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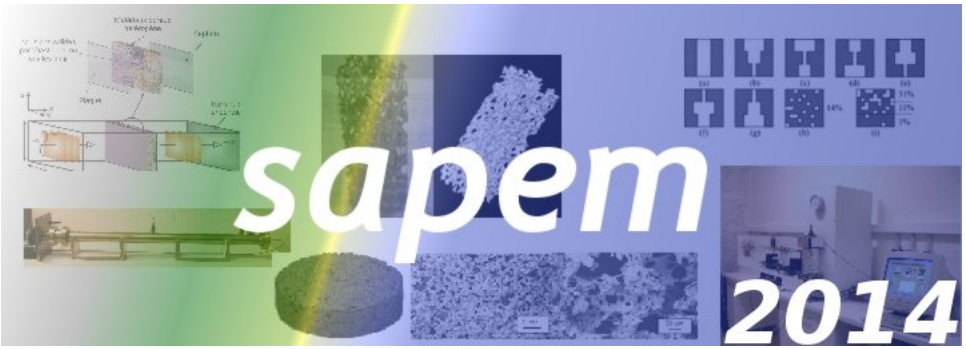

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Sound absorption modelling of granular activated carbon

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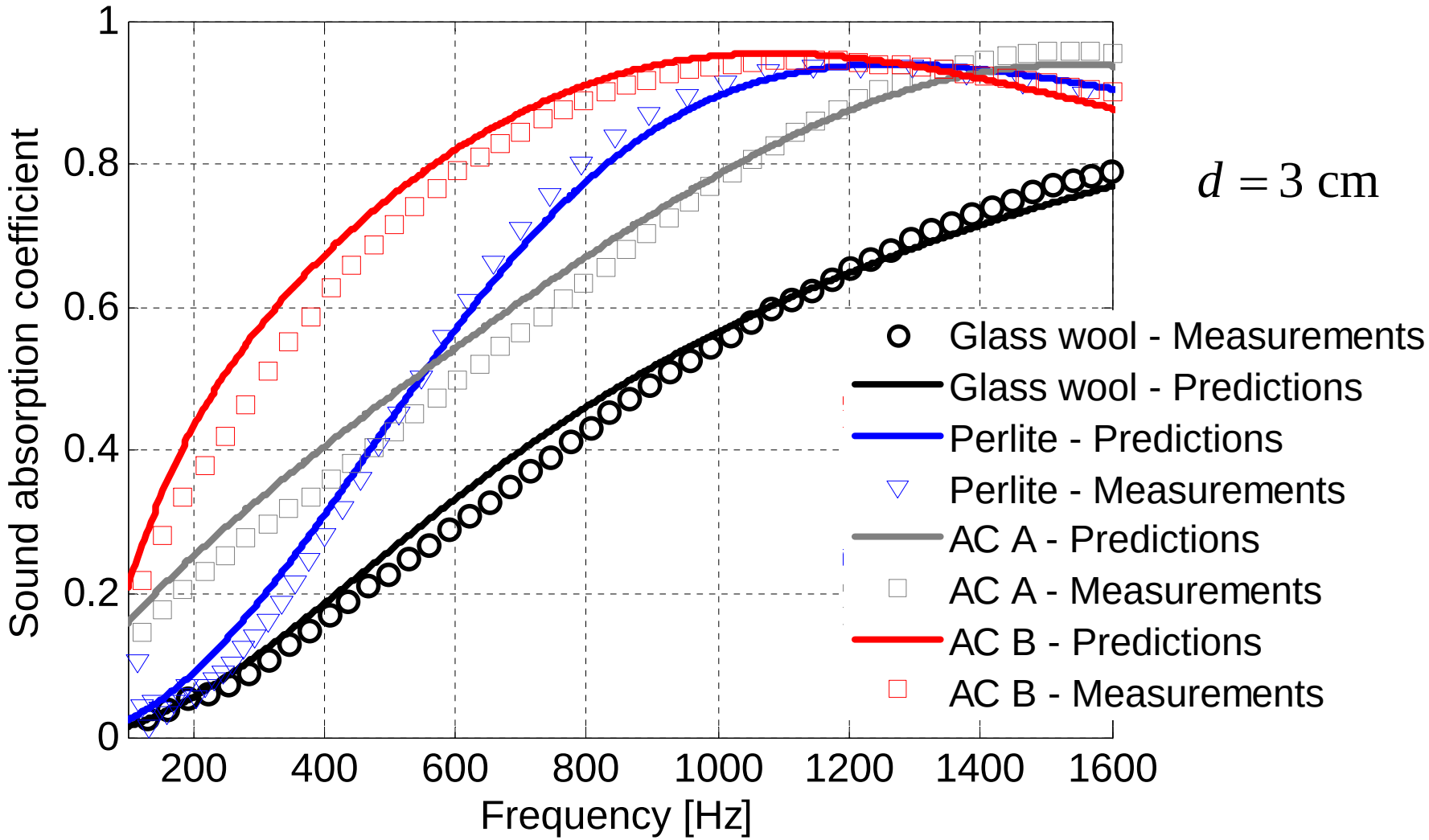
4th symposium on the acoustics of poro-elastic materials, December 16-17-18, 2014, Stockholm, Sweden

