Notes on Fluid Equations and the Lithium Vapor Box

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I. GENERIC EULER FLUID EQUATIONS

The Navier-Stokes equations are often used to describe a general gas (or vapor) or liquid. In the ideal dissipationless limit (collision frequency $\to \infty$, so the visocity and thermal conduction go to 0) these become the Euler Equations, which are conservation laws for mass or particles, momentum, and internal (thermal/random) energy (because these 3 quantities completely specify a local thermodyanmic equilibrium). Denoting the mass density by $\rho(\vec{x}, t)$ the fluid velocity by $\vec{u}(\vec{x}, t)$, and the pressure by $p(\vec{x}, t)$, the Euler equations give the conservation of mass

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{u}), \tag{1}$$

conservation of momentum

$$\frac{\partial \rho \vec{u}}{\partial t} = -\nabla \cdot (\vec{u} \rho \vec{u}) - \nabla p \tag{2}$$

(in the absence of sources, this can also be written in the convective form $\rho d\vec{u}/dt = -\nabla p$, where $d/dt = \partial/\partial t + \vec{u} \cdot \nabla$ is the convective derivative, which is sometimes called the "material derivative", however, most CFD codes use the conservative form because they naturally capture the Rankine-Hugoniot jump conditions at shocks)), and conservation of energy:

$$\frac{\partial E_\mathrm{t}}{\partial t} = -\nabla \cdot (\vec{u}(E_\mathrm{t} + p)) \tag{3}$$

which for an ideal monatomic gas can be written as

$$\frac{\partial}{\partial t}\left(\frac{3}{2}p + \frac{1}{2}\rho u^2\right) = -\nabla \cdot \left(\vec{u}\left(\frac{5}{2}p + \frac{1}{2}\rho u^2\right)\right) \tag{4}$$

where the total energy density $E_\mathrm{t}(\vec{x}, t) = \rho e + (1/2)\rho u^2$ and the "specific internal energy density" e is related to the gas pressure by $p = (\gamma - 1)\rho e$, where γ is known as the "adiabatic index", because it appears in the adiabatic scaling $p \propto \rho^\gamma$ following along a fluid element in the flow. (γ is also known as the "heat capacity ratio" or the "ratio of specific heats", because it is also given by $\gamma = c_P/c_V$, or as the "Poisson constant".) For an ideal gas with N degrees of freedom among which internal energy can be distributed, $\gamma = (N + 2)/N$. (There are generalizations to nonlinear equations of state $p = p(\rho, T)$, accounting for excited states or inter-molecular forces. (This latter is important for treating liquids, where the pressure is a strongly nonlinear function of density, explaining why liquids are hard to compress relative to gases.) But as long as visocity and thermal conduction (and radiation or other dissipative terms) are ignored it is still essentially an ideal fluid.) Lithium vapor in our parameter regime is primarily a monatomic gas (very few dimers or "dilithium") so $N = 3$ and $\gamma = 5/3$. Air is primarily made of diatomic molecules, which have 2 rotational degrees of freedom, so $N = 5$ and $\gamma = 7/5 = 1.4$ is often used for air.

These equations can be found in various places. In the 1-D limit, they are given as Eqs. 1-3 of `https://en.wikipedia.org/wiki/Rankine-Hugoniot_conditions`. They are also given in Sec. 4.4 of `https://en.wikipedia.org/wiki/Euler_equations_(fluid_dynamics)` (though that web page is complicated by a lot of other details not of interest to us at this time.)

These equations are equivalent to the plasma fluid equations in Braginskii and the NRL formulary (where the general stress tensor and thermal conductivity tensor is included), where $\gamma = 5/3$ for protons and for electrons. Instead of the total energy form, Braginskii writes an equation for the evolution of the temperature.

