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Supersonic Molecular Beams with Cycling-Pressure Sources

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Introduction

SUPERSONIC molecular beams that sample from steady sources have been studied analytically and experimentally for two decades. On the other hand, molecular-beam sampling from an unsteady source has not been studied before.[¶] Possible motivations for such studies include a) general investigations of chemical reaction rates and b) specific investigations of chemical processes in combustion chambers of reciprocating internal-combustion engines, useful in efforts to reduce air pollution due to emissions from automobile engines. Both motivations contributed to the initiation of the studies described here.

The investigations of steady supersonic molecular beams indicate that, for a single-species beam operating under ideal conditions (no skimmer interactions and no attenuations due to background gases), the beam density is proportional directly to the source density. It is found^{2,3} that skimmer interference depends on stagnation-chamber conditions, source-chamber conditions, and nozzle-skimmer distance. For a cycling-pressure source, both stagnation-chamber conditions and source-chamber conditions change during the cycle with the result that a given nozzle-skimmer distance is not optimum for all parts of the cycle. A compromise nozzle-skimmer distance might be required.

The main purpose of the present study was to investigate those problems which are unique to a cycling-pressure source. Hence, a single inert species was used. Studies made using inert mixtures and reactive mixtures will be described in subsequent publications.⁴⁻⁶

Analysis of a Simplified Model

The beam source used in this study is a small reciprocating engine driven by a synchronous electric motor. During the

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[¶] Note that the pulsed beam generated by Bier and Hagen¹ used a steady-state source. The beam was pulsed by opening and closing a valve at the nozzle rather than by varying the source condition.

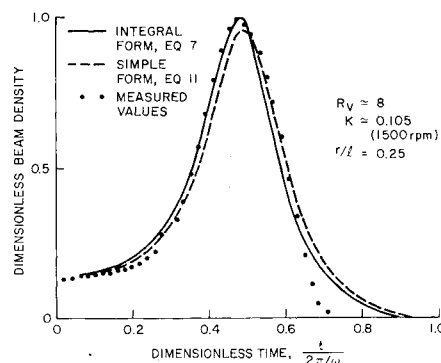


Fig. 1 Comparison between predicted and measured beam densities: The peak of the measured signal is matched to the peak calculated from Eq. (7). The time abscissa is normalized using the engine period.

engine cycle, some of the working gas is expanded through a small orifice located at the center of the cylinder head into a vacuum chamber called the source chamber. A supersonic molecular beam is formed by use of a conventional skimmer and a collimation orifice located downstream of the nozzle (see Fig. 1, Ref. 4).

A. Temporal state of the source gas

The temporal state of the gas inside the engine cylinder was considered for a simplified model in which 1) the velocity of the piston is negligible in comparison with the sound speed of the gas inside the cylinder (hence pressure gradients are not considered); 2) heat transfer between the gas and the cylinder wall is negligible; 3) the effective orifice diameter d^* remains constant throughout the entire cycle; 4) the gas is inert chemically; 5) the gas is perfect thermally and calorically; and 6) the square of the crankshaft radius r divided by the connecting-rod length l is small in comparison with unity. For this model, one may write

$$pV = MRT \quad (1)$$

$$p/T^{\gamma/\gamma-1} = \text{const} \quad (2)$$

$$V \approx V_i - \frac{1}{2}V_i(1 - 1/R_v)(1 - \cos\theta - \frac{1}{2}(r/l)\sin^2\theta) \quad (3)$$

$$\frac{dT}{d\theta} \approx \frac{(\gamma - 1)T}{2} \frac{(1 - 1/R_v)[\sin\theta - \frac{1}{2}(r/l)\sin 2\theta] - K(T/T_i)^{1/2}}{1 - \frac{1}{2}(1 - 1/R_v)[1 - \cos\theta - \frac{1}{2}(r/l)\sin^2\theta]} \quad (4)$$

where p , V , M , R , T , and γ are respectively the pressure, volume, mass, gas constant, temperature, and specific-heat ratio of the gas inside the engine cylinder, θ is the angular position of the crankshaft measured from bottom dead center, V_i is the volume at $\theta = 0$, R_v is the volume compression ratio, ω is the angular speed of the crankshaft, and K is a dimensionless effusion parameter defined by

$$K \equiv (\pi/2)\{\gamma[2/(\gamma + 1)]^{(\gamma+1)/(\gamma-1)}RT_i\}^{1/2}(d^*/\omega V_i) \quad (5)$$

Equation (4) emphasizes that the temperature variation is due to a) the piston motion and b) the gas escaping through the nozzle.

Using Eq. (4), one can determine $T(\theta)$ by numerical integration. Using Eqs. (1-3), one can determine V , p , and M then also as functions of θ .