Outline

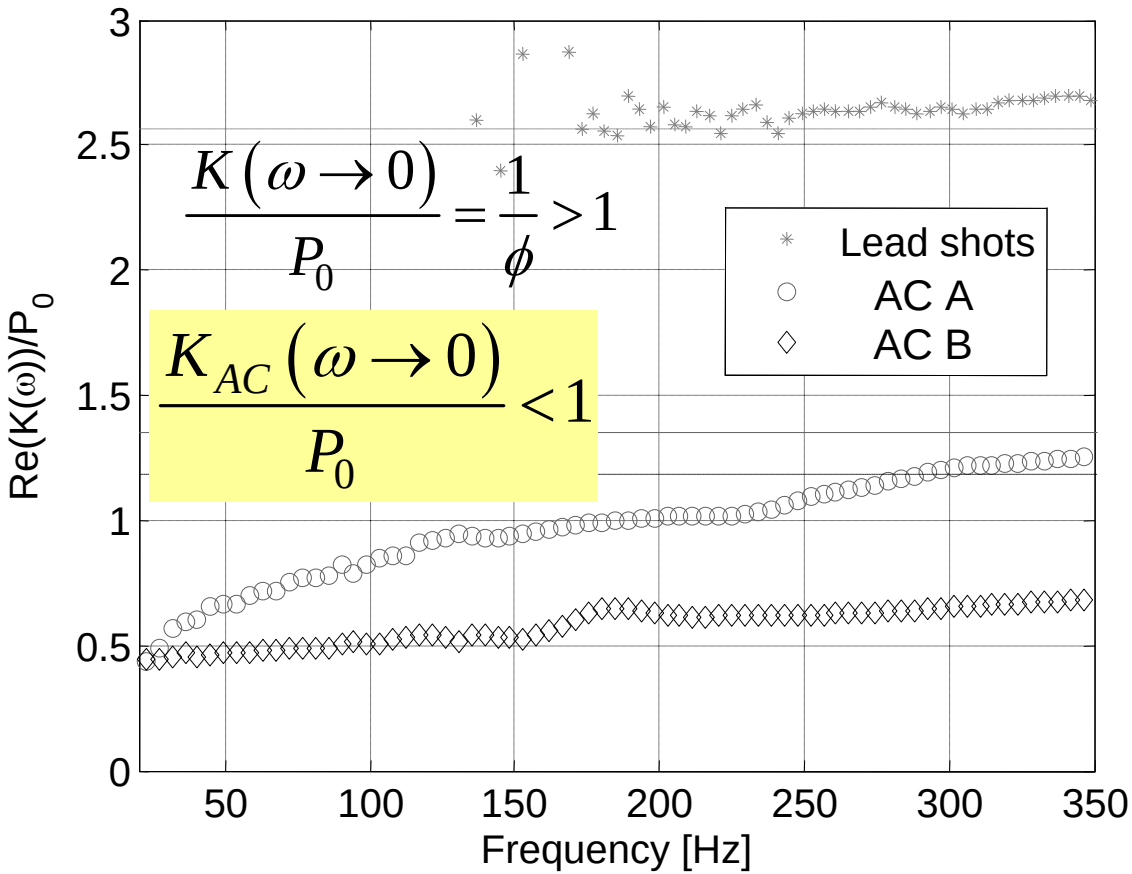
- Motivation
- Dynamic bulk modulus of granular activated carbon (GAC)
- Wave equation upscaling including sorption and rarefaction effects
- A model for sound propagation in GAC
- Acoustic characterisation of GAC
- Sound absorption of GAC - measurements vs predictions
- Future work and conclusions

Granular activated carbon (GAC) has been experimentally shown to exhibit unusually high levels of low frequency sound absorption



R. Venegas, PhD thesis, University of Salford, UK, 2011.

Dynamic bulk modulus of granular activated carbon



$$\frac{K(\omega \to 0)}{P_0} = \frac{1}{\phi} > 1$$

$$\frac{K_{AC}(\omega \to 0)}{P_0} < 1$$

- Rarefaction effects

[Venegas, PhD thesis, UoS, 2011]

- Finite heat capacity of the solid

[Lafarge et al., JASA 102 (4),1997]

- Mass transfer processes

[Raspet et al., JASA 105(1), 1999]

- Particle vibration

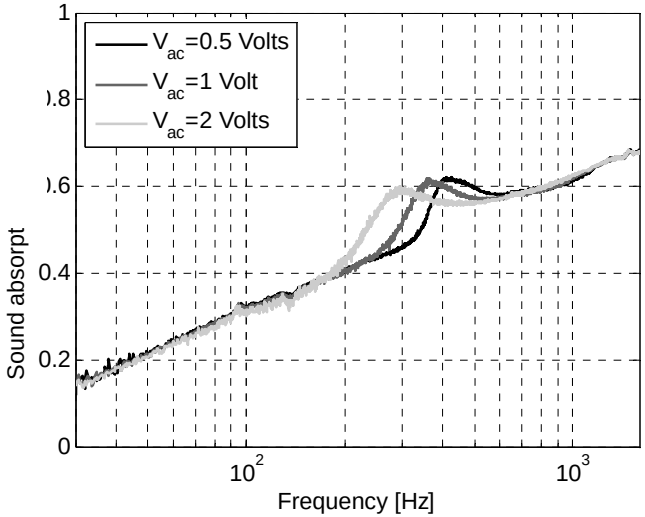
[Okudaira et al. Powder Technol. 77(1), 1993]

