3G03: DETERMINATION OF PYROLYSIS TEMPERATURE FOR CHARRING MATERIALS.

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Comment by Guillermo Rein, The University of Edinburgh, UK
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I think that your conclusions agree with TGA results at different heating rates. These show that temperatures for the onset and the peak of pyrolysis reaction fall within a relatively small range of values for a wide range of heating rates. Also, I think your conclusions are only valid so far for a one-step mechanism. If the degrading solid is subjected to competing reactions, the concept of a pyrolysis temperature might lose meaning. This would be relevant in the context of multi-step pyrolysis, presence of oxidation reactions and smoldering combustion.

Reply by Won Chan Park
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Yes, as presented in our paper, the pyrolysis temperature is determined by comparing with a single-step reaction. The goal is to enable analytical and simpler solutions for more complex geometries and conditions that are dominated by heat and mass transfer. Thus, a systematic method of simplifying the chemistry is presented. As you mention, pyrolysis temperature approximation may not be suitable for problems where chemistry is important.

Interestingly, we started with a multiple-step reaction and found little difference between a single and a multiple-step reaction as long as an appropriate char yield is used. The multiple-step reaction helps determine this char yield through competing reactions. When both mass and energy balances are imposed, the multiple step reaction will help determine the char yield by mass balance and the pyrolysis temperature by energy balance. In this situation, for the energy balance, 'k' in Eq. (8) will have to be replaced by an appropriate sum of $k's$ in the competing reactions.

However, eventually we decided against determining both the char yield and the pyrolysis temperature because there are so many multiple-step reaction mechanisms in the literature with little consensus between them. There may be a good reason for this because more detailed the kinetics, the more material specific it becomes. Thus, one would need to first sort all this out before using a multiple-step reaction. Consequently, we chose char yield from the literature and focused on the pyrolysis temperature.

For the oxidation case you cited, one possibility is to model the solid decomposition as a pyrolysis front and model the char oxidation separately. All this, of course, depends on what you want to accomplish.