

Written Preliminary Exam #1

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1. Constant density flow and incompressible flow are two different things. Constant density implies that a fluid(s) density is constant, but capable of changing (through compression or expansion), whereas incompressible implies the fluid(s) density is incapable of changing but that the density in the flow is not necessarily constant. A good example from the MAE 550 course to distinguish the two is stagnant air in a room, versus an oil/water mixture. Stagnant air in a room is at constant density, but is certainly capable of both compression or expansion; therefore, it is a constant density flow, but not incompressible. An oil/water mixture is not constant density. As illustrated in figure 1, the water and oil are different fluids with different densities, but the fluids are incompressible because both the water and oil are not capable of compression or expansion (at least in a practical sense); therefore, it is not a constant density flow, but it is incompressible.

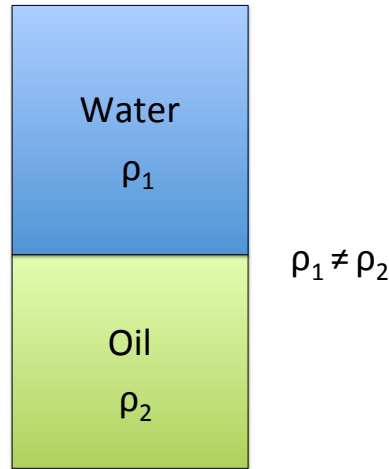


Figure 1: Incompressible Fluid Flow Example

2. The Pohlhausen method is typically defined as a velocity profile polynomial

$$\frac{u}{U_e} = a + b\eta + c\eta^2 + d\eta^3 + e\eta^4 \quad (1)$$
$$\eta = \left(\frac{y}{\delta}\right)$$

where u is the velocity, U_e is the velocity at the edge of the boundary layer, and δ is the boundary thickness. The polynomial coefficients are defined by the boundary conditions

for $u = u(x, y)$, which Pohlhausen specified as

$$u(x, 0) = 0 \quad (2)$$

$$u(x, \delta) = U_e \quad (3)$$

$$\frac{\partial u}{\partial y}(x, \delta) = 0 \quad (4)$$

$$\frac{\partial^2 u}{\partial y^2}(x, 0) = -\frac{U_e}{\nu} \frac{\partial U_e}{\partial x} \quad (5)$$

$$\frac{\partial^2 u}{\partial y^2}(x, \delta) = 0 \quad (6)$$

As discussed in MAE 589, the last boundary condition (Eq. (6)) was a poor choice, because the fact that the first derivative of velocity, $\partial u / \partial y$, is zero at a point does not necessarily mean that the curvature at that point is also zero. A suggested improvement would be to substitute that boundary condition for

$$\frac{\partial^3 u}{\partial y^3}(x, 0) = 0 \quad (7)$$

which comes from differentiating the momentum equation

$$\begin{aligned} \frac{\partial}{\partial y} \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) &= \frac{\partial}{\partial y} \left(-\frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2} \right) \\ \frac{\partial^3 u}{\partial y^3}(x, 0) &= 0 \end{aligned} \quad (8)$$

With this new boundary condition, the polynomial coefficients can be derived as

$$a = 0 \quad (9)$$

$$b = \frac{4 + \lambda}{3} \quad (10)$$

$$c = -\frac{\lambda}{2} \quad (11)$$

$$d = 0 \quad (12)$$

$$e = \frac{\lambda - 2}{6} \quad (13)$$

where $\lambda = \frac{\delta^2}{\nu} \frac{\partial U_e}{\partial x}$ is the Pohlhausen pressure gradient parameter. The separation condition $\tau_w = \mu(\partial u / \partial y)_{y=0} = 0$ is used to determine the value of λ at separation

$$\begin{aligned} \left(\frac{\partial u}{\partial y} \right)_{y=0} &= 0 = \frac{b}{\delta} \\ 0 &= \frac{4 + \lambda}{3\delta} \\ \lambda &= -4 \end{aligned} \quad (14)$$

The same procedure can be used with Eq. (6) in place of Eq. (7) to find that the original Pohlhausen method yields $\lambda = -12$ at separation. The Falkner-Skan equations can be used to verify that Eq. (7) does better at predicting separation for wedge flows, where $U_e = U_1 x^m$. In the literature[6] it is reported that flow separates at $m = -0.0904$, and

$$\frac{\delta}{x} \sqrt{Re_x} = 7.1 \quad (15)$$

at separation. This can be rearranged to give the exact value of the Pohlhausen pressure gradient parameter, λ , at separation

$$\begin{aligned}
\left(\frac{\delta}{x}\sqrt{Re_x}\right)^2 &= \frac{\delta^2}{\nu} \frac{U_e}{x} \\
&= \frac{\delta^2}{\nu} \frac{U_e}{x} \\
&= \frac{\delta^2}{\nu} \frac{\partial U_e}{\partial x} \frac{1}{m} \\
&= \frac{\lambda}{m}
\end{aligned} \tag{16}$$

