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Absolute intensities of supersonic beams

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Introduction

In a molecular beam experiment the center-line intensity $I(0)$ (particles $\text{s}^{-1} \text{sterad}^{-1}$) and the flow rate \dot{N} (particles s^{-1}) of a beam source are important features. To compare the performance of different types of beam sources we introduce the peaking factor κ , defined as the ratio

$$\kappa = \pi(I(0)/\dot{N}) \quad (1)$$

The factor π is added to normalize to $\kappa=1$ for an effusive source. The ideal peaking factor for the supersonic flow from a nozzle follows from continuum theory. Numerical values of κ are available. Experimental values of κ for an argon expansion are presented in this paper, confirming these calculations. The actual center-line intensity of a supersonic beam source with a skimmer is reduced in comparison to this ideal intensity if the skimmer shields part of the virtual source from the detector. Experimental data on the virtual source radius are given, enabling us to predict this shielding quantitatively.

Continuum theory

We consider the flow through an ideal Laval tube sharply cut-off in the sonic plane. In this plane the flow is assumed homogeneous and parallel over the circular nozzle exit. The flow rate \dot{N} is given by

$$\dot{N} = f(\gamma) n_o \alpha_o (\pi R_n^2) n \quad (2)$$

$$f(\gamma) = (\gamma/(\gamma+1))^{\frac{1}{2}} (2/(\gamma+1))^{1/(\gamma-1)}$$

with γ the ratio of specific heats, n_o the reservoir density, $\alpha_o = (2kT_o/m)^{\frac{1}{2}}$ the characteristic velocity in the reservoir with T_o the reservoir temperature and R_n the nozzle radius. Numerical values of $f(\gamma)$ are given in table I, together with the corresponding factor for an effusive source. We see a factor $f(\gamma)2\pi^{\frac{1}{2}}$ increase in flow per unit density when going from free molecular flow to continuum flow (for $\gamma = 5/3$ this equals 1.82).

The ideal peaking factor of the nozzle has to be determined by numerical solution of the hyperbolic differential equation describing the flow downstream of the sonic plane. It appears ⁽¹⁾ that after a distance of a few nozzle diameters the streamlines become straight. Moreover, all streamlines seem to originate from the same point, the virtual source point, located at a position d downstream of the sonic plane. The center-line density in the region of straight streamlines is then given by

$$n(z) = a n_o (z/R_n)^{-2} \quad (3)$$

with z the position on the axis with respect to the virtual source point and a a numerical factor. The values of a and d from the numerical results of Sherman (1,2) are given in table I. The center-line intensity is given by $I(z) = n(z) z^2 u_\infty$, with $u_\infty = (\gamma/(\gamma-1))^{1/2} a_0$ the final value of the flow velocity. The peaking factor is

$$\kappa = a (\gamma/(\gamma-1))^{1/2} / f(\gamma) \tag{4}$$

and is given in table I for Sherman's numerical value of a . Comparison with an effusive source shows that for $\gamma=5/3$ we gain a factor 3.58 in center-line intensity per unit of reservoir density.

Model calculation

The numerical data given above can also be obtained by choosing a suitable model function for the density in the flow field and solving analytically two balance equations, describing the conservation of mass and the axial component of momentum for the flow downstream of the sonic plane. The model function is

$$n(r, \theta) = a n_0 (r/R_n)^{-2} \cos^b((\pi/2)(\theta/\theta_0)) \tag{5}$$

with r and θ the spherical coordinates with respect to the virtual source point. The model function contains three free parameters a , b , and θ_0 of which one has to be fixed by an a priori argument. The remaining two parameters are determined by the balance equations. Using this model Sherman fixed $b=2$, resulting in values of a that are in disagreement with his numerical data. We assume the distribution to scale with the maximum deflection angle of the outer streamlines (3). The Prandtl-Meijer relation gives

$$\theta_{PM} = (\pi/2) \{((\gamma+1)/(\gamma-1))^{1/2} - 1\} \tag{6}$$

for a sharply cut-off nozzle. Solution of the balance equations results in the a and b values given in table I, together with the corresponding peaking factor (4). We see a very good agreement with the κ value derived directly from the numerical data. As a whole, our model fits Sherman's numerical data for the total flow field fairly well.

