Experimental and Numerical Study of Supersonic Jets of N_2 , H_2 , and $N_2 + H_2$ Mixtures

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Abstract. The structure of the shock wave system in underexpanded free jets of pure gases and binary gas mixtures (N_2 , H_2 , $N_2 + H_2$) influenced by strong non-equilibrium processes, such as rotational relaxation, is studied both experimentally and numerically.

Keywords: Underexpanded free jet, barrel shock, rotational relaxation, pressure and temperature measurements, Raman diagnostics, Navier-Stokes equations, gas mixture, diffusion, simulation.

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INTRODUCTION

Gas shock waves are generated in different natural and artificial processes. In a supersonic free jet issuing from the nozzle into a low-pressure space, a system of shock waves adjusts the jet to downstream boundary conditions, changing the flow line directions and reducing the velocity. For axisymmetric jets, such a system is formed by a normal shock wave (Mach disk) perpendicular to the jet axis, and by a barrel shock wave that encapsulates the zone of silence of the jet [1]. Such kind of flow representing a so called underexpanded jet provides the conditions for studying the structure of shock waves in the pure gas or gas mixture. Shock waves are characterized by strong density, temperature, and velocity gradients that in the case of molecular gases results in a strong breakdown of equilibrium between translational and internal degrees of freedom.

In this paper the structure of the shock wave system in underexpanded free jets of pure gases and binary gas mixtures (N_2 , H_2 , $N_2 + H_2$) influenced by strong non-equilibrium processes, such as rotational relaxation, is studied both experimentally and numerically. The experimental data analyzed here were published earlier [2, 3], however the present r/D experimental data have been recalibrated by +0.1 units.

EXPERIMENTAL

One of the two jet diagnostics facility at the Instituto de Estructura de la Materia (CSIC) in Madrid has been employed for the number density and rotational temperature measurements of the jets reported in this work. It consists of **1**) an expansion chamber connected to **2**) a vacuum line for production of steady supersonic free jets through **3**) a home made nozzle fed by a gas (N_2 , H_2 , N_2+H_2) supply line. Raman scattering along selected points of the jet are excited by **4**) a powerful *cw*-laser, being detected by **5**) a high sensitivity Raman spectrometer. Laser source, expansion chamber, and spectrometer are optically connected by means of **6**) a highly efficient transfer optics system. These main elements, and the vacuum system as well, are mounted onto independent structures in order to minimize the effect of vibrations. Nozzle, laser focusing optics, and Raman scattering collection optics inside the expansion chamber are mounted onto **7**) high-accuracy ($\pm 1 \mu m$) xyz-positioning stages operated by remote control.

1. Expansion chamber. Manufactured in welded aluminum 3 cm thick walls and 5 cm thick basis, with dimensions of $55 \times 44 \times 59 \text{ cm}^3$, it is coated inside in order to minimize stray light. Five DN250 and seven DN63 flanges allow for installation of pressure sensors, optical windows, gas feeding line, and electrical connections.

2. Vacuum line. It consists of a 1430 m³/h Roots pump backed by a 70 m³/h rotary pump. A gate valve between the expansion chamber and the Roots pump allows for reference static measurements at known absolute number density.

3. Nozzle and gas supply line. A home made drilled nozzle of diameter $D = 310 \mu\text{m}$ and internal length $L \approx 1.8$ mm operating at 295 K has been employed. $\text{N}_2 + 2\text{H}_2$ and $2\text{N}_2 + \text{H}_2$ mixtures were prepared by means of two Bronkhorst High-Tech mass flow controllers installed online in the feeding line.

4. Laser source. Raman scattering was excited by an Ar^+ cw-laser source delivering 4 W vertical linear polarized radiation at $\lambda = 514.5$ nm. The 1.8 mm wide laser beam was sharply focused onto the chosen points of the jet by means of an $f = 50$ mm Ar14-coated lens.

5. Spectrometer. The spectrometer is a 1-meter additive double monochromator with two gratings of 2400 l/mm equipped with a CCD detector of 2048×512 pixels of $20 \mu\text{m}$ refrigerated by liquid N_2 . Scanning and data acquisition are computer controlled by means of an *ad-hoc* home developed software (REGISTRA, version 3.02).