Thus, the exact value of λ at separation is

$$\begin{aligned}
\lambda_{exact} &= m \left(\frac{\delta}{x}\sqrt{Re_x}\right)^2 \\
&= (-0.0904)(7.1)^2 \\
&= -4.56
\end{aligned} \tag{17}$$

It is therefore clear the Pohlhausen method with Eq. (7), yielding $\lambda = -4$ instead of $\lambda = -12$ at separation, is an improvement over using the original boundary condition (Eq. (6)).

3. There has been significant progress in the recent decades in developing stress models that address second-order closure, where the unique terms in the Reynolds stress tensor are modeled individually and the Boussinesq approximation is not used. Wilcox[8] gives a good description of deficiencies of the Boussinesq approximation, stating that models based upon this “approximation” (actually assumption is more accurate) perform poorly for flows with strong curvature and flows in rotating fluids. Consequently, results from Reynolds Stress Models (RSM) such as the Wilcox stress- ω model[8] and the SSG/LRR- ω [1] have been somewhat encouraging, however they are still lacking when predicting separated flows. This is likely due to poor progress in the development of a truly physics-based length scale equation. Kantha[2] derives a generalized equation for this, and claims to show that current equations used to model the turbulent dissipation rate, ε , and turbulent frequency, ω , are all subsets of a general form. These equations are strongly based on empirical derivations, not physical ones, and are therefore a considerable hinderance to the success of a second-order closure model when applied to complex flows. Thus, a suggestion to improve current RANS methods is to improve the equation used to determine the length scale and couple it with a RSM.

The enstrophy equation in the k- ζ model developed by Robinson and Hassan[4] has potential, since it has a stronger physical basis on vorticity fluctuations. Unfortunately efforts to recast the k- ζ model as an RSM led to issues with convergence[9], and consequently, poor results. Nonetheless, the analysis by Tennekes and Lumley[7] suggests that the energy transfer between large and small turbulent eddies is a vortex stretching process due to nonlinearity, suggesting that enstrophy is a critical component in turbulence. Morinishi et. al. [3] gives a relationship between the turbulent dissipation, ε , and enstrophy, ζ , thus it may be advantageous to replace the ω equation in the SSG/LRR- ω RSM or Wilcox stress- ω RSM, with the enstrophy equation defined in [9]. At the very least, this is useful in determining if the convergence issues previously described can be overcome using a different Reynolds stress tensor formulation, which does not necessarily contract to turbulent kinetic energy, k, equation presented in [4].

4. There are many ways to derive an expression for change in entropy. From a classical thermodynamics perspective, this comes from the definition of Gibbs free energy, G

$$G = H - TS \tag{18}$$

Where H is enthalpy, T is temperature, and S is entropy. It is straightforward to see that the first and second laws of thermodynamics can be used to determine the change of entropy

$$dQ = dH - VdP \quad (19)$$

$$dS = \frac{dQ}{T} + dS_i = \frac{dH - Vdp}{T} + dS_i \quad (20)$$

Where dS_i is entropy generated from irreversible processes. Using the definition of the enthalpy

$$H = E + pV \quad (21)$$

Eq. (20) can be expanded as

$$\begin{aligned} dS &= \frac{dE + pdV + Vdp - Vdp}{T} + dS_i \\ &= \frac{dE + pdV}{T} + dS_i \end{aligned} \quad (22)$$

While this is useful, this derivation is deficient as it does not directly account for multiple species in chemical non-equilibrium. Revisiting Gibbs free energy for multiple species, if a system is considered for each isolated species then

$$G_s = G_s(p, T, N_s) \quad (23)$$

where G_s is the Gibbs free energy of the isolated species s , and N_s is the number of particles of species s . Differentiating Eq. (23) yields

$$dG_s = \left(\frac{\partial G_s}{\partial T} \right)_{(p, N_s)} dT + \left(\frac{\partial G_s}{\partial p} \right)_{(T, N_s)} dp + \left(\frac{\partial G_s}{\partial N_s} \right)_{(p, T)} dN_s \quad (24)$$