SORPTION PROCESSES

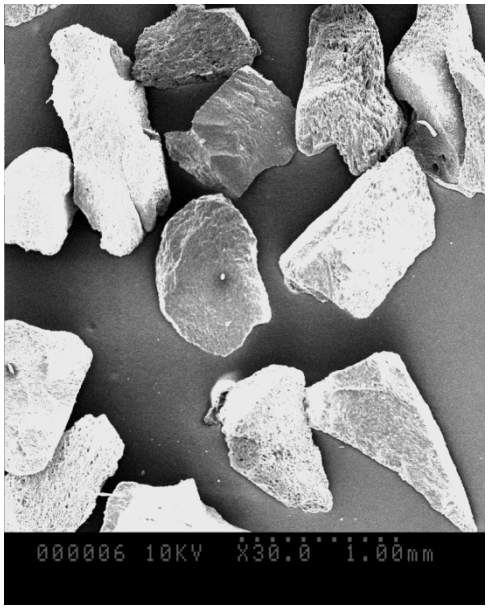
[Venegas, PhD thesis, UoS, 2011]

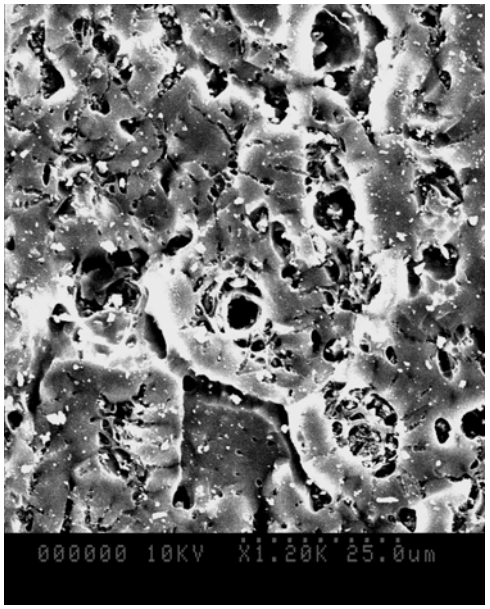
[Bechwati et al. JASA 132(1), 2012]

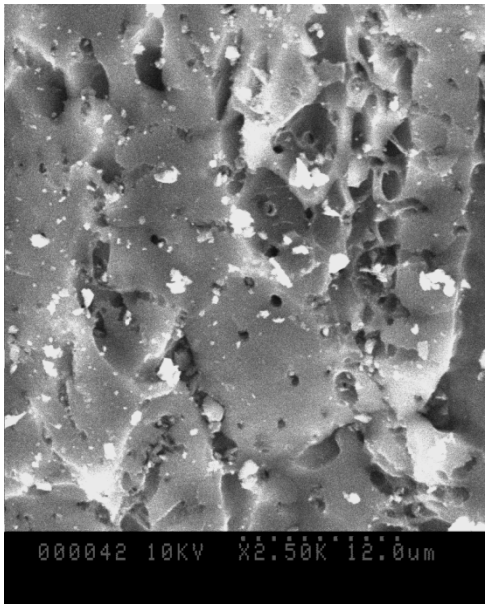
[Mellow et al., Proc of Acoustics 08, CD01. 795, 2008]



Sorption processes = adsorption+desorption







-Adsorption is a physical or chemical process in which the fluid molecules are adhered on to a surface.

- The adherence in physical adsorption is caused by weak van der Waals forces while by chemical bonding in chemical adsorption

- Desorption is the opposite phenomenon whereby the fluid molecules are released from the surface.

- The release of the molecules is caused by either an increase of temperature or a decrease in pressure.

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Langmuir model

- Based on equating the rates of adsorption and desorption.

- Assumptions:
  - The surface of the solid is homogenous - adsorption energy is constant over all sites of the surface.
  - Adsorption is localised - molecules are adsorbed at definite, localised sites (no mobile adsorption).
  - Each site can accommodate only one molecule - monolayer coverage.

$$\frac{d\tilde{\rho}_a}{dt} = k_a \tilde{p}\left(\tilde{\rho}_N - \tilde{\rho}_a\right) - k_d \tilde{\rho}_a$$

$$\rho_a = \frac{k_a k_d \rho_N}{\left(j\omega + \omega_a\right)\omega_a} p$$

ρ_N: maximum density increment

k_a: adsorption coefficient

k_d: desorption coefficient

ω_a : sorption characteristic frequency

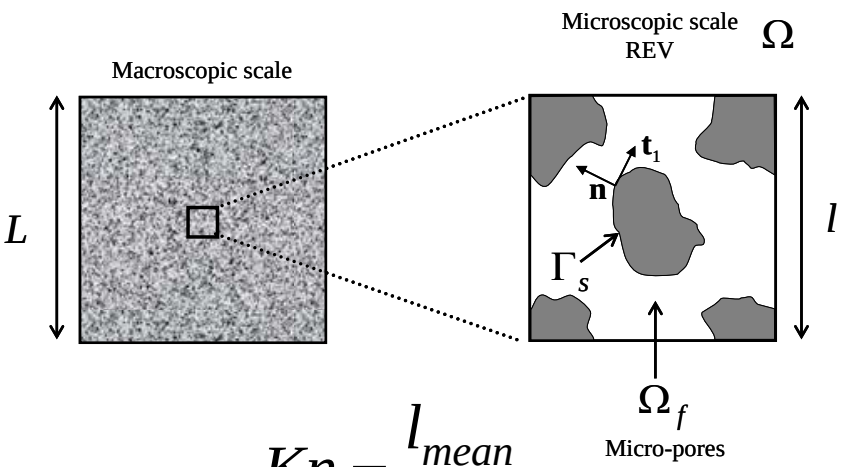
$$\omega_a = k_a P_0 + k_d$$

Rarefaction effects

- Continuum description starts to break down when the characteristic size of the material is comparable to the mean free molecular path.

- No-slip condition is replaced by slip boundary condition - velocity is proportional to the tangential shear stress.

