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The effect of lignocellulosic compounds and monolignols on the soot nanostructure and CO_2 reactivity

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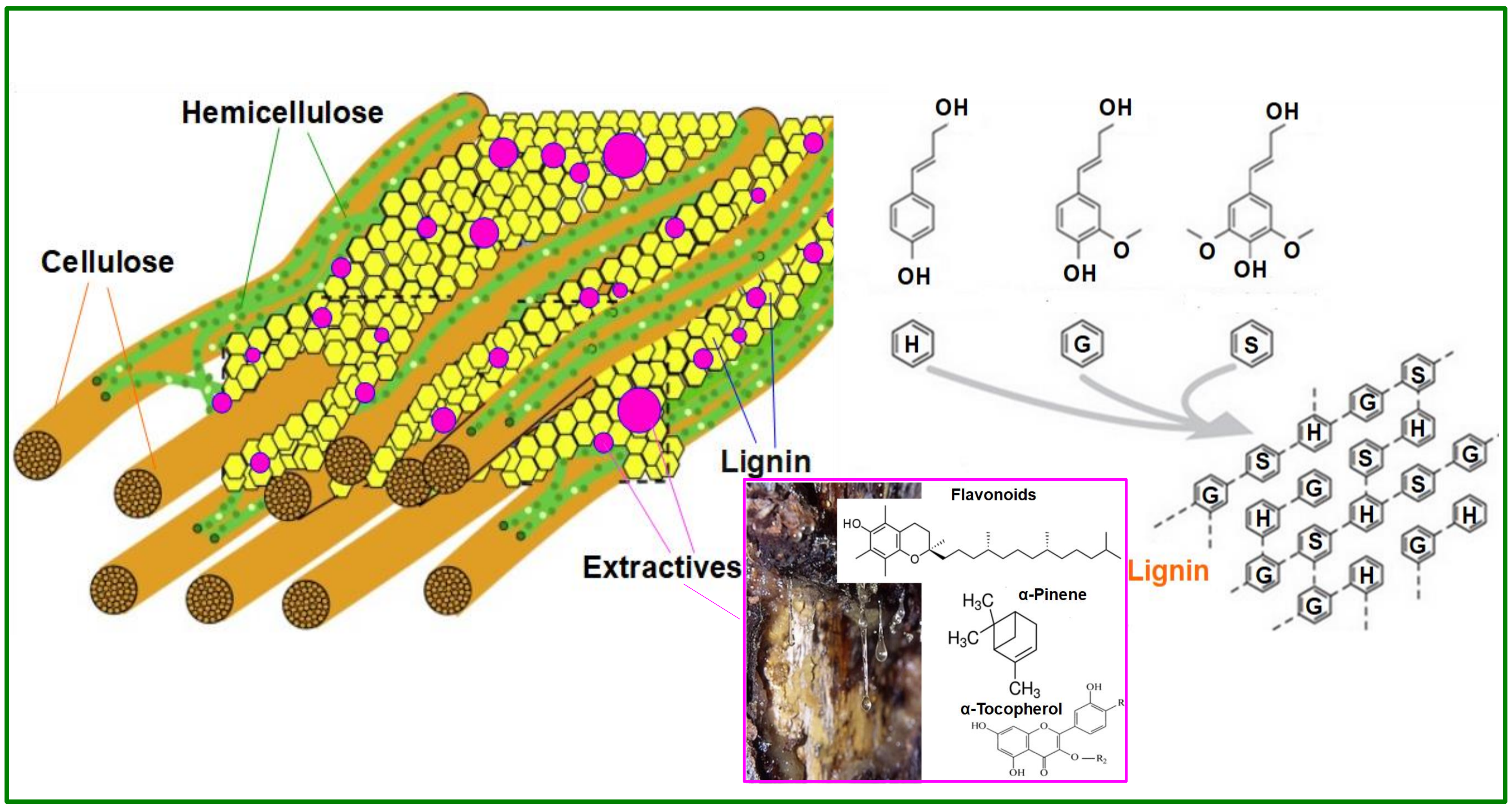
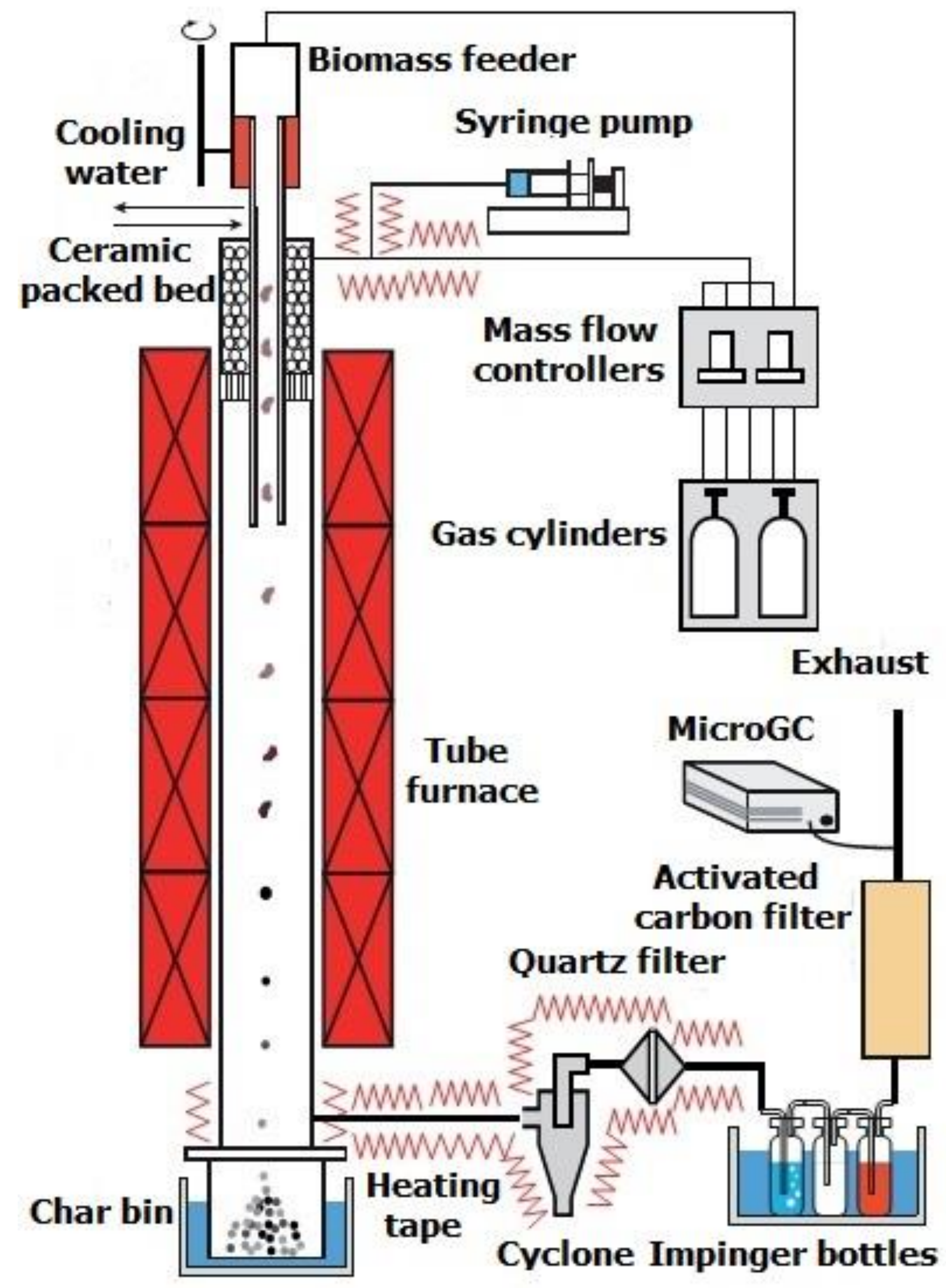
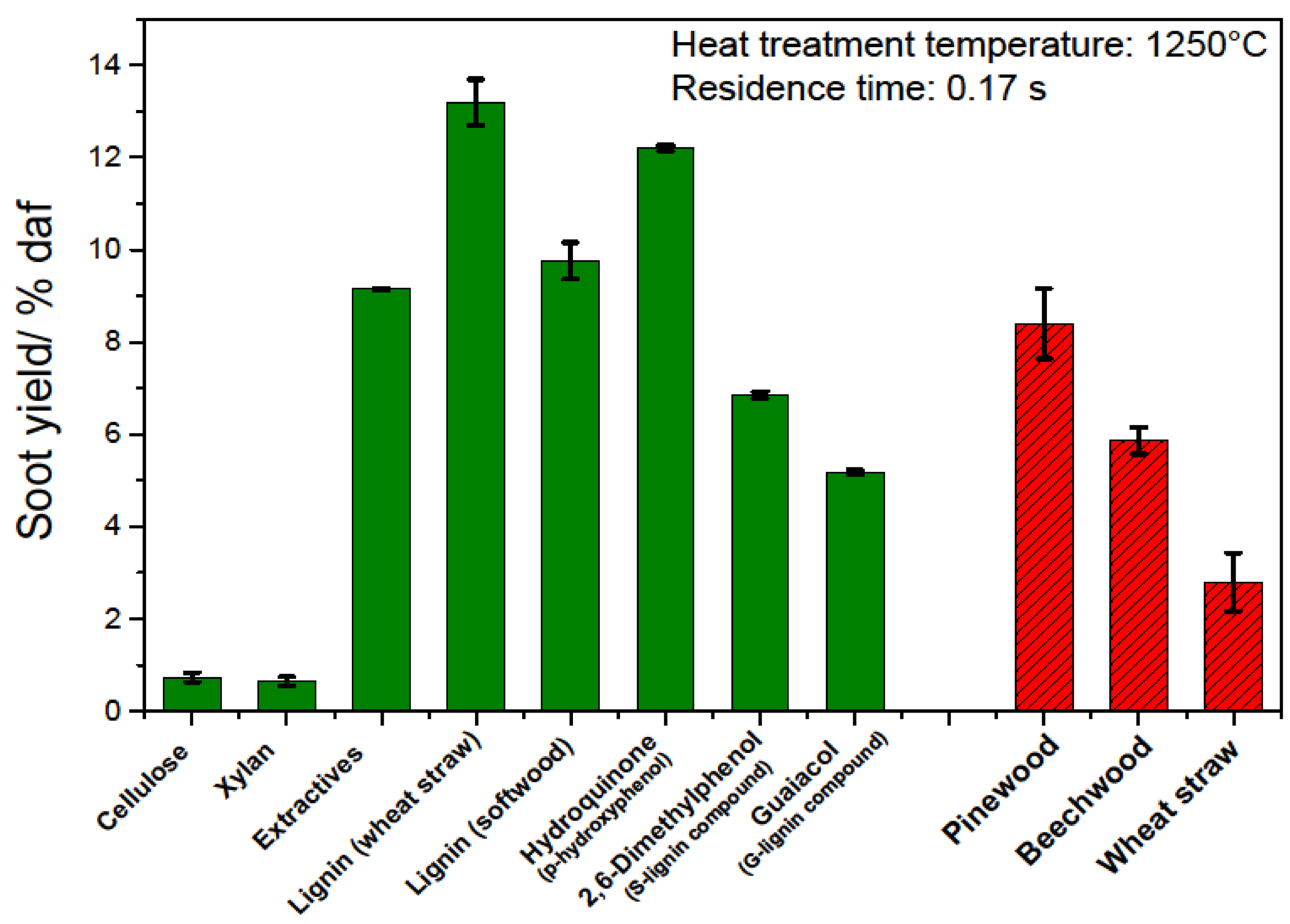
Biomass gasification utilizes biomass in an efficient and sustainable way for a wide variety of applications such as heat, electricity, chemicals and transport fuels [1]. Reducing soot formation combined with production of highly active soot therefore increases overall process efficiency and improves the economic feasibility and reliability of gasification plants. The chemical and structural variance of biomass makes it difficult to identify how the soot yield and composition are affected by specific operating parameters and feedstock composition to optimize entrained-flow gasifiers. Previous investigations showed that low lignin-containing wheat straw generated less soot than the pinewood with the high content of extractives and lignin [2]. Different types of lignin (softwood, hardwood, herbaceous biomass) contain various amounts of methoxy groups depending on how much of each of the three monolignols has been incorporated into the lignin macromolecules [2]. The high concentration of resin acids in wood may reportedly increases soot yields in addition to increasing the formation of PAH precursors [3,4]. Therefore, soot yields and particle properties were correlated with fuel composition and operating conditions in the present study.