Because $G = \sum_{s=1}^{N_{ns}} G_s$, Eq. (24) can be written as

$$dG = \left(\frac{\partial G}{\partial T} \right)_{(p, N_s)} dT + \left(\frac{\partial G}{\partial P} \right)_{(T, N_s)} dp + \sum_{s=1}^{N_{ns}} \left(\left(\frac{\partial G}{\partial N_s} \right)_{(p, T)} dN_s \right) \quad (25)$$

Introducing the concept of chemical potential

$$\mu_s = \left(\frac{\partial G}{\partial N_s} \right)_{p, T} \quad (26)$$

and writing Eq. (18) in differential form and substituting Eq. (22) yields

$$\begin{aligned} dG &= dH - SdT - TdS \\ &= dH - SdT - T \left(\frac{dH - Vdp}{T} + dS_i \right) \\ &= Vdp - SdT - TdS_i \end{aligned} \quad (27)$$

It is clear that in comparing Eq. (27) and Eq. (25) that

$$\left(\frac{\partial G}{\partial T} \right)_{(p, N_s)} = -S, \quad \left(\frac{\partial G}{\partial P} \right)_{(T, N_s)} = V \quad (28)$$

and most importantly

$$dS_i = -\frac{1}{T} \sum_{s=1}^{N_{ns}} \mu_s dN_s \quad (29)$$

Thus, it is now clear that the change of entropy is defined in two components: the entropy generated by the surroundings, S_r , and the entropy generated by irreversible chemical processes, S_i . If Eq. (27) is expanded with $dS_i = 0$ and the definition of enthalpy in Eq. (21) is used, the entropy from reversible processes is given by

$$dS_r = \frac{dE}{T} + \frac{pdV}{T} \quad (30)$$

combining Eq.s (29-30) the change of entropy expression is obtained

$$dS = \frac{dE}{T} + \frac{pdV}{T} - \frac{1}{T} \sum_{s=1}^{N_{ns}} \mu_s dN_s \quad (31)$$

If two gases with the same pressure and temperature are mixed, then Eq. (31) shows that entropy must be generated, regardless of whether chemical reactions occur. Since entropy of a system of gases is additive,

$$dS_{mix} = dS_1 + dS_2 \quad (32)$$

where dS_{mix} is the change of entropy in the mixture, and $dS_{(1,2)}$ are the changes in entropy of species being mixed. If $E = E(T, p)$ and there is no change in temperature or pressure, $dE = 0$ for both species; however, the volume has changed. For two inert gases mixing there will be production of entropy, since

$$dS_{mix} = \frac{p}{T} (dV_1 + dV_2) \quad (33)$$

Where dV_1 and dV_2 are the changes in volume for species 1 and 2, respectively. Using the ideal gas law for the individual inert gases

$$p = \frac{nRT}{V} \quad (34)$$

where R is the universal gas constant and n is the number of moles of the gas, Eq. (33) can be integrated to give the change in entropy when the gases are combined

$$\begin{aligned} \Delta S_{mix} &= \int_{V_1}^{V_1+V_2} \frac{n_1 R}{V} dV + \int_{V_2}^{V_1+V_2} \frac{n_2 R}{V} dV \\ \Delta S_{mix} &= R \left(n_1 \ln \left(\frac{V_1 + V_2}{V_1} \right) + n_2 \ln \left(\frac{V_1 + V_2}{V_2} \right) \right) \end{aligned} \quad (35)$$

The production of entropy is to be expected, intuitively, since the diffusion of one gas into the other happens spontaneously. Each gas will expand into the new volume available after mixing, naturally, and it takes effort to separate them; hence $dS_{mix} > 0$. Likewise, if chemical reactions occur, entropy will also be generated as dictated by Eq. (29).

It should be noted that Eq. (35) can also be derived from statistical mechanics. Beginning with the Boltzmann relation

$$S = k \ln(\Omega) \quad (36)$$

where k is the boltzmann constant and Ω is the ‘‘thermodynamic probability’’. In the boltzmann limit, which is the macro state containing the maximum number of microstates,

$$\ln(\Omega) = N \left(\ln \frac{\sum_j C_j e^{-\beta \epsilon_j}}{N} + 1 \right) + \beta E \quad (37)$$

where C_j is a microstate container, ε_j is a microstate energy, and β is an undetermined multiplier. Substituting Eq. (37) into Eq. (36)

$$S = Nk \left(\ln \frac{\sum_j C_j e^{-\beta \varepsilon_j}}{N} + 1 \right) + \beta E \quad (38)$$

