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A Poro-Elastic Model for Activated Carbon Stacks

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A Poro-Elastic Model for Activated Carbon Stacks

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PURDUE MECHANICAL ENGINEERING

RAY W. HERRICK LABORATORIES

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Content

- Granular Activated Carbon (GAC)
  A review of rigid model for triple porosity particles

- Poro-Elastic Model and Its Stable Approach
  Compare the stability transfer matrix method and the stable approach by Dazel, et. al with an example
  The proposed poro-elastic model for GAC

- Particle Swarm Optimization
  Introduce the settings of the fitting procedure

- Fitting Result
  Show fitted results of two types of particles and compare them with corresponding measurement

- Conclusion

Triple porosity model

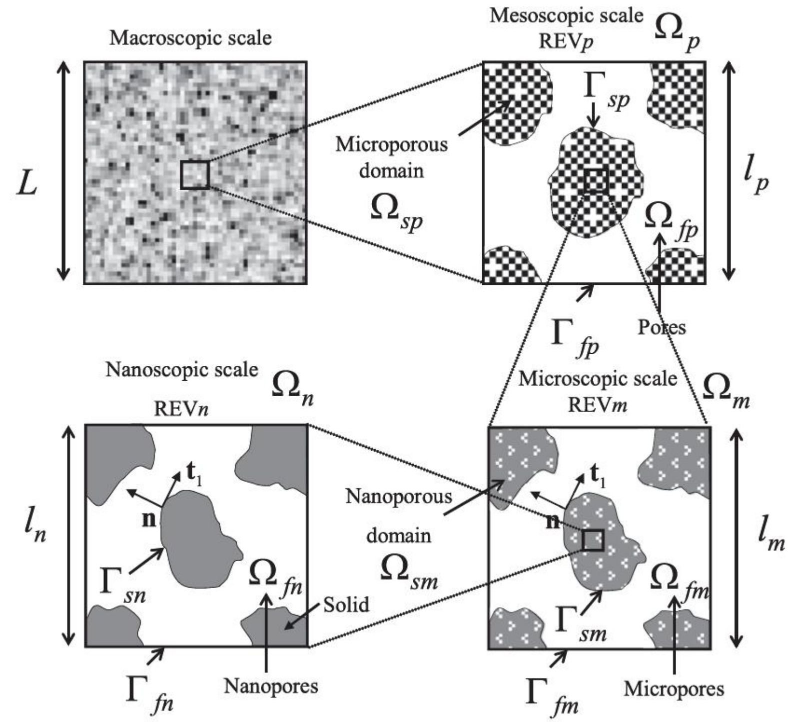
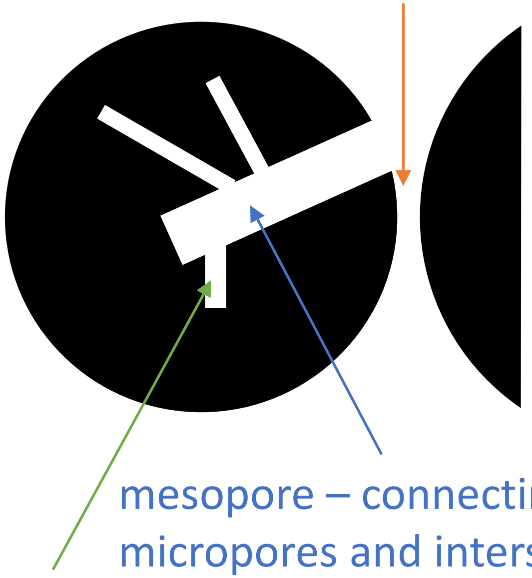


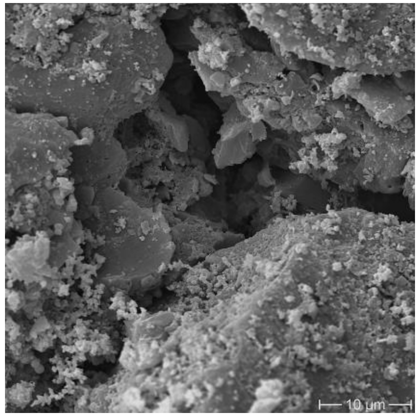
Diagram of the scales of a triple porosity sorptive material from Venegas, R., & Umnova, O. (2016)



macropore – interstice

mesopore – connecting micropores and interstice

micropore – only connected with mesopores, not directly connected to the interstice