B. Predicted beam density at the detector

For a beam with a cycling-pressure source, differences in molecule flight times from the sudden-freezing surface to the detector imply (at least in principle) that molecules detected at the detector at a given time came from different parts of the source cycle. Let bottom dead center of the crankshaft correspond to time zero. Then, at time λ , the number of molecules per unit volume in the speed-ratio range from s to

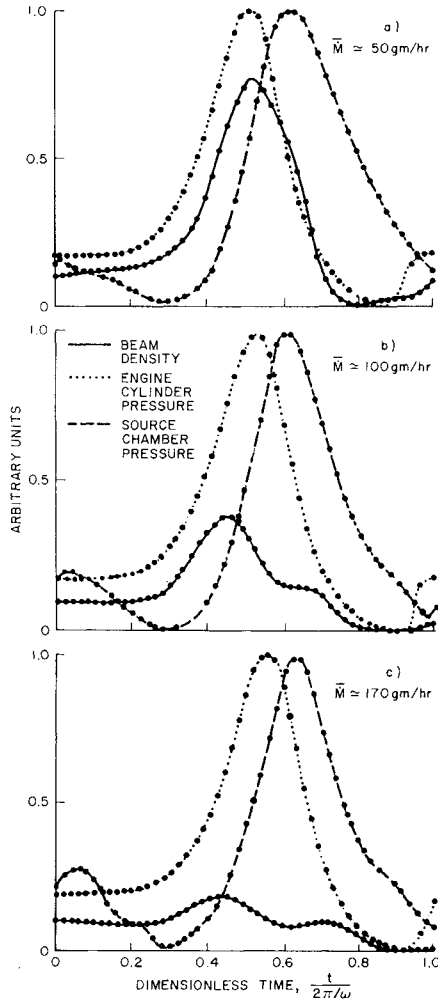


Fig. 2 Measured values of beam density, engine-cylinder pressure, and source-chamber pressure: Both pressure curves are measured from their minima and normalized to unity at their maxima. The abscissa is normalized using the engine period. $K \approx 0.105$ (engine speed = 1500 RPM); $R_s \approx 8$. The mass flow rate \dot{M} is averaged over the engine period.

$s + ds$ emanating from the sudden-freezing surface is

$$dN_{\lambda,s} = n_{f,\lambda} f(s_{f,\lambda}) ds_{f,\lambda} \quad (6)$$

where n is the molecule number density, $f(s)$ is the speed-ratio distribution function, and the subscript f,λ indicates quantities measured at the sudden-freezing surface at time λ . These molecules will arrive at the detector at time $t = L_{sd}/(V_{f,\lambda} s_{f,\lambda}) + \lambda$ where v is the most probable random speed. Then the number density at the detector at time t due to molecules that left the sudden-freezing surface since $t = 0$ is

$$N_{d,t} = \int_0^t n_{d,\lambda} \frac{L_{sd} f(s_{f,\lambda})}{K_{f,\lambda} v_{f,\lambda} (t - \lambda)^2} d\lambda \quad (7)$$

with

$$K_{f,\lambda} \equiv \int_0^\infty f(s_{f,\lambda}) ds_{f,\lambda}$$

where $n_{d,\lambda}$ is the beam density at the detector for a steady beam with source properties the same as for the unsteady beam at time λ . If the expansion to the sudden-freezing surface is isentropic, then the most probable random speed $v_{f,\lambda}$ can be related to the stagnation temperature $T_{o,\lambda}$ inside the

source by

$$v_{f,\lambda} = (2RT_{f,\lambda})^{1/2} = (2RT_{o,\lambda})^{1/2} \{1 + [(\gamma - 1)/2] M_{f,\lambda}^2\}^{-1/2} \quad (8)$$

with $M_{f,\lambda}$ given by the semiempirical expression⁷

$$M_{f,\lambda} \approx 1.17 K n_{o,\lambda}^{-0.4} \quad (9)$$

If the dimensionless speed distribution function $f(s_{f,\lambda})$ is either known or assumed a priori, then Eq. (7) can be integrated numerically.

The forementioned numerical integration, although straightforward, is time consuming. Furthermore, for the system used in the experiments described here, the most probable time of flight is short in comparison with the period of the engine cycle. Hence, consider a simplified model in which all molecules emanating from the source travel with the same (hydrodynamic) speed

$$u_{f,\lambda} = M_{f,\lambda} v_{f,\lambda} (\gamma/2)^{1/2} \quad (10)$$

where $M_{f,\lambda}$ and $v_{f,\lambda}$ are evaluated using Eqs. (8) and (9). Then molecules leaving the sudden-freezing surface at time λ reach the detector at time $t = \lambda + L_{sd}/u_{f,\lambda}$ so that

$$N_{d,t} = N_{d,(\lambda + L_{sd}/u_{f,\lambda})} = n_{d,\lambda} \quad (11)$$

In this simplified model, all molecules detected at the detector at a given time come from the same part of the source cycle. Beam density measurements reported here will be compared with predictions made using both the more general model [Eq. (7)] and the simplified model [Eq. (11)].

Experimental Apparatus

The beam source is a modified model airplane engine with a 1.04-cm bore, a 1.22-cm stroke, and a volume compression ratio of 8. The head was replaced by a 0.025-cm stainless steel diaphragm with a 0.033-cm diam sampling orifice located at its center. Pressure was measured by a semiconductor strain gage mounted on the diaphragm; the average gas temperature was measured by a thermocouple. The engine was driven by a variable-speed synchronous motor. Further details are included in Ref. 4.