- Zero temperature boundary condition is replaced by the temperature-jump boundary condition - temperature is proportional to the normal temperature gradient.



$$Kn = \frac{l_{mean}}{l}$$

$$l_{mean} = \frac{\eta}{p}\sqrt{\frac{\pi R_g \tau}{2}}$$

$$\mathbf{u} = -c_v l_{mean}\left(\mathbf{t}_1 \cdot \left(\nabla \mathbf{u}\right) \cdot \mathbf{n}\right)\mathbf{t}_1$$

$$\tau = c_t \frac{2\gamma}{\left(\gamma+1\right)N_{pr}} l_{mean} \nabla \tau \cdot \mathbf{n}$$

Linearised equations

Conservation of momentum

$$\eta\nabla^2\mathbf{u} - \nabla p = j\omega\rho_0\mathbf{u}$$

Conservation of mass

$$j\omega\left(\rho + \rho_a\right) + \rho_0\nabla\cdot\mathbf{u} = 0$$

Conservation of energy

$$j\omega\rho_0 C_p\tau = \kappa\nabla^2\tau + j\omega p$$

Equation of state

$$\frac{p}{P_0} = \frac{\tau}{\tau_0} + \frac{\rho}{\rho_0}$$

Langmuir equation

$$\rho_a = \frac{k_a k_d \rho_N}{\left(j\omega + \omega_a\right)\omega_a} p$$

Slip and temperature-jump boundary conditions

$$\mathbf{u} = -c_v l_{mean}\left(\mathbf{t}_1\cdot\left(\nabla\mathbf{u}\right)\cdot\mathbf{n}\right)\mathbf{t}_1$$

$$\tau = c_t\frac{2\gamma}{\left(\gamma+1\right)N_{pr}} l_{mean}\left(\nabla\tau\cdot\mathbf{n}\right)$$

R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Dimensionless equations

Conservation of momentum

$$\varepsilon^2 \eta \nabla^2 \mathbf{u} - \nabla p = j\omega\rho_0 \mathbf{u}$$

Conservation of mass

$$j\omega\left(\rho + \frac{k_a k_d \rho_N}{\left(j\omega + \omega_a\right)\omega_a} p\right) + \rho_0 \nabla \cdot \mathbf{u} = 0$$

Conservation of energy

$$\varepsilon^2 \kappa \nabla^2 \tau = j\omega\rho_0 C_p \tau - j\omega p$$

Equation of state

$$\frac{p}{P_0} = \frac{\tau}{\tau_0} + \frac{\rho}{\rho_0}$$

Slip and temperature jump boundary conditions

$$\mathbf{u} = -\varepsilon Kn\left(\mathbf{t}_1 \cdot \left(\nabla \mathbf{u}\right) \cdot \mathbf{n}\right)\mathbf{t}_1$$

$$\tau = \varepsilon \frac{2\gamma Kn}{\left(\gamma + 1\right) N_{pr}}\left(\nabla \tau \cdot \mathbf{n}\right)$$

R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Wave equation including rarefaction and sorption effects

$$\frac{j\omega}{K(\omega, Kn, S)} p^{(0)} = \frac{\mathbf{k}(\omega, Kn)}{\eta} \Delta_x p^{(0)}$$

$$K(\omega, Kn, S) = \left(\frac{1}{K_R(\omega, Kn)} + \frac{1}{K_S(\omega, S)} \right)^{-1}$$

$$K_S(\omega) = \frac{\gamma P_0}{\phi} \left(\frac{\gamma P_0 k_a k_d}{(j\omega + \omega_a)\omega_a} \frac{\rho_N}{\rho_0} \right)^{-1}$$

ρ_N: maximum density increment

k_a: adsorption coefficient

k_d: desorption coefficient

ω_a : sorption characteristic frequency

$$\omega_a = k_a P_0 + k_d$$

$$\frac{K(\omega \to 0)}{P_0} = \frac{1}{\phi} \frac{1}{\left(1 + \frac{P_0 k_a k_d}{\omega_a^2} \frac{\rho_N}{\rho_0} \right)}$$

-The overall flow is not affected by sorption processes.

-The dynamic bulk modulus is modified by sorption processes.

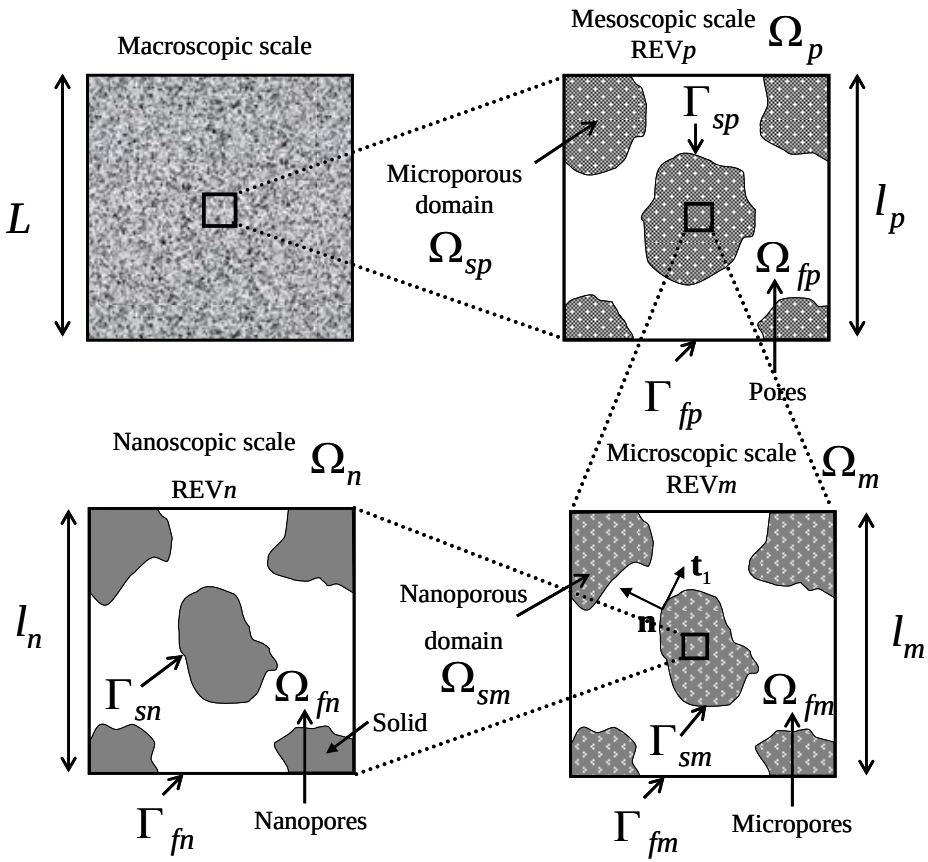
R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Model for sound propagation in granular activated carbon