Scanning electron microscope (SEM) photo of activated charcoal, Mydriatic, 2013. From https://commons.wikimedia.org/wiki/File:Activated_Charcoal.jpg

Such material shows excellent low frequency absorption due to its sorption process inside the pores, which brings this material into our interest to further study its properties.

r_p, r_m, r_n denote the particle radius, mesopore radius, and micropore radius.

ϕ_p, ϕ_m, ϕ_n, and ϕ_{tb} denote the porosity on intergranular scale, mesoscale, microscale, and the overall porosity. The relation between the porosities on different scales is,

$$\phi_{tb} = \phi_p + (1 - \phi_p)[\phi_m + (1 - \phi_m)\phi_n]$$

Poro-elastic model

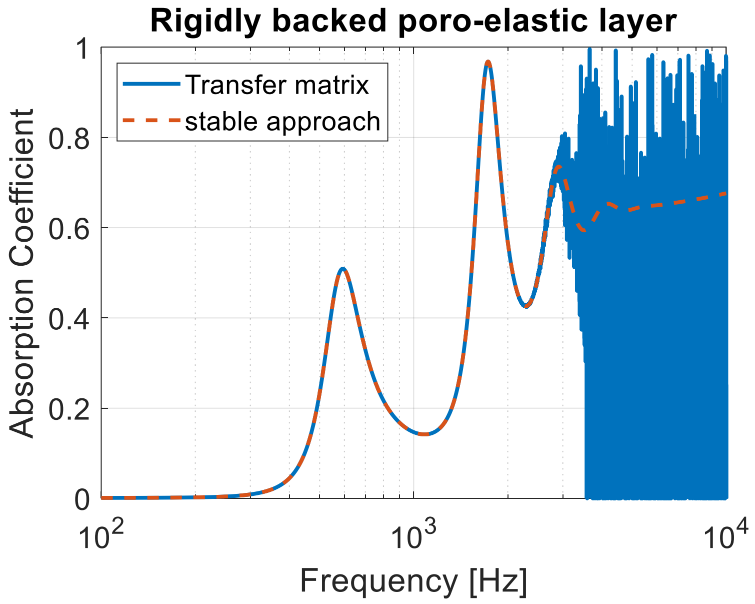
σ[rayls/m]	ϕ	α_∞	ρ_b[kg/m^3]
1.5×10^6	0.92	1.3	24