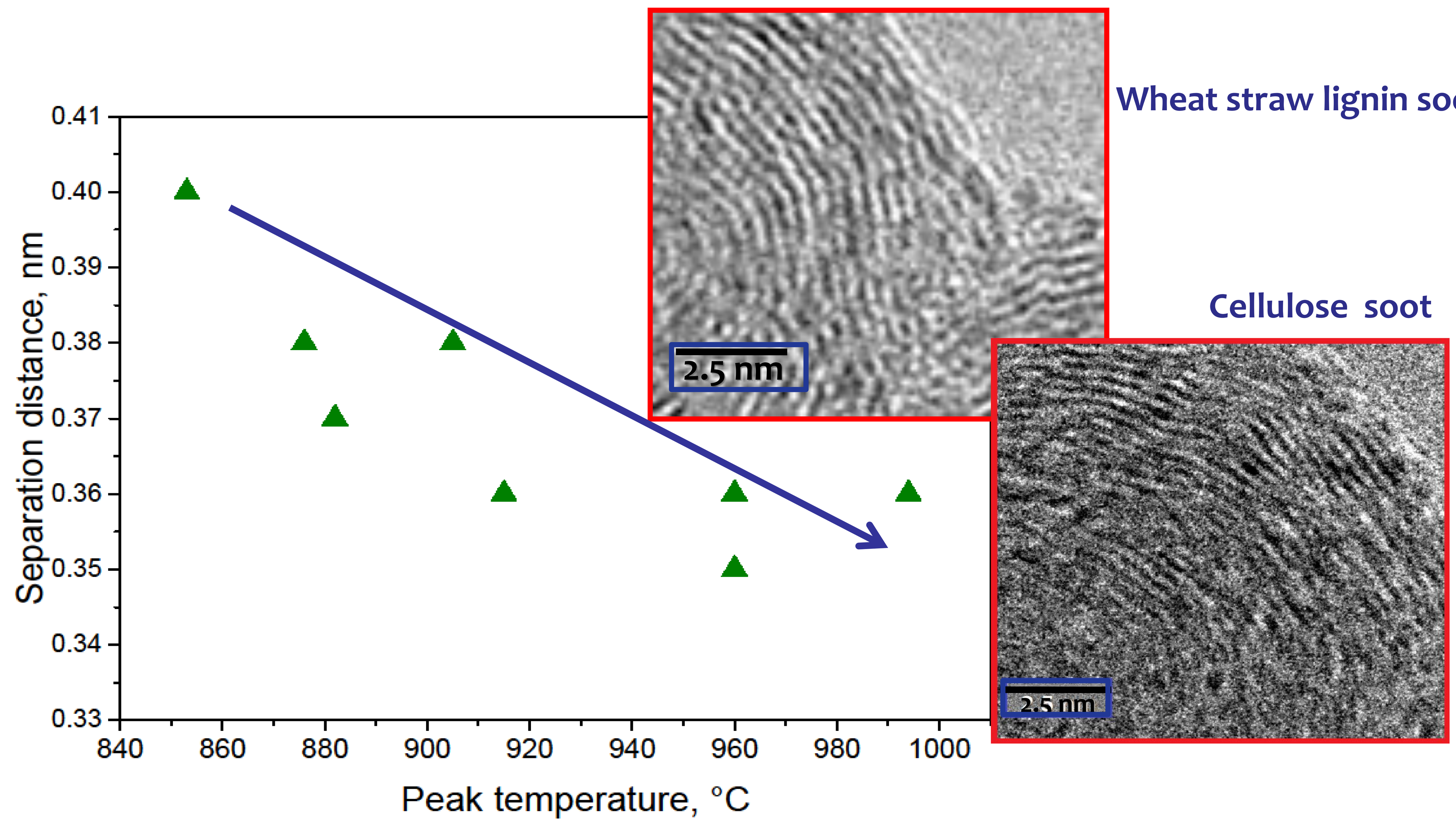
Lignocellulosic compounds and monolignols