6. Transfer optics. Raman scattering from selected points along the jet is collected by a 50 mm f/1.1 Leica objective and then projected onto the entrance slit of the spectrometer by a $f = 500$ mm achromat with a $10\times$ magnification. Spatial resolution of the probed volume element along the jet is determined by the entrance slit width of the spectrometer, and across the jet by the pixel binning system of the CCD detector. Representative values for this work are $15 \mu\text{m}$ along the jet, $70 \mu\text{m}$ across the jet near the nozzle, and $350 \mu\text{m}$ across the jet in the far downstream region.

7. Micropositioning. Points to be probed along and across the jet are selected by moving the nozzle while the laser focus and Raman collection optics remain static. Estimated pointing accuracy within the flow field is $\pm 5 \mu\text{m}$, while repetitivity is $\pm 1 \mu\text{m}$.

The jets were generated at $p_0 = 1$ bar stagnation pressure. Number densities and rotational temperatures along the zone of silence were measured at background pressures p_b as low as possible, namely 0.08 mbar for pure N_2 , 0.10 for $2\text{N}_2 + \text{H}_2$, 0.13 for $\text{N}_2 + 2\text{H}_2$, and 0.35 for pure H_2 . The normal and barrel shock waves were measured at fixed $p_b = 6.1$ mbar employing either the expanded gas as background gas, or pure H_2 or N_2 , in order to investigate penetration effects across the shock boundaries.

Number densities were measured from the integrated intensity of the $\text{Q}(\nu_1)$ vibrational band of either N_2 or H_2 , which is linearly proportional to the number density to a very good approximation. Estimated accuracy is $\approx 5\%$ close to the nozzle, and $\approx 10\%$ far downstream in the jet.

Rotational temperatures of H_2 were measured from the distribution of intensities of the $\text{Q}(0)$, $\text{Q}(1)$, $\text{Q}(2)$, and $\text{Q}(3)$ lines of the $\text{Q}(\nu_1)$ Raman branch, which are proportional to the population of the $J = 0, 1, 2$ and 3 rotational levels, respectively. Temperatures were retrieved from these relative populations. Rotational temperatures of N_2 were obtained from the distribution of intensities of the $J \rightarrow J + 2$ pure rotational Raman lines which are proportional to the populations of the rotational levels J . Rotational temperatures for *para*- H_2 along the zone of silence are expected to be accurate to 1 to 3 K, and for *ortho*- H_2 to 1.5 to 5 K, depending on the region of the jet. Temperature uncertainty of N_2 due to random errors is on the order of 1 %. Rotational temperatures for N_2 within the shock waves are not well defined due to the breakdown of Boltzmann distribution. Values given are just orientative.

NUMERICAL APPROACHES

In this paper the numerical analysis will be made for the following five regimes studied in [3]: $\text{jN}_2\text{-bN}_2$ (the pure N_2 jet against background nitrogen), $\text{jH}_2\text{-bH}_2$, $\text{jN}_2\text{-bH}_2$, $\text{jH}_2\text{-bN}_2$ and $\text{j}(\text{N}_2 + 2\text{H}_2)\text{-b}(\text{N}_2 + 2\text{H}_2)$ with stagnation pressure $p_0 = 1$ bar, background pressures $p_b = 6.1$ mbar and stagnation T_0 and background T_b temperatures both being equal to 295 K for all the regimes.

Among these regimes only the first one may be simulated with the full set of unsteady Navier-Stokes equations written for monocomponent perfect gas (NS-algorithm) [4]. Due to extremely low rate of rotational relaxation of H_2 , the flow field in the jet containing this molecule can not be treated by the full set of Navier-Stokes equations even completed by the bulk viscosity, since its corresponding value should be very high and, therefore, outside the range of applicability of the bulk viscosity concept. This is why the hybrid NS-PNS approach was applied for the numerical analysis of the remaining four regimes. In this approach the NS-algorithm was used for the simulation of the choked flow inside the nozzle in order to obtain the distribution of the flow quantities at the nozzle exit. Such distribution was taken as the starting surface for further calculation of the flow in the free jet using the parabolized Navier-Stokes equations written in so called natural coordinates formed by streamlines and lines normal to them and resolved by a marching procedure (PNS-algorithm) [5]. For the regime $\text{jN}_2\text{-bN}_2$ the flow field was treated by both NS- and NS-PNS- approaches that allows one to estimate the accuracy of the latter approach for describing the

underexpanded free jet flow field including the structure of the barrel shock. As it was found, the NS-PNS-algorithm provides a good description of the jet flow field in the region up to the Mach disk, though the latter itself surely cannot be adequately described by the marching procedure.