E[Pa]	Loss factor	ν	θ	d[m]
6000	0.004	0.27	0	0.03

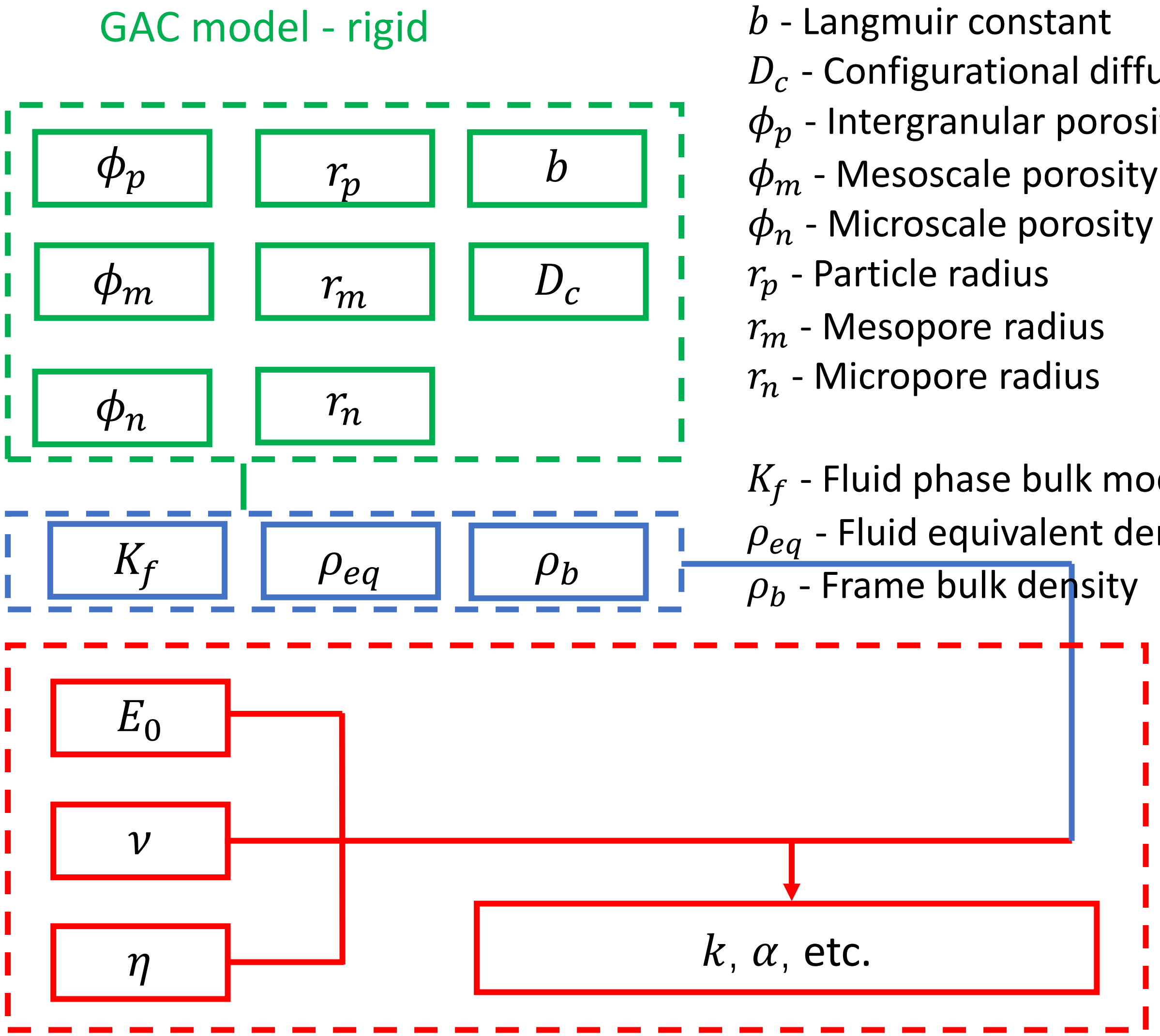
- Three waves are propagating in the porous material:
  Compressional wave in frame
  Compressional wave in fluid phase
  Shear wave in frame

- The poroelastic model was built based on the stable approach, proposed by Dazel, Groby, Brouard, and Potel in 2013.

- By comparing the absorption coefficient obtained from the transfer matrix approach and the stabilized approach, one can find perfect matching at low frequencies, before the transfer matrix approach begins to diverge.



