A Geometric Model for Direct Condensation

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Direct condensation has been established as a well-suited deposition mode for high temperature gas chromatography experiments. Unfortunately, there is no simple model of this process in the literature until now. The model proposed here neglects the exact flow pattern near the deposition foil as well as diffusion processes which might influence the yield. A flow pattern of an underexpanded supersonic jet is formed during the efflux of the reaction gas into a low pressure region, e.g. the ROMA device. Such jets are characterized by a shock cell, the so-called zone of silence, in which the flow velocity is much greater than the local speed of sound and a boundary region between the jet and the ambient gas, in which the gas moves slightly faster than at the exit [1, 2]. The zone of silence consists of a barrel-shaped shock surrounding the jet and a nearly planar normal shock, or Mach disk, downstream. Pressure and temperature decrease dramatically in the zone of silence, whereas the mass flow rate is nearly unchanged. Behind the Mach disk the flow velocity drops down to a subsonic flow. Good conditions for direct condensation of chemical compounds exist within the zone of silence.

The radius of the Mach disk is $r_{mach} = \frac{0.67 \ \mathrm{bar} \cdot r_{in}}{\sqrt{P_0 \ P_{ROMA}}}$

and its distance from the outlet is $d_{mach} = 4\, r_{mach}$

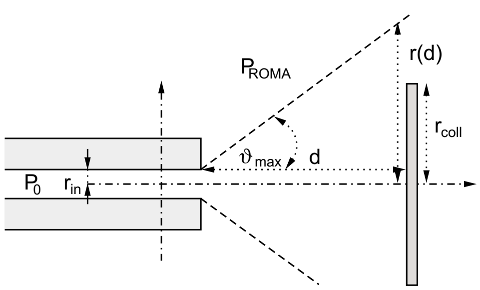

Fig. 1: Geometric model for the evaluation of the deposition yield (symbols are explained below)

A simple geometrical model (Fig. 1) is used to estimate the deposition yield. This model is based on four assumptions:
1) The gas velocity $v_{\parallel}$ in the direction of the axis of the chromatography column after passing the end of the column is constant. 2) The flow pattern is a sharp cone. The axis of the cone has the same direction as the axis of the chromatography column; the cone has an opening angle of $2\vartheta_{max}$. 3) The gas density in a disk perpendicular to the axis of the flow cone is constant. 4) The gas flow perpendicular to the axis of the cone has a constant velocity.

The yield ε is defined by $\varepsilon = \frac{\dot{m}_{coll}}{\dot{m}_{out}}$. The mass flow rates $\dot{m}_{coll}$ and $\dot{m}_{out}$ can be calculated by integrating the local gas density $\rho(d)$ over the collection and the outlet cross section, respectively.

This leads to

$$\dot{m}_{out} = \pi \ r_{in}^2 \ v_{\parallel} \ \rho_L$$

$$\dot{m}_{coll} = \int_0^{r_{coll}} 2\pi \ r \ v_{\parallel} \ \rho(d) \ dr$$

The mass flow rate is constant. $\rho(d)$ can be calculated by

$$\rho(d) = \left(\frac{r_{out}}{r(d)}\right)^2 \rho_L$$

The exit velocity $v_{\parallel}$ of the gas for $P_{ROMA} < P_0$ is given by

$$v_{\parallel} = \sqrt{\kappa \frac{P_L}{\rho_L}}$$

and the velocity component $v_{\perp}$ perpendicular to the direction of the out flow can be calculated by

$$v_{\perp} = \sqrt{\frac{2\kappa}{\kappa - 1} \cdot \frac{P_L}{\rho_L} \cdot \left[1 - \left(\frac{P_{ROMA}}{P_L}\right)^{\frac{\kappa-1}{\kappa}}\right]}$$

The opening angle ϑ_{max} of the flow cone can be calculated by

$$\tan(\vartheta_{max}) = \frac{v_{\perp}}{v_{\parallel}}$$

Combining these formulas yields

$$\dot{m}_{coll} = \begin{cases} \pi \ r_{in}^2 \ v_{\parallel} \ \rho_L & \text{for} \quad r(d) < r_{coll} \\ \pi \left(\frac{r_{coll}}{r(d)}\right)^2 r_{in}^2 \ v_{\parallel} \ \rho_L & \text{for} \quad r(d) > r_{coll} \end{cases}$$

for the collected mass flow.
Finally, the yield ε can be obtained by

$$\varepsilon = \begin{cases} \frac{\kappa - 1}{2} \cdot \left(\frac{r_{coll}}{d}\right)^2 \cdot \left[1 - \left(\frac{P_{ROMA}}{P_L}\right)^{\frac{\kappa-1}{\kappa}}\right]^{-1} & \text{for} \quad r(d) > r_{coll} \\ 1 & \text{for} \quad r(d) < r_{coll} \end{cases}$$

Experimental data (ε, optimum d, spot diameter) could be reproduced well with the proposed geometrical model [3]. For instance, the spots observed experimentally at the pressure optimum can be explained by the zone of silence. The Mach disk has a diameter of 3.3 mm close to the observed diameter of about 3 mm.

Acknowledgments

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References

[1] Trigg, G., L. (ed.): Encyclopedia of Applied Physics, Vol. 4, VCH, Weinheim 1992, pp. 43
[2] Tejeda, G. et al., Phys. Rev. Lett. 76, 34 (1996)
[3] Vahle, A. et al., submitted to Nucl. Instr. Meth.

Symbols: m_{coll} = mass collected on the catcher foil, m_{out} = mass flowing out of the tip of the chromatography column (cc), r_{in} = inner radius at the end of the cc, $\rho(d)$ = density at the distance d from the outlet, r_{coll} = radius of the catcher foil, d = distance between cc and catcher foil, r(d) = radius of the cone = d tan(ϑ_{max}), κ = POISSON coefficient = C_p / C_v, P_0 = back pressure in the cc, P_{ROMA} = ambient pressure in the ROMA device, ρ_0 = gas density at P_0, P_L = Laval pressure = $P_0 \left(\frac{2}{\kappa+1}\right)^{\frac{\kappa}{\kappa-1}}$, ρ_L = Laval density = $\rho_0 \left(\frac{2}{\kappa+1}\right)^{\frac{1}{\kappa-1}}$