II. ENTHALPY

Note that while the RHS of the particle conservation equation $\partial\rho/\partial t = -\nabla \cdot (\rho\vec{u})$ just represents simple advection of particles at the velocity $\vec{u}$, the RHS of the energy conservation equation contains an additional term in the energy flux $\vec{u}p$ in addition to the convective term $\vec{u}E_t$, which is related to the pdV work done during compression. The energy conservation equation can be written as $\partial E_t/\partial t = -\nabla \cdot (\vec{u}\rho H)$, where $H = (E_t + p)/\rho = (1/2)u^2 + e + p/\rho$ is the "total enthalpy". Perhaps more carefully, H is the "specific total enthalpy", because it is the total enthalpy density (total enthalpy per unit volume) divided by the mass density, i.e., it is the enthalpy per unit mass (the term "specific" is sometimes used to denote something that has been divided by the mass density). The total energy E_t is related to the "internal energy" or "thermal energy" e by

$$E_t/\rho = e + (1/2)u^2$$

and the total enthalpy H is related to the "enthalpy" $h = e + p/\rho$ (i.e., just the thermal contribution) by

$$H = h + (1/2)u^2$$

or in other words, the enthalpy $h = e + p/\rho$ does not include the fluid flow energy $(1/2)u^2$. This is consistent with the terminology in some MIT course notes[1]. The enthalpy h is definied in the same way in the wiki page `https://en.wikipedia.org/wiki/Euler_equations_(fluid_dynamics)#Enthalpy_conservation`

Interestingly, the total enthalpy is constant along flow trajectories in steady-state flow, even for compressible flows. I.e., consider $\partial/\partial t = 0$, so $\nabla \cdot (\rho \vec{u}) = 0$. Then the energy conservation equation becomes $\rho \vec{u} \cdot \nabla H = 0$. For a $\gamma = 5/3$ fluid, this means

$$H = (1/2)u^2 + (5/2)T/m \tag{5}$$

is constant along flow trajectories. This is true even across shocks, since the particle flux and energy flux are constant across a shock, and the enthalpy is essentially the ratio of the energy flux to the particle flux. (Enthalpy is constant across shocks in the frame where the shock is stationary, which is the only case in which things are truly steady-state, $\partial/\partial t = 0$.) (One might have thought that $(1/2)u^2 + (3/2)T$ would be constant along flow trajectories, since that would seem to be the sum of the kinetic and thermal energy, but one also needs to account for pdV work, which gives the extra factor of T. Maybe another way to think of it is that $(1/2)u^2 + (3/2)T + p/\rho$ is kind of like kinetic energy plus thermal energy plus a potential energy. ?? Not sure about that...)

III. THE RANKINE-HUGONIOT SHOCK JUMP CONDITIONS

Consider a steady-state flow in 1D, then the flux of mass, momentum, and energy must be constant:

$$\rho(x)u(x) = \Gamma \tag{6}$$

$$\rho(x)u^2(x) + p(x) = p_t \tag{7}$$

$$(1/2)\rho(x)u^3(x) + (5/2)u(x)p(x) = \Gamma_E \tag{8}$$

where the constants Γ, p_t, and Γ_E are the mass, momentum, and energy fluxes. (One could also use the symbol Γ_u for the momentum flux, but it can be confusing to distinguish this from the oft-appearing factor of Γu, and it has the same units as pressure so I used p_t instead.)

This gives us 3 equations in the 3 unknowns ρ, u, and p, so this gives us the possibility of a solution (though solutions do not exist for some values of Γ, p_t and Γ_E). However, note that these are nonlinear equations, so there is also the possibility of multiple solutions. In fact one finds that there are two possible solutions, which is related to the existence of shocks.

Using the mass conservation equation $\rho u = \Gamma$ to rewrite the momentum equation as $\Gamma u + p = p_r$, we can solve for u as

$$u = (p_t - p)/\Gamma \tag{9}$$

Inserting this into the energy equation we get

$$4p^2 - 3p_t p - (p_t^2 - 2\Gamma\Gamma_E) = 0 \tag{10}$$

The two possible solutions for the pressure are

$$p = \frac{3p_t \pm \sqrt{25p_t^2 - 32\Gamma\Gamma_E}}{8}. \tag{11}$$

The corresponding solutions for the velocity are

$$u = \frac{p_t - p}{\Gamma} = \frac{5p_t \mp \sqrt{25p_t^2 - 32\Gamma\Gamma_E}}{8\Gamma} \tag{12}$$

These correspond to the low flow (high pressure and high density) and high flow (high pressure and high density) sides of a shock, i.e., these are essentially the Rankine-Hugoniot jump conditions across a shock, in the frame of reference moving with the shock front, so the discontinuity is stationary in this frame. Once u is known on the two sides of the shock, one can find ρ on the two sides from $\rho = \Gamma/u$.