Poro-elastic model



GAC model - rigid

ϕ_p r_p b

ϕ_m r_m D_c

ϕ_n r_n

K_f ρ_{eq} ρ_b

E_0

ν

η

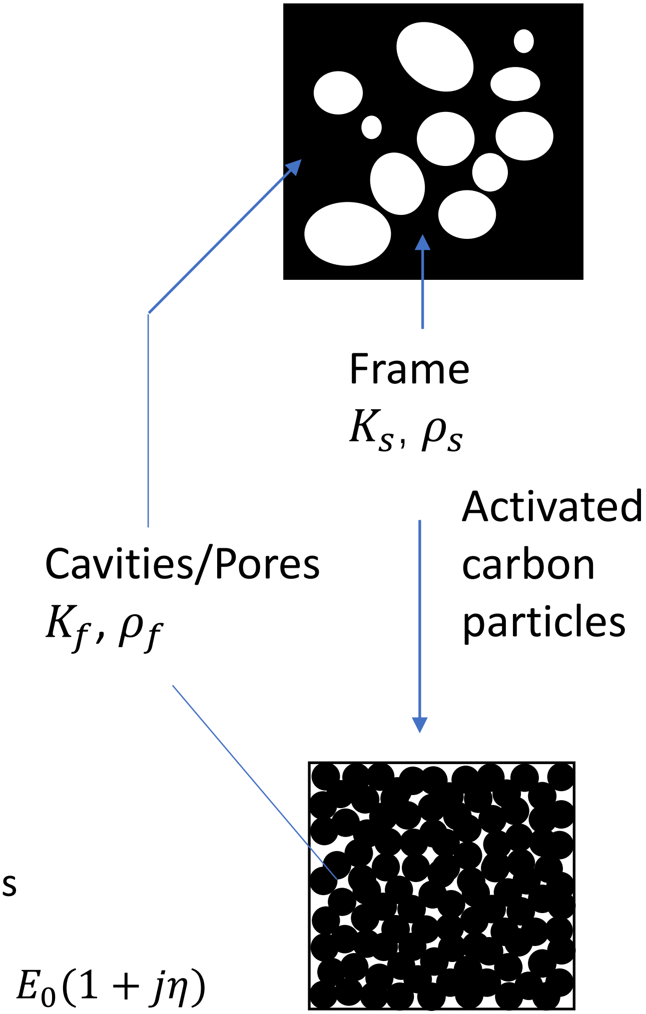
k, α, etc.

b - Langmuir constant
D_c - Configurational diffusivity
ϕ_p - Intergranular porosity
ϕ_m - Mesoscale porosity
ϕ_n - Microscale porosity
r_p - Particle radius
r_m - Mesopore radius
r_n - Micropore radius

K_f - Fluid phase bulk modulus
ρ_{eq} - Fluid equivalent density
ρ_b - Frame bulk density