The main features of NS-algorithms are described in detail in [4]. The peculiarity of applying the PNS-algorithm [5] for simulation of the flow of a binary mixture of rotationally relaxing gases, which is not described in [5], will be clarified below briefly. The basic system of gas dynamic equations together with the diffusion and relaxation equations in natural coordinates for axisymmetric flow has the form

$$\rho u A = \text{const}, \quad (1)$$

$$\rho u \frac{\partial u}{\partial s} + \frac{\partial p}{\partial s} = \frac{1}{r} \frac{\partial}{\partial n} (r \mu \frac{\partial u}{\partial n}) - \frac{4}{3} \mu u (\frac{\partial \varphi}{\partial n})^2, \quad (2)$$

$$\rho u^2 \frac{\partial \varphi}{\partial s} + \frac{\partial p}{\partial n} = \frac{4}{3} \frac{\partial}{\partial n} (\mu u \frac{\partial \varphi}{\partial n}) + 2 \mu u \frac{\cos \varphi}{r} (\frac{\partial \varphi}{\partial n} - \frac{\sin \varphi}{r}), \quad (3)$$

$$\rho u \frac{\partial}{\partial s} (h + e_r + \frac{u^2}{2}) = \frac{1}{r} \frac{\partial}{\partial n} \{ r [u \mu \frac{\partial u}{\partial n} + \lambda \frac{\partial T}{\partial n} + c_1 \lambda_{r1} \frac{\partial T_{r1}}{\partial n} + c_2 \lambda_{r2} \frac{\partial T_{r2}}{\partial n} - J_{1n} (h_1 - h_2 + R_1 T_{r1} - R_2 T_{r2} + D_T \alpha \frac{R_0 m}{m_1 m_2} T)] \}, \quad (4)$$

$$\rho u \frac{\partial T_{ri}}{\partial s} = \rho \frac{T - T_{ri}}{\tau_{ri}} + \frac{1}{r} \frac{\partial}{\partial n} (r \lambda_{ri} \frac{\partial T_{ri}}{\partial n}), \quad (5)$$

$$p = \rho R T, \quad (6)$$

$$\rho u \frac{\partial c_1}{\partial s} = - \frac{1}{r} \frac{\partial}{\partial n} (r J_{1n}), \quad (7)$$

$$J_{1n} = - \rho D_{12} [\frac{\partial c_1}{\partial n} + c_1 c_2 (D_p \frac{m_2 - m_1}{m} \frac{\partial \ln p}{\partial n} + D_T \alpha \frac{\partial \ln T}{\partial n})], \quad (8)$$

$$h = c_1 h_1 + c_2 h_2,$$

$$h_i = \frac{5}{2} R_i T,$$

$$e_r = c_1 R_1 T_{r1} + c_2 R_2 T_{r2},$$

$$\lambda_{ri} = \rho D_{ii} R_i,$$

where s and n are the coordinates along the streamlines and lines normal to them, respectively, ρ is the density, p is the pressure, T is the translational temperature, A is the streamtube area, h , h_i are the specific enthalpy of mixture and of i^{th} species over translational degrees of freedom, respectively, φ is flow angle with respect to the axis, μ is the dynamic viscosity of the mixture, λ is the contribution of translational degrees of freedom to the heat conductivity of the mixture, r is the distance from the symmetry axis, c_i is the mass fraction of i^{th} species in the mixture, T_{ri} is the rotational temperature of i^{th} species, D_{12} is the binary diffusion coefficient, D_{ii} is the self diffusion coefficient for i^{th} species, τ_{ri} is rotational relaxation time of i^{th} species, R , R_i are the gas constant of mixture and of i^{th} species, respectively, R_0 is the universal gas constant, m_i is the molecular mass of i^{th} species, m is the mean molecular mass of mixture, J_{1n} is the diffusion flux of species 1, e_r is the specific rotational energy of mixture, α is the thermal diffusion factor, λ_{ri} is the rotational heat conductivity of i^{th} species, D_p , D_T are auxiliary values being equal 1 or 0 determining the accounting for or neglecting the effects of pressure- (D_p) or thermal (D_T) diffusion on the flow field.

