Equilibrium/Frozen Flow Modeling and Nonequilibrium

Problem Introduction
You have been asked to examine the design and operation of a high-enthalpy wind tunnel intended to simulate hypersonic flight conditions with a 2:1 mixture (by mole) of O₂ and CO₂. The hypersonic flow is to be produced by a high-enthalpy gas expanded through a supersonic (converging-diverging) nozzle that exits into a constant-area test section.

Starting Assumptions
For the purposes of THIS PROJECT, you should assume the following:
- the upstream source for the nozzle is an equilibrium mixture with the required C:O ratio and a temperature of 4100 K and a pressure of 25 atm;
- the only species that exist in your mixture are CO₂, O₂, CO and O;
- the flow is quasi-one dimensional, inviscid and adiabatic throughout the nozzle and test section;
- the nozzle expands the flow to a test-section pressure of 0.0005 atm.

Molecular Data
For CO, O₂, CO₂, and O use the molecular parameters used in homework sets #2 #3.

Goals
I. Equilibrium/Frozen Flow Calculations
Your first goal is to determine the following set of nozzle geometric and flow properties based on various flow assumptions. Use a partition function-based approach for determining state relations (e.g., as you used in homework set #3).
1) the design nozzle expansion ratio (exit area to throat area ratio);
2) the flow properties as a function of the local area ratio (local nozzle area to throat area), specifically:
   a) the gas composition (i.e., the mass fractions, \( y_i \));
   b) the gas temperature;
   c) the gas pressure;
   d) the gas density;
   e) the gas velocity
3) the mass flux (mass flow rate per unit area) at the nozzle throat;
4) the speed of sound and the frozen speed of sound at the nozzle throat;
5) the Mach number at the nozzle exit.
You need to find the above values for each of three assumptions about the flow behavior:

1. fully equilibrium flow;
2. flow with frozen chemistry (but all other energy modes in equilibrium); and
3. frozen flow (i.e., only translational and rotational modes in equilibrium).

II. Vibrational Nonequilibrium Estimates

Your next goal is to provide information to determine the likelihood for nonequilibrium to exist for the vibrational mode of O\textsubscript{2}. Specifically, we want to know if the O\textsubscript{2} vibrations are likely to be out of equilibrium with the translational energy.

To make estimates of the relaxation time constants, use the model described in class, based on the paper by Millikan and White,\textsuperscript{1} for the vibrational relaxation time, \( \tau_v \) (sec), for a vibrating species \( i \) with a collision partner \( j \)

\[
p \tau_{v,i-j} = \exp \left[ 1.16 \times 10^{-3} \mu_{ij}^{1/2} \theta_v^{4/3} \left( T^{-1/3} - 0.015 \mu_{ij}^{1/4} \right) - 18.42 \right]
\]

where, \( p \) is the total pressure (in atm), \( \theta_v \) is the characteristic vibrational temperature (in K), \( T \) is the (translational) temperature (in K) of the gas, and \( \mu \) is the unitless reduced mass for a given pair,

\[
\mu_{ij} = \frac{m_i m_j}{m_i + m_j}.
\]

where the \( m_i \) are unitless molecular masses. The total vibrational relaxation time for a given species in a mixture of gases is given by summing over all the collision partners, i.e.,

\[
\frac{1}{\tau_{v,i}} = \sum \frac{\chi_j}{\tau_{v,i-j}}.
\]

where \( \chi_j \) is the mole fraction of species \( j \) in the mixture.

Calculations

a) Vibrational Relaxation Time Constant: Estimate the characteristic vibrational relaxation time constant for O\textsubscript{2} in the supersonic portion of the nozzle using our simplified flow assumptions. Specifically, provide two estimates: one based on the flow properties you found using the equilibrium flow assumption and the other based on the chemically frozen flow assumption. (NOTE: this does not mean you are supposed to find that the relaxation time that is consistent with

each flow assumption – you are just using the flow properties based on that assumption to calculate the time constant.)

b) **Vibrational Freezing Estimate**: Assuming the nozzle is conical with an expansion half-angle of 15° and a throat diameter of 1 cm, estimate at what region of the expanding nozzle (i.e., what approximate \( A/A_{\text{throat}} \) range) you think the \( \text{O}_2 \) in the flow might be reasonably considered to be vibrationally in equilibrium.

### III. Test Section Shock

Your last goal is to determine what would happen in the test section downstream of the supersonic nozzle if a blunt body was placed in the flow. Specifically, you need to determine the conditions that might exist just downstream of the centerline of a 2-d bow shock sitting in front of the body. You can model the center of the bow shock as a normal shock.

Assuming that **AFTER the shock**, the flow **reaches equilibrium**, find the following:

1. the pressure ratio across the shock and the post-shock pressure;
2. the ( translational) temperature ratio across the shock and the post-shock temperature;
3. the density ratio across the shock and the post-shock density;
4. the normalized entropy increase, \( (s_2-s_1)/R_{\text{init}} \) across the shock, where \( R_{\text{init}} \) is the gas constant for the initial mixture (before the shock).

Find the above for each of the three **pre-shock** (i.e., nozzle exit) conditions you determined in Goal I.

**Cooperation/Teaming**

You can work on this project either individually or in a group of two members. If you work in a group, the group should turn in a single report.

**Project Report**

You need to turn in a hardcopy report in class AND a digital version online (T-square). Note, this report is **NOT** to be written in the standard homework format. There should be a **SINGLE** report for all the parts (goals) of this assignment that must include the following items. Please use the section titles indicated below (except for the cover page – which should not be titled).
Cover Page

Should include (at least): a report title, author name(s), date

Introduction

A BRIEF overview of all the goals/issues of this assignment in your own words.

Approach

Describe (and include) the equations you are solving and your solution method - not just what computer tool you used, but a brief but descriptive outline of the solution methods that you used. You should include here the approach(es) used for ALL parts of this assignment (you can choose to have subsections for each different goal).

Results and Discussion

Present ALL your results in this section (you may have subsections if you like). You should present your results primarily as tables or plots, whichever is more appropriate for a given result. For plots and tables, present your results so that it is easy to compare the different flow assumptions, e.g., by plotting all the flow cases for a given flow variable on a single graph. Also, make sure the graph does not "lose information," e.g., consider semi-log or log-log scaling if needed to expand the dynamic range of the plot. Include a running discussion/interpretation of your results as you present them.

Conclusions

Summarize your results and draw interesting and relevant conclusions from them.