

Evaluating Calorimetric Capabilities of Laboratory Automates

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David Bretz, Mathieu Roch, Pauline Sanglard, Reto Sommerhalder
Jean-Nicolas Aebischer



Goal

Measuring calorimetric data with the EasyMax™ system from Mettler Toledo.

Potential Benefits

Quick access to calorimetric data; Small quantities of chemicals; (Safety).

Method

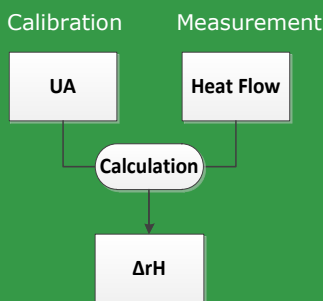
Calibration of the UA coefficient by programming a temperature step for a given solvent.

$$(m_{\text{solvent}} \cdot C_{p,\text{solvent}} + C_w) \cdot \Delta T_1 = \int_{t_{\text{ini}}}^{t_{\text{fin}}} U \cdot A \cdot \Delta T_2(t) \cdot dt$$

with $\Delta T_1 = T_{r,\text{fin}} - T_{r,\text{ini}}$ and $\Delta T_2(t) = T_j(t) - T_r(t)$

Measuring the heat flow under isothermal conditions and determining the reaction enthalpy by calculating the following integral. Beware of the stirring speed and the volume must be identical between calibration and measurement.

$$\Delta_r H = \int_{t_{\text{ini}}}^{t_{\text{fin}}} U \cdot A \cdot \Delta T_2(t) \cdot dt$$



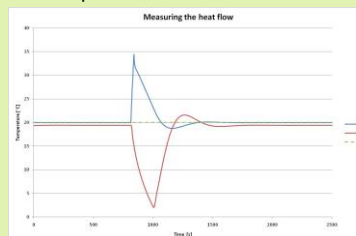
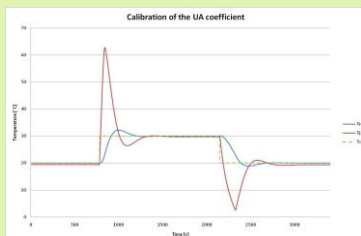
Results

UA coefficient : UA = **1.373 +/- 0.043 W/K** (+/- 3.1%)

- 48 experiments
- 100ml of water
- T-Step 10K (from 20°C to 30°C and from 30°C to 20°C)
- 325 rpm

Reaction enthalpy : Δ_rH = **- 62'298 +/- 5360 J/mol** (+/- 8.6%)

- 3 experiments
- Isothermal dilution of H₂SO₄ (5 ml 98% in 95ml water)
- Tr = 20 C
- 325 rpm



Comparison

To check the method a comparison is made with the reaction performed in the RC1e.

Δ_rH(RC1e) = **- 62'409 +/- 2930 J/mol**