Table I	γ	5/3	7/5	9/7	Effusive source
Reduced flow rate	$\dot{m}/a n_0 (\pi R_n^2)$	0.513	0.484	0.474	0.282
Numerical data,	a	0.643	0.357	0.246	
Sherman (1,2)	d/R_n	0.15	0.80	1.70	
	κ	1.98	1.38	1.10	
Model function	a	0.613	0.319	0.212	
with $b=2$,	b	2	2	2	
	θ_0	1.37	1.66	1.89	
Sherman (1,2)	κ	1.89	1.23	0.95	
Model function	a	0.650	0.349	0.240	0.25
with $\theta_0 = \theta_{PM}$	b	3	4.32	5.47	1
(this work)	θ_0	$\pi/2$	2.28	2.87	$\pi/2$
	d/R_n	0	0.85	3.62	0
	κ	2	1.35	1.08	1
Experimental	κ	1.95 ± 0.10			

Shielding effect of skimmer

In the case of a supersonic beam source without skimmer the center-line intensity is directly given by $I(o)_\infty = (\kappa/\pi) \dot{N}$. Using a skimmer the influence of the perpendicular temperature has to be taken into account. A useful representation of the perpendicular velocity distribution is given by the virtual source model⁽⁴⁾. From the free molecular region of the expansion the particle trajectories are prolonged backwards to find a virtual source distribution radiating isotropically (in the paraxial approximation) along straight lines. A Boltzmann distribution of the perpendicular velocities results in a virtual source distribution given by

$$f(x,y) dx dy = (\pi R_v^2)^{-1} \exp -((x^2+y^2)/R_v^2) dx dy \quad (7)$$

with x and y coordinates in the plane at $z=0$, $R_v = z(\alpha_\perp(z)/u_\infty)$ the virtual source radius and $\alpha_\perp(z)$ the characteristic velocity of the perpendicular velocity distribution at position z . For free molecular flow we have geometrical cooling $T_\perp \sim z^{-2}$ and R_v is constant.

The center-line intensity $I(o)_s$ with a skimmer is reduced as compared to the ideal intensity $I(o)_\infty$ by the shielding effect of the skimmer, and is given by

$$I(o)_s = I(o)_\infty \iint_A f(x', y') dx' dy' \quad (8)$$

where the integration is performed over the area A "visible" from the detector. If the nozzle-detector distance is much larger than the nozzle-skimmer distance, we obtain

$$I(o)_s = I(o)_\infty \{1 - \exp-(r_s/R_v)^2\} \quad (9)$$

for a circular skimmer of radius r_s and

$$I(o)_s = I(o)_\infty \operatorname{erf}(\alpha_s/R_v) \quad (10)$$

for a slit skimmer of infinite height and with α_s the half-width of the slit.

Experimental

All measurements have been performed with our time-of-flight molecular beam machine. The detector has been carefully calibrated for beam detection, by using an effusive source. A 20 K cryo-expansion chamber is used to pump the supersonic beam source. Measurements of the ideal peaking factor have been done for a converging (60° full angle) cut-off nozzle with an optical diameter of 87 μm . The flow diameter is 85.0 μm , as determined from the measured flow rate and Eq.2. A 3 mm diameter orifice in the end wall of the 20K cryo-expansion chamber (160 mm downstream of the nozzle) replaced the skimmer. The reservoir conditions are $T_o = 295$ K and $p_o = 100$ Torr which lies within the range where $I(o)$ is proportional to \dot{N} (no clustering, no large dimer concentrations). The experimental value $\kappa = 1.95 \pm 0.10$, determined by repeated calibrations and intensity measurements for Argon, is in good agreement with the numerical value of κ .

