Supporting Information for: A Multiplexed Paper Analytical Device for Measuring Airborne Metal Particulates Using Distance-Based Detection

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Lab on a Chip Manuscript

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Abstract
Important details from the main text are further discussed in this supplemental information. Information for gradient printing from empirically derived equations is provided, as well as a description of weighting for response curves. Tables of z-values for common solvents and a list of metal alloy composition are given. Figures detailing the fabrication of ink reservoirs, results from single channel devices, and the effect of increasing reagent concentration are provided.

Table S1 | Z values for common solvents. Values were quantified using Oh^{-1} based on a print head nozzle diameter of 90 µm.

Solvent Name	Vapor Pressure (Torr)	Viscosity (N s/m^2)	Density (kg/m^3)	Surface Tension (N/m)	Z value
n-Butyl Alcohol	4.4	0.00298	809.7	0.02457	14.1994
Isobutyl Alcohol	8.8	0.00285	801.6	0.02298	14.2866
Isopropyl Alcohol	32.4	0.0024	785.4	0.02179	16.3525
n-Propyl Alcohol	15	0.0023	803.7	0.0237	18.0017
Dimethyl Acetamide	1.3 (25°C)	0.00214	941.5	0.03243	24.4958
2-Methoxyethanol	6.2	0.00172	964.6	0.0318	30.5478
Dimethylsulfoxide	0.42	0.00199	1100	0.04354	32.992
Ethanol	40	0.001144	789	0.0221	34.6282
Ethyl Alcohol	43.9	0.0011	789.2	0.02232	36.1967
1,4-Dioxane	29	0.00137	1033.6	0.03445	41.3211
Cyclohexane	77.5	0.001	778.5	0.02498	41.8357
o-Dichlorobenzene	1.2	0.00132	1305.8	0.02684	42.5478
o-Xylene	6.6	0.000812	880	0.0301	60.1298
Pyridine	18	0.00095	983.2	0.03688	60.1332
o-Xylene	6	0.00081	880.2	0.03003	60.215
n-Butyl Acetate	7.8	0.00074	879.6	0.02509	60.2258
N,*N*-Dimethylformamide	2.7	0.00092	948.7	0.03676	60.8956
Methanol	97	0.00059	791.3	0.02255	67.9224
Iso-Octane	41	0.0005	691.9	0.01877	68.3762
Methyl Isobutyl Ketone	16	0.00058	800.8	0.02364	71.1671
Chlorobenzene	8.8	0.0008	1105.8	0.03328	71.9385
m-xylene	8.3	0.00062	860	0.0289	76.283
Ethylene Dichloride	83.35	0.00079	1253	0.03223	76.3132
Toluene	28.5	0.00059	866.9	0.02853	79.9659
Water	17.54	0.001	998.2	0.0728	80.8715

Table S2 | Common metal alloys used for welding and their chemical composition (% m/m).

Alloy	% Nickel	% Chromium	% Copper	% Iron	% Manganese	% Zinc
SS301	6-8	16-18	Trace	> 70	0-2	Trace
SS304	8-10.5	18-20	0-1	> 60	0-2	Trace
SS308	10-12	19-21	Trace	> 65	0-2	Trace
SS309-EL	12-15	22-24	Trace	> 55	0-2	Trace
SS17-4 PH	3-5	15-17.5	3-5	> 60	0-1	Trace
SS20	32-38	19-21	3-4	> 30	0-2	Trace
Brass	0.2-1	Trace	55-95	0-2	0-1.8	4-43.5
INCONEL® (Ni alloy)	72	15.5	0.5	8	1	Trace

