SUPPLEMENTARY MATERIALS: A TWO-WAY COUPLED MODEL OF VISCO-THERMO-ACOUSTIC EFFECTS IN PHOTOACOUSTIC TRACE GAS SENSORS*

ALI MOZUMDER†, ARTUR SAFIN‡, SUSAN MINKOFF†, AND JOHN ZWECK†

SM1. Supplementary Materials.

SM1.1. The effective absorption coefficient. The heat source, S, on the right hand side of (2.1) is given by $S = H/(\rho_F\, C_p)$, where H is the heat power density deposited into the gas due to the interaction between the laser and the trace gas [SM1]. Because quartz tuning forks are sharply resonant, we may assume that H is time harmonic. As in Petra [SM2], we model the laser as a Gaussian beam so that

$$S = \Re\left[C_S\, e^{-r^2/2\,\sigma^2}\; e^{-i\,\omega\, t}\right], \tag{SM1.1}$$

where $\Re(w)$ denotes the real part of a complex number w, r is the radial distance from the axis of the beam, σ is the beam width, ω is the angular frequency of the periodic interaction between the laser and the trace gas, and

$$C_S = \frac{\alpha_{\text{eff}}}{\rho_F C_p}\frac{W_L}{4\pi\sigma^2}. \tag{SM1.2}$$

Here W_L is the laser power, and α_{eff} is the effective absorption coefficient.

We now discuss how the effective absorption coefficient, α_{eff}, depends on the ambient pressure, P_0. In a trace gas sensing experiment, the wavelength of the laser is chosen to excite a particular absorption line of the trace gas. By the Beer-Lambert law, the absorption per unit length of light intensity at wavelength, λ, is of the form

$$\alpha(\lambda) = A\kappa(\lambda)N, \tag{SM1.3}$$

where A is the line strength, κ is the line-shape function, and N is the number density of the trace gas. In a typical trace gas sensing experiment, molecules of a trace gas such as ammonia are mixed with molecules of nitrogen in a fixed molecular ratio. This ratio is preserved when the gas sample is depressurized for experiments at low ambient pressure. Consequently, by the ideal gas law, the number density, N, of the trace gas is proportional to the ambient pressure, P_0. Furthermore, because of pressure-broadening effects, the width of the line-shape function also depends on P_0. In a QEPAS or ROTADE trace gas sensor, the wavelength of the laser is sinusoidally modulated about the central wavelength, λ_c, of a targeted absorption line, so that $\lambda(t) = \lambda_c + \lambda_{\text{amp}}\sin(2\pi f t/2)$, where f is the resonance frequency of the tuning fork. Therefore, as in Petra et al. [SM2], the effective absorption coefficient is of the form

$$\alpha_{\text{eff}} = \widetilde{A}P_0 \left| \int_{-\pi}^{\pi} \kappa(\lambda_c + \lambda_{\text{amp}}\sin s)e^{2is}\, ds\right|, \tag{SM1.4}$$

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†Department of Mathematical Sciences, University of Texas at Dallas (axm164531@utdallas.edu, sminkoff@utdallas.edu, zweck@utdallas.edu, https://math.utdallas.edu).

‡Swiss Federal Institute of Aquatic Science and Technology (asafin@gmail.com).

for some pressure-independent constant, $\widetilde{A}$. If we assume that the targeted absorption line is well separated from the other absorption lines, it is reasonable to assume that the line-shape function is a Lorentzian, with a half width at half maximum, γ, that depends on P_0. If the laser modulation amplitude is chosen so that $\lambda_{\text{amp}} = \beta\gamma$, then

$$\alpha_{\text{eff}}(\beta) = \widetilde{A} P_0 \left| \int_{-\pi}^{\pi} \frac{e^{2is}}{1 + (\beta \sin s)^2}\, ds \right|, \tag{SM1.5}$$

where the integrand is now independent of P_0 and is maximized at $\beta \approx 2$. Under these assumptions, we conclude that

$$C_S = \frac{\alpha_{\text{eff,ref}}\, R_0 T_0}{P_{\text{ref}}\, C_p} \frac{W_L}{4\pi\sigma^2}, \tag{SM1.6}$$

where $\alpha_{\text{eff,ref}}$ is the absorption coefficient at ambient pressure, P_{ref}, and where R_0 is the ideal gas constant and T_0 is the ambient temperature. We caution however that in practice the targeted absorption line may not be sufficiently well separated from neighbouring lines to ensure the accuracy of (SM1.6) once the ambient pressure exceeds some threshold [SM3].