For a quantitative evaluation of the shielding effect of the skimmer we need accurate data on the virtual source distribution. The measured distributions, as determined by a least squares analysis of measured beam profiles, is more complex

than assumed in the previous discussion. The sum of two gaussian shapes is necessary and sufficient to describe the data. For measurements on Argon, using a nozzle with $R_n = 26 \mu\text{m}$ and a slit skimmer at a distance of 10 mm, the radii of the two virtual source components and the population ratio α_1/α_2 (with $\alpha_1 + \alpha_2 = 1$) are given in figure 1 (4,5). In the lower part of figure 1 we have calculated the resulting

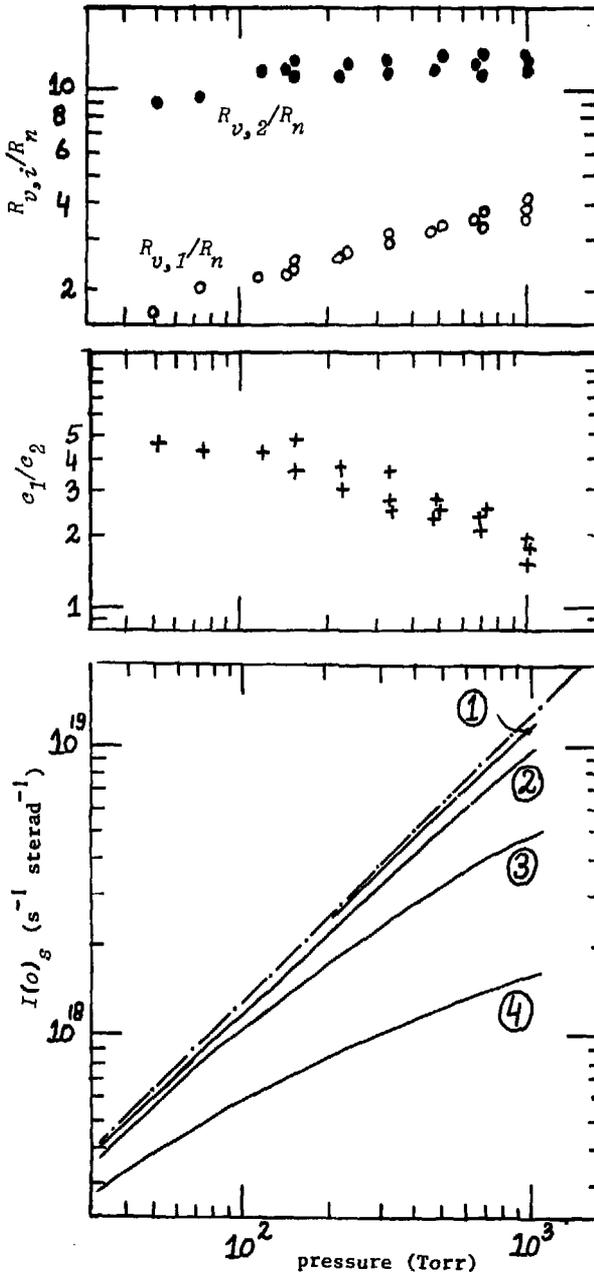


Figure 1.

center-line intensity $I(o)_s$ for this nozzle ($R_n = 26 \mu\text{m}$) for different circular skimmers. For case 4,3,2 and 1 the skimmer radius r_s is equal to 0.05, 0.1, 0.25 and 0.5 mm, respectively. This shielding effect is in agreement with our measurements of $I(o)_s$ (4). We see that the increasing population of the wide virtual source explains the empirical design rule $r_s = 20R_n$. As it is likely that (R_v/R_n) and (α_1/α_2) scale with the product $n_o R_n T_o^{-1/3}$ (4,5), the experimental results on $R_{v,i}$ and α_i can be used to predict the performance of other beam systems.

The shielding effect of the skimmer also explains why the center-line intensity of the monomers levels off at the onset of clustering. This behaviour is caused mainly by the increase of both virtual source radii and an increasing population of the wide virtual source component due to the release of the heat of formation, as measured for an Argon expansion (4,5). Decrease of the monomer population in the expansion is only a minor effect.

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