The method is based on the decomposition of the whole flow field into a number of streamtubes [6]. The 2-D character of the flow is taken into account by normal momentum equation (3), which defines the local curvature $\frac{\partial \varphi}{\partial s}$ of the streamline. The continuity equation (1), the streamwise momentum equation (2), and the energy equation (4) together with relaxation equations (5) and equation of state (6) define the 1-D evolution of the flow in each streamtube. In the diffusion equation (7) with expression (8) for the diffusion flux the contributions of concentration, pressure and thermal diffusion fluxes on the flow field are taken into account. The last term in the energy equation (4) describes the diffusion thermoeffect [7].

Under the assumption that the pressure above the streamline corresponding to the jet boundary is constant and equals to the pressure in the flooded space the algorithm allows one to simulate the whole flow field in the underexpanded jet by the marching procedure. For this simulation the background gas is assumed to have small

axial velocity with corresponding Mach number $M_b \ll 1$ (usually $M_b = 0.02$). The algorithm is suitable to describe the flow field of binary gas mixtures in a wide range of conditions, including those of oblique shock waves such as the barrel shock.

The values of rotational relaxation time for considered species were estimated as $\tau_{ri} = Z_{ri}\tau_{ti}$ where $\tau_{ti} = \frac{\pi}{4} \frac{\mu_i}{p}$ and μ_i is the dynamic viscosity of i^{th} species. The calculations were performed for the collision numbers $Z_r = 5$ for N_2 and $Z_r = 600$ for H_2 [8].

The temperature dependence of the transport coefficients for the considered gases and their binary mixtures was assumed to be described by Lennard-Jones (6 – 12) potential [7] with parameters $\sigma = 2.968 \text{ \AA}$, $\varepsilon / k = 33.3 \text{ K}$ for H_2 and $\sigma = 3.681 \text{ \AA}$, $\varepsilon / k = 91.5 \text{ K}$ for N_2 and the combination rules commonly used to describe the interaction between unlike molecules [7]. The exact expressions for the first approximation of the transport properties of a gas mixture (viscosity, heat conductivity, diffusion, thermal diffusion) were used [7].

RESULTS AND DISCUSSION

FIGURE 1. Axial (a) and radial at $z/D = 5.4$ (b) distributions of number density in pure N_2 jet. Solid lines – NS-algorithm, dashed lines – PNS-algorithm, symbols – experiment.

FIGURE 2. Axial (a) and radial at $z/D = 5.4$ (b) distributions of temperatures in pure N_2 jet. 1 – NS-algorithm (T), 2 – PNS-algorithm (T_r), 3 – PNS-algorithm (T), symbols – experiment (T_r).

Figure 1(a) illustrates the axial distribution of number density in pure N_2 jet (jN_2 - bN_2). As it is seen, the predictions of NS-algorithm are in good agreement with the measured data in the whole flow field including the region of Mach disk. As mentioned above, the predictions of PNS-algorithm failed to describe the Mach disk region, though in the region of silence the predictions of both algorithms are practically identical.

Figure 1(b) illustrates the radial distribution of number density in the same jet at $z/D = 5.4$ (here and below all the radial profiles of parameters will be presented at this axial distance, the precise dimensional value of which is $z = 1.66$ mm). Again the predictions of both algorithms are very close, noticeable difference ($\sim 10\%$) between them is observed only for maximum value of number density in the barrel shock. An overestimation of both algorithms of ~ 0.2 (in units of r/D) with respect to the experimental data is observed. However, the shape of the calculated profiles is in excellent agreement with the shape of the experimental ones.

Figure 2(a) illustrates the axial distributions of temperatures. As in the number density case (see Figure 1(a)), the predictions of NS-algorithm for temperature are in good agreement with the measured data in the whole flow field including the region of Mach disk and the predictions of both algorithms are very close in the region of silence. In contrast with NS-algorithm which predicts only one temperature T that may be interpreted as translational temperature, the PNS-algorithm predicts two temperatures: translational, T , and rotational, T_r , though the difference between them is very small due to high rate of rotational relaxation of nitrogen.

