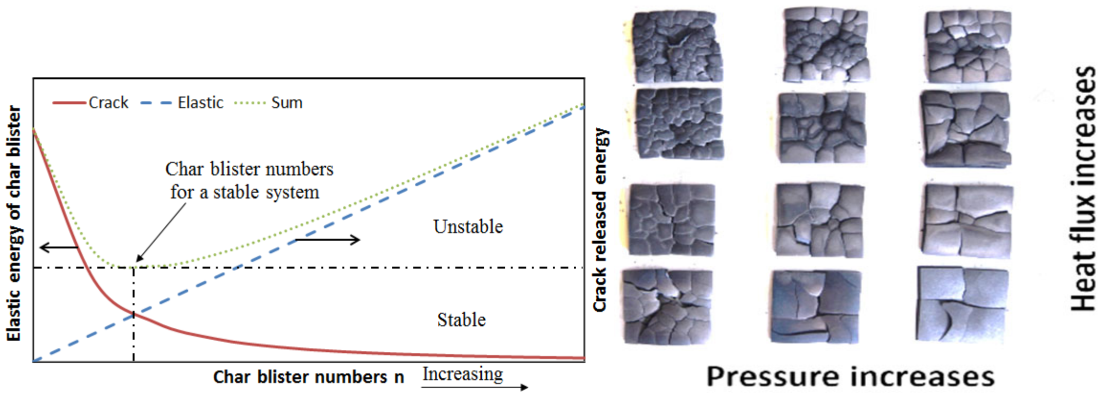
STSM report COST FP1404

/Kaiyuan Li/, From /Aalto University/ to /Imperial College London/ (03.07-18.07.2016)

- The purpose of this STSM is to develop a simplified calculation method for kinetic properties determination in pyrolysis model and to predict the pyrolysis process and stress field which explain the formation of char cracks (fissures) in timber fires.
- Short summary of performed STSM: In pyrolysis modelling of timber materials, the kinetic properties have to be determined. By resolving the reaction order using the product logarithm function (Lambert W function), a simplified method is developed simultaneously determining A, E and n. The properties were further implemented in FDS to predict the charring process to investigate the char shrinkage and cracking behaviours during timber combustion.
- Description of the main results obtained: A simplified calculation method is developed. The surface stresses of char blisters after cracking are found similar under different heat fluxes and the values of which are close to the tensile strength. This finding indicates that cracking will release the elastic strain energy caused by tension and the size of char blister is determined by the char depth at the cracking time.
- Future collaboration with the host institution. The simplified calculation method will be used for predicting the charring rate of timber structure under travelling fire. The effects of char shrinkage and cracking on the heat transfer process will be investigated in the future.
- Foreseen publications/articles resulting from the STSM: The results of this STSM were further discussed with Dr. Xinyan Huang from Imperial College London during the 36th International Symposium on Combustion. Based on the results, a short communication for the simplified method and a journal paper for cracks formation are scheduled to be prepared.
- Confirmation by the host institution of the successful execution of the STSM is attached (annex 1)
- Other comments (if any)


Crack
Elastic
Sum
Elastic energy of char blister
Crack released energy
Char blister numbers for a stable system
Unstable
Stable
Char blister numbers n
Increasing
Heat flux increases
Pressure increases

Annex 1 – Confirmation by Host Institution

Imperial College London

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Reader in Thermal Energy

August 10, 2016

To: Whom Responsible for the Short Term Scientific Mission (STSM) of the COST Action FP 1404

Confirmation Letter of Short Term Scientific Mission (STSM) of the COST Action FP 1404 entitled "the role of char cracking in timber fires" performed by Dr. Kaiyuan Li from Aalto University to Imperial College London, 03.07-18.07.2016

Dear Sir,

The purpose of this letter is to confirm that Dr. Li Kaiyuan from Aalto University has accomplished the Short Term Scientific Mission (STSM) entitled "the role of char cracking in timber fires" at Imperial College London from 3 July to 18 July 2016.

Since his entrance in our lab, Dr. Li has been working on the projects which contain: (1) Developing simplified calculation method for kinetics properties, (2) CFD modelling of pyrolysis wood, (3) Effect of wood cracking on development of timber fires. Dr. Li finished the research works successfully and obtained many useful results. He did computational and experimental researches simultaneously and had excellent performance in both aspects. He is very familiar with the pyrolysis models such as FDS, which is the most applicable tool in fire industry.

I am deeply impressed by his quick grasp of new ideas and collaborations with other researchers and look forward to have him in the group again in the near future.

