Scott et al 2025: Development of the SiMPLE-PAS

Supplemental Information

Contents

1 Cell Photos

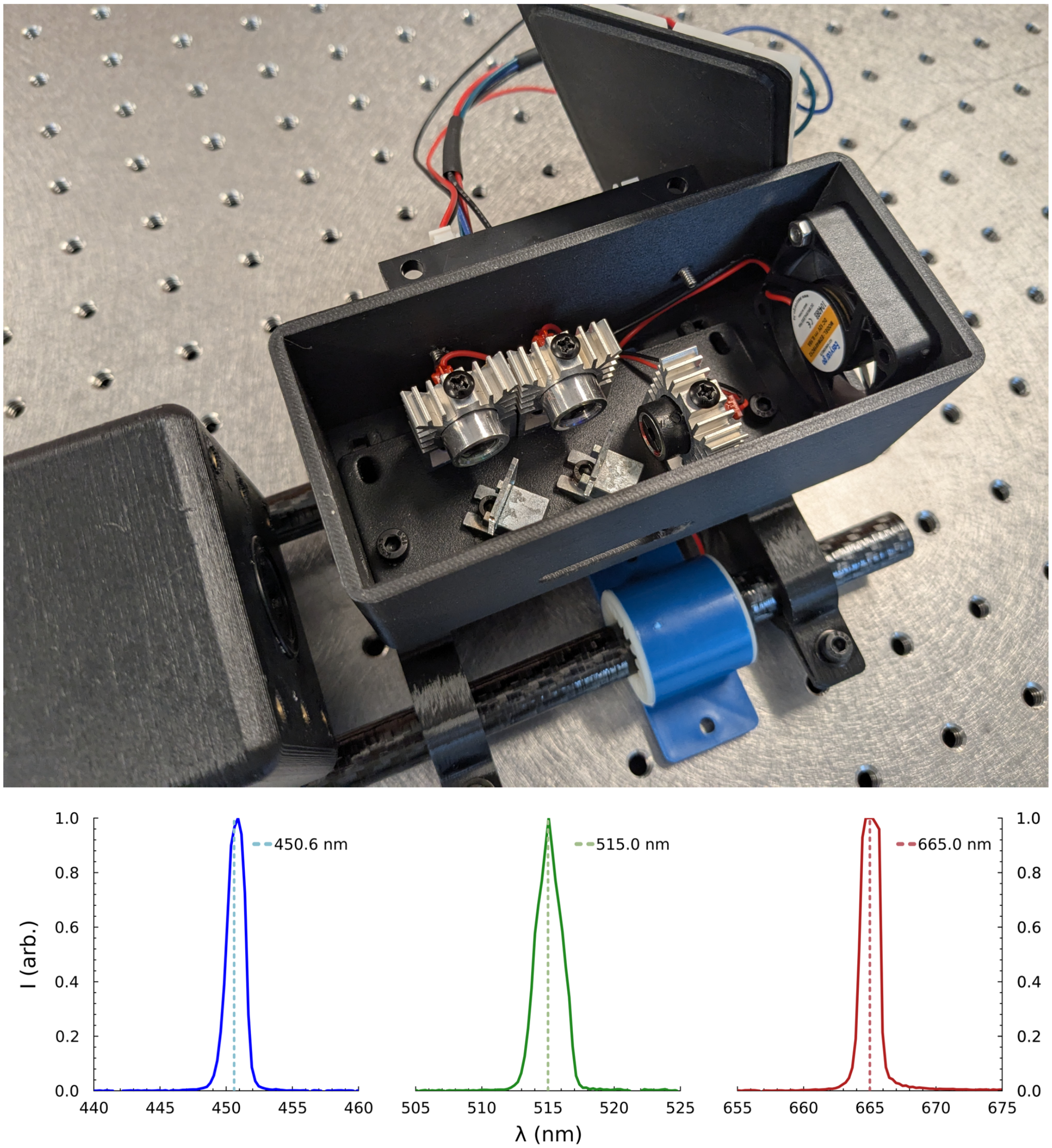

Figure S1: RGB laser module used in the SiMPLE-PAS, shown in its 3D-printed case with the control board mounted on the back (top) and spectra of the lasers used in the SiMPLE-PAS (bottom). Laser spectra were measured with an Ocean Optics QE65000 UV-visible spectrometer.