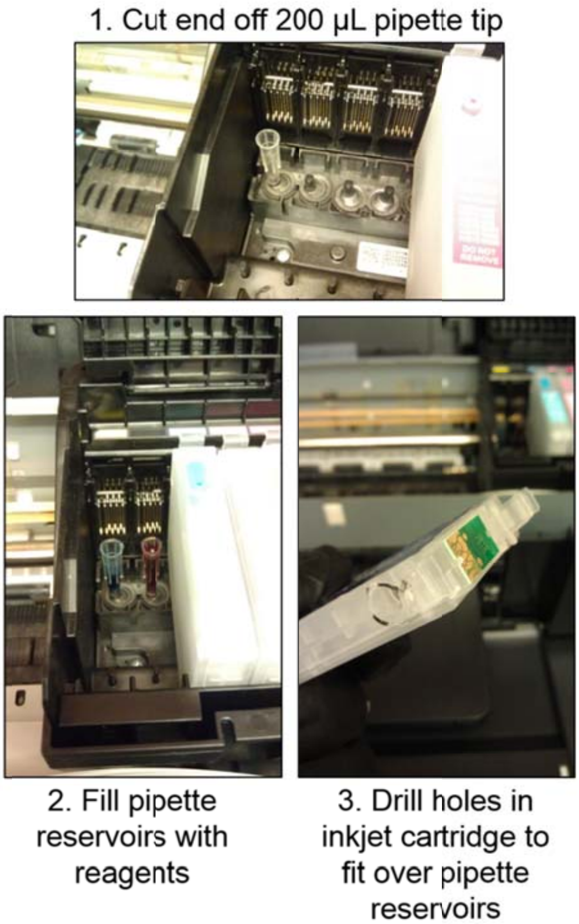

Figure S1 | To create a reservoir for inkjet printing, the end of a 200 µL pipette tip was cut and placed over a nozzle for each color channel. Third-party refillable cartridges were cored to create space for the pipette tip. The reservoir holds approximately 180 µL of printable liquid.