Sincerely yours,

Guillermo Rein

Dr. Guillermo Rein
Editor-in-Chief of Fire Technology The research journal of NFPA and SFPE by Springer Nature https://twitter.com/FireTechnology
Imperical College London

Annex 2 – Scientific Report

Fire safety use of bio-based building products

The role of char cracking in timber fires

Scientific report of STSM at Imperial College London,

Department Mechanical Engineering

03.07-18.07.2016

Author:

Kaiyuan Li, Aalto University, Finland

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Introduction

Fire continues to be a global problem, causing about 1% loss of global GDP and 4000 deaths per year in Europe [1]. In U.S. the total cost of fires in 2011 was about $330 Billion [2]. Most fire deaths (70-90%) occur in domestic housing, and thus more fire-safe materials for construction and consumer goods are needed. However, out of environmental reasons, new bio-based materials are being developed, which are inherently combustible. There is also a renewed interest in wood as a construction material but in most countries, its use is restricted by the fire safety regulations of the building code. A notable example in these codes is Eurocode 5 [3].

Fire safety and fire resistance of both bio-based and synthetic materials have been studied extensively [4]. In case of timber materials, their fire behaviour consists of two aspects: reaction-to-fire (i.e. how much it contributes to the fire) and fire resistance (i.e. the capability to fulfil the function). Most of the previous research has aimed at improving the reaction-to-fire behaviour. Possibilities to improve the fire resistance by modifying the material itself have been studied rarely, which is surprising as the trend towards high stage-of-completion products would enable effective physical treatments during the manufacturing process. We believe that a missing key element in our understanding of fire resistance is the quantitative description of the role of char cracking in timber fires.

The appearance of characteristic cracks in timber undergoing fire exposure can be examined in light of both chemical process data (i.e. thermal degradation of component polymers) and crack propagation theory as studied in plastics technology. The cracks apparently provide paths of low resistance for flow of reactants and products to and from outer areas of the char layer. Despite significant research on timber constructions with regard to fire safety, they are still designed in an oversized manner. This is due to natural variance in physical and mechanical properties of wood and deficient understanding of temperature- and moisture-dependent changes that come from biological origin.

In addition, it should be noted that high accuracy numerical models are demanded in modern timber structure design. These models can improve the physical predictions of timber structures, for example, the proposed charring rate of 0.65 – 0.70 mm/min in Eurocode 5 [3] might be modified by detail pyrolysis modelling, and also estimate the contribution of bio-based materials to the fire scenario. So far, many computational studies have also been conducted with different in-house codes [5-8] and other standard pyrolysis codes such as FDS [9], ThermaKin [10], Gpyro [11]. Although a better understanding on the pyrolysis dynamics has been gained in the last few decades, modelling charring materials is still challenging because of the anisotropic nature of both physical and chemical properties as well as a lack of knowledge on material behaviours and measuring techniques. More specifically, the state-of-the-art pyrolysis modelling has mostly ignored the charring behaviours and no char fissure effect has been taken into account, due to the limited understanding on charring of various materials.

The collaboration of Aalto University and Imperial London College brings together the required computational tools and experimental characterization techniques that need for solving the multi-scale and multi-physics problem at hand, for charring behaviours. Aalto University provides experimental data and be responsible of multi-scale (FDS [12]) simulations while Imperial College London has a necessary competence on chemical kinetics experiments and modelling. The current collaboration aims to develop a simplified calculation method for kinetics properties which can be implemented in FDS pyrolysis model. The model is further used to predict the pyrolysis processes and the stress field for cracks formation. The collaboration leads to scientific benefits to both parties and the topic meets the goal of COST Action FP 1404, i.e. improving the understanding on

−Contribution of bio-based materials to the fire scenario.

−Modelling combustible products in FSE-tools.

Overview of performed work

The research group in Imperial College London developed a simplified calculation method for determining the kinetics properties of wood materials. Based on their previous researches on pre-exponential factor and activation energy, the current method resolves the reaction order using the product logarithm function (Lambert W function). The kinetic triplets are finally expressed as

$$A_{cp}(T_p) = \frac{\beta E_{cp}}{\exp\left(-\frac{E_{cp}}{RT_p}\right) RT_p^2} \tag{1}$$

$$E_{cp} = -R \frac{n\sum_{i=1}^{n} \ln\left(\frac{\beta}{T_{pi}^{\ 2}}\right)\frac{1}{T_{pi}} - \sum_{i=1}^{n} \ln\left(\frac{\beta}{T_{pi}^{\ 2}}\right)\sum_{1}^{n}\frac{1}{T_{pi}}}{n\sum_{i=1}^{n}\left(\frac{1}{T_{pi}}\right)^2 - \left(\sum_{i=1}^{n}\frac{1}{T_{pi}}\right)^2} \tag{2}$$

$$n = 0.7318B - 0.9147, \qquad 1 < B < 5.5 \tag{3}$$

The method was validated using the thermogravimetry experimental results of birch from Finland and compared to the optimized searching results obtained by genetic algorithm. The K-GA comparison will be presented in the next section.

