

# Numerical model for nanoporous silica and discrete simulation of their mechanical comporment for building insulation applications

Étienne Guesnet\*, Rémy Dendievel<sup>ø</sup>, David Jauffrès<sup>ø</sup>, Christophe L. Martin<sup>ø</sup> and Bernard Yrieix<sup>†</sup>.

\* <sup>ø</sup>: Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France  
e-mail: etienne.guesnet@simap.grenoble-inp.fr,  
web page: <http://simap.grenoble-inp.fr/>

<sup>†</sup> EDF R&D

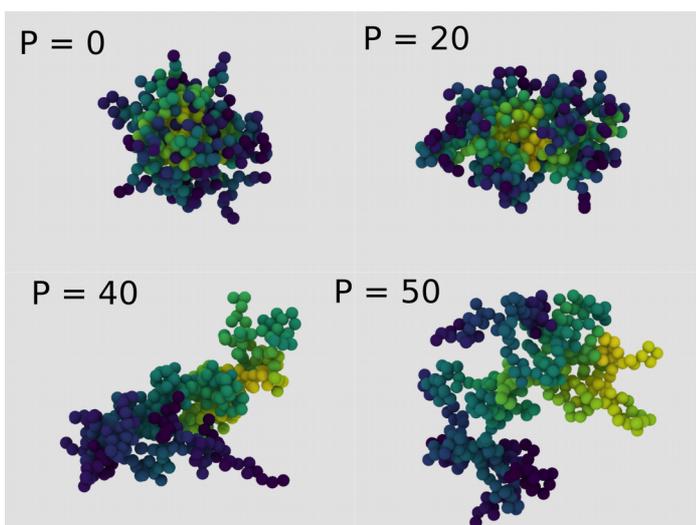
## ABSTRACT

Nanoporous materials are a natural choice for insulation materials. In particular, nanostructured silica powders are the preferred material for vacuum insulated panels (VIP) cores, with a thermal conductivity as low as  $5 \text{ mW.m}^{-1}.\text{K}^{-1}$  versus  $30 \text{ mW.m}^{-1}.\text{K}^{-1}$  for standard materials. The large amount of nanoporosity of these materials greatly decreases the thermal conductivity.

However, it comes at the price of poor mechanical properties. Here, we model and simulate the mechanical behavior of various types of nanostructured porous silica considered for VIP applications, to better understand the origin of their brittleness and to optimize their microstructure for the best strength / low thermal conductivity compromise.

Generation of numerical nanostructured silica is based on a modified Eden model [1]. In this model, the aggregate morphology is controlled by a single parameter  $P$ . The relationships between this parameter  $P$  and conventional morphology metrics (aggregate size, porosity, fractal dimension) are investigated. The suitability of our model to generate realistic aggregates is discussed with regards to experimental observations of real nanostructured silica powders.

Mechanical simulations are carried out using the discrete element method (DEM) on these numerical microstructures. DEM method is particularly well-suited to model damage and fracture behavior of porous materials with granular character [2]. Nanosilica aggregates are isostatically compacted to obtain numerical samples representing VIP core material with realistic microstructures. These samples are then characterized for strength via numerical tensile loading. In particular, the effect of aggregate morphologies is discussed. Mechanical properties and aggregate morphologies are compared with experimental results [3].



*Different aggregates generated for different  $P$ . Black particles are generated later.*

## REFERENCES

- [1] Eden, M., 1961, A two-dimensional growth process.
- [2] Pizette, P. et al., 2013, *J. Eur. Ceram. Soc.* **33**, 975–984.
- [3] Roiban, L., et al. "Advanced three dimensional characterization of silica-based ultraporous materials." *RSC Advances* 6.13 (2016): 10625-10632.