The radial temperature profiles shown in Figure 2(b) reveal the same features as the number density profiles in Figure 1(b). Thus, the comparison between model predictions and the results of measurements, illustrated in Figures 1 and 2, confirm, that in the case of pure nitrogen jet both NS- and PNS-algorithms provide quite similar description of axial and radial profiles of number density and temperature. This allows us to hope for a similar description of the flow field in the H_2 -containing jets by using the PNS-algorithm.

FIGURE 3. Axial (a) and radial at $z/D = 5.4$ (b) distributions of number density in pure H_2 jet. Solid lines – model (PNS), symbols – experiment.

Figure 3(a) illustrates the axial distribution of number density in pure H_2 jet (jH_2-bH_2). As it is seen, the profile obtained by PNS-algorithm is in good agreement with the data measured in the zone of silence.

Figure 3(b) illustrates the radial distribution of number density in the same jet. As in the case of pure N_2 jet (see Figure 1(b)) the shape of the profile obtained by the PNS-algorithm agrees well with the experimental one, while the predicted radius of the barrel shock is again ~ 0.2 (in units of r/D) larger than the measured one. Comparison of the

FIGURE 4. Axial (a) and radial at $z/D = 5.4$ (b) distributions of temperatures in pure H_2 jet. Lines – model (PNS): solid lines – T_r , dashed lines – T ; Symbols – experiment for T_r : solid circles – *para*- H_2 , open circles – *ortho*- H_2 .

measured profiles in the jets of N_2 and H_2 (see Figures 1(b) and 3(b)) reveals the difference in the barrel shock radiuses (the H_2 jet is thinner than the N_2 jet) that seems to be caused by the extremely low rate of rotational relaxation in H_2 that results in the intermediate behaviour of this gas between that of monatomic and diatomic gases in expanding flow.

Figure 4(a) illustrates the axial distributions of temperatures in pure H_2 jet. As in the number density case (see Figure 3(a)), the profile of rotational temperature obtained by PNS-algorithm is in agreement with measured data in the zone of silence. The measurements reveal some difference in rotational temperatures of *para*- and *ortho*- H_2 which are ignored in the used model. Large difference between rotational and translational temperatures is caused by the extremely low rate of rotational relaxation of H_2 .

The same features are observed in Figure 4(b) where the radial temperature profiles for pure hydrogen jet are shown.

FIGURE 5. Radial distributions of total number density (a) and of mole fraction of background gas (b) in jN_2 - bH_2 and jH_2 - bN_2 jets at $z/D = 5.4$. Lines – model (PNS): 1 – jN_2 - bH_2 jet, 2 – jH_2 - bN_2 jet; Symbols – experiment: closed circles – jN_2 - bH_2 jet, open circles – jH_2 - bN_2 jet.

Figure 5(a) illustrates the radial profiles of total number density in jN_2 - bH_2 and jH_2 - bN_2 jets. As in Figures 1(b) and 3(b) the shape of the numerical profiles agrees very well with experiment and, again, the predicted radiuses are overestimated by ~ 0.2 (in r/D units). As in Figures 1(b) and 3(b) the jH_2 - bN_2 jet is thinner than the jN_2 - bH_2 jet.

FIGURE 6. Radial distributions of temperature at $z/D = 5.4$ in jH_2 - bN_2 (a) and $j(N_2+2H_2)$ - $b(N_2+2H_2)$ (b) jets. Lines – model (PNS): 1 – T , 2 – T_r of N_2 , 3 – T_r of H_2 ; Symbols – experiment for T_r : solid circles – *para*- H_2 , open circles – *ortho*- H_2 , triangles – N_2 .

FIGURE 7. Radial distributions of total number density (a) and of mole fraction of N_2 (b) in $j(N_2+2H_2)$ - $b(N_2+2H_2)$ jet at $z/D = 5.4$. (a): Lines – model (PNS), symbols – experiment; (b): Lines – model (PNS): 1 – $D_T = D_p = 0$; 2 – $D_p = 0$, $D_T = 1$; 3 – $D_p = 1$, $D_T = 0$; 4 – $D_T = 1$, $D_p = 1$; Symbols – experiment.