SM1.2. Eigenfrequency of the undamped structure. We compute the eigenfrequency of the undamped structure by solving the eigenproblem

$$\begin{aligned} \nabla \cdot C[\nabla \mathbf{u}] + \rho_S\, \omega_0^2\, \mathbf{u} &= 0 \quad \text{in} \quad \Omega_S, \\ \mathbf{u} &= 0 \quad \text{on} \quad \partial\Omega_S^{\text{Fixed}}, \\ C[\nabla \mathbf{u}]\mathbf{n} &= 0 \quad \text{on} \quad \partial\Omega_S^{\text{Free}}, \end{aligned} \tag{SM1.7}$$

where $\mathbf{n}$ is the normal vector field on $\partial\Omega_S^{\text{Free}}$ and ω_0 is an undamped eigenfrequency to be determined. With the annular geometry, the eigenproblem (SM1.7) reduces to

$$\begin{aligned} r^2\, u'' + r\, u' + \left(\kappa_0^2\, r^2 - 1\right) u &= 0, \qquad \text{for } R_1 \le r \le R_2, \\ u &= 0, \qquad \text{for } r = R_2, \\ \frac{\lambda_S}{r}\, u + (\lambda_S + 2\,\mu_S)\, u' &= 0, \qquad \text{for } r = R_1, \end{aligned} \tag{SM1.8}$$

where $\kappa_0 = \sqrt{\frac{\rho_S\, \omega_0^2}{\lambda_S + 2\,\mu_S}}$ and $\lambda_S,\ \mu_S$ are the Lamé parameters. The general solution of (SM1.8) is

$$u(r) = d_1\, J_1(\kappa_0\, r) + d_2\, Y_1(\kappa_0\, r), \tag{SM1.9}$$

where d_1 and d_2 are arbitrary constants. The undamped eigenfrequencies, ω_0, correspond to values of κ_0 for which (SM1.8) has a nontrivial solution, i.e., to nontrivial solutions of the boundary interface condition equations

$$\begin{bmatrix} J_1(\kappa_0\, R_2) & Y_1(\kappa_0\, R_2) \\ \frac{\xi_1\, J_1(\kappa_0\, R_1)}{R_1} - \kappa_0\, \xi_2\, J_2(\kappa_0\, R_1) & \frac{\xi_1\, Y_1(\kappa_0\, R_1)}{R_1} - \kappa_0\, \xi_2\, Y_2(\kappa_0\, R_1) \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{SM1.10}$$

where $\xi_1 = 2(\lambda_S + \mu_S)$ and $\xi_2 = (\lambda_S + 2\mu_S)$. We use a numerical root finding method to determine the smallest positive value of ω_0 for which the determinant of the matrix in (SM1.10) is zero.

SM1.3. Interface and boundary conditions for the two-way coupled model. In this appendix we provide formulae for the entries in the matrix $\mathbf{A}$ and vector $\mathbf{F}$ in (3.18) for the two-way coupled model.

The first row of $\mathbf{A}$, which is obtained using the continuity condition (2.6) for the temperature at the interface, together with formulae (3.10) and (3.12) for the temperature in the fluid and in the structure, is given by,

$$a_{11} = -\, J_0(\kappa_p \tilde{R}_{1F}), \quad a_{12} = -\, J_0(\kappa_t \tilde{R}_{1F}), \quad a_{13} = \; J_0(\lambda \tilde{R}_{1S}), \quad a_{14} = \; H_0^{(1)}(\lambda \tilde{R}_{1S}),$$

and

$$\begin{aligned} F_1 = & c_1(\tilde{R}_{1F})\; J_0(\kappa_p \tilde{R}_{1F}) + c_2(\tilde{R}_{1F})\; H_0^{(1)}(\kappa_p\; \tilde{R}_{1F}) + c_3(\tilde{R}_{1F})\; J_0(\kappa_t \tilde{R}_{1F}) \\ & + c_4(\tilde{R}_{1F})\; H_0^{(1)}(\kappa_t\; \tilde{R}_{1F}), \end{aligned}$$

where, $\widetilde{R}_{1F} \; = \; R_1/r_c$ with $r_c = c/\omega$ and $\widetilde{R}_{1S} \; = \; R_1/r_s$ with $r_s \; = \; \sqrt{\frac{\lambda_S + 2\mu_S}{\rho_S\, \omega^2}}$.

The second row of $\mathbf{A}$, which is obtained by assuming the temperature at the outer surface of the annulus is zero, together with formula (3.12) for the temperature in the structure, is given by

$$a_{23} = \; J_0(\lambda \tilde{R}_2) \qquad \text{and} \qquad a_{24} = \; H_0^{(1)}(\lambda \tilde{R}_2),$$

where $\widetilde{R}_2 \; = \; R_2/r_s$.