As stated, these results are in the frame of reference where the shock location is stationary. In physical systems we often think of a case where there is a high density gas flowing rapidly into a stationary low density gas, so the shock front is moving. But the analysis is easier in the frame where the shock front is stationary and one can think of the low density gas flowing into the shock, getting compressed, and coming out on the other side with a higher density (and lower velocity). Going from the frame where the low-density region is stationary to the frame where the shock is stationary means the velocity in the high-density region reverses sign. Note that pressure and density are invariant to changing the frame of reference, but the velocity u on one side of a shock can be made aribtrary by changing frames of reference, though the velocity jump $u_2 - u_1$ across a shock is invariant. Merely the fact that there is a flow with $\mathcal{M} > 1$ somewhere is not sufficient to mean there is a shock, because one could always go to a frame of reference where $\mathcal{M} = 1$. But it is boundary conditions or interactions with other things (which give a preferred frame) that cause shocks to occur.

From the constraint that p must be positive on both sides of the shock, it can be shown that the maximum density ratio from the compression in a shock is 4 (for $\gamma = 5/3$), though the pressure ratio can get arbitrarily large for arbitrarily high incoming Mach number.

The two solutions merge when $25p_t^2 = 32\Gamma\Gamma_E$, which corresponds to $u = \sqrt{\gamma T/m}$, i.e., it corresponds to the Mach number $\mathcal{M} = 1$ (in the frame where the shock front is stationary). For other values of parameters, one solution has $\mathcal{M} > 1$ and the other has $\mathcal{M} < 1$.

When following a fluid element (a point moving with the fluid) in the flow, one can see a transition from a low pressure state to a high pressure state (corresponding to compression from going through a discontinuity in the flow velocity with large negative $\partial u/\partial x$). In the frame where the shock front is stationary, this corresponds to transitioning from a high flow state to a low flow state. If viscosity and/or thermal conduction is included, this will broaden the shock width to a finite size (of order the mean free path for large Mach numbers, but that means that fluid equations have broken down). The reverse transition, a discontinuous transition from a high pressure state to a low pressure state is physically not allowed. It turns out that there is entropy production in the shock. (One way to see this is to note that the relation $p \propto \rho^\gamma$, or more precisely $d(p/\rho^\gamma)/dt = (\partial/\partial t + \vec{v} \cdot \nabla)(p/\rho^\gamma) = 0$, which holds for continuous flows, breaks down in the jump across the shock.) This is due to irreversible heating by the viscosity and/or thermal conduction. In the limit that the viscosity and thermal conductivity go to zero, this dissipation remains finite (because the gradients become infinite as the shock width goes to zero). This can be seen by working out the entropy production in a shock. If one starts a flow with an initial condition of a discontinuity corresponding to a reverse shock, one finds that it instead broadens over time into a "rarefaction fan" (which is the reverse of the wave steepening that can occur that can cause continuous initial conditions in flow to turn into the discontinuous state of a shock).

These and other interesting properties of shocks are discussed at `https://en.wikipedia.org/wiki/Rankine-Hugoniot_conditions`, LeVeque's book on numerical methods for hyperbolic equations. and other sources.

Shocks are a rich and fascinating subject. Shocks become much more complicated in plasmas, where a magnetic field is also involved and shocks depend on the angle of the shock relative to the background magnetic field or the relative electron and ion temperatures and the electron-ion mass ratio. In magnetic fusion energy we usually don't need to consider shocks. There was a time when some people had the idea that shocks were generically unimportant in low-collisionality plasmas because hydrodynamic shocks have a width of order the mean-free path, which is very large at low collisionality. However, when a high velocity plasma flows into a low velocity plasma, one can excite all kinds of 2-stream instabilities (and other variants like Weibel instabilities) or other velocity-space instabilites that act as a kind of enhanced collisionality. These kinds of "collisionless" shocks are probably very important in supernova explosions expanding into the low density interstellar medium, or other astrophysical systems, and are an active area of astrophysical research. Important questions include the amount of relative electron vs. ion heating, the generation of magnetic fields and their spectra, the acceleration of some particles to ultra high energies to cause cosmic rays, etc. Shocks are of course important in IFE and the study of laser-plasma interactions. (As I write this, I wonder if magnetic field generation in IFE shocks is ever important enough to mess up assumptions about heating of particles to fusion temperatures. Presumably this has been studied, though some work on magnetic field generation in collisionless shocks is quite recent, see work by Spitkovsky and others.)