Results

A. Numerical predictions

Values of $T(\theta)$, $p(\theta)$, and $M(\theta)$ were calculated using Eqs. (1, 2, and 4) and an IBM Model 360/91 digital computer. It was found that increasing R_s increases significantly the

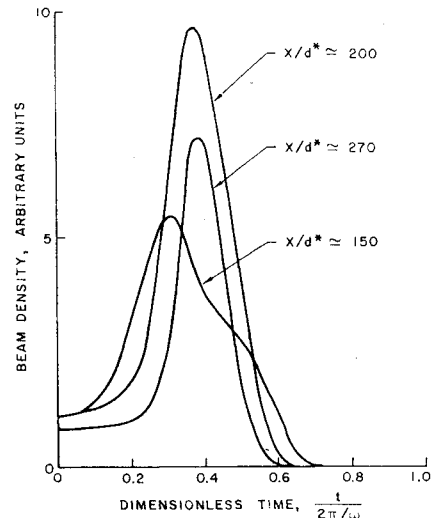


Fig. 3 Measured values of beam density for several nozzle-to-skimmer distances.

pressures and temperatures during the central portion of the cycle but decreases them during the last 35% of the cycle; increasing the effusion parameter K decreases the pressures and temperatures during all parts of the cycle.

The beam density at the detector was calculated numerically for both Eqs. (7) and (11). Typical predicted values are compared with measured values in Fig. 1. The results justify the use of the simplified model for cases in which the most probable time of flight is less than about 5% of the cycle period.

B. Experimental results

Data taken to demonstrate the increasing skimmer-interference effects due to increasing mass-flow rates are presented in Figs. 2a-2c. It is seen that the beam density decreases dramatically, particularly in the vicinity of the top dead center, as the mass-flow rate increases. An analysis of source-chamber flows indicates that the observed lag of the source-chamber pressure peak behind the source pressure peak is determined by the ratio of the booster-pump characteristic time and the source-cycle period. The smaller source-chamber pressure peak appearing in the early part of the cycle is due to a superpositioning of residual gas from the previous cycle and gas from the present cycle.

Consequences of varying the nozzle-skimmer distance x are shown in Fig. 3. For small nozzle-skimmer distances, strong skimmer interference occurs near the peak density of the cycle; for large nozzle-skimmer distances, the beam density is attenuated throughout the cycle.

Beam densities observed for three different engine speeds are compared in Fig. 4. It is seen that the peak beam density increases with engine speed, which speed is inversely proportional to the effusion parameter K .

Discussions

Agreement between the measured and predicted signals is good except near the end of the cycle (see Fig. 1). The relatively low beam density observed near the end of the cycle might be due to background scattering resulting from the relatively high source-chamber background density during this part of the cycle.

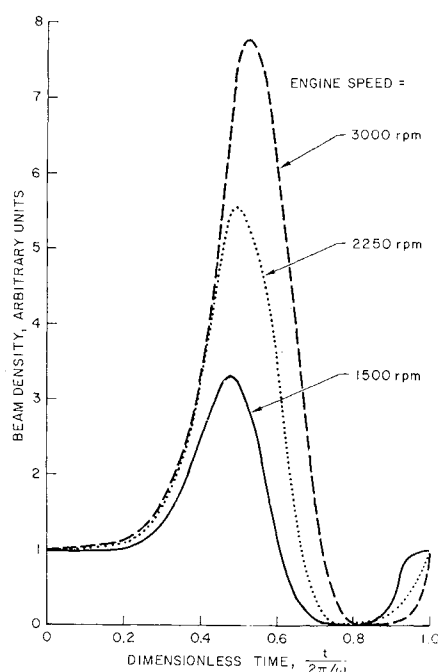


Fig. 4 Measured values of beam density for several engine speeds. The signals are measured from their minima and normalized using the values evaluated at $t = 0$.

The measured peak source pressures (Fig. 2) are substantially smaller than the predicted values. It is possible that the measured peak pressure was decreased by a) gas leakage between the piston and the cylinder wall and b) heat transfer from the gas to the cylinder wall.

Continuations of these studies have shown that skimmer interference affects the relative densities in a multicomponent beam less than it affects the absolute density. For details of these additional studies, see Refs. 4-6.

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Vortices Induced in a Jet by a Subsonic Cross Flow

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Nomenclature

- d = nozzle diameter
 I = impulse
 K' = empirical constant
 K = vortex strength constant
 U = velocity
 x, y, z = coordinates in Fig. 1
 $2y_0$ = vortex spacing
 Y_v = vortex spacing constant
 μ = angle between jet trajectory and freestream direction
 ξ, η, ζ = coordinates in Fig. 1
 ρ = density
 σ = freestream-to-jet exit velocity ratio
 ϕ = velocity potential

Subscripts

- ∞ = freestream conditions
 e = jet exit conditions

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