E_0 - Frame modulus
ν - Poisson's ratio
η - Loss factor, $E = E_0(1 + j\eta)$

poroelastic model



Frame
K_s, ρ_s

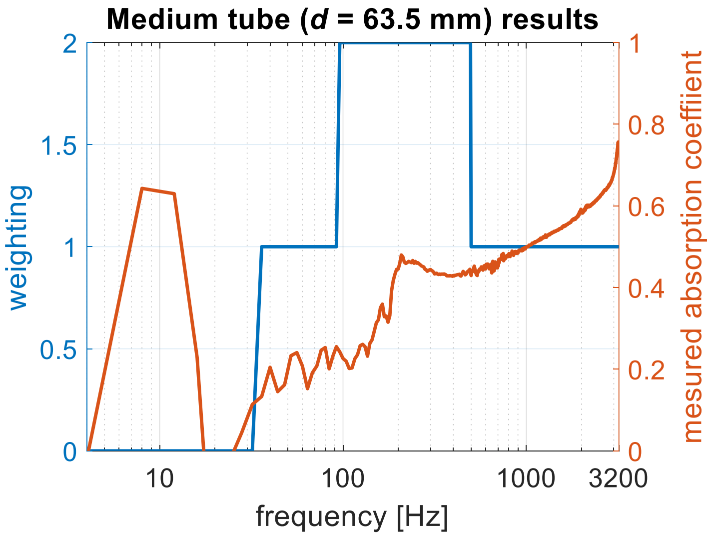
Cavities/Pores
K_f, ρ_f

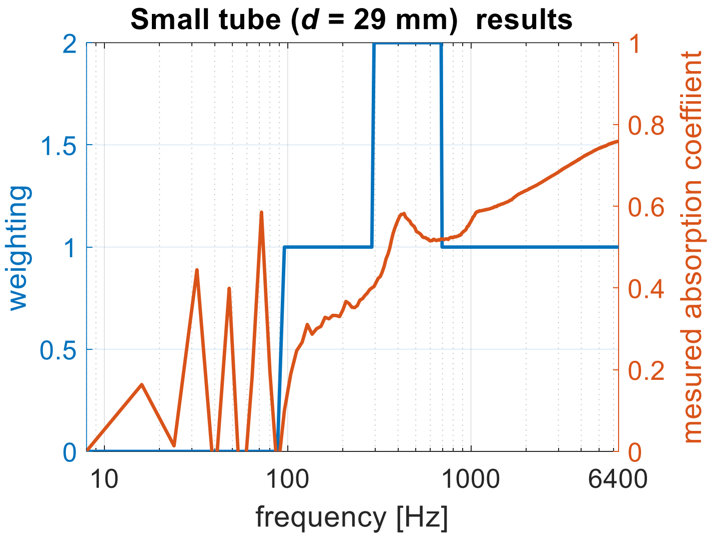
Activated carbon particles

Particle swarm optimization

All parameters are fitted with constrained particle swarm algorithm, which is realized by a package available at https://github.com/sdnchen/psomatlab or https://www.mathworks.com/matlabcentral/fileexchange/25986-constrained-particle-swarm-optimization

The frequency range corresponding to resonance peak is given higher weight to capture the feature better. The weighting plot for medium tube tests and small tube tests are given at right side.


Medium tube (d = 63.5 mm) results


Small tube (d = 29 mm) results

Target function is the weighted mean of square error between fitted and measured absorption coefficient.

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}(\mathbf{a} - \mathbf{a}_m)^2/N$$

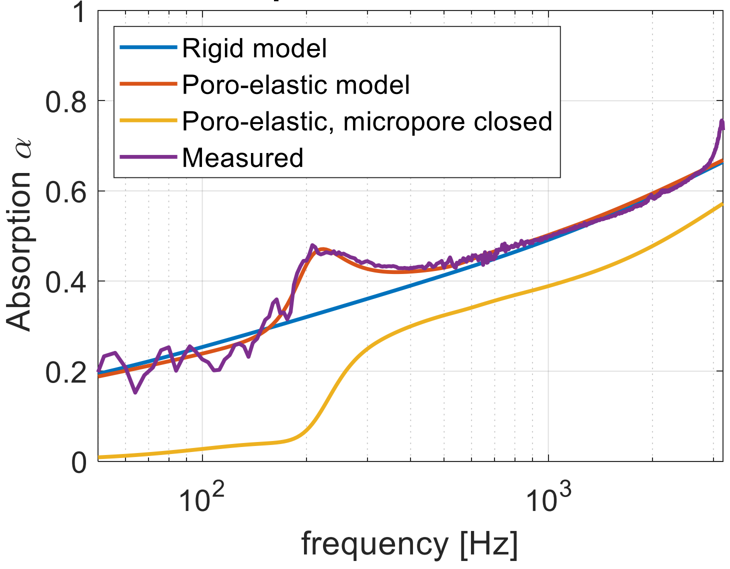
$$\text{s.t.} \quad \mathbf{x}_{lb} < \mathbf{x} < \mathbf{x}_{ub}$$

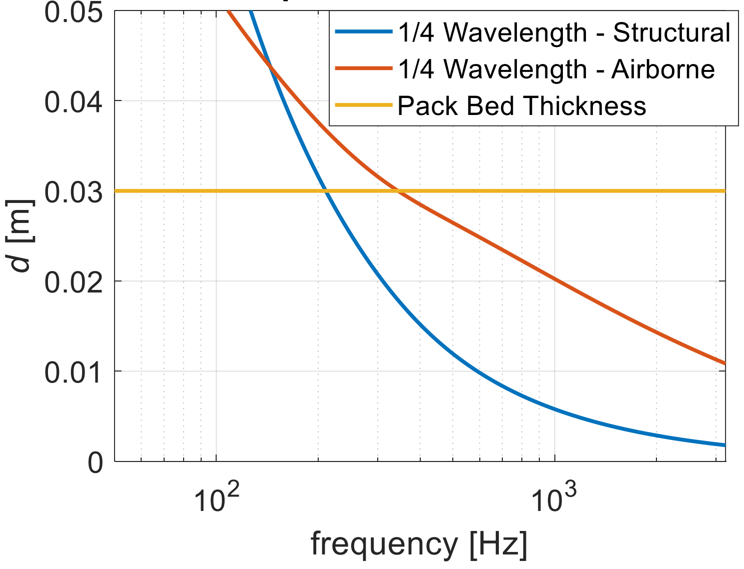
$$\rho_{lb} < \rho_c\left(1 - \phi_p - (1-\phi_p)(\phi_m + (1-\phi_m)\phi_n)\right) < \rho_{ub}$$