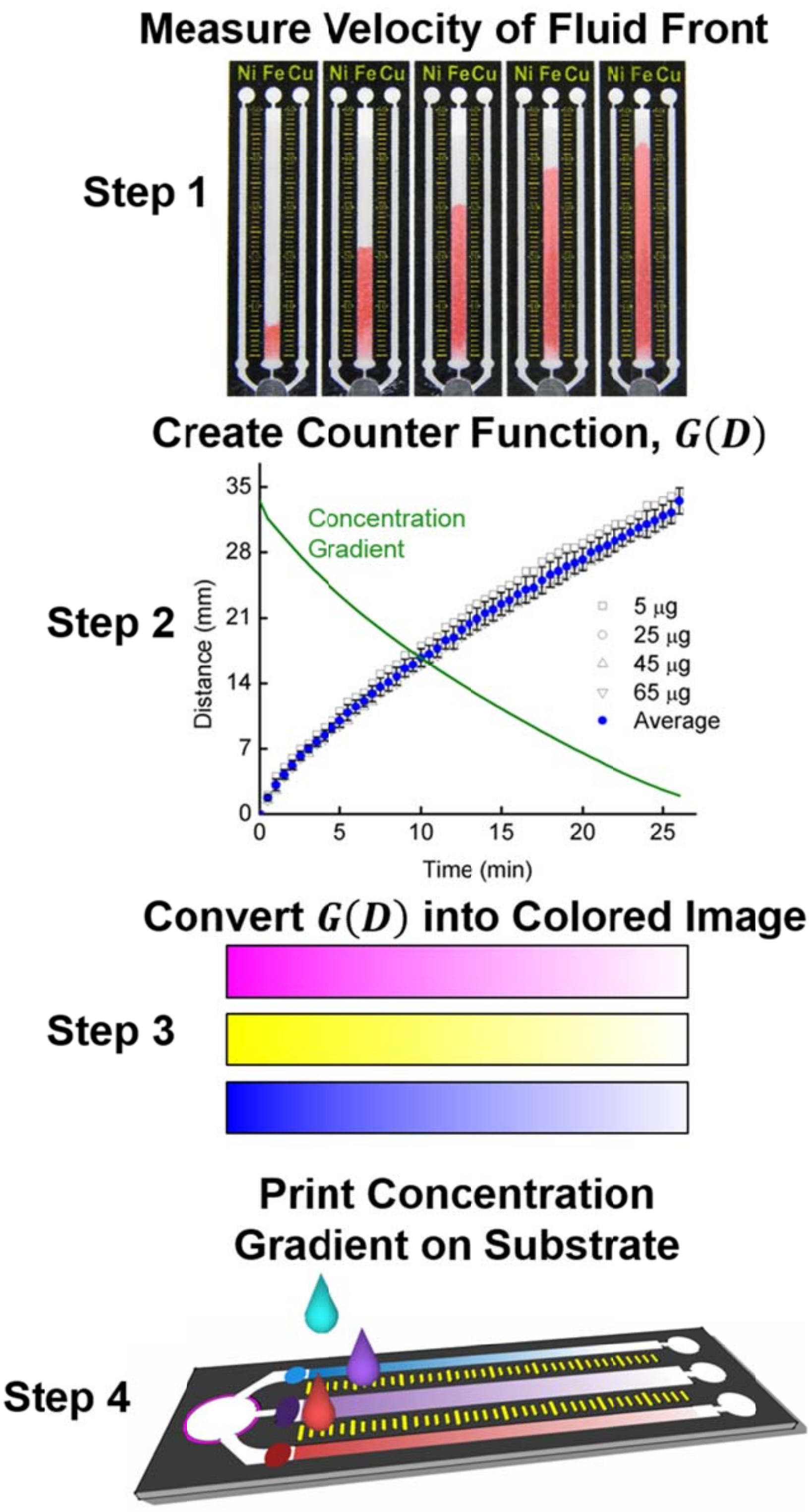

Figure S2 | Steps to create a printable reagent gradient.

Concentration Gradients of Reagents

Empirically derived equations given below were used to print colorimetric gradients for measuring Ni, Cu, and Fe. For each equation, eluent flow rates were first measured in the multi-channel device for several analyte concentrations. The equations below were normalized to 255, the maximum intensity in RGB space for a given color. For the following equations, the units on the vertical and horizontal axes were RGB intensity and distance in pixels, respectively.

Equation for Ni: $y = -7.6 \times 10^{-8}x^4 + 4.4 \times 10^{-5}x^3 - 1.0 \times 10^{-2}x^2 + 2.1x + 5.7$
Equation for Cu: $y = -7.0 \times 10^{-8}x^4 + 4.0 \times 10^{-5}x^3 - 1.1 \times 10^{-2}x^2 + 2.2x + 6.3$
Equation for Fe: $y = -6.0 \times 10^{-8}x^4 + 4.0 \times 10^{-5}x^3 - 9.6 \times 10^{-3}x^2 + 2.1x + 4.1$

Weighted Regression Analysis

For analysis in this work, weighting was given to distance (y) to the −1 power, according to eq. 1.

$$w_i = \frac{n{y_i}^{-1}}{\sum_{i=1}^{n} {y_i}^{-1}} \qquad \text{(Eq. 1)}$$

Confidence and prediction intervals were calculated from eqs. 2 and 3 with respect to the best-fit regression line.

$$CI = \pm t_{\alpha/2,DOF}\hat{s}\sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}} \qquad \text{(Eq. 2)}$$

$$PI = \pm t_{\alpha/2,DOF}\hat{s}\sqrt{\frac{1}{w_i} + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}} \qquad \text{(Eq. 3)}$$

Here, $t_{\alpha/2,DOF}$ corresponds to a two-tail distribution of the *t* distribution and DOF are the degrees of freedom equal to n-2 for linear fits. S-hat is a function of the sum of squared error (SS_E), given by eq. 4.

$$\hat{s} = \sqrt{\frac{SS_E}{DOF}} \qquad \text{(Eq. 4)}$$

X-bar corresponds to the weighted x-centroid given by eq. 5.

$$\bar{x} = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i} \qquad \text{(Eq. 5)}$$

S_{xx} corresponds to the weighted sum of squares between x_i and x-bar, given by eq. 6.