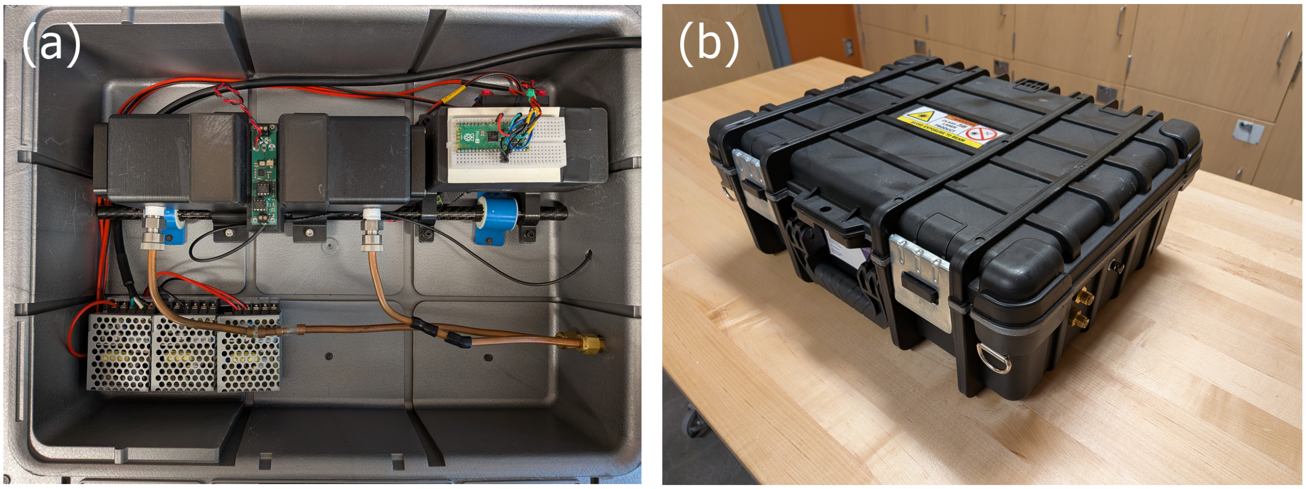

Figure S2: Photos of the (a) inside and (b) of the SiMPLE-PAS case.

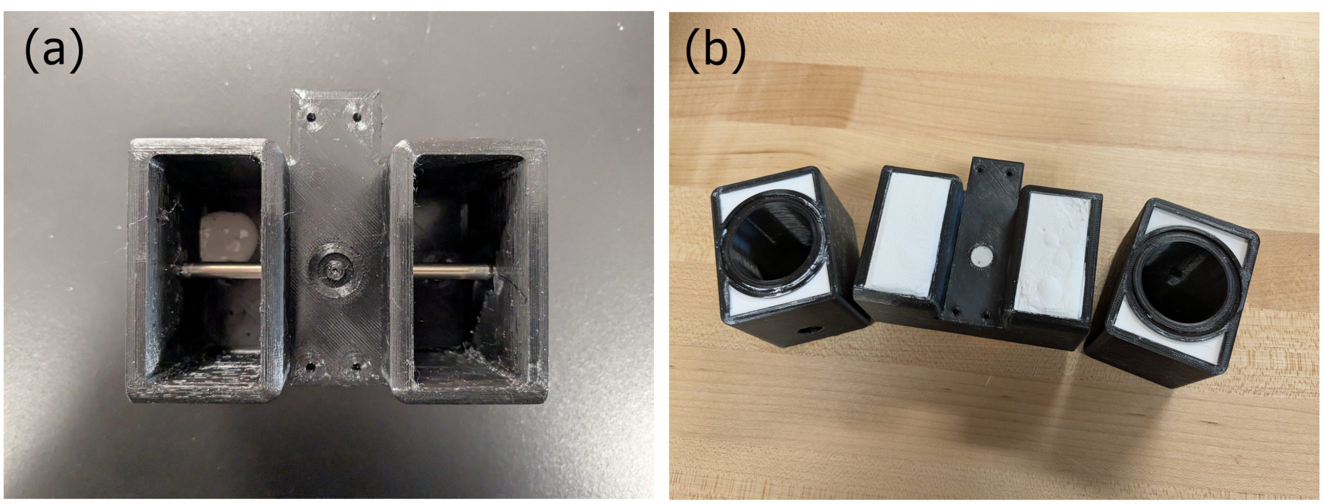

Figure S3: Photos of the assembly process. (a) Photo of the 3D-printed shell before filling with plaster, showing the stainless steel resonator that has been pressed into the shell. (b) Photo after filling with plaster but before glue-up; note that an error with the 3D printer caused the central microphone port to break through during assembly in (b), but the port and o-ring groove typically appears as in (a) even after filling.

