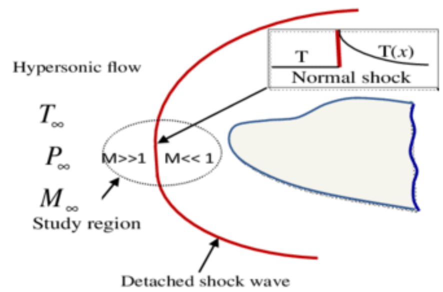
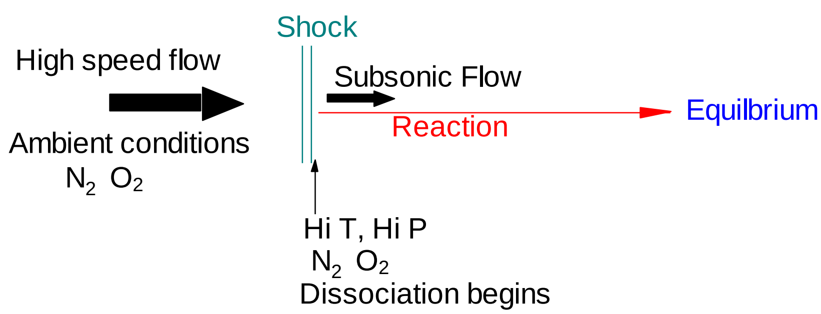
ME 501 Homework 4 Due 2/25/25

The problem of erosion due to oxidiation by atomic species generated by incident shocks during hypersonic travel is a very active area of research. In front of the leading edge of the vehicle is a bow shock. Consider the center streamline as a normal shock in 1-D compressible flow, similar what is depicted here:



The shock process occurs very rapidly such that the gas on downstream side of the shock does not have time to react, and the gas composition is unchanged from the upstream side. This schematic depicts the general situation along the central streamline:



The conditions immediately downstream of the shock represent the "Frozen" conditions. After this point, the flow begins to dissociate towards equilibrium, eventually attaining the "Equilibrium" solution. Pressure, temperature, velocity, composition, and density all change as the flow progresses towards equilibrium.

The degree of dissociation of the flow as it passes over the craft is important since atomic oxygen is orders of magnitude more reactive than molecular oxygen. Thus, it's desirable to know the oxygen mole fraction as a function of time (and distance) from the incident normal shock, as well as the other thermodynamic parameters. This is a fully coupled reacting flow problem, and you'll do a somewhat simplified, but still very relevant simulation using the skills you've learned so far.

The goal of this assignment is to calculate the profiles of temperature, pressure, and atomic oxygen mole fraction with time and distance from the incident shock.

Consider a hypersonic vehicle traveling at 3 km/s at 30 km altitude where the pressure is 1.172 kPa and the temperature is -46.5 °C.

1) Using Gordon McBride or CEA, solve the shock problem for X_{O2}=.21 and X_{N2}=.79 at the conditions listed above. Obtain both frozen and equilibrium solutions. For the input file, add the command

only N2 O2 O

to make the nitrogen non-reactive. It makes no difference for the frozen case, and doesn't really affect how you do the problem, but the equilibrium for that case will be what your simulation is working towards.

The 1-D equations for compressible flow are the conservation of energy, mass, and momentum, and they can be represented as follows:

$h + \frac{1}{2}u^2$ = constant (c_1) ρu = constant (c_2) and $P + \rho u^2$ = constant (c_3). The ideal gas law also applies.

2) Using the frozen solution, solve for these constants (c(1),c(2),and c(3)).
3) Assuming that N_2 does not react, derive an expression (or set of equations) from which one can calculate h as a function of only X_O and temperature. Note that this h is energy per unit mass.
4) Obtain the rate constants for the oxygen dissociation and recombination that are valid in this temperature range.
5) Generate an expression for dX_O/dt as a function of X_O, T, and P, similar to what you did in the previous homework. This will look similar but include both recombination and dissociation pathways.

At this point, you have all the equations you need to solve the problem. You can proceed using a program or spreadsheet or other tool, but you'll follow the general procedure:

i) Choose a timestep. I'd suggest 10 μs or less to start.
ii) Assume that during a timestep, T and P are fixed. Assume furthermore that $dXo/dt = \Delta Xo/\Delta t$.
iii) Calculate a new X_O (new X_O = original $X_O + \Delta X_O$) at the end of the timestep using the equation that you developed in 5).
iv) Now you need to find out how T, P, and u have changed as a result of the new composition. You'll need to do this by ensuring that $h + \frac{1}{2}u^2 = c_1$, $\rho u = c_2$, and $P + \rho u^2 = c_3$ for the new composition that you have calculated in iii). There are many ways to do this, but I suggest something like setting up an objective function like:

$$|(h + \frac{1}{2}u^2) - c_1| + |\rho u - c_2| + |(P + \rho u^2) - c_3|$$

which will be minimized (zero) for the correct new T, P, and u. This solution is easily done in excel using the solver functionality. You can do some substitutions and make this a 1-D optimization, which may be easier for you.

v) Start the next calculation with the new composition, T, P, and u, and repeat from step ii).

6) In this way, solve for X_O, T, P, and u as a function of time, and plot these values. Plot X_O, T, P, and u versus distance as well. Run the calculation out to at least 10 ms. Depending on how you do the

calculation, repeating individual timesteps may be tedious if you're unable to automate the process. However, after I set it up on excel, I could run about 6 steps per minute, so you can run the 100 or more timesteps (which is probably enough) in a half hour or so. Most of the time will be spent getting to that half hour of grinding. If you're doing this via programming, use a smaller timestep for better accuracy. I ran my program with Δt = 1 us, and it was pretty smooth. For the spreadsheet approach, I'd suggest the first 10 iterations at Δt = 10 us, the 2nd 10 at 20 us, the 3rd 10 at 50 us, then 100us out to 5 ms, the 500 us thereafter. With that, you get to 10 ms in 80 iterations.