in the shock location, there is agreement between numerical and analytical pressure jumps. Figure 2 is the axial distribution of Mach-number profiles, where the agreement between the numerical and analytical shock jump is apparent. The effect of the sharp expansion corner after the flat nozzle throat is reflected in the Mach-number profiles. Figure 3 is the numerical void fraction profiles. Despite the wide range of pressure ratio and inlet void fractions among the four runs, there is again agreement between numerical and analytical shock jumps.

V. Conclusion

Numerical mass-flux results have been compared to experimental and analytical mass-flux values. The amount of inlet void fraction, together with inlet total pressure and temperature, sets the mass-flux level. Analytic and numerical shock jumps of pressure, Mach number, and void are in close agreement.

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Influence of $O_2(v) + N = NO + O$ on NO Formation in One-Dimensional Air Nozzle Flow

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IN a recent investigation[1,2] we have studied the nonequilibrium state-to-state air vibrational kinetics of air mixtures in one-dimensional nozzle expansion. The main result of this investigation was the strong non-Arrhenius behavior of the NO formation rate through the reaction between vibrationally excited molecules [$N_2(v)$] and atomic oxygen:

$$N_2(v) + O \leftrightarrow NO + N \tag{1}$$

In turn this was caused by the preferential pumping of high energy levels of nitrogen by the gas-phase recombination reaction generating non-Boltzmann vibrational distributions along the axis of the nozzle. In this Note we present results relative to a further study of the same nozzle expansion. In particular we have inserted the reaction between vibrationally excited O_2 molecules and atomic nitrogen, i.e., the process

$$O_2(v) + N \leftrightarrow NO + O \tag{2}$$

with the double intent to detect any variation of the NO formation rate as well as to understand better the kinetics of O_2/O components in the air mixture.

Process 2 is then inserted in the state-to-state vibrational kinetics reported in Refs. 1 and 2, which in turn is coupled to the fluid dynamics equations describing nozzle expansion. We use the same nozzle geometries (parabolic and F4 nozzle) discussed in Refs. 1 and 2, whereas the state-to-state rate coefficients are those discussed in Refs. 3 and 4.

Complete results of this study have been reported in Ref. 5. In this Note we want to emphasize the differences in the relevant results that occur after introduction of reaction 2.

The calculations performed for a 1-m-long parabolic nozzle (see Fig. 1 of Ref. 1) with reservoir pressure P_0 of about 1 atm and

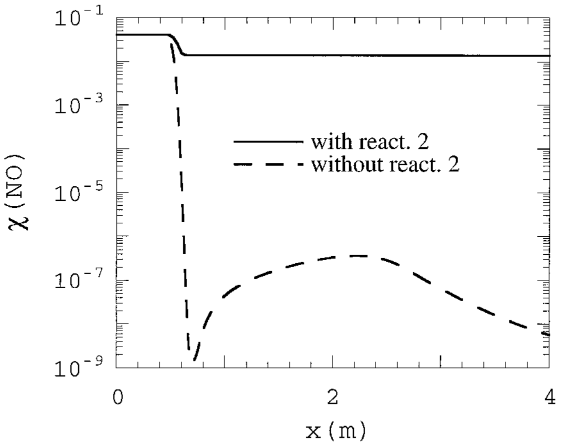
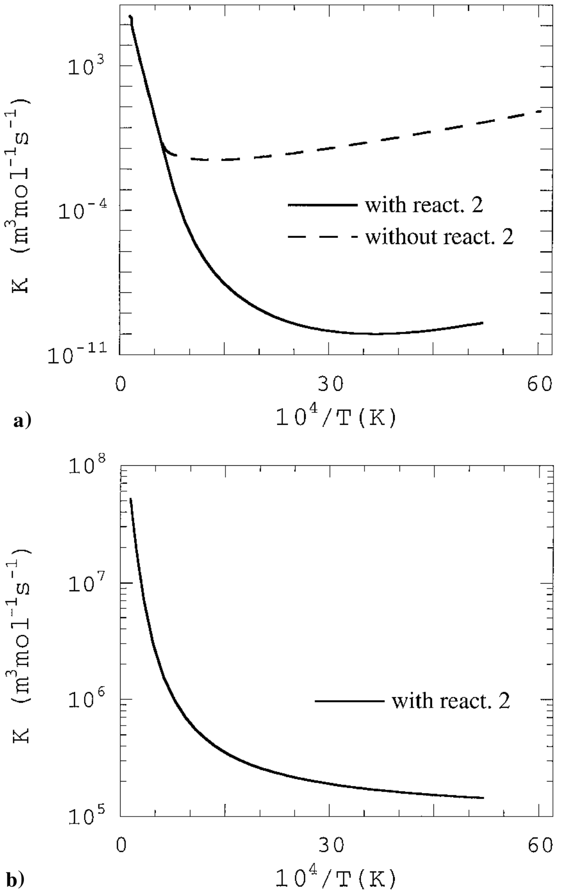


Fig. 1 **NO molar fraction profile in F4 nozzle calculated with and without reaction 2.**



a)

b)