2 PAS GUI

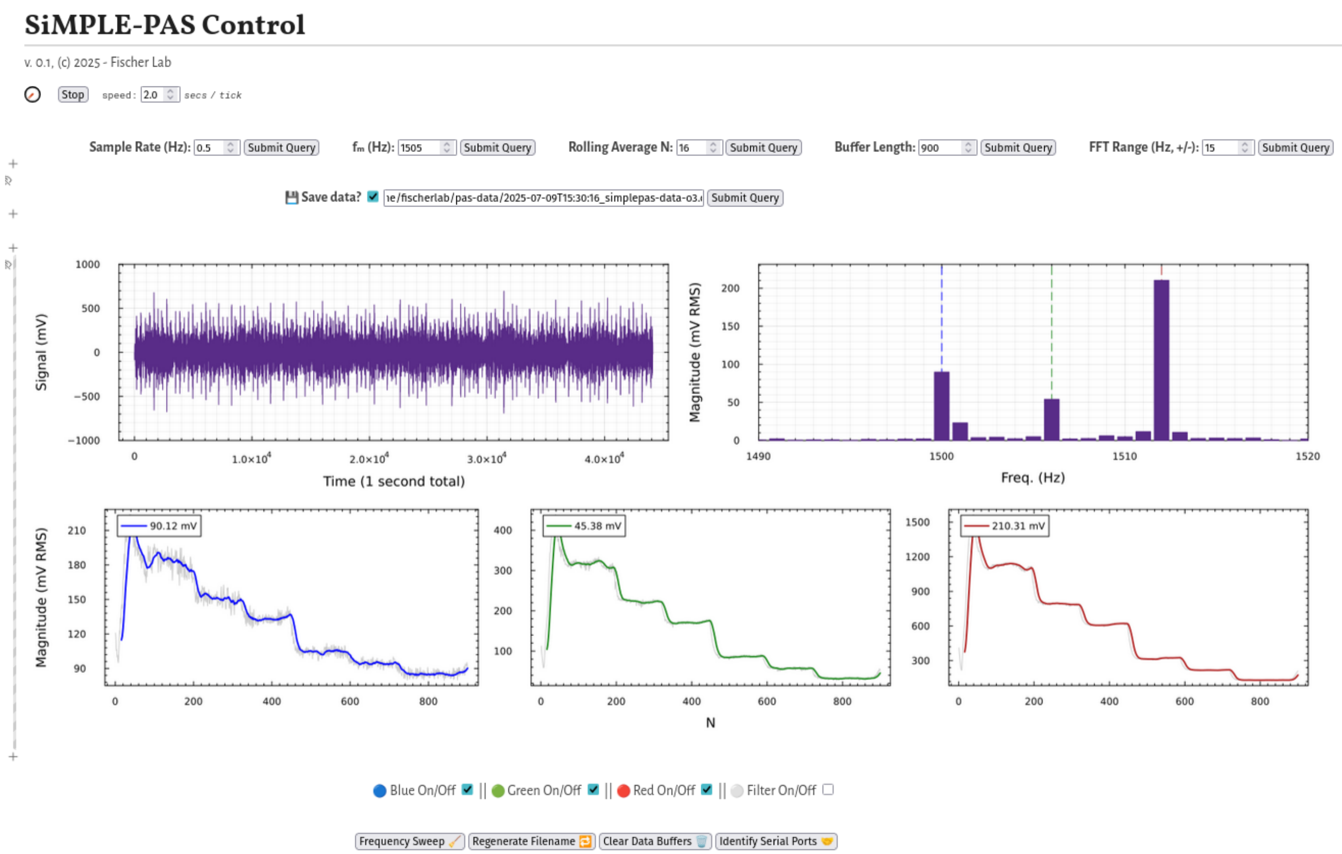

Figure S4: Screenshot of the Pluto/Julia SiMPLE-PAS GUI showing the front panel slide.

