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# Simulation of the pyrolysis of charring polymers: influence of the porous media properties

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Fire spreading along cable trays in Nuclear Power Plants (NPP) has been widely studied in large scale facilities. Yet, the cable sheath material has been identified as an influent factor on the fire spreading, with significant differences between experiments involving halogenated (e.g. PVC) and non-halogenated (e.g. PE/EVA compounds filled with a mineral fire-retardant load) sheaths. In this respect, many efforts are currently made to improve the simulation and the modelling of the pyrolysis of such materials. In particular, special attention is paid on the characterization of these materials residuals conductivity, which has rarely been studied so far, but which may have a strong influence on the temperature rise in the virgin part of the pyrolysing material. In this context, the present communication aims at presenting a methodological approach to model the thermal conductivity of these porous residuals and simulate their thermal degradation. This approach mainly consists in three steps.

1. Build a 3D representation of the degraded polymer at the most significant steps of its pyrolysis. In this purpose, naked eye visualizations, high-resolution photo and scanning electron microscope (SEM) can provide enough information to define a relevant synthetic porous medium; ultimately, 3D tomography can directly provide such a representation.
2. Evaluate the effective thermal conductivity of the residuals. First estimates can be obtained from general empirical or theoretical models, such as the usual parallel and perpendicular Wiener's bounds, or the Hashin & Strickman bounds for isotropic materials. Improved precision can be sought for by a direct solution of the Laplace's equation, either in a model geometry devised from and conditioned by the observations, or in a tomographic image of the residual, though the latter involves sampling and methodological issues [1].
3. Use this effective conductivity in the complete simulation of the material pyrolysis, accounting for the coupled heat and mass transfers and chemical reactions. The fire simulation software CALIF<sup>3</sup>S-ISIS[2] developed at IRSN will be used in this purpose. Of prominent interest is the accurate prediction of the heat release rate (HRR), which is actually a measure of the emission rate of combustible pyrolytic gases, expressed in terms of the energy released when it burns, as usual in the field of fire safety.

The analysis of the residuals of PE/EVA/ATH and PVC cable sheaths already tested in large-scale facilities [4] has exhibited two opposite trends (Fig. 1): the PE/EVA/ATH compound residual was composed of a microporous structure of 2  $\mu\text{m}$  typical pore/grain size observed under SEM, which probably corresponds to the initial ATH load contained in the polymer matrix [3]; conversely, PVC cables residuals showed large pores visible to the naked eye [4]; other PVC tested in the literature generally exhibit similar features and intumescence [5]. Further studies are currently in progress to obtain a 3D representation of these porous media and proceed with this approach so as to compare pyrolysis simulations to cone calorimeter experiments involving these materials.

Meanwhile, preliminary simulations of reference cone calorimeter experiments carried out on PVC samples [5] are performed. Thermal conductivity is modelled by Wiener's or Hashin & Strickman's bounds based on the volume fractions and properties of the various components. A Rosseland-like radiative conductivity  $\lambda_{\text{rad}}^r$  is also added: its general form is  $\lambda_{\text{rad}}^r = F\sigma\bar{T}^3$  where  $F$  is a prefactor [m],  $\sigma$  is the Stefan-Boltzmann constant, and  $\bar{T}$  is the local average temperature. Indeed, conduction alone leads

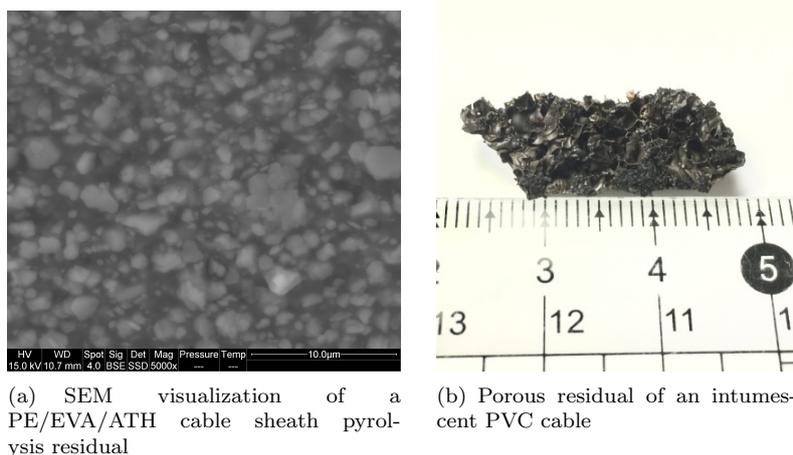


Figure 1: Illustration of the morphology of pyrolysis residuals for two different materials

to a strongly underestimated heat release rate (Fig. 2(a)). The amplitude of the radiative conduction determined by the prefactor  $F$ , which strongly depends on pore size, is large in this intumescent material. Thus,  $\lambda_{\text{rad}}^r$  has a major influence on the HRR, whereas the response is weakly sensitive to the choice of the model chosen to represent the effective conductivity (Fig. 2(b)).

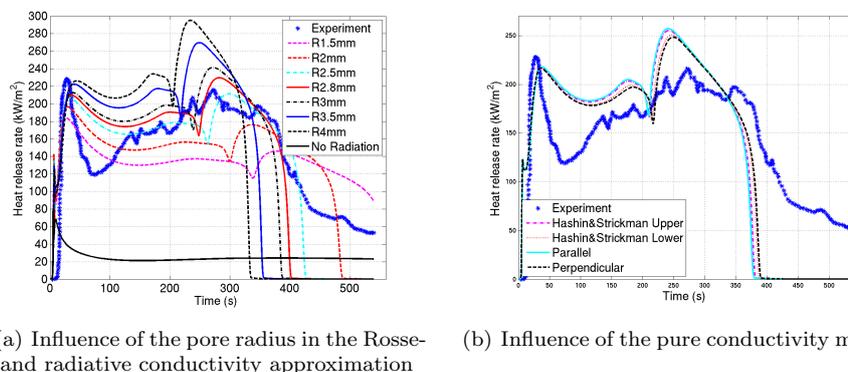


Figure 2: Comparison of heat release rate per unit area between cone calorimetry experiment and numerical simulations. Imposed heat flux:  $92 \text{ kW/m}^2$ ; 6 mm thick PVC sample.

To sum up, the present state of this work shows that the porous residuals morphology may have a strong influence on the material conductivity and induce strong radiative effects, in particular when the medium pore size is large as observed for PVC. Conversely, non-intumescent compounds filled with mineral fire retardants are expected to induce highly conductive mineral residuals with limited radiative effects if the pores are small. In this case, more attention should be paid on the modelling of the pure effective conductivity. Progress on the characterization of the porous media morphology and conductivity and comparison between cone calorimeter experiments and pyrolysis simulations will be addressed in the presentation in the case of an example of such a material.

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