Model published in [Venegas & Umnova, JASA 130 (5), 2011] is extended to account for an additional scale, and sorption and rarefaction effects

$$\phi_{tb} = \phi_p + \left(1-\phi_p\right)\phi_u = \phi_p + \left(1-\phi_p\right)\left(\phi_m + \left(1-\phi_m\right)\phi_n\right)$$



High permeability contrast between the mesoscopic and microscopic and nanoscopic scale.

$$\mathbf{k}_{tb}\left(\omega\right) \approx \mathbf{k}_p\left(\omega\right)$$

$$K_{tb}\left(\omega, Kn, S\right) = \left(\frac{1}{K_p} + \frac{\left(1-\phi_p\right)}{K_u} F_d\left(\frac{P_0}{\phi_u}\frac{\omega}{K_u}\right)\right)^{-1}$$

Low permeability contrast between the microscopic and nanoscopic scale.

$$K_u\left(\omega, Kn, S\right) = \left(\frac{1}{K_m} + \frac{\left(1-\phi_m\right)}{K_n}\right)^{-1}$$

$$\frac{K_{tb}\left(\omega \to 0\right)}{P_0} = \frac{1}{\phi_{tb}} \frac{1}{\left(1 + \left(\frac{\omega_n}{\omega_a}\right)^2\right)}$$

R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Model for sound propagation in GAC

- Granular activated carbon is modelled as a packing of spherical porous grains
- Two inner-particle scales (e.g. microscopic and nanoscopic scales) are both modelled as arrays of cylindrical pores

$$\mathbf{k}_{tb}(\omega) \approx \mathbf{k}_p(\omega)$$ ← [Boutin & Geindreau, JASA, 124 (6),2008]

[Venegas & Umnova, JASA 130 (5), 2011]

$$K_{tb}(\omega, Kn, S) = \left(\frac{1}{K_p} + \frac{(1-\phi_p)}{K_u} F_d\left(\frac{P_0}{\phi_u} \frac{\omega}{K_u} \right) \right)^{-1}$$

[Boutin & Geindreau, Phys. Rev. E 82, 2010]

$$K_u(\omega, Kn, S) = \left(\frac{1}{K_m} + \frac{(1-\phi_m)}{K_n} \right)^{-1}$$

[Kozlov et al. JASA, 117, 2005]

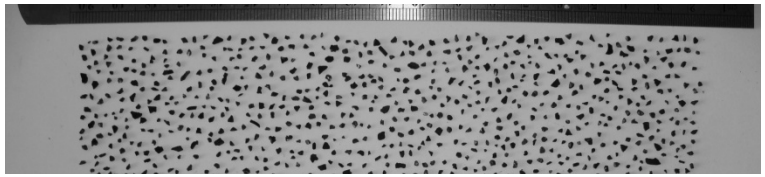
[Mellow et al., Proc of Acoustics 08, CD01. 795, 2008]

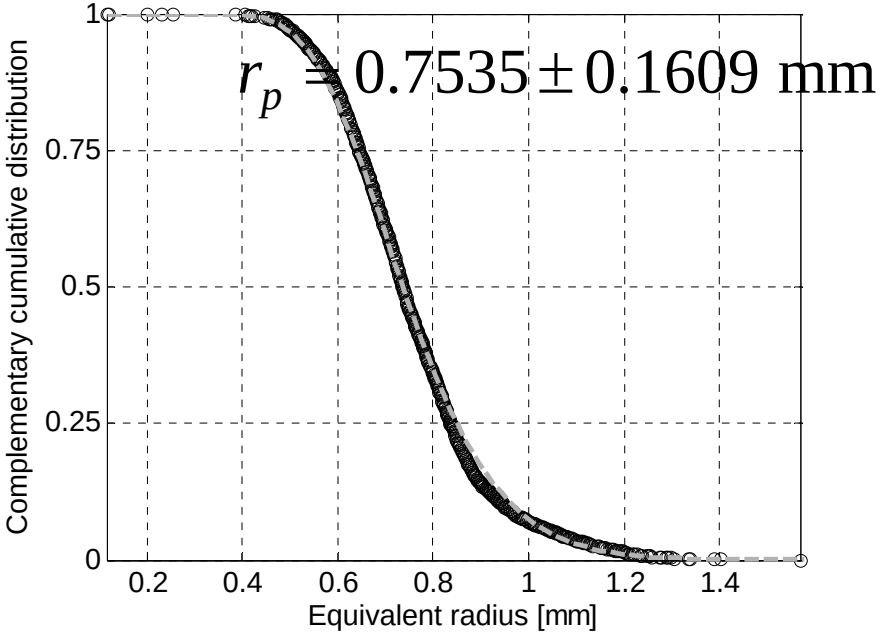
R. Venegas and O. Umnova, JASA, to be submitted