3 Cell Frequency Response

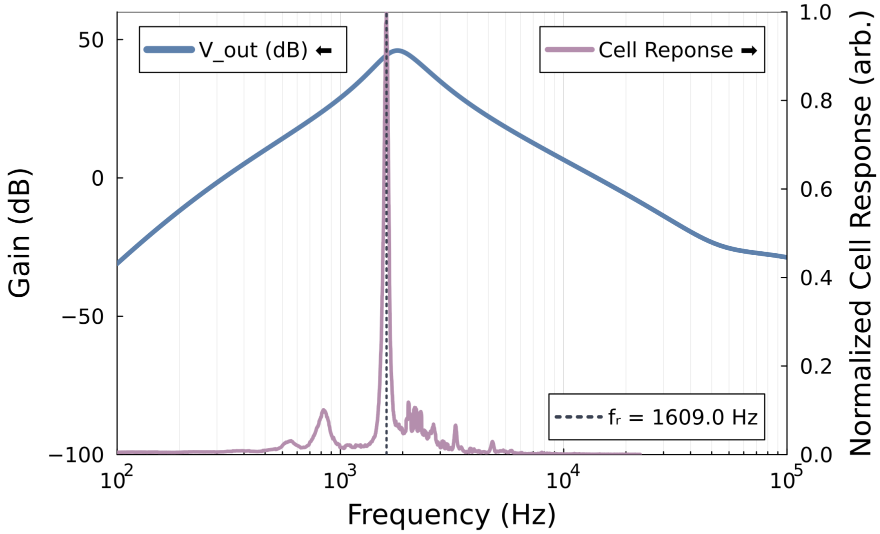

Figure S5: Simulation results for preamplifier performance (left axis) and the measured frequency response of the cell and preamp combined, determined using the new method described herein (right axis). Simulation results indicate strong amplification around the resonant frequency (f_r) with less amplification and attenuation at frequencies away from the f_r. The frequency response shows a sharp peak around 1609 Hz, representing f_r. The FWHM of the resonance peak is approximately 50 Hz, indicating $Q \approx 30$.

4 Error Analysis

For calibration curves (Fig. 4), we estimate the indeterminate error on each point as the standard deviations of a single 2-minute average of the PAS signal and background added in quadrature, which works out to an average absolute uncertainty of 2.7, 2.7, and 1.9 Mm^{-1} for the blue, green, and red channels, respectively; the indeterminate error appears invariant with the magnitude of absorption. We estimate the maximum determinate error in y as the propagated error on the ratios of the absorption cross section for NO_2 ($\sigma_{\lambda_{\mathrm{PAS}}}/\sigma_{446\mathrm{nm}}$) reported by Bogumil (2003) (4.5 % total) and add the determinate and indeterminate errors in quadrature to obtain the error bars shown on the plots. For the indeterminate error in x, we again take 1 standard deviation of τ and τ_0 and propagate these accordingly for an average total indeterminate error in x of 2.5 %. We add this value to the maximum determinate error of 3.5 %, which is obtained from the uncertainty on R_L (estimated at 2 %) and the uncertainty on the total flow and CRDS purge flow. The rotameter used to control the 300 sccm total flow has an uncertainty on accuracy of 8 % at 300 sccm that dominates the error on the flows and the calibration itself. We therefore calibrated the rotameter using a TSI 5150 flow meter and assume the uncertainty on the total flow becomes the flow meter's 2 % error combined with the 0.25 % precision of the rotameter, yielding the 2.02 % error on the 300 sccm flow used in our error analysis. This provides a final error of 5.8 % on the x values in the calibration.

For ozone measurements (Fig. 5), we did not use a purge flow and therefore present the propagated 1 standard deviation of τ and τ_0 as the uncertainty on x. For y, we calculate the standard deviation of the absorption coefficients retrieved from the calibration curve via inverse prediction ($s_{b_{abs,\mathrm{PAS}}}$) according to:

$$s_{b_{abs,\mathrm{PAS}}} = \frac{s_r}{k}\sqrt{\frac{1}{m} + \frac{1}{n} + \frac{(\bar{y}_{\mathrm{O_3}} - \bar{y}_{\mathrm{NO_2}})}{k^2 \sum_{i=1}^{n} \left(b_{\mathrm{NO_2,CRDS}_i} - \bar{b}_{\mathrm{NO_2,CRDS}}\right)^2}} \tag{1}$$

where y represents the PAS signal (in mV), k is the slope of the calibration line, m is the number of data points used in each average measurement (here we consider each average to be $m = 1$ since the measurements of a single concentration are not truly independent), n is the number of calibration points used for the regression, and s_r is the standard deviation of the regression for the calibration:

$$s_r = \sqrt{\frac{\sum_{i=1}^{n} \left(y_{i,\mathrm{NO_2}} - \hat{y}_{i,\mathrm{NO_2}}\right)^2}{n-2}} \tag{2}$$