Understanding that 2 possible flow states are possible for a given set of conditions is related to other interesting If one considers 1-D flow in a pipe with a varying cross-section, then then this is related to how de Laval nozzles work, where there is a transition between a low flow velocity in a high-pressure reservoir to a supersonic flow. `http://web.mit.edu/16.unified/www/SPRING/fluids/Spring2008/LectureNotes/f20.pdf` looks like it has a good, detailed treatment of the de Laval nozzle flow (including a discussion of "jet shock diamonds" that can be seen in the exhaust of some figher jets or rockets, due to underxpanded or overexpanded nozzles).

Another related variation of this problem is to consider 1D radial flows in cylindrical or spherical geometry, like the Parker solar wind problem, where Parker showed the solar wind can transition to a supersonic outflow. (I'm told that this transition is easier with an isothermal equation of state for the electron pressure).

?? The main results in this section are in the frame of reference where the shock is stationary. It would be useful to put in the generalizations to a moving shock.

IV. 1-D FLOW WITH A GAS SOURCE AND ABSORBING END WALLS

Here we consider an idealized problem with a uniform source of gas for $|x| < L_s$, which flows out to walls at $|x| = L$ which are assumed to be perfect absorbers. This is motivated by considering the flow of hot lithium vapor in a box that is injected near $x \sim 0$ and flows to the ends of a box where it hits a cold plate and condenses onto the plate. (This is like the steam condensing on a bathroom mirror when taking a shower. This is also related to cryopumps which are used in fusion devices.) There are also similarities between this probem and a simple model of the 1D dynamics along a scrape-off-layer (SOL) in a fusion device, though thermal conduction and electric fields play an important role there also.

Modify the fluid equations to include, for $x < L_s$, a uniform mass source S_ρ and energy source $S_E = (3/2)T_s S_\rho/m$, where T_s is the temperature of the gas source and m is the mass of the gas atoms. For $x < L_s$, in steady state we have

$$0 = -\frac{\partial}{\partial x}(\rho u) + S_\rho \tag{13}$$

$$0 = -\frac{\partial}{\partial x}(\rho u^2 + p) \tag{14}$$

$$0 = -\frac{\partial}{\partial x}\left(u\left((1/2)\rho u^2 + (5/2)p\right)\right) + S_E \tag{15}$$

(u is now the velocity in the x direction.) Note there is no momentum source (the injected gas has a temperature but no mean flow in the x direction), but pressure gradients that will arise will accelerate the flow. (Note that viscosity and thermal conduction are being neglected, as is viscous drag with the walls in the y direction.)

Integrate these equations from $x = 0$ to an arbitrary position $x < L_s$, and use the boundary condition that $u = 0$ at $x = 0$, to get

$$\rho u = x S_\rho \tag{16}$$

$$\rho u^2 + p = p_0 \tag{17}$$

$$(1/2)\rho u^3 + (5/2)up = x S_E \tag{18}$$

The source rates S_ρ and S_E are assumed known, but the pressure p_0 at $x = 0$ is unknown at present and will need to be set by other considerations (discussed later). These 3 equations are of the same form as Eqs.(6-8), the 3 equations we started with for the shock jump. Substituting for the parameters of our 1-D source region, $\Gamma = x S_\rho$, $p_t = p_0$, and $\Gamma_E = x S_E$, we get

$$p(x) = \frac{3p_0 \pm \sqrt{25p_0^2 - 32x^2 S_\rho S_E}}{8} \tag{19}$$

$$u(x) = \frac{5p_0 \mp \sqrt{25p_0^2 - 32x^2 S_\rho S_E}}{8x S_\rho} \tag{20}$$

Note that for small x, the only physical solution is the positive branch. As the fluid flows out to larger x, the negative branch would seem to be a possibility, but is still excluded because jumping to that lower-pressure branch would correspond to a reduction in entropy, which is not physical. Plots of the both the physical and unphysical solutions for $p(x)$ and $u(x)$ are shown in Fig.1. This is the solution from $x = 0$ to $x = L_s$, and then for $x > L_s$ one has $p =$ constant and $u =$ constant. (The gradients of p and u become infinite right at $x = L_s$. Presumably introducing a finite amount of viscosity and thermal conduction will smooth out the profiles around the $x \sim L_s$ region. This is not a shock, because u and p are continuous, so there is no entropy production or dissipation expected here in the limit that the viscosity and thermal conduction go to 0.)