Soot was generated at 1250℃







Wheat straw lignin soot

Cellulose soot

The present results indicate that both lignin samples from softwood and wheat straw provide greater soot yields than holocelluloses and extractives, consistent with the aromatic content of lignin. Moreover, soot reactivity decreases with increasing feedstock lignin content. Tests with representative monolignols suggest that hydroquinone - rather than 2,6-dimethylphenol and guaiacol - plays an especially important role in soot formation. Thermogravimetric analysis results showed that the soot reactivity towards CO_2 depends mainly on the soot nanostructure, as determined by TEM and Raman spectroscopy, and less on the particle size and radical concentrations. In particular, cellulose and hemicellulose soot consisted of graphene sheets spaced at approximately 0.4 nm, whereas the graphene spacing of the lignin-derived soot was approximately 0.25 nm. These results provide a clear basis for understanding the effects of feedstock on soot formation, showing that increasing the lignin content of the feedstock increases the soot yield while decreasing the soot reactivity - both potentially negatively impacting gasifier operation and emissions. Differences in reactivity can be ascribed in part to differences in soot nanostructure. Based on this work, selection of gasification feedstocks should emphasize biomass with low lignin content [5]. ***Future molecular level studies using Density Functional Theories (DFT) are planned to confirm the experimental observations.***

References

[1] C.F. Mhilu, *Modeling Performance of High-Temperature Biomass Gasification Process*, Chem. Eng. J. **2012**, 1-3 (2012).
[2] A. Trubetskaya, P.A. Jensen, A.D. Jensen, A.D. Garcia Llamas, K. Umeki, P. Glarborg, *Effect of fast pyrolysis conditions on biomass solid residues at high temperatures*, Fuel Process. Tech. **143**, 118-29 (2016).
[3] W.F. Rogge, M.A. Mazurek, J.M. Hildemann, *Quantification of urban organic aerosols at a molecular level: identification, abudance and seasonal variation*, Atmos. Environ. **27**(A), 1309-30 (1993).
[4] J.J. Schauer, M.J. Kleeman, G.R. Cass, B.R.T. Simoneit, *Measurement of Emissions from Air Pollution Sources. 2.* C_1*-*C_{29} *Organic Compounds from Fireplace Combustion of Wood*, Environ. Sci. Technol. **35**, 1716-28 (2001).
[5] A. Trubetskaya, A. Brown, M.T. Timko, J.Kling, M. Larsen Andersen, K. Umeki and etc., *Characterization and reactivity of soot from fast pyrolysis of lignocellulosic compounds and monolignols*, Appl. Energy **212**, 1489-500 (2018).

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