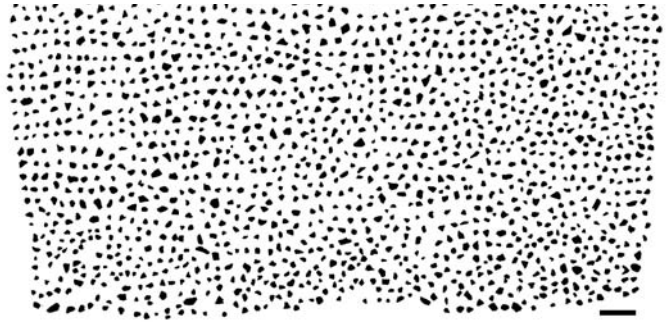
R. Venegas, PhD thesis, University of Salford, UK, 2011.

Characterisation of GAC – particle radius - optical granulometry

A







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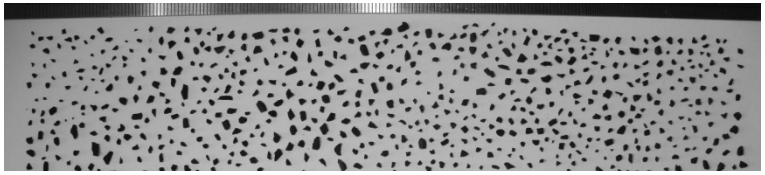
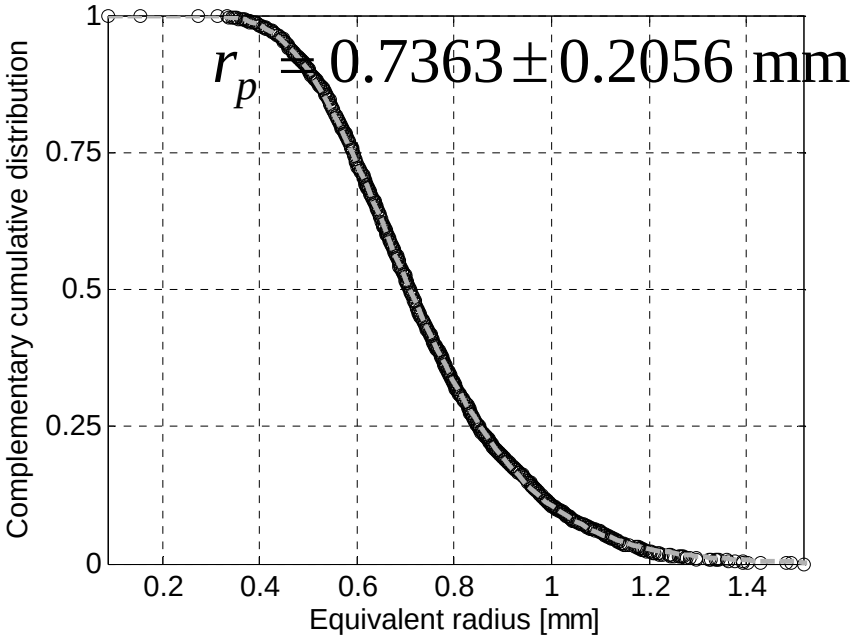
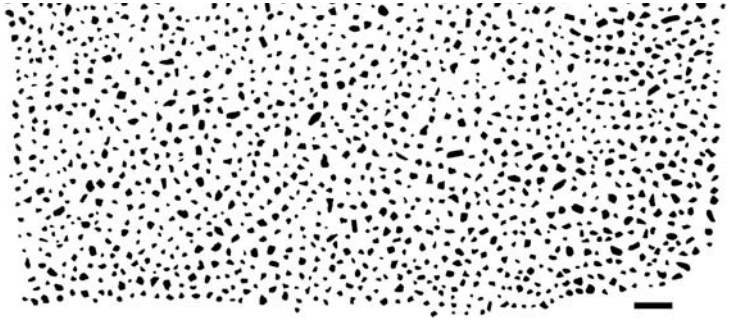






R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Characterisation of GAC – Flow resistivity and mesoporosity

- Flow resistivity measured using BS EN 29053:1993

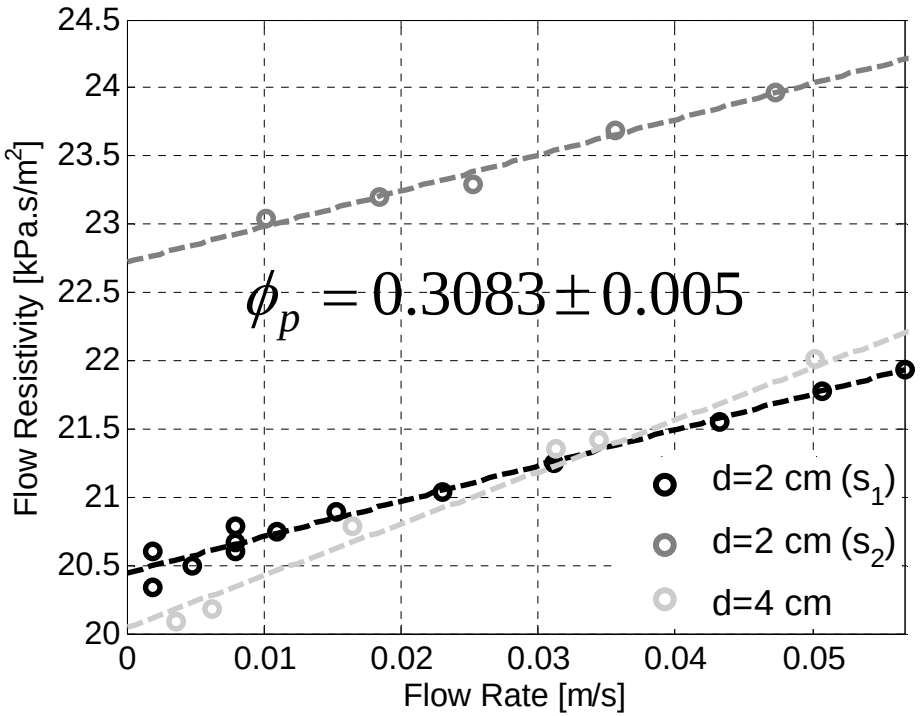
- Mesoporosity calculated by inverting:

$$k_0 = \left(\frac{r^2}{3\beta^2}\right)\left(\frac{2+3\beta^5}{\beta\left(3+2\beta^5\right)}-1\right)$$

[Boutin & Geindreau JASA,124 (6),2008]

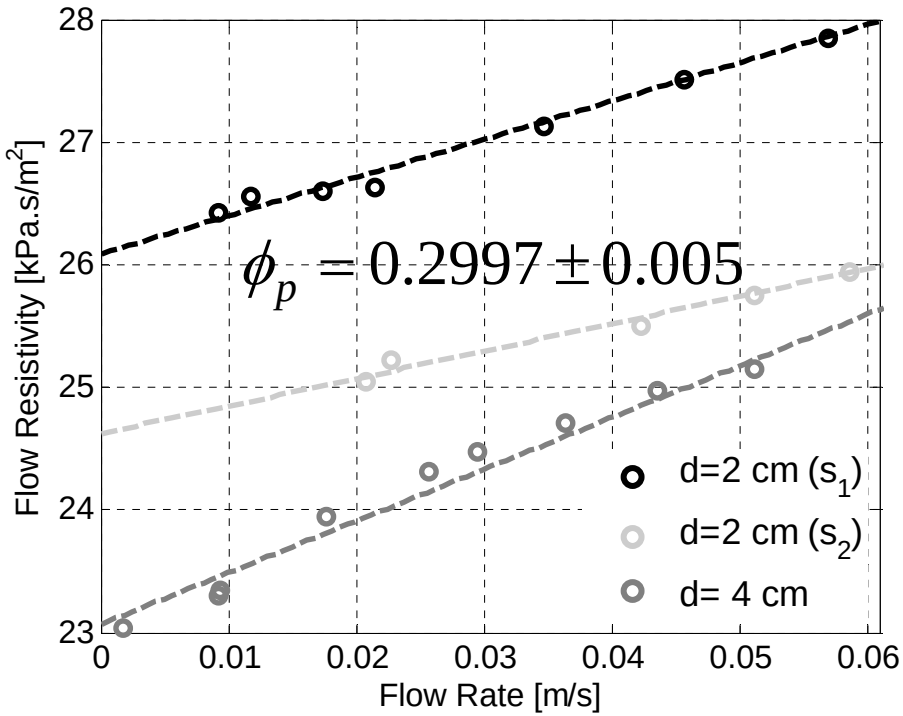
$$\beta = \left(1-\phi_p\right)^{1/3}$$

A



$$\sigma = 21.068 \pm 1.444 \text{ kPa.s.m}^{-2}$$

B



$$\sigma = 24.592 \pm 1.510 \text{ kPa.s.m}^{-2}$$

R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Characterisation of GAC – remaining parameters

- Overall porosity calculated from measured bulk density

- Nanoporosity measured from isotherms (Nitrogen @ 77K) using the Dubinin-Radushkevich method

- Microporosity calculated from the other porosity values

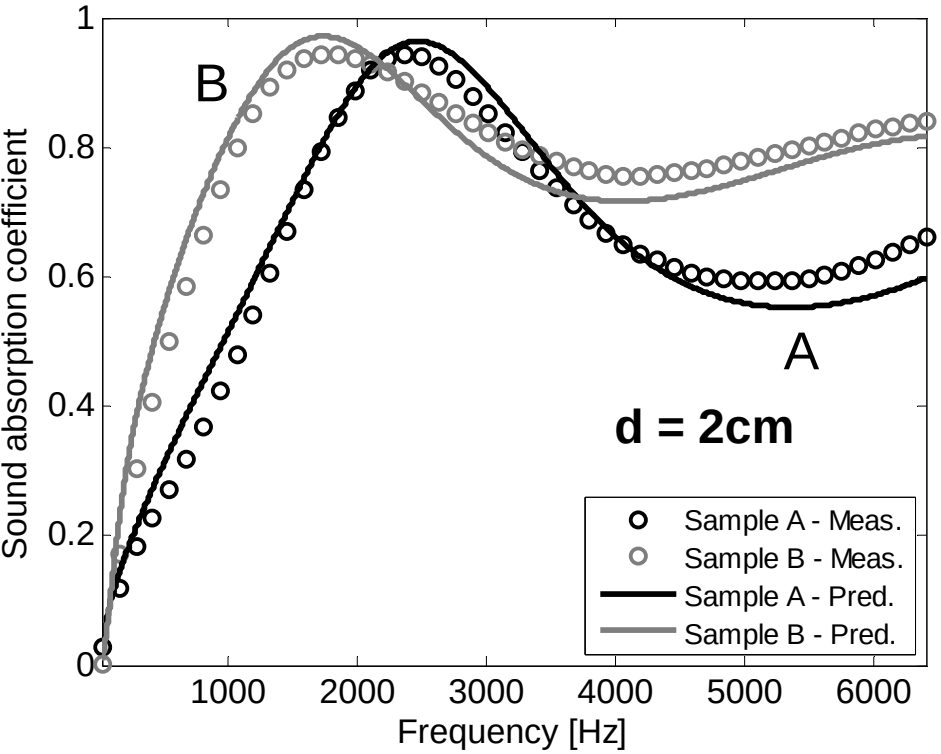
- Nanopore radius, micropore radius, and adsorption and desorption coefficients are adjusted through a best fitting routine