The third row of $\mathbf{A}$, which is obtained using the continuity of heat flux condition (2.7) at the fluid-structure interface, together with formulae (3.10) and (3.12) for the temperature in the fluid and in the structure, is given by

$$\begin{aligned} a_{31} \; &= \; -\frac{K_F}{r_c}\, \kappa_p\; J_1(\kappa_p \tilde{R}_{1F}), & a_{32} \; &= \; -\frac{K_F}{r_c}\, \kappa_t\; J_1(\kappa_t \tilde{R}_{1F}), \\ a_{33} \; &= \; \frac{K_S}{r_s}\; \lambda\;\; J_1(\lambda \tilde{R}_{1S}), & a_{34} \; &= \; \frac{K_S}{r_s}\; \lambda\;\; H_1^{(1)}(\lambda \tilde{R}_{1S}). \end{aligned}$$

and

$$\begin{aligned} F_3 = \frac{K_F}{r_c} \Big[& c_1'(\tilde{R}_{1F})\; J_0(\kappa_p \tilde{R}_{1F}) - \kappa_p\; c_1(\tilde{R}_{1F})\; J_1(\kappa_p \tilde{R}_{1F}) + c_2'(\tilde{R}_{1F})\; H_0^{(1)}(\kappa_p\; \tilde{R}_{1F}) \\ & - \kappa_p\; c_2(\tilde{R}_{1F})\; H_1^{(1)}(\kappa_p\; \tilde{R}_{1F}) + c_3'(\tilde{R}_{1F})\; J_0(\kappa_t \tilde{R}_{1F}) - \kappa_t\; c_3(\tilde{R}_{1F})\; J_1(\kappa_t \tilde{R}_{1F}) \\ & + c_4'(\tilde{R}_{1F})\; H_0^{(1)}(\kappa_t\; \tilde{R}_{1F}) - \kappa_t\; c_4(\tilde{R}_{1F})\; H_1^{(1)}(\kappa_t\; \tilde{R}_{1F}) \Big]. \end{aligned}$$

The fourth row of $\mathbf{A}$ is obtained by using the fact that the structure is clamped at the outer boundary, $\mathbf{u}(R_2) \; = \; 0$. Together with the formula (3.6) for the displacement of the structure, we obtain

$$a_{43} = \tfrac{\lambda \pi}{2} \left[J_1(\kappa_u \tilde{R}_2) \int_{\tilde{R}_{1S}}^{\tilde{R}_2} s Y_1(\kappa_u\, s)\, J_1(\lambda\, s) ds - Y_1(\kappa_u \tilde{R}_2) \int_{\tilde{R}_{1S}}^{\tilde{R}_2} s\, J_1(\kappa_u\, s)\, J_1(\lambda\, s) ds \right]$$

$$a_{44} = \tfrac{\lambda \pi}{2} \left[J_1(\kappa_u \tilde{R}_2) \int_{\tilde{R}_{1S}}^{\tilde{R}_2} s Y_1(\kappa_u s) H_1^{(1)}(\lambda s) ds - Y_1(\kappa_u \tilde{R}_2) \int_{\tilde{R}_{1S}}^{\tilde{R}_2} s J_1(\kappa_u s) H_1^{(1)}(\lambda s) ds \right]$$

$$a_{45} \; = \; J_1(\kappa_u \tilde{R}_2), \quad a_{46} \; = \; Y_1(\kappa_u \tilde{R}_2).$$

The fifth row of $\mathbf{A}$ is obtained from the interface condition (3.3) for the fluid pressure and temperature on the structure. Together with the formulae (3.9), (3.10) and (3.3) for the pressure and temperature in the fluid and displacement of the structure, we obtain

$$a_{51} = \frac{p_0}{r_c}\,\kappa_p\; J_1(\kappa_p\,\tilde{R}_{1F})\;[(1-i\,\gamma\,\Lambda)\,m_p + i\;\gamma\,\Lambda]\,,\quad a_{55} = u_c\,\rho_F\,\omega^2\; J_1(\kappa_u\,\tilde{R}_{1S})$$

$$a_{52} = \frac{p_0}{r_c}\,\kappa_t\; J_1(\kappa_t\,\tilde{R}_{1F})\;[(1-i\,\gamma\,\Lambda)\,m_t + i\;\gamma\,\Lambda]\,,\qquad a_{56} = u_c\,\rho_F\,\omega^2\; Y_1(\kappa_u\,\tilde{R}_{1S}),$$