It is not completely clear to me how to set the parameter p_0. I'm guessing that perfectly absorbing boundary conditions means that fluid flows out at the fastest velocity possible. (For partially absorbing boundary conditions, or hotter plates where the evaporation flux is a nonnegligible fraction of the condensing flux, one will need to consider more complicated boundary conditions.) The outflow velocity $u(L_s)$ is maximized by setting p_0 as small as possible while $p(x)$ is still real for all $x < L_s$. This means that p_0 will be set by the criterion that the descriminant in Eq.19 vanishes at $x = L_s$, i.e.,

$$p_0^2 = \frac{32}{25} L_s^2 S_\rho S_E = \frac{32}{25} L_s^2 (3/2) T_s S_\rho^2 / m \tag{21}$$

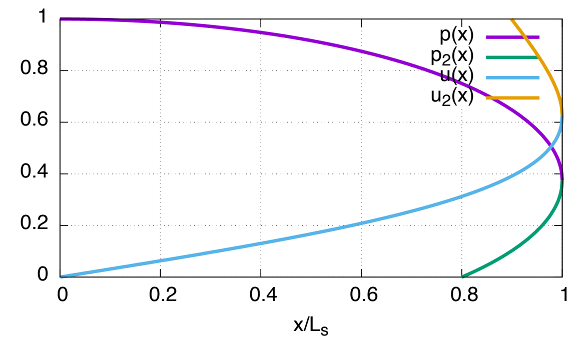

FIG. 1. The pressure and velocity profile in the source region. (The p_2 and u_2 solutions are unphysical.)

With this assumption, the pressure profile in the source region $0 < x < L_s$ takes the form

$$p(x) = p_0 \frac{3 + 5\sqrt{1 - (x/L_s)^2}}{8} \tag{22}$$

We will instead write this in terms of the mass and energy flux to each end plate, $\Gamma_\rho = S_\rho L_s$, $\Gamma_E = S_E L_s$ (note the total mass flux summed over both plates at either end is $2\Gamma_\rho$), so

$$p_0^2 = \frac{32}{25}\Gamma_\rho \Gamma_E = \frac{32}{25}(3/2) T_s \Gamma_\rho^2 / m \tag{23}$$

Interestingly, this is independent of L, the distance to the absorbing plate. From $\rho u = S_\rho x$, one can show that the density at the midplane ($x = 0$) is

$$\rho_0 = \rho(0) = (5/2)(S_\rho/S_E) p_0 = (5/3)(p_0/T_s) m. \tag{24}$$

Noting $p_0 = T_0 \rho_0 / m$, we find this means that the midplane temperature

$$T_0 = (3/5) T_s, \tag{25}$$

where T_s is the temperature of the gas source. One might have guessed that $T_0 = T_s$, but in reality it is colder because the hot particles leave faster than the cooler particles (another way to think of it is probably in terms of expansion cooling). (One has to be a little careful about applying this. If the gas is injected in the y direction through slots near $x = 0$, the flow velocity through the slot will eventually be converted to thermal energy and accounted for in the source temperature. This is discussed more in Sec.IV A.))

?? Somewhere, probably later, put in the solution for the de Laval nozzle and the temperature in a choked-flow injection source?

Once one knows the midplane parameters, one can determine the downstream parameters in the main flow to the plates

$$p_d = (3/8) p_0 \tag{26}$$

$$\rho_d = (1/2)\rho_0 \tag{27}$$

$$T_d = (3/4)T_0 = (9/20)T_s \tag{28}$$

$$u_d = \sqrt{(5/3)p_d/\rho_d} \tag{29}$$

(The last equation is equivalent to $\mathcal{M} = 1$.)