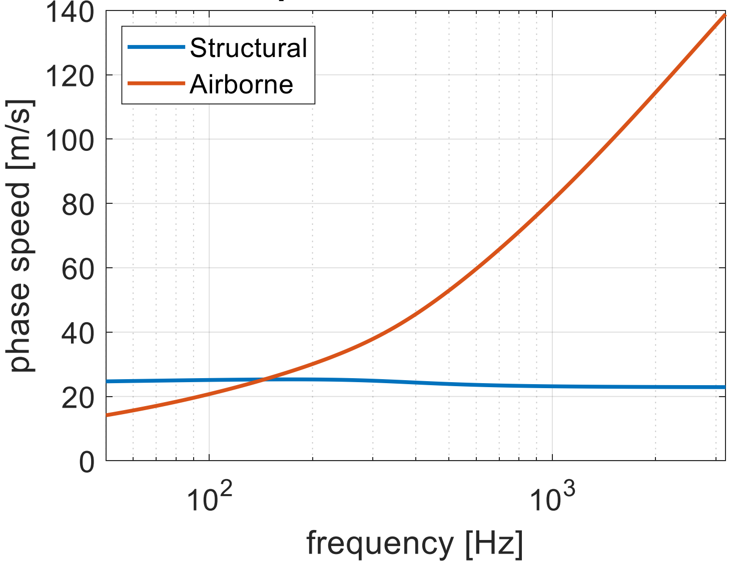
Nonlinear constrain is given on the porosities, so the predicted bulk density is in $\pm 5\%$ range of measured value for most cases.

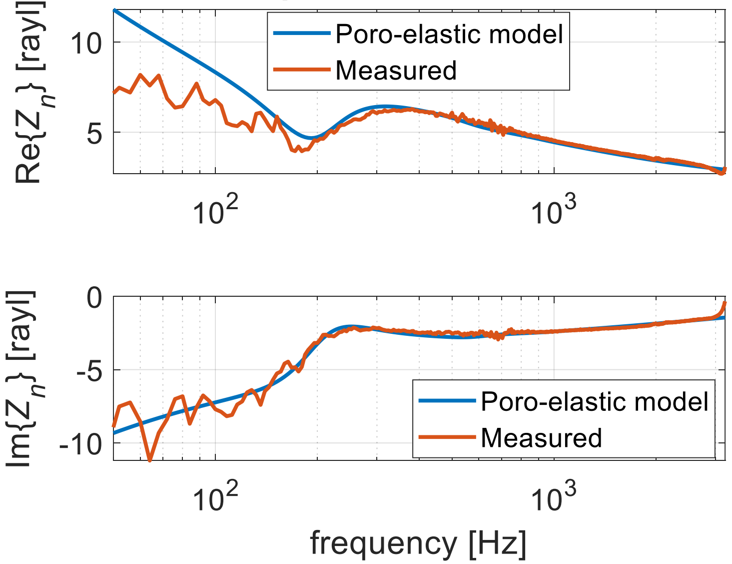
where N denotes the number of measured data points, $\mathbf{w}$ denotes the weighting vector applied, $\mathbf{x}$ denotes the poro-elastic model parameters, $\mathbf{x} = (E, \nu, \eta, \phi_p, \phi_m, \phi_n, r_p, r_m, r_n, b, D_c)$, $\mathbf{a}$ and $\mathbf{a}_m$ denote predicted and measured absorption coefficient.