and

$$\begin{aligned}
F_5 = {}& (1-i\,\gamma\,\Lambda)\,\Big[m_p\,c_1'(\tilde{R}_{1F})J_0(\kappa_p\,\tilde{R}_{1F}) - m_p\,\kappa_p\,c_1(\tilde{R}_{1F})J_1(\kappa_p\,\tilde{R}_{1F})\\
&+m_p\,c_2'(\tilde{R}_{1F})H_0^{(1)}(\kappa_p\,\tilde{R}_{1F}) - m_p\,\kappa_p\,c_2(\tilde{R}_{1F})H_1^{(1)}(\kappa_p\,\tilde{R}_{1F}) + m_t\,c_3'(\tilde{R}_{1F})J_0(\kappa_t\,\tilde{R}_{1F})\\
&-m_t\kappa_t c_3(\tilde{R}_{1F})J_1(\kappa_t\,\tilde{R}_{1F}) + m_t c_4'(\tilde{R}_{1F})H_0^{(1)}(\kappa_t\,\tilde{R}_{1F}) - m_t\,\kappa_t c_4(\tilde{R}_{1F})H_1^{(1)}(\kappa_t\tilde{R}_{1F})\Big]\\
&+i\,\gamma\,\Lambda\Big[\,c_1'(\tilde{R}_{1F})J_0(\kappa_p\,\tilde{R}_{1F}) - \kappa_p\,c_1(\tilde{R}_{1F})J_1(\kappa_p\,\tilde{R}_{1F}) + c_2'(\tilde{R}_{1F})H_0^{(1)}(\kappa_p\,\tilde{R}_{1F})\\
&-\kappa_p\,c_2(\tilde{R}_{1F})H_1^{(1)}(\kappa_p\,\tilde{R}_{1F}) + c_3'(\tilde{R}_{1F})J_0(\kappa_t\,\tilde{R}_{1F}) - \kappa_t\,c_3(\tilde{R}_{1F})J_1(\kappa_t\,\tilde{R}_{1F})\\
&+c_4'(\tilde{R}_{1F})H_0^{(1)}(\kappa_t\,\tilde{R}_{1F}) - \kappa_t\,c_4(\tilde{R}_{1F})H_1^{(1)}(\kappa_t\,\tilde{R}_{1F})\Big]\,.
\end{aligned}$$

The sixth row of $\mathbf{A}$ is obtained by the interface condition (2.16) on the structure due to the fluid. Together with the formulae (3.9), (3.10), (3.12), and (3.3) for the pressure and temperature in the fluid and the temperature and displacement in the structure, we obtain,

$$a_{61} = p_0\,m_p\;J_0(\kappa_p\tilde{R}_{1F}),\qquad a_{62} = p_0\,m_t\;J_0(\kappa_t\tilde{R}_{1F}),$$

$$a_{63} = -\frac{\zeta_1\,p_0}{\alpha}\,J_0(\lambda\,\tilde{R}_{1S}),\qquad a_{64} = -\frac{\zeta_1\,p_0}{\alpha}\,H_0^{(1)}(\lambda\,\tilde{R}_{1S}),$$

$$a_{65} = (\zeta_0 + i\omega\,\zeta_2)\,\frac{u_c}{r_s}\,\zeta_4 + (\lambda_S + i\,\omega\,\zeta_3)\,\frac{u_c}{r_s\,\widetilde{R}_{1S}}\,J_1(\kappa_u\,\widetilde{R}_{1S}),$$

$$a_{66} = (\zeta_0 + i\omega\,\zeta_2)\,\frac{u_c}{r_s}\,\zeta_5 + (\lambda_S + i\,\omega\,\zeta_3)\,\frac{u_c}{r_s\,\widetilde{R}_{1S}}\,Y_1(\kappa_u\,\widetilde{R}_{1S}),$$

where,

$$\zeta_0 = (\lambda_S + 2\mu_S),\quad \zeta_1 = \alpha_S(3\lambda_S + 2\mu_S),\quad \zeta_2 = (\eta_F + \frac{4}{3}\mu_F),\quad \zeta_3 = (\eta_F - \frac{2}{3}\mu_F),$$

$$\zeta_4(\tilde{R}_{1S}) = \kappa_u\,\left[\frac{1}{\kappa_u\,\tilde{R}_{1S}}J_1(\kappa_u\,\tilde{R}_{1S}) - J_2(\kappa_u\,\tilde{R}_{1S})\right],$$

$$\zeta_5(\tilde{R}_{1S}) = \kappa_u\,\left(\frac{1}{\kappa_u\,\tilde{R}_{1S}}Y_1(\kappa_u\,\tilde{R}_{1S}) - Y_2(\kappa_u\,\tilde{R}_{1S})\right],$$