A. A source treated as a sonic flow.

The above results depend only on the source mass flux Γ_ρ and the energy flux Γ_E. This source might be due to small holes in the tube in the region $|x| < L_s$ that inject gas from a higher-pressure region. The injection is in the y direction, and the gas bounces off of the far wall and converts the initial y-directed flow energy into thermal energy, which then by pressure gradients flows in the x direction to the absorbing plates. If we treat this injected gas as if it was from a similar Mach 1 incoming flow, then we can work out a couple of curious relations.

In the previous section, we defined a source temperature T_s via $S_E = (3/2)T_s S_\rho/m$, or equivalently in terms of the fluxes by $\Gamma_E = (3/2)T_s\Gamma_\rho/m$. If the source flow through the holes is a Mach 1 flow, where $u_{in}^2 = (5/3)T_{in}/m$, then we have $\Gamma_{E,in} = u_{in}((1/2)\rho_{in}u_{in}^2 + (5/2)p_{in}) = 2\rho_{in}u_{in}^3$. Inserting this into $T_s = (2/3)\Gamma_E m/\Gamma_\rho$, we get $T_s = (20/9)T_{in}$, which is exactly the inverse of the relation between the downstream temperature and the source temperature in Eq.28. I.e., this means that $T_d = T_{in}$, the downstream temperature in the main flow is equal to the temperature in the incoming injected gas before its velocity is thermalized.

Another way to see this is the following conservation relation. The total mass injection rate is $A_{in}\rho_{in}u_{in} = A_{out}\Gamma = A_{out}\rho_{out}u_{out}$, where A_{in} is the area of the holes injecting gas into the tube and A_{out} is the area of the absorbing plates at the end of the tube. The total energy injection rate, assuming the injection is at Mach 1 just like the outflow, is $A_{in}2\rho_{in}u_{in}^3 = A_{out}2\rho_{out}u_{out}^3$. The solution to this pair of conservation equations is

$$\rho_{out} = \frac{A_{in}}{A_{out}}\rho_{in} \tag{30}$$

$$u_{out} = u_{in} \tag{31}$$

i.e., that $T_{out} = T_{in}$. There is no net expansion cooling of the flow (though it went up from T_{in} to T_0, and then back down to $T_{out} = T_d$).

This is fundamentally different than the expansion cooling that occurs in a de Laval nozzle or the expansion of radial flow in cylindrical or spherical geometry that can lead to supersonic outflows. The difference might lie in assumptions that the source and exit flows have exactly $\mathcal{M} = 1$ and/or something about the walls of the tube converting any y-directed energy in the original injected source into thermal energy. The differences might be related to the fact that the model explored in these notes is strictly 1-D so the maximum acceleration that can be obtained leads to a local Mach number of 1, while for radial flow in cylindrical (or spherical) coordinates or the expansion in a de Laval nozzle can give expansion to arbitrarily low temperature and thus arbitrarily high Mach number. As the flow comes out of a hole (a slit in 3d) it is expanding with a kind of cylindrical symmetry in 2 dimensions, and so we might get more expansion cooling there. I.e., the side walls in a lithium vapor box are also absorbing, and expansion in this 2cd direction may give larger pressure drops so the (local) Mach number can reach larger values.

If the constant temperature regime is approximately true, $\rho_{out} = \frac{A_{in}}{A_{out}}\rho_{in}$, then to get the density to fall by a factor of 3400 after going through 4 holes from the first boxen to the 5th boxen (as it does in Rob's vapor box paper), we need the ratio of the bottom absorbing wall to the hole attaching adjacent boxes to have $A_{out} \sim 8A_{in}$, which appears to be roughly correct from the figure in the paper.

V. EXPANDING FLOW IN CYLINDRICAL AND SPHERICAL GEOMETRY

?? It would be useful to put here the solutions for expanding flow in cyclindrical and spherical geometry, to illustrate the expansion cooling that occurs (or can occur, depending on the boundary conditions at large r), and the relation with the famous Parker solar wind model, showing that the solar wind can transition to become supersonic at large distances.

VI. SUPERSONIC FLOW FROM DE LAVAL NOZZLES

?? It would be useful to put the standard results from de Laval Nozzles here, or some links to where it is worked out.

