Supporting Information

Electrothermal Metallic Furnace Atomic Absorption Spectrometry.

Ezequiel Morzan, Guillermo Carrone, Mabel Tudino* and Roberto Etchenique*

Departamento de Química Inorgánica, Analítica y Química Física, INQUIMAE, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria Pabellón 2 AR1428EHA Buenos Aires, Argentina.

Script used for temperature modelling with FlexPde

title "EMFAAS temperature distribution"

select
nominmax = on
{ stages = 3
  errlim = staged(1e-3,1e-4,1e-5)
  autostage=off
 }
coordinates
xcylinder('Z','R')

Variables
Temp { Identify "Temp" as the system variable }

definitions
  K = 1 { define the conductivity }
  source = 0 { define the source }
  Tzero = 0 { define the coolant temperature }
  flux = -K*grad(Temp) { define the thermal flux vector }

Initial values
Temp = 0

equations
  div(K*grad(Temp)) + source = 0 { define the heatflow equation }

boundaries

REGION 1 'air'
{MESH_DENSITY = 1}
k=0.19
START(-10,-0)
natural(Temp)=0 {adiabatic at center }
LINE TO (-10,0) TO (10,0)
value(Temp)=25 {25 C air around}
LINE TO (10,10)
line to (-10,10)
line to close

region 2 'pared del tubo'
{MESH_DENSITY = 10}
k=0.034
source=1200
start (-2.5,0.5)
(NATURAL(Temp) = -k*Temp^4)
line to (2.5,0.5) to (2.5,0.6) to (-2.5,0.6) to close

region 10 'aleta izq'
{MESH_DENSITY = 10}
k=0.004
source=1000
start (-2.5,0.6)
(NATURAL(Temp) = -k*Temp^4)
line to (-2.4,0.6) to (-2.4,1.9) to (-2.5,1.9) to close
Temperature imaging calibration

Consumer digital cameras employ several strategies to deal with the occurrence of dark and illuminated zones within the frame. A typical way to diminish over and under exposition is the use of a nonlinear light flux to pixel value scale. To calibrate this relationship in order to linearize the camera response to light a primary calibration was performed as follows:

A set of pictures of the EMFAAS cell, heated to 835 °C at the maximum, were taken at different exposure times between 1 and 1/30 seconds. The obtained images were stacked into ImageJ and a zone was chosen to perform the calibration as shown in Figure S1 for the G channel.
Figure S1. Images of the heated EMFAAS cell (T = 835 ºC) taken at 1, 1/2, 1/4, 1/10,1/15 and 1/30 seconds from top to bottom. The indicated square area was taken as a calibration point.

A similar calibration was done for the R channel at a zone of lower temperature to avoid image saturation. Since the goal of this calibration is merely to map the integrated light intensity (taken from
the exposure times) to the pixel values, the exact temperature of the used zones are irrelevant, but pixel values near saturation (255) must be avoided. The results are depicted in Figure S2.

The plots show a strong nonlinearity in both channels R and G. Cubic polynomials were chosen to fit the pixel values between 30 and 220 digital units. The results are the following:

\[
R = 9.854 \times 10^{-5} r^3 - 8.021 \times 10^{-3} r^2 + 1.029 r + 30.8 \quad \text{Eq. s1}
\]

\[
G = -3.305 \times 10^{-5} g^3 + 2.762 \times 10^{-2} g^2 + 0.686 g + 31.9 \quad \text{Eq. s2}
\]

Once obtained R and G values in arbitrary units (linearly related to exposure times), the Temperature vs. intensity calibration was done. Images of the heated EMFAAS cell from 724 ºC to 990 ºC were taken under the same conditions at adequate exposure times for imaging the very variable emission. The temperature was taken with a K thermocouple introduced into the cell through the injection hole. The temperature for calibration was taken from a 4 mm² zone directly in contact with the thermocouple. The results are shown in figure S3.

Figure S2. Relationship between pixel value and light intensity for the images of Fig. S1. Squares: Red channel. Circles: Green channel. The curves were fitted with cubic polynomials (see text).
Figure S3. Relationship between R or G values and temperature. Squares: Red channel. Circles: Green channel.

The linear relationship between temperature and \( \ln(R) \) or \( \ln(G) \) was fitted with the following equations:

\[
T = 56.572 \ln\left(\frac{R}{t_{\text{exp}}}\right) + 351.64 \quad \text{Eq. s3}
\]

\[
T = 49.554 \ln\left(\frac{G}{t_{\text{exp}}}\right) + 494.65 \quad \text{Eq. s4}
\]

where R and G are the values obtained using Eq. s1 and Eq. s2 and \( t_{\text{exp}} \) the exposure time of the picture measured in seconds.

Once obtained the calibration curves, the complete procedure to obtain a temperature image is summarized as follows:

1) Take a picture at a exposure time that generates pixel values between 30 and 220.
2) Use equations s1 or s2 to obtain the R or G intensity values.
3) Multiply the light intensity by the reciprocal of the exposure time in seconds.
4) Use the respective s3 or s4 equations to obtain the temperature.

Note that different cameras even of the same model can have different calibration curves.
Table s1: Error analysis of T measurement at different exposure times and temperatures.

<table>
<thead>
<tr>
<th>T/C</th>
<th>Green channel raw pixel values (g)</th>
<th>G intensity values (obtained with Eq. s2)</th>
<th>Light intensity (G / ( t_{exp} ))</th>
<th>Temperature (obtained with Eq. s4)</th>
<th>Temperature (% Kelvin relative error)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T/C</td>
<td>T/C</td>
<td>T/C</td>
<td>T/C</td>
<td>T/C</td>
</tr>
<tr>
<td>724</td>
<td>0.0</td>
<td>89.6</td>
<td>179.1</td>
<td>751.7</td>
<td>0.0%</td>
</tr>
<tr>
<td>752</td>
<td>35.5</td>
<td>196.8</td>
<td>393.7</td>
<td>790.8</td>
<td>-0.9%</td>
</tr>
<tr>
<td>800</td>
<td>68.2</td>
<td>502.2</td>
<td>1004.4</td>
<td>837.2</td>
<td>0.2%</td>
</tr>
<tr>
<td>835</td>
<td>127.9</td>
<td>1245.8</td>
<td>2491.7</td>
<td>882.2</td>
<td>-1.1%</td>
</tr>
<tr>
<td>895</td>
<td>2296</td>
<td>826.4</td>
<td>3305.7</td>
<td>899.4</td>
<td>-0.1%</td>
</tr>
<tr>
<td>942</td>
<td>254.5</td>
<td>1245.8</td>
<td>804.2</td>
<td>940.3</td>
<td>-0.1%</td>
</tr>
<tr>
<td>990</td>
<td>255.0</td>
<td>826.4</td>
<td>1077.0</td>
<td>974.8</td>
<td>-1.2%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t_{exp} / s</th>
<th>0.500</th>
<th>0.250</th>
<th>0.100</th>
<th>0.067</th>
<th>0.033</th>
</tr>
</thead>
<tbody>
<tr>
<td>shutter</td>
<td>2</td>
<td>4</td>
<td>10</td>
<td>15</td>
<td>30</td>
</tr>
</tbody>
</table>