where again y represents the PAS signal in the calibration such that the numerator is the residual sum of square of the regression. We consider this to represent the indeterminate error in the calibration and so again add to this the determinate error from the calibration and indeterminate error from the measurement (1 SD of the PAS signal and background) to obtain the error bars on the plot. We also calculate the 95 % confidence interval (CI) for the slop of the regression of the PAS data vs. CRDS data as Student's t value times the standard error of the predicted slope. Because the CIs of the slopes overlap with literature values, and the uncertainties on each point overlap with literature sources, we conclude the SiMPLE-PAS is accurate within the precision of the instrument and uncertainty of the calibration and literature values. We compute the uncertainty for b_{abs} values from G-WISE 2 data (Fig. 7) in the same way as those for ozone for the SiMPLE-PAS; for MultiPAS-IV data, we assume a nominal error of 3.3 % obtained from a similar error analysis for that instrument.

5 Bill of Materials

SiMPLE-PAS Bill of Materials (c) 2025, Fischer Lab, fischer-lab.com (CC-BY-SA-NC)				
Item	**QTY**	**QTY Unit**	**As-built Cost**	**Low-cost Option**
Cell				
PET-G Filament, for cell	0.5	kg	$13.97	$13.97
CaSO4 (s)	0.5	kg	$1.15	$1.15
Coating, Polycrylic	0.25	can	$3.49	$3.49
X-ring, 1", Buna-N	2	ea	$0.37	$0.37
O-ring, 1/4", Buna-N	1	ea	$0.03	$0.03
Threaded inserts, heat-set, M2	4	ea	$0.87	$0.87
Threaded inserts, heat-set, M3	12	ea	$2.51	$2.51
Screws, M2, SHCS, 12 mm	4	ea	$1.19	$1.19
Screws, M3, BHCS, 16 mm	12	ea	$1.13	$1.13
Tubing, SS, 1/4" O.D., 6 ga	100	mm	$5.08	$5.08
Fittings, 1/4", press-to-connect	2	ea	$10.20	$10.20
Windows, BK-7, 25 mm x 5 mm	2	ea	$220.52	
or Glass Slide	*2*	*ea*		*$2.91*
Case & Mounting System				
Case, 18", Plastic, VOYAGER	1	ea	$39.99	
Heat-set Inserts, M2	8	ea	$1.73	
Screws, M2, SHCS, 12 mm	4	ea	$1.19	
Filament, for mounts	0.1	kg	$2.79	$2.79
Screws, M4, SHCS	8	ea	$0.96	$0.96
Nuts, flange, M4, 12 mm	8	ea	$0.69	$0.69
Rod, carbon fiber, 1/2"	2	ea	$50.48	
or PVC Pipe, 1/2"	*2*	*ea*		*$3.31*
Mounts, isolation, 1/2"	4	ea	$9.48	$9.48
Fitting, compression, bulkhead, 1/4"	2	ea	$40.81	
Connector, BNC, bulkhead	1	ea	$1.80	
Cable, BNC, RG-78	0.3	m	$2.93	
Tubing, copper, 1/4"	0.5	m	$3.90	
Preamp & DAQ				
Sound Card, USB	1	ea	$27.19	$27.19
Printed circuit board	1	ea	$0.47	$0.47
Microphone	1	ea	$3.24	$3.24
Op-amp, precision	2	ea	$2.54	$2.54
Instrumentation Amp	1	ea	$2.90	$2.90
Misc passives	1	ea	$1.00	$1.00
Potentiometer, 5K, SMD	1	ea	$3.24	$3.24
Laser Module				
Laser module, RGB	1	ea	$21.90	$21.90
Filament, for case	0.05	kg	$1.40	$1.40
MCU, Raspberry Pi Pico 2	1	ea	$4.99	$4.99
Power Supply				
Power supplies, +/- 3.3 VDC	2	ea		
or OEM option	*2*	*ea*	$17.20	*$17.20*
Power supply, 12 VDC	1	ea		
or 12V wall adapter	*1*	*ea*	$8.60	*$8.60*
		Total Cost:	**$511.92**	**$154.78**

Figure S6: Bill of materials for the SiMPLE-PAS. The As-built option shows the cost for the version presented in the paper, not including bench power supplies. The Low-cost option presents what we consider the bare minimum cost for a working instrument, replacing expensive components with recommendations for lower-cost options and eliminating not strictly necessary components. All costs are given in US dollars and represent cost at the time of purchase (2020-2025).