VII. KINETIC APPROACH TO ABSORBING WALL BOUNDARY CONDITIONS

?? Could put here some details of my current thoughts on absorbing wall boundary conditions. I think there is a steady-state boundary layer transition near an absorbing wall (where $F(v_{||}) = 0$ for $v_{||} < 0$ only for certain conditions on the incoming fluid. Somehow this boundary solution adjusts to keep a constant input flux of partilces, momentum, and energy. But this steady-state solution probably only exists if the incoming flow velocity is about Mach 1 or greater. For more general time-dependent problems, things get more complicated. In particular, for flows below Mach 1, there is probably a rarefaction fan expanding into the absorbing region, until eventually the flow becomes supersonic at the boundary.

Consider a 1-D problem (ignoring velocity in other directions, which will lead to some additional viscosity effects if included)...

Resolving the details of the mean-free-path boundary layer or time-dependent expansion fronts is probably not necessary in many cases. One way is perhaps to work out the boundary fluxes based on integrals over $v_{||} > 0$ of a shifted Maxwellian reconstructed from the local values of n, u, and T, and perhaps corrections from heat flux q as well. (Have to be a bit careful. I think the particle flux is exactly nu in steady state (if $u > c_s$) because the correction to the one-sided distribution function exactly offsets the missing part of the shifted-Maxwellian tail.

VIII. RIEMANN PROBLEM APROACH TO ABSORBING WALL BOUNDARY CONDITIONS

I finally found an answer in one useful limit, where we think of it in terms of what is called a "Riemann problem", the solution of the ideal Euler fluid equations for discontinuous initial conditions. This is widely used in hydrodynamic codes for shock capturing algorithms (and is discussed in Leveque's book "Finite Volume Methods for Hyperbolic Problems"). For general discontinuous initial conditions, the solution gives a propagating shock wave, a contact discontinuity, and a rarefaction fan. But if one side of the initial conditions is a vacuum, then one gets only a rarefaction fan, and the solution at x=0 has a simple form, discussed below.

Physically, what is the picture we are thinking of? Think of a uniform as for $x < 0$ next to a perfectly absorbing wall at $x = 0$. The wall acts as if it instantenously removes any gas that crosses to $x > 0$ so that it can't return. This is like the gas at $x < 0$ is adjacent to a vacuum at $x > 0$. Even if the fluid is initially stationary, there is a pressure gradient from the gas at $x < 0$ to no pressures at $x > 0$, and this will accelerate fluid across the $x = 0$ boundary. In fact, if we really start with a discontinuous pressure that drops to 0 in an infinitely thin width at $x = 0$, then there is an infinite pressure gradient that will accelerate fluid across to $x > 0$. Although the pressure gradient is infinite there, is is an integrable Dirac delta function, and it will accelerate the gas to a finite velocity across the $x = 0$ boundary. As we will find below, if we start with a stationary uniform gas at density ρ_0 at $x < 0$ at $t = 0$, then at a short time later, $t = 0+\epsilon$, the pressure drop will accelerate the fluid to 3/4 of the sound speed across the $x = 0$ boundary at a density which is $(3/4)^3$ of the initial density, giving a mass flux of $(3/4)^4\rho_0 c_s$. The more general result is given below.

I found the general solution for the version of the Riemann problem of expansion into vacuum in a paper by Munz:

"A Tracking Method for Gas Flow into Vacuum Based on the Vacuum Riemann Problem" C.-D. Munz, Math. Meth. in the Applied Sciences 17, 597 (1994) `http://onlinelibrary.wiley.com/doi/10.1002/mma.1670170803/abstract`

The general solution is given in Eqs. 5&6, and is plotted in Fig. 5. The actual solution for a perfectly absorbing wall isn't exactly the same, because in Fig. 5 at $t > 0$ there is gas at $x > 0$ with inertia and pressure that impedes the flow of gas from $x < 0$ into the the $x > 0$ region, while if there is a perfectly absorbing wall, then the gas at $x > 0$ is constantly being removed so there is no gas at $x > 0$ to push back on the incoming gas from $x < 0$. Nevertheless, one can use the solution In Eq. 6 at $x = 0$ (for $t = 0+\epsilon$, though the results are independent of t in this case for any $t > 0$) to infer what the flux would be into a perfect absorbing wall. The result is a simple form.