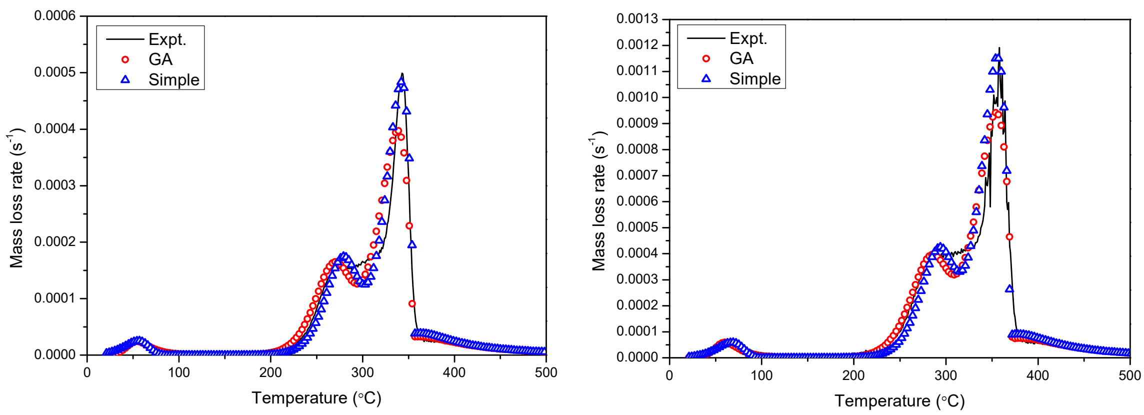
The derived kinetics properties were implemented in FDS pyrolysis model to predict the inert charring processes of wooden materials in nitrogen. The surface stresses with and without cracking were determined using the shrinkage gradient predicted by FDS at the sample surface. The thermal shock theory for most of the sudden shrinkage processes was used to analyse the cracking mechanism while the Griffith theory was used to reveal (or further confirm) the mechanism based on system energy balance.

Results and discussions

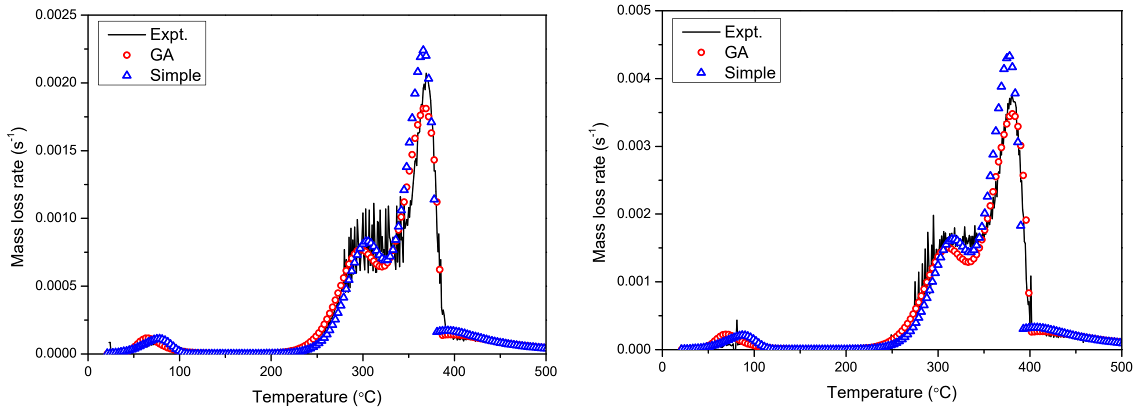
Birch samples with a moisture content of approximately 2.6% were decomposed using TG in nitrogen atmosphere. The results were used to validate the proposed simplified method and the modelling accuracy was evaluated through the comparison of the experimental and predicted mass loss rates produced by GA. In order to quantify the agreement of MLR curves between experiment and prediction, the Pearson correlation coefficient (PCC)