Fig. 2 **Arrhenius plot of NO formation rates by a) reaction 1 and b) reaction 2 in F4 nozzle.**

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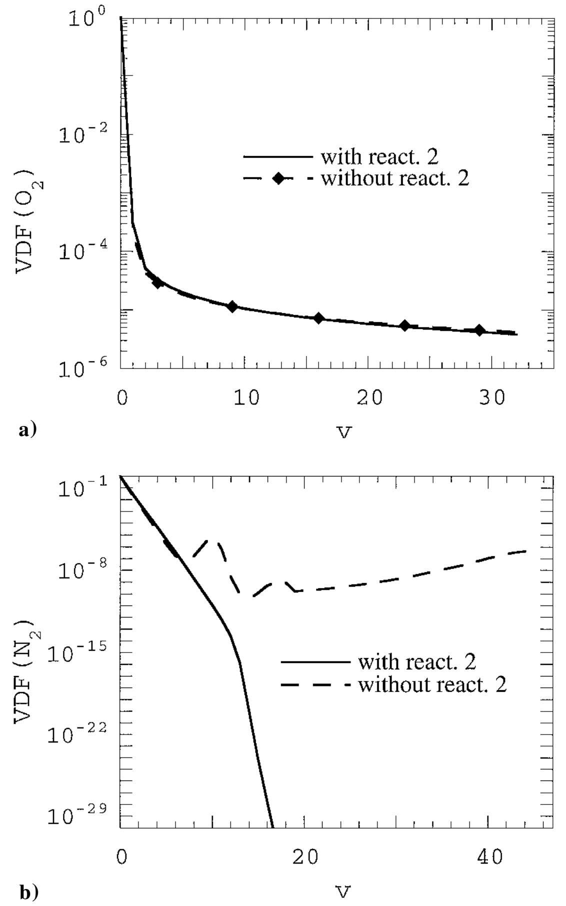

Fig. 3 Vibrational distribution functions of a) oxygen and b) nitrogen at the outlet ($x = 4$ m) of the F4 nozzle calculated with and without reaction 2.

reservoir temperature T_0 values ranging from 4000 to 8000 K show a substantial agreement with the previous results obtained by neglecting reaction b. In particular the translational and vibrational temperature profiles along the nozzle axis for different reservoir temperatures (4000–8000 K) are within 3% in all of the studied cases. The only exception is represented by the O_2 vibrational temperature for $T_0 = 8000$ K, which presents larger deviation: in this case, however, the molar fraction of O_2 is very small.

Concerning the molar fraction profiles of the different components along the nozzle axis, differences up to 35% are observed in the NO profile, whereas the introduction of process 2 has a negligible role in affecting the molar fraction of the other components.

The vibrational distributions of N_2 and O_2 calculated in the presence of process 2 still present the strong deviations from the Boltzmann behavior because of the recombination process: the differences with the results of Refs. 1 and 2 are up to 30% for N_2 and up to 15% for O_2.

These differences propagate in the global rates. As an example, the formation rate of NO through reaction 1 keeps its non-Arrhenius behavior as shown in Refs. 1 and 2, and the insertion of process 2 has a small effect.

The situation completely changes for the high enthalpy F4 nozzle ($P_0 = 300$ atm; $T_0 = 7000$ K) operating at ONERA (see Fig. 16 of Ref. 5). In particular, the NO profile is dramatically affected by reaction 2 as can be appreciated by looking at Fig. 1, where we have reported the NO profile calculated with and without reaction 2. The profile of atomic nitrogen is strongly affected by reaction 2 (Ref. 5).

Interesting also is the behavior of global NO formation rates through reaction channels 1 and 2. Both rates present a non-Arrhenius behavior caused by the corresponding non-Boltzmann vibrational distributions (Fig. 2). The insertion of process 2 dramatically affects the formation rate of NO from vibrationally excited N_2 molecules and atomic oxygen (i.e., from process 1): in particular, differences up to several orders of magnitudes are observed in the two cases (Fig. 2a) as a consequence of the corresponding differences in the N_2 vibrational distributions (Fig. 3b). In Fig. 3a we have reported the corresponding vibrational distributions of O_2, which are not affected by the presence of reaction 2 with similar consequences on the global dissociation rates of O_2.

The present results confirm those reported in Refs. 1 and 2, i.e., the strong nonequilibrium character of vibrational distribution functions of diatomic species as well as the strong non-Arrhenius behavior of global rates for their dissociation and for NO formation. Inclusion of process 2 does not modify the situation reported in Refs. 1 and 2 for the parabolic nozzle.

In different reservoir conditions and geometry (i.e., the F4 nozzle) the role of process 2 is completely different, a dramatic one.

As a conclusion, we want to stress the importance of state-to-state kinetics in characterizing high-enthalpy flows along nozzle axis. Future improvement in this direction can be obtained either improving the input data or using two-dimensional nozzle flow solvers. In addition, dedicated experiments for measuring nozzle profiles of the vibrational distributions as well as of the global concentrations of the different species appear necessary to confirm the importance of the present physical model.

Acknowledgment

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