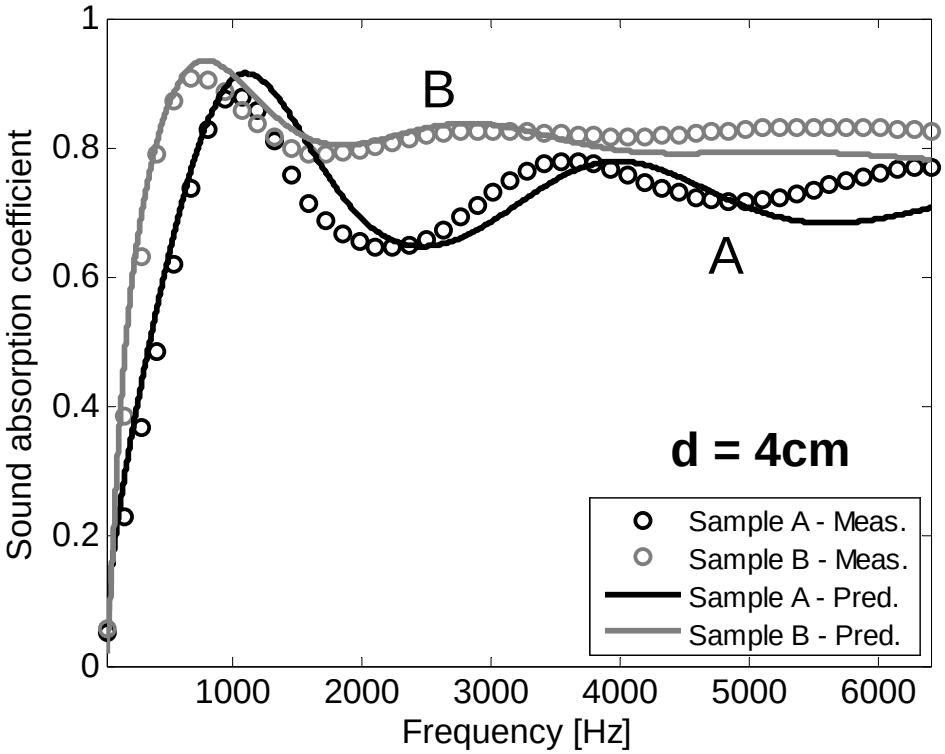
- Values of adsorption and desorption coefficients match the measured static bulk modulus

R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Sound absorption coefficient of GAC – prediction vs measurements





Sample	ϕ_p	r_p *[mm]*	ϕ_m	r_m *[μm]*	ϕ_n	r_n *[nm]*	k_a [1/Pa/s]	$k_d \times 10^{-3}$ [1/s]
A	0.3083	0.7536	0.5571	0.2048	0.1602	1.5696	1.4830	0.9881
B	0.2997	0.7363	0.7064	0.4976	0.2593	1.2868	13.8479	8.3216

- Micropore and nanopore radii in the order of those commonly found in activated carbon

- Sorption characteristic time is proportional to the square of the particle radius when the particle is “large” [Do, Imperial College Press, 1998]

R. Venegas and O. Umnova, JASA, to be submitted

R. Venegas, PhD thesis, University of Salford, UK, 2011.

Future work

- Several physical processes are likely to accompany sound propagation in granular activated carbon:
  - Diffusion [Nori & Brandani,JASA 135(5), 2014] [Crank, Clarendon press, Oxford, 1975]
  - Multi-layer sorption [Do, Imperial College Press, 1998]
  - Surface diffusion [Do, Imperial College Press, 1998]
  - Film and capillary condensate flow [Do&Do, Chem. Eng. J. 84, 2001]
  - Phase change (evaporation-condensation) [Raspet et al., JASA 105(1), 1999]
  - Competitive sorption of multiple species
  - Multi-phase flow
  - Poroelasticity [Dazel&Tournat, JASA 127(2),2010]
- Upscale the wave equation for multiscale materials including the above physical phenomena.
- Use sound as a probe.
- Too many open questions…

Conclusions

- A model for sound absorption of activated carbon has been introduced in a phenomenological manner.
- The model:
  - accounts for the multi-scale nature of the material, physical processes specific to small pores, and the interaction among several scales.
  - depends on several parameters that can be measured independently.
  - provides satisfactory predictions of sound absorption coefficient of activated carbon
- Some of the parameters have been adjusted. However, their values are representative to those normally found in activated carbon.
- Several research topics have been mentioned.

Acknowledgements

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- The authors are grateful to Chemviron for supplying the samples investigated in this work, and to Dr. T. Simpson for conducting isotherm measurements.

MANY THANKS FOR YOUR ATTENTION. YOUR QUESTIONS ARE MORE THAN WELCOME!

"THERE'S PLENTY OF ROOM AT THE BOTTOM", R. FEYNMAN, Caltech, December 29th, 1959