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Multi-scale modelling of heat transfer in polyurethane foams

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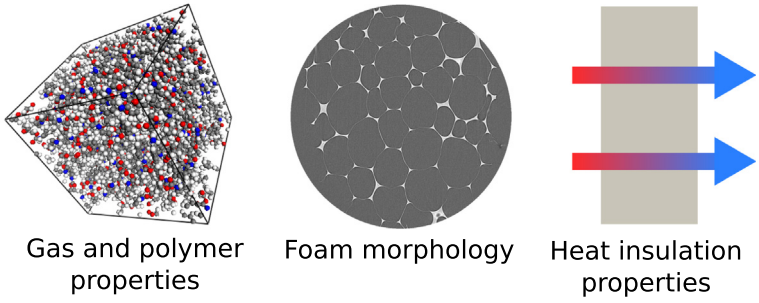
HIGHLIGHTS

- Model for the prediction of heat insulation properties of PU foams is presented.
- Absorption spectrum of PU is computed by quantum chemical density functional theory.
- Thermal conductivity of PU, gas and gas mixtures is calculated by molecular dynamics.
- Equivalent conductivity of foam is determined by homogeneous phase approach.
- Validation by experimental data showed the successfulness of proposed model.

GRAPHICAL ABSTRACT



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ABSTRACT

The influence of morphology and cell gas composition on heat insulation properties of polyurethane (PU) foams was investigated using a multi-scale mathematical model. The polymer absorption coefficient was determined from quantum chemical computations. Reverse non-equilibrium molecular dynamics was used to calculate the thermal conductivity of polymer and gas mixtures relevant to PU foams. The equivalent foam conductivity was calculated using homogeneous phase approach. The individual models were coupled together using suitable surrogate models within MoDeNa framework. To validate the proposed model 9 foam samples were prepared using different recipes, their morphology was characterized and their thermal conductivity was measured. The difference between experimental and predicted values was comparable to experimental error. Developed multi-scale model was used to identify the most suitable relation for the calculation of thermal conductivity of gas mixtures in PU foams and to quantify the influence of foam density, cell size, and strut content on heat insulation properties of PU foams.

1. Introduction

The insulation properties of PU foams are derived from their morphology, i.e., porosity, cell size, strut content, etc., and from the material properties of the polyurethane and the cell gases, i.e., their thermal conductivities and the complex index of refraction of the polymer. Conduction and radiation are the primary modes of heat transfer, because the cells of PU foams are too small for the onset of free convection (Mills, 2007; Klempner et al., 2004). In this work, we employed quantum chemical density functional theory and molecular dynamics simulations to predict material properties of gas and polymer phases.

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Nomenclature

Subscripts

C	cold slab
c	cell
f	foam
g	gas
H	hot slab
p	polymer
s	strut
w	wall

Greek letters

β	extinction coefficient (m^{-1})
κ	absorption coefficient (m^{-1})
λ	wavelength (m)
ν	wavenumber (cm^{-1})
ω	frequency (s^{-1})
ρ	density ($kg\ m^{-3}$)
ε	porosity

Latin letters

$\mathbf{q}$	heat flux ($W\ m^{-2}$)
$\mathbf{v}$	velocity (ms^{-1})
A	surface (m^2)
A_{ij}	Wassiljewa coefficients
c_p	specific heat capacity ($J\ kg^{-1}\ K^{-1}$)
$E_{b\lambda}$	spectral blackbody emissive power ($W\ m^{-3}$)
E_b	blackbody emissive power ($W\ m^{-2}$)
f_s	strut content
G	incident radiation ($W\ m^{-2}$)
G_λ	spectral incident radiation ($W\ m^{-3}$)
k	thermal conductivity ($W\ m^{-1}\ K^{-1}$)
L	domain size (m)
M	molar mass ($kg\ mol^{-1}$)
m	mass (kg)
R	gas constant ($J\ mol^{-1}\ K^{-1}$)
S	Sutherland constant (K)
T	temperature (K)
t	time (s)
V	volume (m^3)
y	molar fraction

We take special care in predicting the thermal conductivity of gas mixtures, because one of future applications of the model is the study of long-term evolution of foam insulation properties. In literature, the thermal conductivity of gas mixtures is often estimated from the conductivities of individual gases using various mixing rules. Although this approach was extensively tested for monoatomic gases and small polyatomic molecules, its precision often suffers for the prediction of conductivity of gas mixtures consisting of larger gas molecules, which are often employed as blowing agents (Dohrn et al., 2007). Accordingly, we compared the predictions of the several frequently used mixing rules and direct molecular dynamics simulations. The conductive–radiative heat transfer in foams is modelled using homogeneous phase approach (Coquard et al., 2011). Polystyrene foams were studied in the literature much more extensively than PU foams. Thus, we mainly focus on typical morphological aspects of PU foams like the strut content.

Under this perspective, the goal of this paper is to develop a multi-scale model capable of predicting the insulation properties of complex materials like PU foams based on first principles with the morphology of the material and the chemical composition of gas and solid phases being the only inputs. Papers usually describe only some aspects of the multi-scale modelling; here, we design and report a multidisciplinary strategy, in which several advanced modelling techniques are combined, yielding a multifaceted, multi-scale description of the phenomena under investigation. The models are coupled together using the MoDeNa platform (MoDeNa-EUProject, 2015). This framework utilizes concept of surrogate models for microscopic codes to enable efficient transfer of information across scales. We compare calculated results with experimental measurements and demonstrate that it is possible to create accurate and efficient predictive tool by linking models from quantum through atomistic to continuum scale.

2. Experimental

2.1. Foam preparation

The chemical components used in PU foam preparation and characterization are reported in Table 1.

The polyurethane foams characterized in this paper were prepared according to the following procedure:

Component A of the reactive foam mixture was obtained by blending polyols and additives such as foam stabilizers (surfactant), catalyst and chemical (water) and physical (cyclopentane) blowing agents in the desired ratio (see Table 2). Component B of the reactive foam mixture was an aromatic isocyanate in all cases.

For the foam preparation component A and B were mixed in a beaker in the specific ratio given in Table 2 using a Vollrath laboratory mixer with a Lenart-disc of diameter 6.5 cm at 1500 rpm for 6 s. The reaction mixture was then poured into a suitable container and left to expand and cure.

2.2. Measurement of equivalent heat conductivity

The equivalent heat conductivity of the foams was measured with a TCA 300 DTX device of the company TAURUS instruments GmbH.

The measurement is based on the principle of heat flow measurement according to ISO 8301.

2.3. Morphological analysis of foams

First, we should emphasize that this work focuses on closed-cell PU foams. Density of the foams ρ_f was determined according to

Table 1
Materials used to prepare the foam samples.

Chemical	Description/Properties	Supplier
Polyol 1	Sucrose based polyether polyol, OH value 400 mg KOH/g	BASF SE
Polyol 2	Glycerol based polyether polyol, OH value 400 mg KOH/g	BASF SE
Polyol 3	Glycerol based polyether polyol, OH value 805 mg KOH/g	BASF SE
Isocyanate	Polymeric MDI, NCO content 31.5%	BASF SE
Surfactant 1	Tegostab B 8467, silicone surfactant	Evonik Goldschmidt
Surfactant 2	Dabco DC 193, silicone surfactant	Air Products
Blowing agent	Cyclo pentane	
Catalyst	N,N-Dimethylcyclohexylamine	