Chemical Composition Description

- The chemical composition of a sys mixture may be specified in many different ways:

1) $\underset{\text{of species } i}{\text{Mole Fraction}} \equiv X_i \equiv \frac{n_i}{n} \equiv \frac{\#\text{ of moles of species } i}{\#\text{ of moles of mixture}}$

2) $\underset{\text{of species } i}{\text{Concentration}} \equiv [X_i] \equiv \frac{n_i}{V} \equiv \frac{\#\text{ of moles of species } i}{\text{volume of mixture.}}$

3) $\underset{\text{of species } i}{\text{Mass fraction}} \equiv c_i \equiv \frac{\rho_i}{\rho} = \frac{\text{density of species } i}{\text{density of mixture}}$

4) $\underset{\text{of species } i}{\text{Mole-mass Ratio}} \equiv \eta_i = \frac{[X_i]}{\rho} = \frac{\#\text{ moles of species } i}{\text{mass of mixture}}$

4) $\underset{\text{of species } i}{\text{Partial pressure}} \equiv P_i$

Note: $P_i = \rho_i \left(\frac{\hat{R}}{\bar{M}_i}\right) T = \underbrace{n_i}_{\text{\# density of } i = \frac{N_i}{V}} KT = X_i P = [X_i] \hat{R} T$

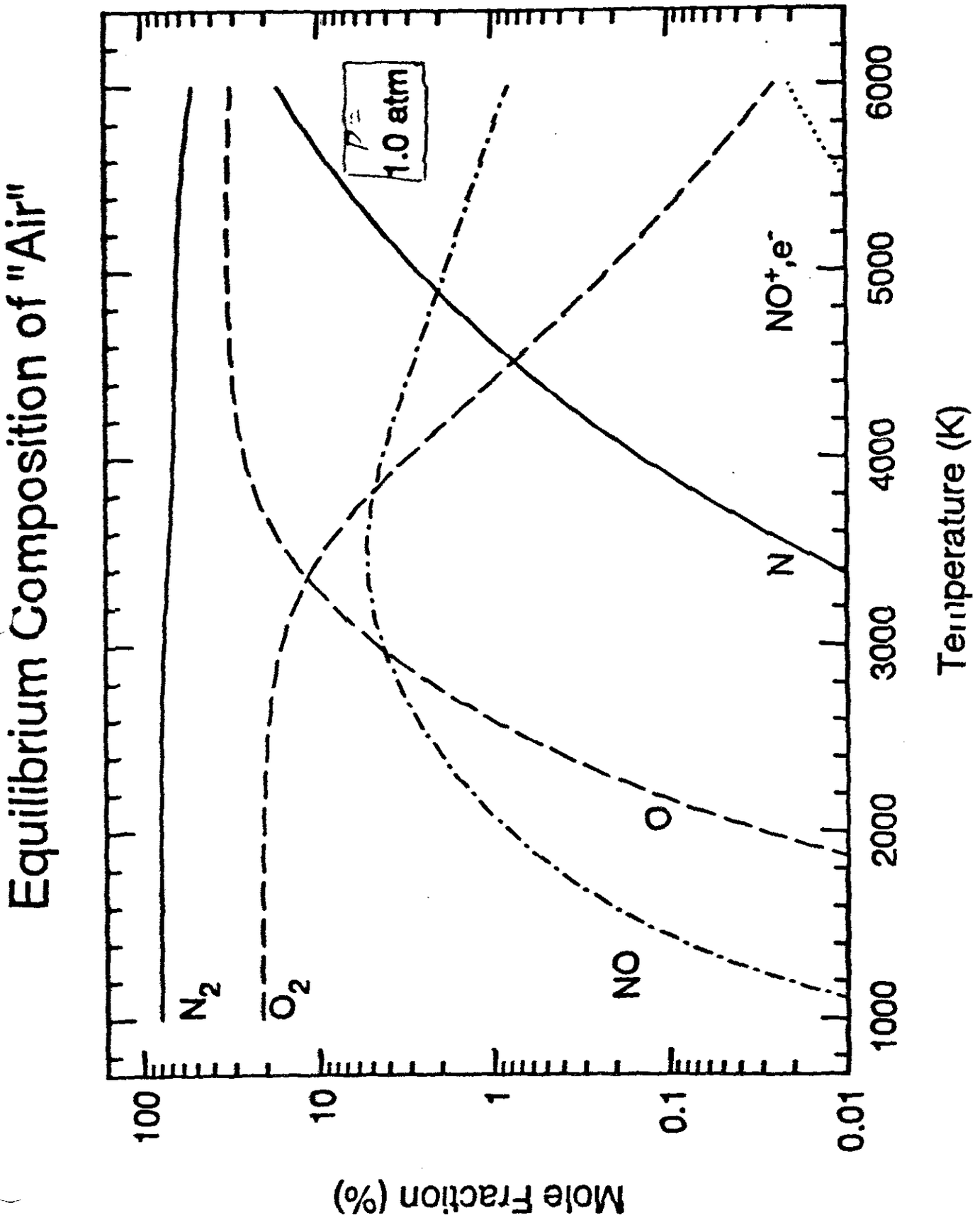
(for mixture of thermally perfect gases) P