Using Eq. (22) to solve for β , Eq. (38) can be rewritten in terms of the the partition function, Q , as

$$S = Nk \left(\ln \frac{Q}{N} + 1 \right) + \frac{E}{T} \quad (39)$$

$$Q = \sum_j C_j e^{-\varepsilon_j/kT} \quad (40)$$

Because the partition functions is the product of all the energy modes

$$Q = Q_{trans} Q_{rot} Q_{vib} Q_{elec} \quad (41)$$

and the only volume dependence that Q has is in the translational mode

$$Q_{trans} = V Q'(T) \quad (42)$$

$$Q = V Q'(T) \quad (43)$$

where $Q'(T)$ is used to denote a partition function's temperature dependence. Substituting Eq. (43) into Eq. (40) gives a relation for entropy with a clear dependence on T and V

$$S = Nk \left(\ln \frac{V Q'(T)}{N} + 1 \right) + \frac{E}{T} \quad (44)$$

Since the entropy change of the mixture is the sum of the individual gases' entropy changes, and there is no change in temperature or pressure when mixing occurs

$$\begin{aligned} \Delta S_{mix} &= N_1 k \left(\ln \frac{(V_1 + V_2) Q' T}{N_1} - \ln \frac{V_1 Q' T}{N_1} \right) \\ &\quad + N_2 k \left(\ln \frac{(V_1 + V_2) Q' T}{N_2} - \ln \frac{V_2 Q' T}{N_2} \right) \\ \Delta S_{mix} &= N_1 k \left(\ln \frac{(V_1 + V_2)}{V_1} \right) + N_2 k \left(\ln \frac{(V_1 + V_2)}{V_2} \right) \end{aligned} \quad (45)$$

Since $R = N_A k$, where N_A is avogadro's number and $n = N/N_A$, Eq. (45) is equivalent to Eq. (35).

5. As stated previously, gibbs free energy is defined as

$$G = G(T, p, N_1, N_2, \dots, N_{ns}) = H - TS \quad (46)$$

Using the definition of G in Eq. (46), it was previously shown that

$$S = - \left(\frac{\partial G}{\partial T} \right)_{(p, N_s)} \quad (47)$$

Where G and S are defined as Gibbs free energy and entropy per mole of the mixture, respectively, and N_s is the number of particles of species i per mole of the mixture. Likewise, enthalpy, H , and specific heat at constant pressure, C_p , per mole of mixture can be

determined from Eq.s (46-47) as

$$H = G - T \left(\frac{\partial G}{\partial T} \right)_{(p, N_s)} \quad (48)$$

$$C_p = \left(\frac{\partial H}{\partial T} \right)_{(p, N_s)} = \left(\frac{\partial G}{\partial T} \right)_{(p, N_s)} - \left(\frac{\partial G}{\partial T} \right)_{(p, N_s)} - T \left(\frac{\partial^2 G}{\partial T^2} \right)_{(p, N_s)} \quad (49)$$

These thermodynamic quantities can also be found for each species (per mole of mixture) by substituting G_s in place of G , where G_s is the Gibbs free energy of species s per mole of the mixture, and

$$G = \sum_{s=1}^{ns} \chi_s G_s \quad (50)$$

where χ_s is the mole fraction of species s . Thus, if the variables T , p , N_1 , \dots , N_{ns} are known, Gibbs free energy can be used to derive all the thermodynamic quantities needed for a reacting gas solver. Likewise, if the mixture composition is not known, and needs to be determined at chemical equilibrium for a given p and T , this can be done by free energy minimization. Gordon and McBride[5] explain this in detail, and have developed a chemical equilibrium solver based on this principle.

One other useful quantity that the Gibbs free energy provides is the reaction equilibrium constant in partial pressures, K_p

$$K_p = \prod_{i=1}^{ns} p_i^{(\nu_i'' - \nu_i')} = e^{-\Delta G / RT} \quad (51)$$

$$\Delta G = \sum_{i=1}^{ns} (\nu_i'' - \nu_i') G_i \quad (52)$$

where ν_i'' is the stoichiometric coefficient of the product species i , ν_i' is the stoichiometric coefficient of the reactant species i , and R is the universal gas constant. Converting this to the more useful reaction equilibrium constant in concentrations, K_c , assuming the partial pressure is in units atm

$$K_c = \left(\frac{101325}{RT} \right)^{(m'' - m')} K_p \quad (53)$$

$$m'' = \sum_{i=1}^{ns} \nu_i'', \quad m' = \sum_{i=1}^{ns} \nu_i'$$

This is a more useful quantity, as it can be used to obtain the backward reaction rate constant, k_b , based on the forward reaction rate coefficient, k_f , where

$$k_b = \frac{k_f}{K_c} \quad (54)$$

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