$$S_{xx} = \sum_{i=1} w_i (x_i - \bar{x})^2 \qquad \text{(Eq. 6)}$$

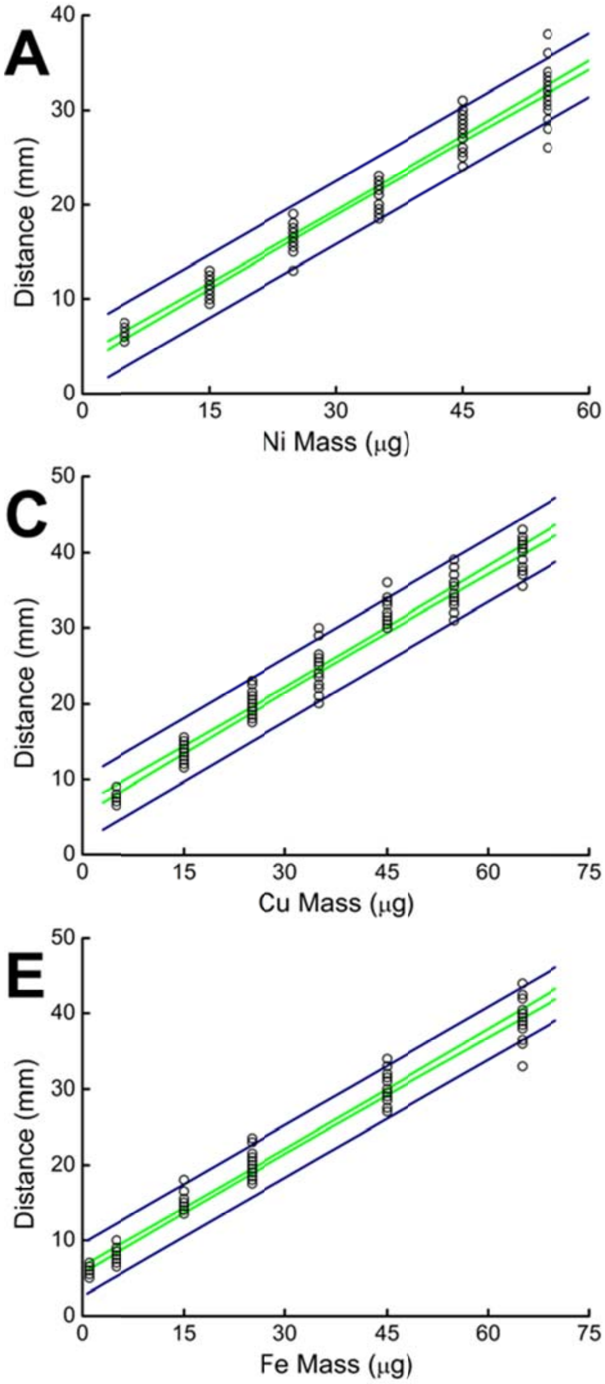

Figure S3 | Unweighted (A, C, E) and weighted (B, D, F) linear regression fits for Ni, Cu, and Fe showing 95% prediction (blue) and confidence (green) intervals.

