Electronic Supplementary Material (ESI) for Analyst

SUPPORTING INFORMATION

Detection of Trace Amounts of Water in Hydrocarbon Matrices with Mid-infrared Fiberoptic Evanescent Field Spectroscopy

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Determining stirring speed (RPM) in the blender cell

To measure the number of rotations per minute (RPM) of the blender cell, a small magnet was attached to the mixer rotor with aid of super glue and an electromagnetic coil was placed in the proximity of the rotor. If the magnet passes the coil, a current pulse is generated in the coil. To estimate the pulse frequency (which corresponds to the RPM), the signal from the coil was digitized with a computer sound card. The pulse frequency was estimated by Fourier

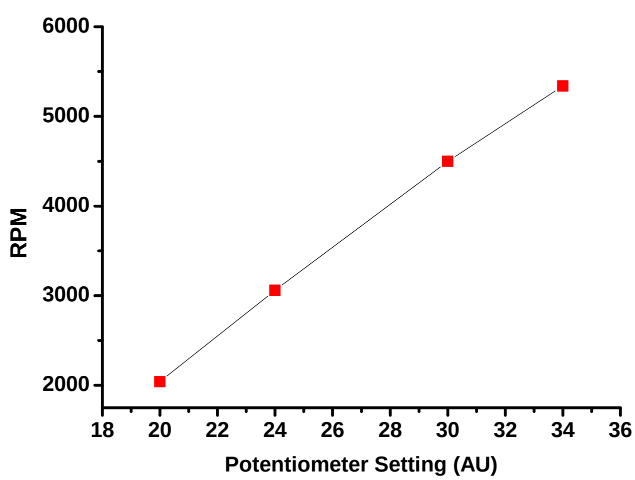

Fig. S-1: Revolutions per minute (RPM) in the blender cell as a function of potentiometer settings.

transformation of the current pulses in Labview. **Fig. S-1** presents the RPM as a function of the potentiometer settings. In this study, setting 24 was used producing approximately 3,000 RPM.

Table S-1: Parameters for establishing calibration curves (± number represents standard deviation).

Concentration (%)	Concentration (ppm)	Peak Area (AU)
Unmodified AgX fiber (Range 0-600 ppm)		
0	0	0±0.49
0.02	200	6.48±0.52
0.03	300	11.66±1.13
0.04	400	16.68±1.58
0.06	600	23.56±1.1
y=-0.43+405.7*x, R=0.995		
PAA-modified AgX fiber (Range 0-3500 ppm)		
0	0	0
0.01	100	3.30
0.02	200	22.71
0.03	300	31.19
0.04	400	33.93
0.06	600	43.78
0.08	800	50.71
0.1	1000	58.80
0.15	1500	67.22
0.25	2500	74.38
0.35	3500	76.62
y=93.78(15.65*x)/(1+15.65*x)		
PAA-Sn-modified AgX fiber (Range 0-1500 ppm)		
0	0	0±2.4
0.00007	0.7	0.73±1.06
0.00014	1.4	0.96±1.06
0.001	10	2.56±1.36
0.003	30	3.17±2.07
0.005	50	3.61±0.8
0.01	100	10.38±0.33
0.02	200	16.88±1.39
0.03	300	22.67±2.1
0.04	400	30.31±5.28
0.06	600	38.13±2.98
0.08	800	47.90±1.85
0.10	1000	51.64±5.56
0.15	1500	55.37±5.49
y=88.35(12.84*x)/(1+12.84*x)	LOD 76 ppm & LOQ 170 ppm	Threshold sensitivity: 10 ppm

Estimation of droplet/fiber contact area for a droplet placed on the fiber surface

To estimate contact area of a droplet with constant volume, yet different contact angle following considerations were used. The droplet of the liquid (grayed in the F**ig. S-2**) is assumed to be enclosed by a sphere of arbitrary radius R. The radius of the droplet circle in contact with the surface, r, and the height of the droplet h or h+h1 were expresses via the contact angle Θ, and the radius R of the enclosing sphere around the droplet.

For contact angle values less than 90^o, r and h are:

$r=R*\cos(90-\Theta);\ h=R*(1-\sin(90-\Theta))$.

For contact angle values more than 90^o, r and h are:

$r=R*\cos(\Theta-90);\ h=R*\sin(\Theta-90)$.

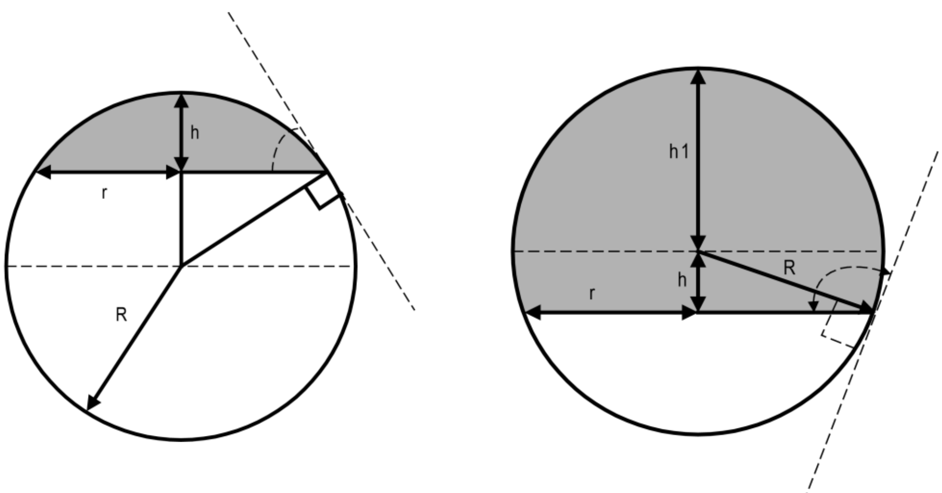

Fig. S-2 Schematic representation of the liquid droplet (gray) at different wetting angles at the surface.

With h and r as function of R, the volume of the droplet can be expresses solely in terms of R and the contact angle value.

For contact angle values less than 90^o, the volume of the droplet corresponds to:

$$V(\theta < 90) = \frac{1}{6}\pi h(3r^2 + h^2) = \frac{1}{6}\pi h(3[R\cos(90-\theta)]^2 + [R(1-\sin(90-\theta))]^2)$$

For contact angle values more than 90^o, the volume of the droplet corresponds to:

$$
\begin{aligned}
V(\theta > 90) &= \frac{1}{6}\pi h(3R^2 + 3r^2 + h^2) + \frac{4}{6}\pi R^3 \\
&= \frac{1}{6}\pi h(3R^2 + 3[R\cos(\theta - 90)]^2 + [R\sin(\theta - 90)]^2] + \frac{4}{6}\pi R^3
\end{aligned}
$$

Setting volume of the droplet to be V=1 for known contract angles, the corresponding radii of the enclosing sphere, R, can be determined (using e.g., Excel Solver). Thus, the corresponding radii of droplet contact circles, r, can then be derived. Finally, the area of contact for the droplet can be estimated.