$$PPC(\%)=\frac{\sum\left(\dot{m}''_{\text{pred}}-\overline{\dot{m}''_{\text{pred}}}\right)\left(\dot{m}''_{\text{exp}}-\overline{\dot{m}''_{\text{exp}}}\right)}{\sqrt{\sum\left(\dot{m}''_{\text{pred}}-\overline{\dot{m}''_{\text{pred}}}\right)^2\sum\left(\dot{m}''_{\text{exp}}-\overline{\dot{m}''_{\text{exp}}}\right)^2}}\times 100\% \tag{4}$$

was used. In this case, the mass fraction of each sub-reaction and its residue yield has been set exactly the same as the GA properties. The MLR curves in Figure 1 show no significant difference between these two methods while the PCC values of GA are slightly greater than the ones of simplified method. This is understandable since after all the GA properties were generated using computer optimizing method which should have led to the most comparable results to the experimental curves. Nevertheless, the simplified method led to a set of PCC values over 0.96 at multiple heating rates and an average value of approximately 0.97 which is definitely acceptable for engineering use. Besides, it should be noted that GA consumed several hours from setting up the model to finishing the searching process whereas simplified method used less than 10 min to come up with the properties.



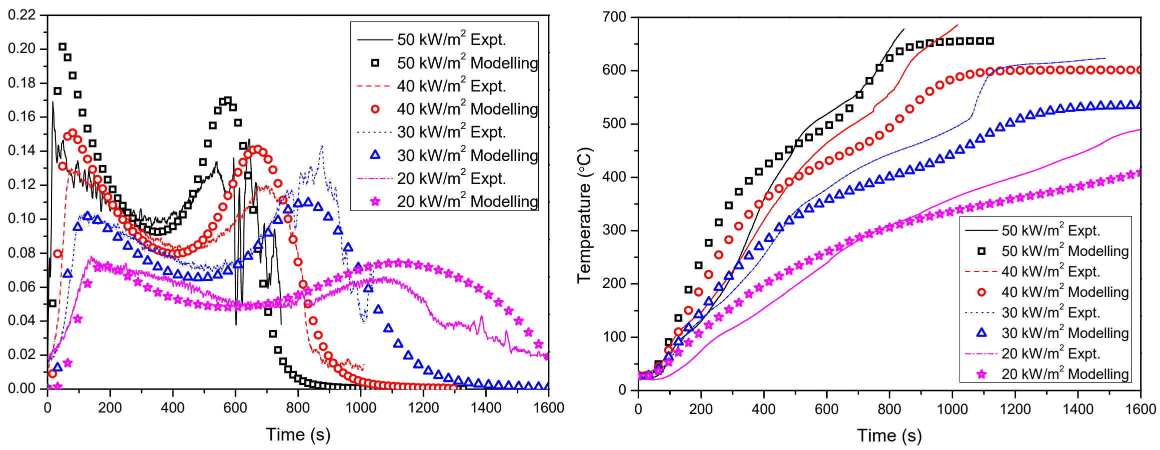
(a) 2 K/min *(b) 5 K/min*



(c) 10 K/min *(d) 20 K/min*

Figure 1: Birch TG results in nitrogen

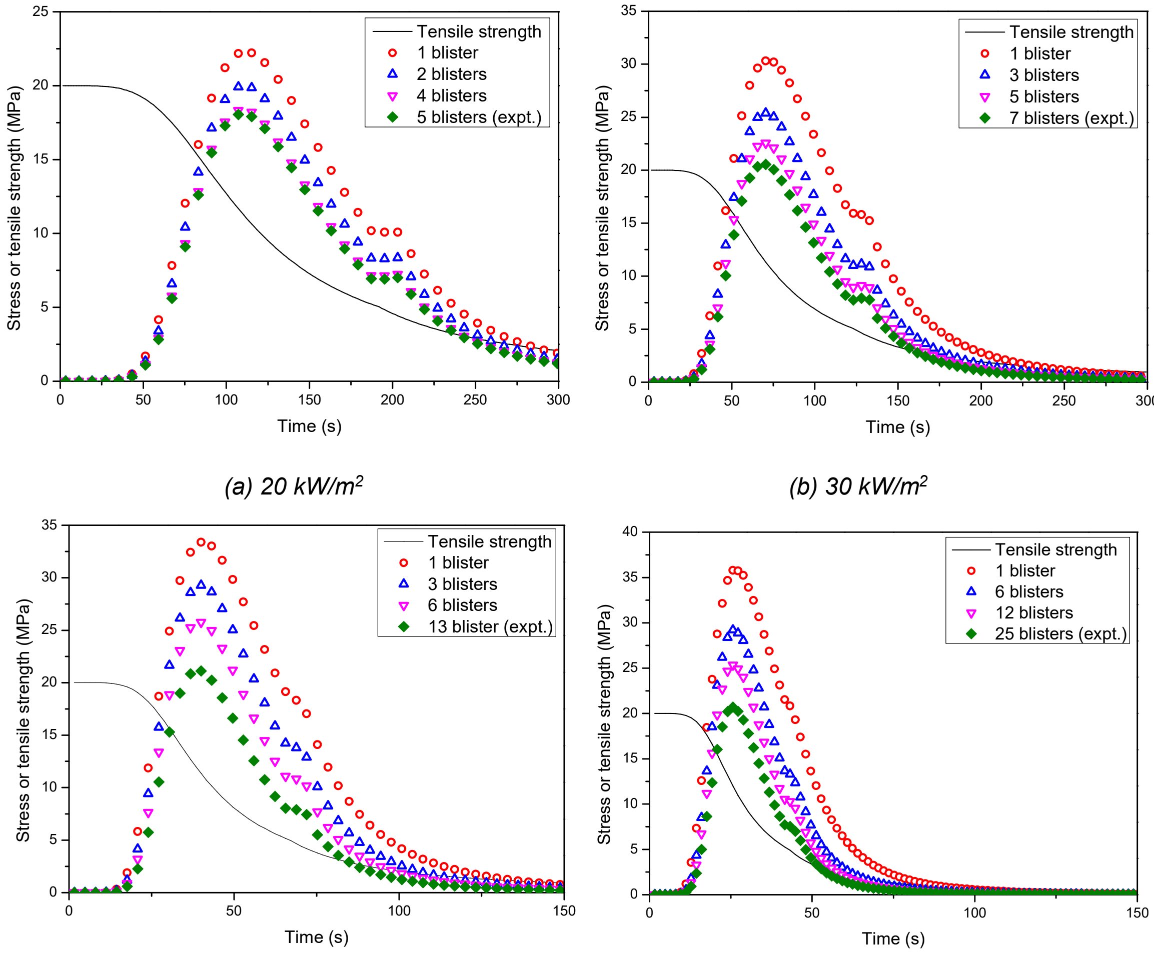
Figure 2 shows the pyrolysis modelling results. It can be seen that the current pyrolysis model gives reasonably good predictions to the overall mass loss rate and the temperature in the sample center, although at the later stages the measured center temperatures are under-predicted owing to the sample deformation which enhances the thermocouple positions in the experiments.



(a) Mass loss rate *(b) Center temperatures*

Figure 2: Pyrolysis modelling results

