Equilibrium/Frozen Flow Modeling and Nonequilibrium

Problem Introduction

You will examine the flowfield around a body with a simple airfoil shape intended to fly at hypersonic conditions in an atmosphere composed of O_2 (85% mole fraction) and CO_2 (15%). The airfoil is traveling at 6200 m/s, and the ambient temperature and pressure ahead of the airfoil are 220 K and 0.001 atm. Figure 1 provides the geometry of the airfoil, which has a 2 m chord.



Figure 1. Airfoil geometry shown at 0° angle of attack.

Starting Assumptions

For the purposes of this project, you will assume the following:

- the only species that can be present in the mixture are O₂, CO₂, CO, and O;
- the body is two-dimensional (so constant cross-section);
- the flow is inviscid (except within shocks) and adiabatic; and
- the airfoil will only operate at positive angles of attack.

Molecular Data

You should use the molecular parameters from homework set #2. To avoid calculating negative values for enthalpies/energies in this problem (a convenience only), you may want to consider setting an appropriate system energy zero.

Goals

In this project, you need to determine the following results.

1. Approach Flow

Determine the Mach number of the flow approaching the airfoil, as well as its enthalpy and entropy.

2. Leading Edge Oblique Shock

For angles of attack that will produce an attached oblique shock, determine the **oblique shock angle** and the following flow properties at point A (i.e., post-shock properties) *as a function of the angle of attack*:

- a) velocity
- b) temperature
- c) pressure

- d) density
- e) composition (mass fractions)
- f) entropy

Calculate these shock properties for three flow assumptions:

- equilibrium flow after the shock (using a *partition function-based* approach like that used in homework set #2);
- chemically frozen flow after the shock, i.e., all energy modes in equilibrium except chemical composition, which remains the same as before the shock (using a *partition function-based* approach like that used in homework set #2); and
- frozen flow after the shock, i.e., all molecular energy modes do not change through the shock except for the translational and rotational modes, which are in equilibrium after the shock.

3. Detached Bow Shock Estimates

If the airfoil was operated at an angle of attack beyond which an attached oblique shock could exist, then a detached bow shock would form.

For each of the three flow assumptions defined above (equilibrium, chemically frozen, and frozen flow), determine the following post-shock properties (i.e., immediately behind the shock) near the center of the bow shock, where the bow shock could be modeled as a normal shock:

- a) velocity
- b) temperature
- c) pressure
- d) density
- e) composition (mass fractions)
- f) entropy

4. Expansion

For the airfoil *operating at a zero angle of attack*, determine the following flow properties as a function of turn angle as the flow goes through the expansion turn around the bottom of the airfoil:

- a) velocity
- b) temperature
- c) pressure
- d) density
- e) composition (mass fractions)
- f) Mach number

Just before the turn, assume the oncoming (post-shock) flow conditions are the equilibrium flow assumption results from Goal 2. For the expansion results, however, perform the calculations for each of the three flow assumptions defined above, i.e., calculate results as the flow goes through the turn for each assumption.

5. Vibrational Nonequilibrium Estimates

In the previous results, you assumed that the vibrational energy modes were either frozen or in equilibrium. Now you will investigate the likelihood for nonequilibrium to exist for the vibrational mode of O₂. Specifically, we want to know if the O₂ vibrations are likely to be out of equilibrium with the translational energy mode.

To do this you will need to make **estimates** of the relaxation time constants; **use the model described in the class lecture notes** for the vibrational relaxation time, τ_v , based on the paper by Millikan and White.¹ In addition, you will need to make estimates of appropriate flow times.

Required Nonequilibrium Estimates

a) **Oblique Shock**

Determine the characteristic vibrational relaxation time constant for O_2 just behind the leading edge oblique shock *at the zero angle of attack condition*, based on the flow conditions (temperature, pressure, and composition) that you determined using each of the three flow assumptions (equilibrium, chemically frozen, and frozen flow). So you will provide three values of the vibrational relaxation time constant τ_{ν,O_2} : one for each post-shock condition predicted by a given flow assumption.

Then use these three time constants to determine whether the O_2 will likely reach vibrational equilibrium before the downstream expansion turn. Hint: use the airfoil dimensions to help determine this.

b) Expansion

Based on the flow conditions (temperature, pressure, and composition) determined in Goal 4, determine the characteristic vibrational relaxation time constant for O_2 through the expansion at the bottom of the airfoil *as a function of turn angle* through the expansion. You will do this three times (one for each of the flow assumptions).

Then assuming the O₂ vibrational energy was in equilibrium before the expansion, provide an estimate of when (i.e., at what angle through the turn) the O₂ is likely to no longer be in vibrational equilibrium as it goes through the expansion along a streamline that passes through point A (see Figure 1), which is $\delta=3$ cm from the airfoil surface.

¹R. C. Millikan and D. R. White, "Systematics of Vibrational Relaxation," Journal of Chemical Physics, Vol. 39, No. 12, pp. 3209-3213, December, 1963.

Cooperation/Teaming

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

Project Report

You need to submit a pdf version of your report on Canvas. Note, this report **should not** be written in the standard homework format. There should be a single report that covers all the parts (goals) of this assignment. Furthermore, the report must include the following sections. 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* but meaningful overview of the problem and the goals/issues explored in your report, *in your own words*.

Approach

Describe (and include) the equations you are solving and a clear description of your solution method/approach - not just what computer tool you used, but a brief but descriptive outline of the methods you used. Include the approaches used for all parts of this assignment (subsections for each different goal might be helpful). Note: the approach section *should not* be a listing of your code.

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 necessary 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 (based on the discussion you already presented in the previous section).