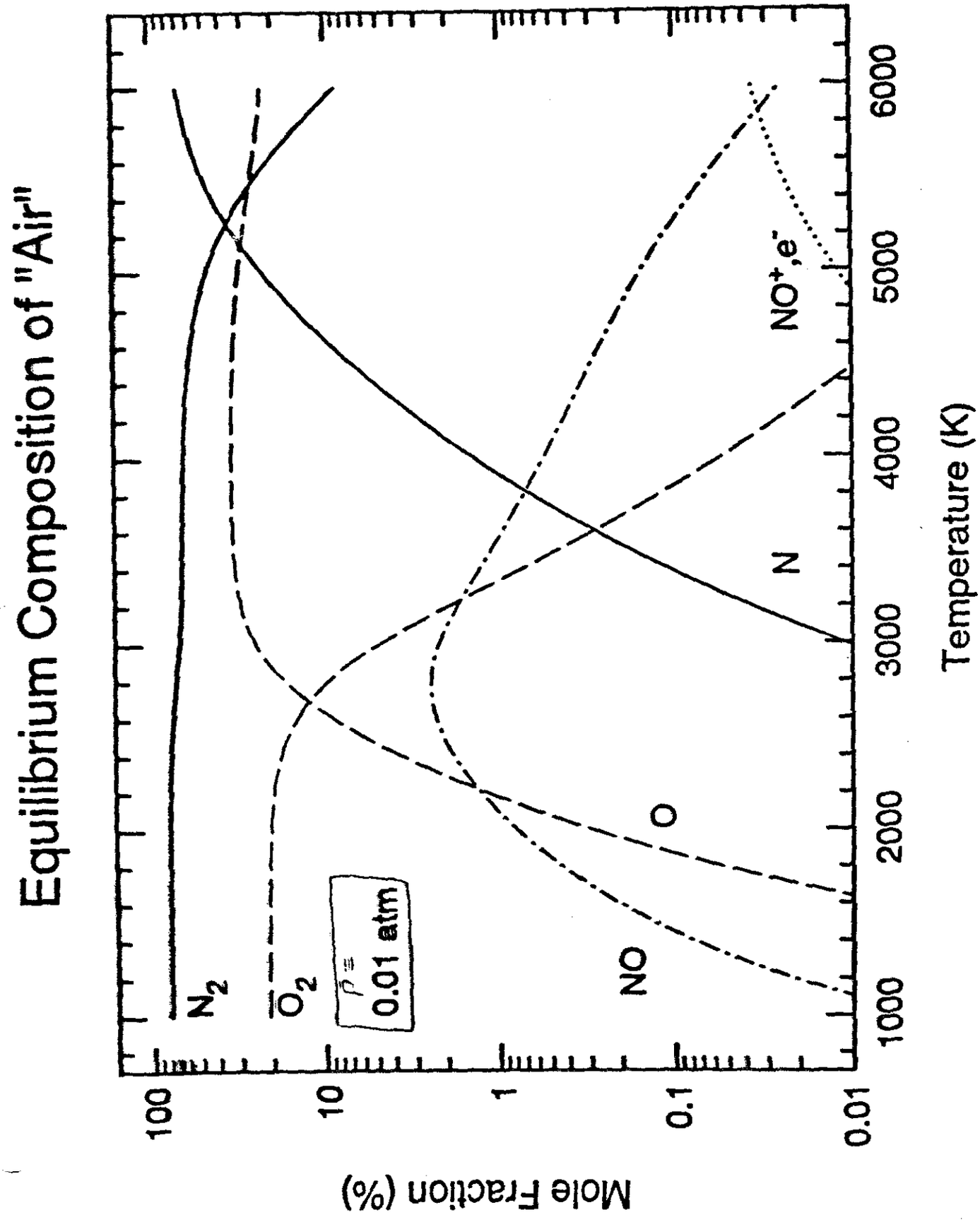
- If any one of the above variables is known for all species, the chemical composition is uniquely defined.

- Note: Pressure = Sum of Partial Pressures

$$P = \sum P_i$$

- Mole Fraction: $X_i = \frac{P_i}{P}$


Equilibrium Composition of "Air"
Mole Fraction (%)
100
10
1
0.1
0.01
Temperature (K)
1000
2000
3000
4000
5000
6000
N_2
O_2
NO
O
N
NO^+, e^-
p = 1.0 atm


Equilibrium Composition of "Air"
Mole Fraction (%)
100
10
1
0.1
0.01
1000
2000
3000
4000
5000
6000
Temperature (K)
N2
O2
NO
O
N
NO+,e-
p = 0.01 atm