the particle conversion model will be included in LOGEsoft through an additional user subroutine. This work will start after char gasification validation is completed and the work required for publications scheduled for spring and summer (see below) are finished.

It is the belief of both LOGE and NTNU that this STSM has greatly enhanced the usability of the LOGEsoft gasification model and that updates made will be of benefit also to other parties wishing to model biomass pyrolysis and char gasification at a simpler scale and affordable CPU cost.

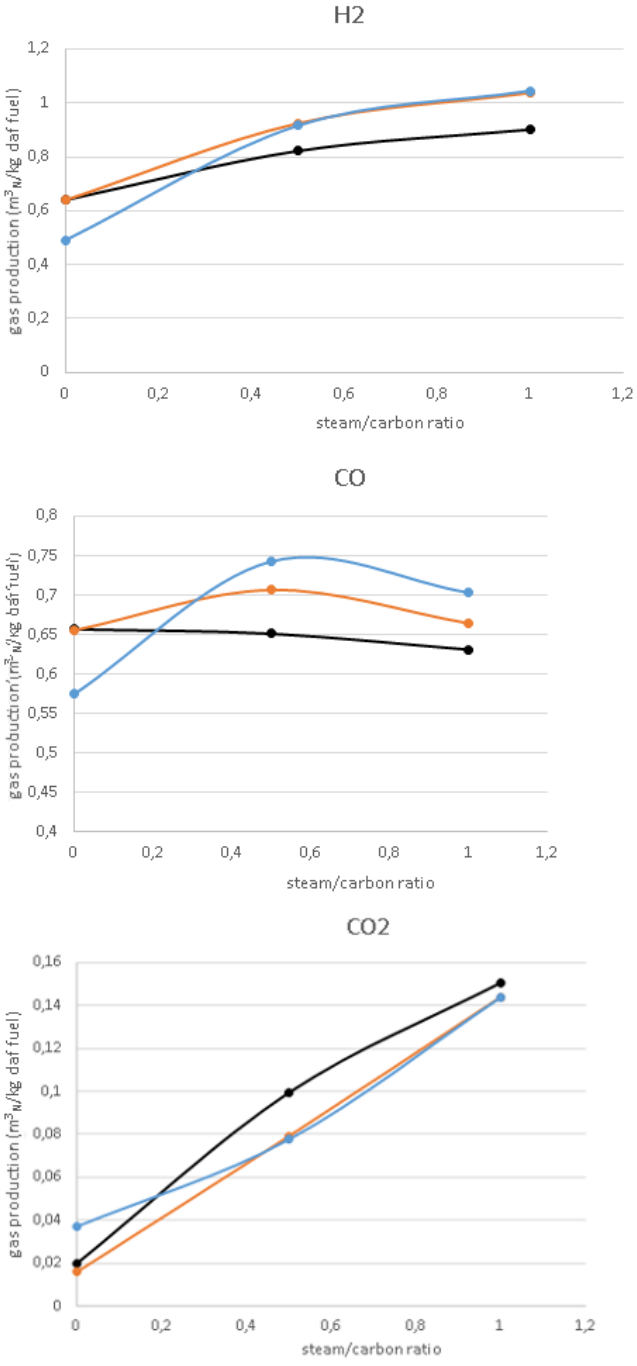

Figure 1: Preliminary results of pyrolysis cases using updated LOGEsoft gasification model together with char gasification user subroutine. Black lines are experimental data, orange lines are results from CFD and blue lines are results from LOGEsoft.

3 Publications Derived from the STSM

The work carried out during the STSM will be featured in a conference paper for the Pyro2016 conference in France (http://www.pyro2016.com/), where there will be a poster presentation. In conjunction with this a paper will also be submitted to the *Journal of Applied and Analytical Pyrolysis*.

In addition, there will be a poster presentation at the 2016 European Biomass Conference and Exhibition (http://www.eubce.com/home.html).

References

[1] Ström H., Thunman H., "CFD Simulations of Biofuel Bed Conversion: A Submodel for the Drying and Devolatilization of Thermally Thick Wood Particles", *Combust. Flame*, 160, (2013)

[2] Li T., Ku X., Løvås T., "Eulerian-Lagrangian Simulation of Thermochemical Degradation of Thermally Thick Biomass Particles", *accepted for presentation at EUBCE 2016*