Let ρ_1, v_1, and p_1 represent the density, fluid velocity, and pressure of the fluid at $x < 0$. (Munz uses an "l" for left subscript, but l and 1 don't distinguish well.) Also denote $c_s = \sqrt{((5/3)p_1/\rho_1)}$ as the sound speed in the fluid, and $M = v_1/c_s$ as the Mach number of the fluid. Then the corresponding gas crossing the $x = 0$ surface into the perfect absorber has the parameters:

For $-3 < M < 1$:

$$v_0 = c_s(M + 3)/4 \tag{32}$$

$$\rho_0 = \rho_1(v_0/c_s)^3 \tag{33}$$

$$p_0 = p_1(v_0/c_s)^5 \tag{34}$$

For $M > 1$, we just have

$$v_0 = v_1 \tag{35}$$

$$\rho_0 = \rho_1 \tag{36}$$

$$p_0 = p_1 \tag{37}$$

i.e., the fluid flows into the absorbing wall so fast that there is no propagation of information to the left, so the incoming fluid parameters are constant.

For $M < -3$, the result is

$$v_0 = 0 \tag{38}$$

$$\rho_0 = 0 \tag{39}$$

$$p_0 = 0 \tag{40}$$

i.e., the fluid is flowing away from the absorbing wall faster than the expansion fan is broadening the edge of the fluid, so no fluid ever gets to the absorbing wall.

Once ρ_0, v_0, and p_0 are known, one can work out the fluxes into the absorbing wall from the standard relations:

$$\text{mass flux} = \rho_0 v_0 \tag{41}$$

$$\text{momentum flux} = \rho_0 v_0^2 + p_0 \tag{42}$$

$$\text{energy flux} = v_0((1/2)\rho_0 v_0^2 + (5/2)p_0) \tag{43}$$

Note that if $v_1 = 0$, i.e., the fluid is initially stationary, there is still a finite v_0 and thus a finite mass, momentum, and energy flux into the wall. (This is related to the fact that a centered Maxwellian gives a finite flux if integrated only over $v > 0$.) This will lower the fluid pressure near the wall, and the resulting pressure gradient will accelerate fluid towards the wall so that v_1 near the wall doesn't remain at 0. There will be a rarefaction wave that spreads to the left, lowering the density and temperature of the fluid to the left and increasing it's velocity. The final steady state is presumably $M = 1$ into the wall (or more generally $M >= 1$). By comparing the upstream and boundary fluxes, I'm pretty sure one can show the only steady-state solution is $M >= 1$.

Ammar's fluid code does a Riemann solve (or an approximate Riemann solve) for more general cases (not just the vacuum limit), which is useful for handling cases with a finite wall temperature so the equilibrium vapor pressure from the wall is finite, but it should automatically recover the above result in the vacuum limit.

One can try to do a more refined kinetic theory (which I now understand how to do), which will give a boundary layer with a width of order the mean-free path near $x = 0$ and some modest modifications to the above results if $M < 1$ (but that is not a steady-sate regime). This may be important for some SOL / sheath plasma problems, particularly because of fast electron thermal conduction, but for high density lithium vapor condensing onto a cold surface, I think the above results are probably quite good.

IX. SUMMARY

Sec. III and IV solve for the flow with a source region and how that depends on p_0, the central pressure, which can apparently only be determined in steady-state by the boundary conditions at the end plate wall. Fig. 1 shows the results if we hypothesize that the outflow in steady state for a perfect absorbing wall must be at Mach 1 (the maximum possible outflow velocity that can physically be produced in the source region, since a shock jump to a higher flow velocity is not allowed by entropy constraints). Sec VIII discusses the Riemann problem approach to handling absorbing wall boundary conditions. The only steady sate solutions is Mach number $>= 1$ for the flow incident on the absorbing wall, thus confirming the $M = 1$ hypothesis in Fig. 1.

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[1] http://ocw.mit.edu/courses/aeronautics-and-astronautics/16-901-computational-methods-in-aerospace-engineering-spring-2005/projects/proj2.pdf.