Fitting Results


Sample A in Medium Tube


Sample A in Medium Tube

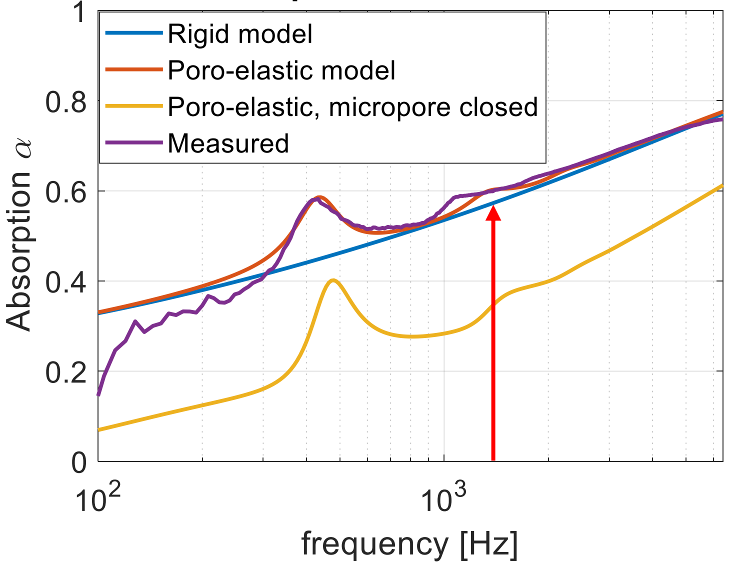

Sample A in Medium Tube

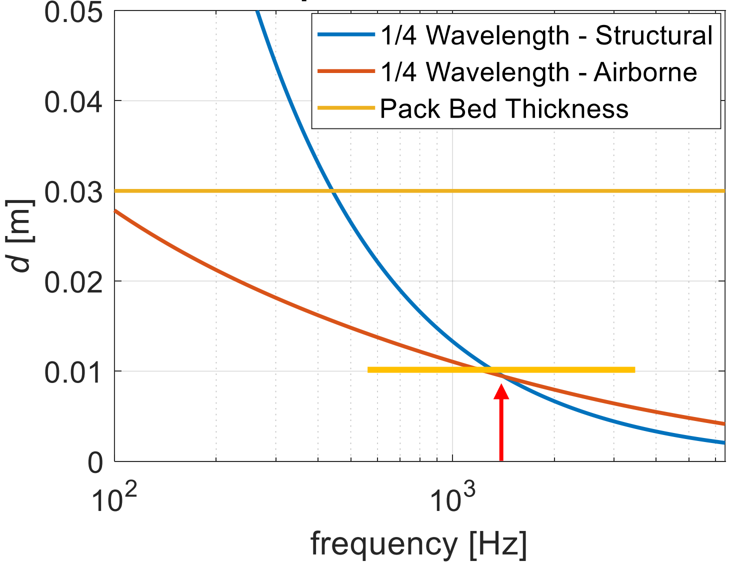

Sample A in Medium Tube

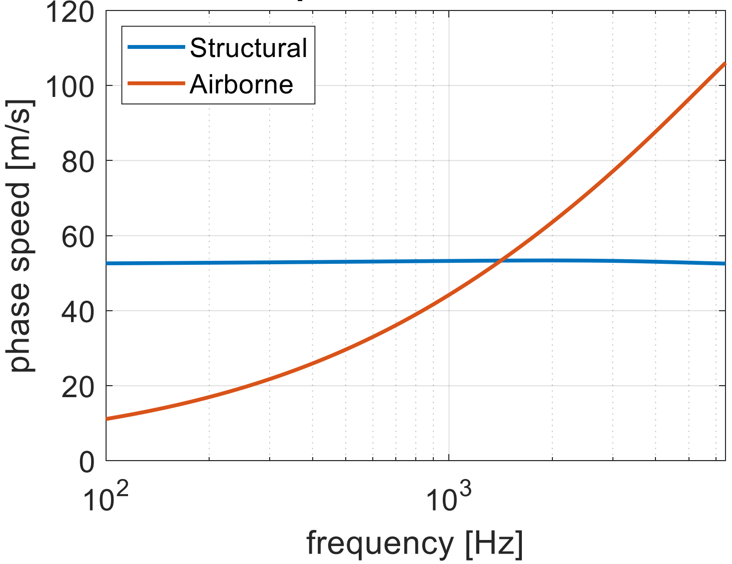
	Lower bound	Fitted value	Upper bound
r_p [mm]	0.105	**0.1111**	0.2125
r_m [μm]	0.01	**5.2526**	10
r_n [nm]	0.2	**0.3637**	0.5
ϕ_p	0.260	**0.4278**	0.476
ϕ_m	0.1	**0.1671**	0.4
ϕ_n	0.3	**0.5518**	0.8
b[Pa^{-1}]	5×10^{-7}	$\mathbf{5.3967 \times 10^{-6}}$	1×10^{-5}
D_c [m^2/s]	5×10^{-11}	$\mathbf{2.6404 \times 10^{-10}}$	5×10^{-10}
E_0 [Pa]	1×10^5	$\mathbf{2.3090 \times 10^5}$	5×10^5
η	0.01	**0.2963**	1
ν	0	**0.0357**	0.45