and

$$\begin{aligned}
F_6 = -p_0\,\Big[&m_p\,c_1(\widetilde{R}_{1F})\,J_0(\kappa_p\,\widetilde{R}_{1F}) + m_p\,c_2(R_{1F})\,H_0^{(1)}(\kappa_p\,\widetilde{R}_{1F})\\
&+m_t\,c_3(\widetilde{R}_{1F})\,J_0(\kappa_t\,\widetilde{R}_{1F}) + m_t\,c_4(\widetilde{R}_{1F})\,H_0^{(1)}(\kappa_t\,\widetilde{R}_{1F})\Big]\,.
\end{aligned}$$

SM1.4. Interface and Boundary conditions for the one-way coupled model. For the one-way coupled model, the last two rows of $\mathbf{A}$ and $\mathbf{F}$ are given as follows. The fifth row of $\mathbf{A}$, which is obtained using the zero Neumann boundary condition for the fluid pressure at the fluid-structure interface, together with the formula (3.9) for the pressure in the fluid, is given by

$$a_{51} = m_p\,\kappa_p\; J_1(\kappa_p\,\tilde{R}_{1F}) \quad \text{and} \qquad a_{52} = m_t\,\kappa_t\; J_1(\kappa_t\,\tilde{R}_{1F}),$$

and

$$\begin{aligned}
F_5 = {} & m_p\,c_1'(\tilde{R}_{1F})J_0(\kappa_p\,\tilde{R}_{1F}) - m_p\,\kappa_p\,c_1(\tilde{R}_{1F})J_1(\kappa_p\,\tilde{R}_{1F}) + m_p\,c_2'(\tilde{R}_{1F})H_0^{(1)}(\kappa_p\,\tilde{R}_{1F}) \\
& - m_p\,\kappa_p\,c_2(\tilde{R}_{1F})H_1^{(1)}(\kappa_p\,\tilde{R}_{1F}) + m_t\,c_3'(\tilde{R}_{1F})J_0(\kappa_t\,\tilde{R}_{1F}) - m_t\,\kappa_t\,c_3(\tilde{R}_{1F})J_1(\kappa_t\,\tilde{R}_{1F}) \\
& + m_t\,c_4'(\tilde{R}_{1F})H_0^{(1)}(\kappa_t\,\tilde{R}_{1F}) - m_t\,\kappa_t\,c_4(\tilde{R}_{1F})H_1^{(1)}(\kappa_t\,\tilde{R}_{1F}).
\end{aligned}$$

The sixth row is obtained using the interface condition (2.16) on the structure due to the fluid. Together with formulae (3.9), (3.10), (3.12), and (3.3) for the pressure and temperature in the fluid and the temperature and displacement in the structure, we obtain,

$$\begin{aligned}
a_{61} &= p_0\,m_p\; J_0(\kappa_p\tilde{R}_{1F}), & a_{62} &= p_0\,m_t\; J_0(\kappa_t\tilde{R}_{1F}), \\
a_{63} &= -\frac{\zeta_1\,p_0}{\alpha}\,J_0(\lambda\,\tilde{R}_{1S}), & a_{64} &= -\frac{\zeta_1\,p_0}{\alpha}\,H_0^{(1)}(\lambda\,\tilde{R}_{1S}), \\
a_{65} &= \frac{u_c}{r_s}\,\zeta_0\,\zeta_5 + \frac{u_c}{r_s\,\widetilde{R}_{1S}}\,\lambda_S\,J_1(\kappa_u\,\widetilde{R}_{1S}), & a_{66} &= \frac{u_c}{r_s}\,\zeta_0\,\zeta_4 + \frac{u_c}{r_s\,\widetilde{R}_{1S}}\,\lambda_S\,Y_1(\kappa_u\,\widetilde{R}_{1S}),
\end{aligned}$$

and

$$\begin{aligned}
F_6 = -p_0 \Big[& m_p\,c_1(\widetilde{R}_{1F})\,J_0(\kappa_p\,\widetilde{R}_{1F}) + m_p\,c_2(R_{1F})\,H_0^{(1)}(\kappa_p\,\widetilde{R}_{1F}) \\
& + m_t\,c_3(\widetilde{R}_{1F})\,J_0(\kappa_t\,\widetilde{R}_{1F}) + m_t\,c_4(\widetilde{R}_{1F})\,H_0^{(1)}(\kappa_t\,\widetilde{R}_{1F}) \Big].
\end{aligned}$$

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