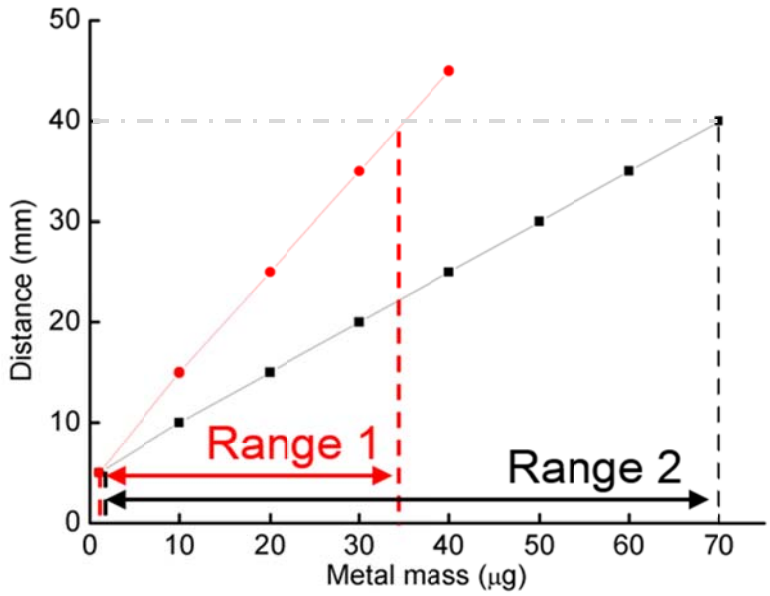

Figure S4 | Hypothetical curves showing changes in dynamic range as a result of slope. The lines on the horizontal were drawn to intersect the vertical axis at 40 mm, which represented the distance at which the eluent velocity was approximately zero.

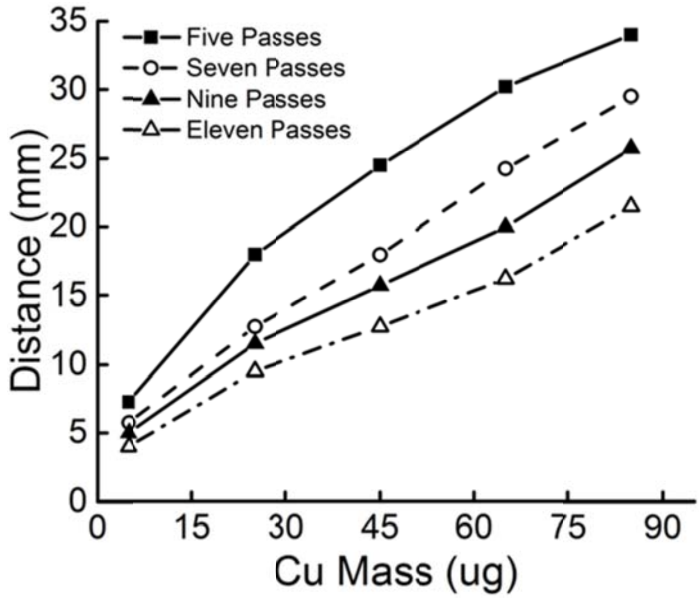

Figure S5 | Response curves for detection of Cu in single-channel devices. As the concentration of printed dithiooxamide was increased on the paper substrate, the slope of the response curve decreased.

