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Modelling the implementation process of blown rigid tannin-based foams

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1 Introduction

The considerable progress made in recent years to develop non-flammable and cheap bio-based insulation foams for building now requires a thorough review of their implementation process, a prerequisite for standardization and ultimately to industrialization. Indeed, the complexity of the physical phenomena (thermo-chemo-rheological coupling) involved in the formation of these materials may be the source of some problems related to the final product quality: collapse of the material or non-optimal development of the structure. To optimize the process, a modelling approach is proposed. The objective is to develop a multi-physic model taking into account the involved phenomena and to compare it to the experimental results.

2 Foam preparation

The method for preparing rigid tannin-based foams has already been described elsewhere [1–3]. In short, mimosa bark tannin extracts (kindly supplied by SilvaChimica, St. Michele Mondovi, Italy), is mixed with furfuryl alcohol as a co-reagent, then water is added with or without formaldehyde as an additional crosslinker and with or without diethyl ether as blowing agent. Such additives are premixed with the furfuryl alcohol and the blend is mechanically stirred until a homogeneous viscous liquid is obtained. Finally, a 65% solution of p-toluenesulphonic acid (pTSA) is added as catalyst. The exotherm caused by the self-polymerization of furfuryl alcohol and its reaction with tannin leads to the boiling of the blowing agent and to the quasi-simultaneous foaming and setting of the resultant resin.

3 Physical Model

Many models have already been implemented to simulate polymerised foam [4–7]. The porous foam structure is considered as a homogeneous medium comprising three phases: gas, solid and liquid. In a first approach, only the blowing agent is considered in the liquid (1) and gas phase (2). The rest of the matter belongs to the solid phase (3). Changes of densities are calculated from mass conservation equations, and depend on local expansion \vec{u} and diethyl ether phase change K_{de} , which itself is a function of the local temperature. Diethyl ether is considered as a liquid or as a gas below and above the phase change temperature T_{de} (34°C), respectively.

$$\frac{\partial \rho_{de;l}^a}{\partial t} + \vec{\nabla} \cdot (\rho_{de;l}^a \vec{u}) = -K_{de} \quad (1)$$

$$\frac{\partial \rho_{de;g}^a}{\partial t} + \vec{\nabla} \cdot (\rho_{de;g}^a \vec{u}) = K_{de} \quad (2)$$

$$\frac{\partial \rho_s^a}{\partial t} + \vec{\nabla} \cdot (\rho_s^a \vec{u}) = 0 \quad (3)$$

where $\rho_{de;l}^a$ and $\rho_{de;g}^a$ are densities of liquid and gas diethyl ether, respectively, and ρ_s^a is the density of solid matter.

Temperature is calculated from the energy conservation equation as follows:

$$\frac{\partial H}{\partial t} + \vec{\nabla} \cdot (\vec{Q} + H\vec{u}) = 0 \quad (4)$$

With \bar{Q} the conductive heat transfer calculated by the Fourier's law:

$$\bar{Q} = -\lambda \bar{\nabla} T \quad (5)$$

A momentum equation, including gravity \bar{g} , is used to calculate the mechanical matrix velocity. The foam is considered as a viscous medium wherein the dynamic viscosity changes with the degree of polymerisation. Gas pressure P is calculated from the gas diethyl ether density $\rho_{de:g}^a$ by using the ideal gas law.

$$\frac{\partial(\rho \bar{u})}{\partial t} + \bar{\nabla} \cdot \left(\bar{\tau} + (P - P_{atm}) \bar{I} + \rho \bar{u} \bar{u} \right) = \rho \bar{g} \quad (6)$$

where $\bar{\tau} = \eta \left(-(\bar{\nabla} \bar{u} + \bar{\nabla} \bar{u}^t) + \frac{2}{3} (\bar{\nabla} \cdot \bar{u}) \bar{I} \right)$ is the viscous stress tensor.

In addition, an equation of polymerisation is used [6].

A symmetry condition is applied on the left side boundary. There is no mass exchange with the atmosphere and a natural convective heat flux is applied at the rest of the geometry. Moreover, vertical boundaries are allowed to move only with the y direction, the top one is free and a zero velocity is imposed at the bottom.

4 Results

Experimental data were provided with a FOAMAT apparatus Model 281 (Foamat Messtechnik GmbH, Karlsruhe, Germany) for a standard test at 20°C under atmospheric pressure [1]. Simulation will be compared to experimental evolutions for temperature and expansion (Figure 1).

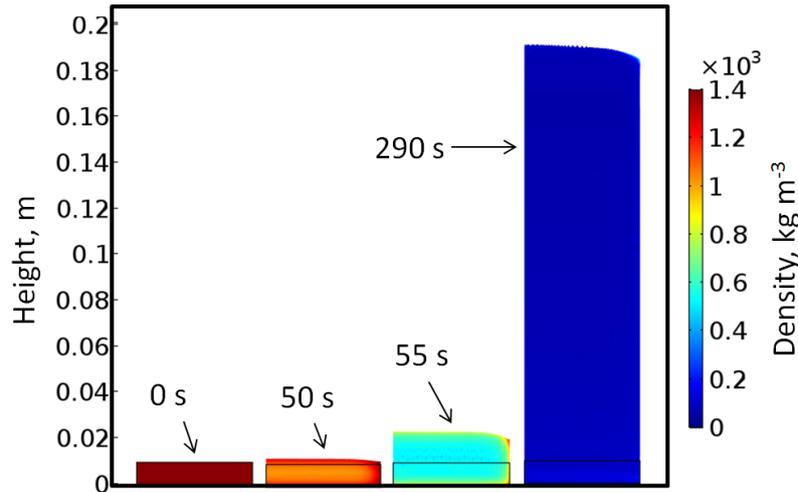


Figure 1: shape and density of simulated foams at different times

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