From Fig. 3, it can be seen that the surface stress decreases with increasing number of char blisters. If there is no crack (1 blister), the surface has the maximum strain which leads to the highest stress being a lot higher than the tensile strength of wood. As the char fissures increase, the number of char blisters increases, which reduces the surface stress. For all heat fluxes, the peak stresses were reduced to approximately 20 MPa with the number of char blisters measured experimentally, which is close to the estimated tensile strength of wood. Moreover, it is surprisingly found that the surface stresses with the experimentally measured number of char blisters are almost the same at different heat fluxes, while the highest stresses with no crack are quite different at different heat fluxes. This indicates that the final pattern of char fissures is determined by the size of char blisters generating a stress less than the tensile strength.



(a) 20 kW/m² *(b) 30 kW/m²*

(c) 40 kW/m² *(d) 50 kW/m²*

Figure 3: Surface stress and tensile strength

Conclusions

High accuracy pyrolysis modelling will benefit the fire designs for timber structures, such as leading to more accurate charring rate and estimation to contribution of bio-based materials to the fire scenario. Understanding the char cracking can further improve the accuracy of current pyrolysis models. To determine the kinetic properties in pyrolysis models, a simplified method is developed which simultaneously solves A, E and reaction order using the product logarithm function (Lambert W function). The validation shows the simplified method can give comparable predictions to experimental data. The derived properties were then implemented in FDS pyrolysis model to predict the charring process of wood. Based on the results, the char shrinkage and cracking behaviours were analysed. The surface stresses of char blisters after cracking are found similar under different heat fluxes and the values of which are close to the tensile strength. This finding indicates that the final pattern of char fissures is determined by the size of char blisters generating a stress less than the tensile strength.

References

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