Radial profiles of mole fraction of background gas in these jets are shown in Figure 5(b), the numerical profiles are again in agreement with the measured data. The penetration of H_2 in the jet of N_2 is more pronounced than the penetration of N_2 in the jet of H_2 , which is well reproduced by the model. At distance $z/D = 5.4$ the concentration of the background gas in the jet axis is negligibly small. The numerical experiments show that for considered case when the jet gas and the background gas are different (jN_2 - bH_2 , jH_2 - bN_2) the structure of the barrel shock is completely determined by concentration diffusion, with negligibly small effects of pressure- and thermal diffusion fluxes.

Figure 6(a) illustrates the radial profiles of temperatures in jH_2 - bN_2 jet. The comparison of this profiles with those for pure H_2 jet (see Figure 4(b)) reveals the effect of the nature of the background gas – as it is seen, the replacement of H_2 by N_2 as the background gas resulted in slow decrease of rotational temperatures of both *ortho*- and *para*- H_2 species. The same behaviour is observed for numerical profiles of rotational temperature of H_2 .

Figure 6(b) illustrates the radial profiles of temperatures in $j(N_2+2H_2)$ - $b(N_2+2H_2)$ jet. Now the comparison of this profiles with those for pure H_2 jet (see Figure 4(b)) reveals the effect of the dilution of H_2 by 1/3 mole fraction of N_2 – this procedure leads to noticeable decrease of rotational temperatures of both H_2 species. The same behaviour observed for numerical profiles of rotational temperature of H_2 is caused by slower decrease of translational temperature in $j(N_2+2H_2)$ - $b(N_2+2H_2)$ jet compared to that in pure H_2 jet. Rotational temperature of N_2 is significantly lower than that for H_2 and is close to the numerical curve, which in turn is close to the translational temperature.

The radial profiles of total number density in $j(N_2+2H_2)$ - $b(N_2+2H_2)$ jet shown in Figure 7(a) are intermediate between the corresponding profiles for pure N_2 and pure H_2 jets shown in Figures 1(b) and 3(b), respectively.

The plots in Figure 7(b), where the radial profiles of mole fraction of N_2 in $j(N_2+2H_2)$ - $b(N_2+2H_2)$ jet are shown, illustrate the effect of pressure, thermal and concentration diffusion fluxes on mixture composition in this jet. Neglecting the pressure and thermal diffusion ($D_T = D_p = 0$, curve 1) leads to constant mixture composition in the whole flow field. In spite of the small effect of thermal diffusion itself ($D_p = 0$, $D_T = 1$, curve 2), which is visible only in the barrel shock region, the accounting of this component of total diffusion flux ($D_p = 1$, $D_T = 1$, curve 4) noticeably improves the agreement between model and experiment in the barrel shock region compared to the case when only pressure diffusion is taken into account ($D_p = 1$, $D_T = 0$, curve 3).

CONCLUSIONS

The developed hybrid NS-PNS approach to simulate the structure of underexpanded jet of binary gas mixture with accounting for diffusion processes and the rotational relaxation of both species proved to be an effective tool to clarify the main features of the flow.

In spite of an overestimation in the model of the barrel shock radius of ~ 0.2 (in r/D units), which is well below 10%, the numerical results concerning the shape of the barrel shock are in excellent agreement with the experiment.

For the same stagnation p_0 and background p_b pressures the nature of the background gas doesn't effect on the position of the barrel shock ($jN_2-bN_2 = jN_2-bH_2$; $jH_2-bH_2 = jH_2-bN_2$).

For the same stagnation p_0 and background p_b pressures the radial size of H_2 jet is noticeably lower compared to the size of N_2 jet. Due to extremely low rate of rotational relaxation in H_2 the behaviour of this gas in expanding flow is intermediate between that of monatomic and diatomic gases.

For the case when the jet gas and the background gas are different (jN_2-bH_2 , jH_2-bN_2) the structure of the barrel shock is completely determined by concentration diffusion with negligibly small effects of pressure- and thermal diffusion fluxes.

For the case when the mixture composition in the jet and in the background gas is the same ($j(N_2+2H_2)-b(N_2+2H_2)$) the mixture composition in the barrel shock is completely determined by pressure- and thermal diffusion, though the influence of the thermal diffusion is much lower than the effect of pressure diffusion.

In principle the developed approach allows one to estimate the rotational relaxation rate of H_2 , pure, and mixed with N_2 and we plan to do this in the future.

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