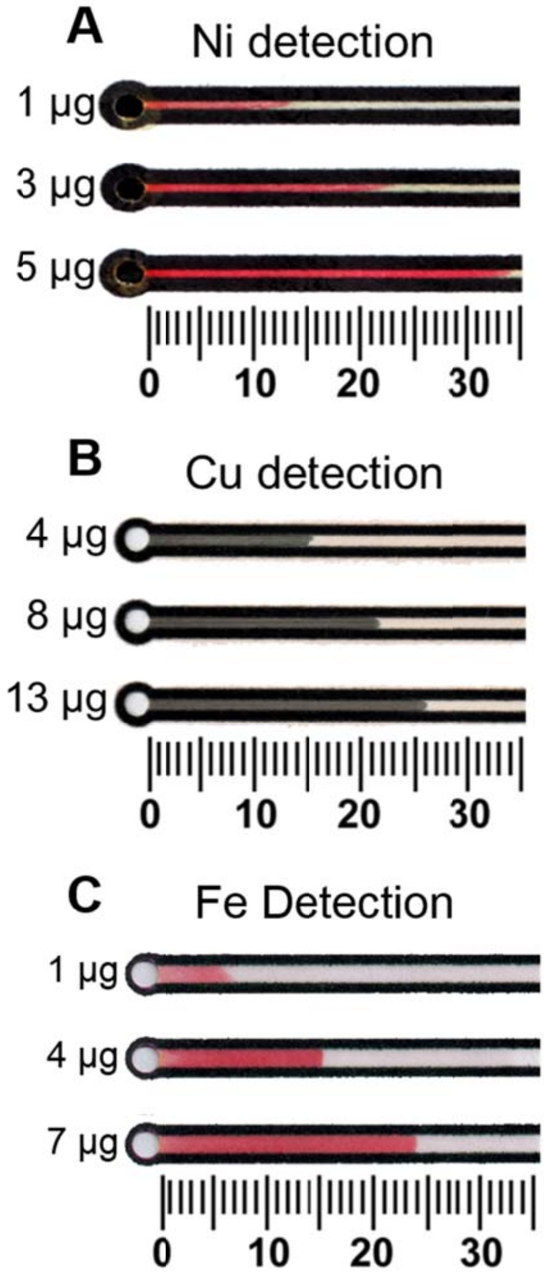

Figure S6 | Distance-based detection of (A) Ni, (B) Cu, and (C) Fe in single channels.

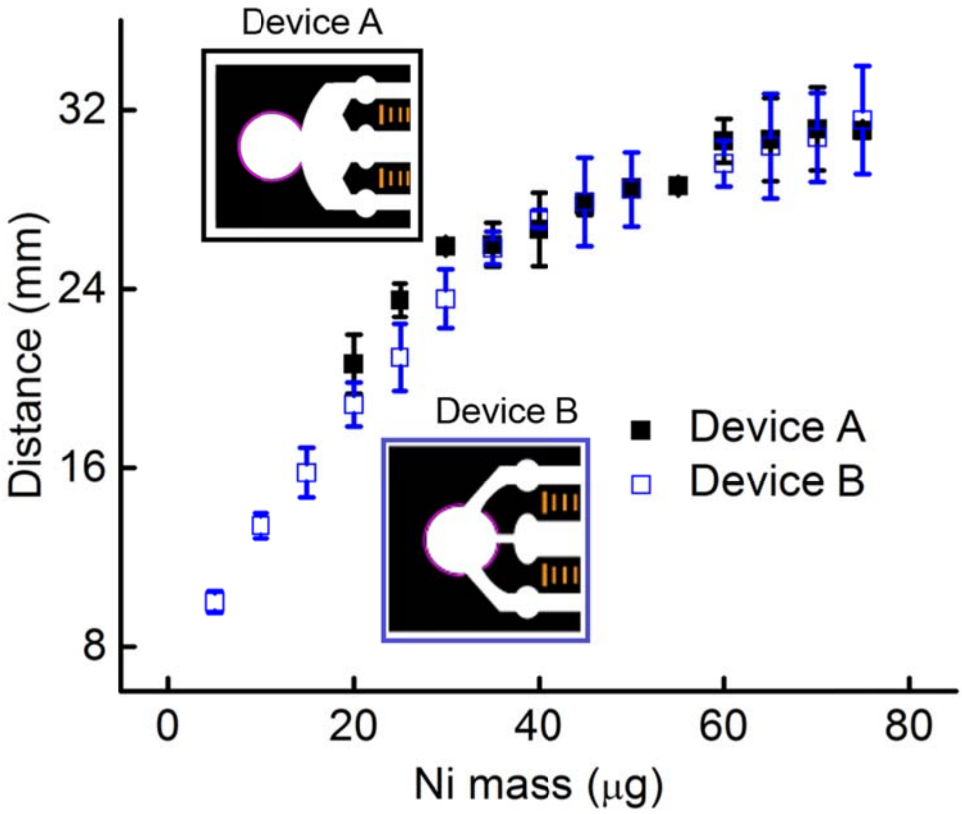

Figure S7 | Dynamic range increased for multi-channel detection of Ni when the inlet surface area was reduced.

Movie S1 | Time-lapse video showing detection of 15 and 10 μg Ni and Cu, respectively, in a two-channel device. The total runtime of the video was ~40 min. The video is available online for viewing.

Movie S2 | Time-lapse video showing detection of 5, 5, and 15 μg Ni, Cu, and Fe, respectively, in a three-channel device. The total runtime of the video was ~45 min. The video is available online for viewing.