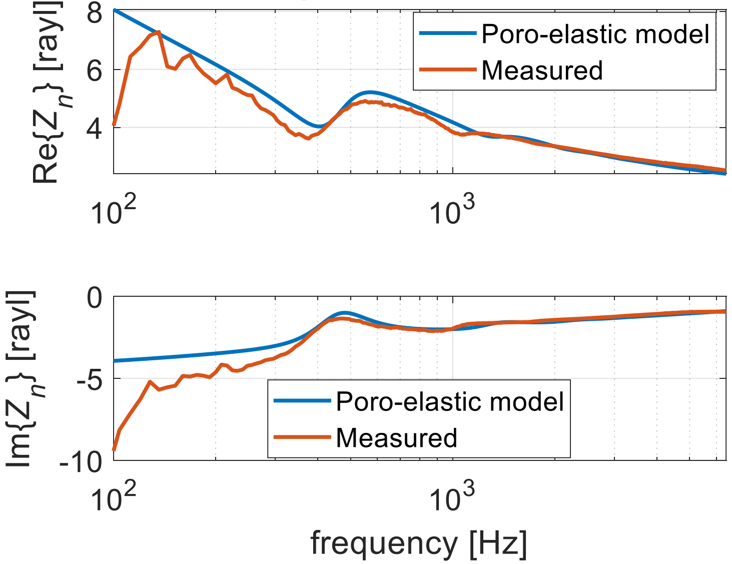
ρ_b measured in [kg/m^3]	484.73		
	Lower bound	**Fitted value**	**Upper bound**
ρ_b[kg/m^3]	460.49	469.87	508.97

Fitting Results


Sample B in Small Tube


Sample B in Small Tube


Sample B in Small Tube


Sample B in Small Tube

	Lower bound	Fitted value	Upper bound
r_p [mm]	0.075	**0.1160**	0.161
r_m [μm]	0.01	**4.5014**	10
r_n [nm]	0.2	**0.2000**	0.5
ϕ_p	0.260	**0.3524**	0.476
ϕ_m	0.2	**0.4668**	0.8
ϕ_n	0.35	**0.4989**	0.55
$b[\mathrm{Pa}^{-1}]$	5×10^{-7}	$\mathbf{7.2657 \times 10^{-6}}$	1×10^{-5}
D_c [m^2/s]	5×10^{-11}	$\mathbf{8.8559 \times 10^{-11}}$	5×10^{-10}
E_0 [Pa]	1×10^5	$\mathbf{5.2113 \times 10^5}$	5×10^5
η	0.01	**0.3552**	1
ν	0	**0.3753**	0.45

ρ_b measured in [kg/m^3]	390.42		
	Lower bound	**Fitted value**	**Upper bound**
ρ_b[kg/m^3]	370.90	380.68	409.94

Conclusions

- The poro-elastic model can predict the behavior of the particle stack at high frequencies,
  where rigid model generates similar results.
- The poro-elastic model can capture the resonance peak,
  at the frequency where the stack thickness corresponds to a quarter wavelength of structural wave.
- In some cases, a second peak in absorption coefficient is also predicted by the poro-elastic model,
  at the frequency where the stack thickness corresponds to three quarter wavelengths of structural wave.
- The fitting results from poro-elastic model gives reasonable bulk density prediction,
  in these two cases, this prediction is constrained in $\pm 5\%$ range of measured value.
- The absorption coefficient is significantly benefited from the micropores,
  which is consistent with the conclusion drew from the rigid model.

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