

ME 451C  
Winter Quarter, 2004-05  
Week # 9 Homework Answers

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**Abstract**

I am generally happy with the quality of this homework. However, several of you went down the wrong track on question (d). So take a more careful look at it.

**Homework**

1. For our toy problem of unsteady two-dimensional stagnation point flow, let's consider the no chemistry case  $\mathbf{W} = 0$  with a scalar unknown  $\mathbf{X} = X$ . In addition, we limit ourselves to the one-dimensional unsteady case so that  $X = X(\xi, \tau)$  only. Find a transformation to transform this PDE into the usual constant coefficient unsteady one-dimensional diffusion PDE.

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The PDE for  $X(\xi, \tau)$  is:

$$\frac{\partial X}{\partial \tau} = D \frac{\partial^2 X}{\partial \xi^2} \exp\left(-\frac{2\Omega}{\omega} \sin(\omega\tau)\right). \quad (1)$$

We introduce a new set of independent variables  $\xi_*, \tau_*$  as follows:

$$\xi_* = \xi, \quad (2)$$

$$\tau_* = \int_0^\tau \exp\left(-\frac{2\Omega}{\omega} \sin(\omega\tau')\right) d\tau'. \quad (3)$$

Note that  $\tau_*(\tau)$  when plotted looks like a staircase with slanted steps.

The PDE for  $X(\xi_*, \tau_*)$  is now:

$$\frac{\partial X}{\partial \tau_*} = D \frac{\partial^2 X}{\partial \xi_*^2}. \quad (4)$$

The solution depends on  $\tau_*$  smoothly, but its dependence on  $t$ , the physical wall clock time, is jerky.

2. Consider the toy problem in §1 of Week #8 Notes: Eqs.(1,2,3) and Eqs.(12,13) with  $w_2 = w_3 = 0$  and  $D_{11} \neq D_{22} \neq 0$ .

We shall consider an unsteady one-dimensional  $(y, t)$  problem—the domain of interest is  $0 \leq y \leq L, t \geq 0$ . The initial conditions are:

$$X_1(y, 0) = c_1(y), \quad (5)$$

$$X_2(y, 0) = c_2(y). \quad (6)$$

The boundary conditions at  $y = 0$  and  $y = L$  are:

$$X_1(0, t) = b_1(t), \quad (7)$$

$$X_2(0, t) = b_2(t), \quad (8)$$

$$D_{11} \frac{\partial X_1}{\partial y}(L, t) = 0, \quad (9)$$

$$D_{22} \frac{\partial X_2}{\partial y}(L, t) = 0. \quad (10)$$

Assume that  $c_1(0) \neq b_1(0), c_2(0) \neq b_2(0)$ .

- a Write down the leading order reduced chemistry PDE for  $X_1$  and  $X_2$  in the limit of asymptotically small  $\epsilon$ . Where in our domain of interest does this PDE apply? By dimensional analysis, there are two characteristic diffusion time scales:  $L^2/D_{11}$  and  $L^2/D_{12}$ . What can you say about the general qualitative picture of the solution for  $t$  small in comparison to these values, and for  $t$  of this order of magnitude or larger?

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The original PDEs are:

$$\frac{DX_1}{Dt} = W_1 + W_2, \quad (11)$$

$$\frac{DX_2}{Dt} = -2W_1 + W_3, \quad (12)$$

$$W_1 = \frac{X_2^2 - X_1}{\epsilon}, \quad (13)$$

$$W_2 = w_2(X_1, X_2) + \nabla \cdot D_{11} \nabla X_1, \quad (14)$$

$$W_3 = w_3(X_1, X_2) + \nabla \cdot D_{22} \nabla X_2. \quad (15)$$

where  $W_2(X_1, X_2)$  and  $W_3(X_1, X_2)$  are some differentiable functions of their arguments and are independent of  $\epsilon$ —which is a positive small parameter.

The  $\epsilon \rightarrow 0$  reduced chemistry PDE for  $X_2$  is given by eq.(14) of Week # 8 Notes:

$$\frac{DX_2}{Dt} = \frac{\nabla \cdot (4X_2 D_{11} + D_{22}) \nabla X_2}{1 + 4X_2} \quad (16)$$

using  $w_2 = w_3 = 0$ . Now, in the small  $\epsilon$  limit, we have  $X_1 = X_2^2$  so  $X_1$  can be obtained after  $X_2$  is found. Alternately, the reduced chemistry PDE for  $X_1$  can be derived:

$$\frac{DX_1}{Dt} = 2X_2 \frac{\nabla \cdot (4X_2 D_{11} + D_{22}) \nabla X_2}{1 + 4X_2}. \quad (17)$$

We can eliminate the  $X_2$ 's on the right hand side by  $X_2 \approx \sqrt{X_1}$  to yield a single PDE for  $X_1$ .

These reduced chemistry PDEs are valid only when  $X_2^2 - X_1 = O(\epsilon)$  is valid. Certainly the initial conditions for  $X_1$  and  $X_2$  may not satisfy this condition in general, so the PDEs are not applicable at and near  $t = O(\epsilon)$ . So the brief initial transient period is excluded. In addition, at the sidewalls of the problem, the boundary conditions may not satisfy reduced chemistry in general. Certainly if  $b_1 \neq b_2^2$ , this condition is not satisfied at the lower wall  $y = 0$ . So a thin layer of thickness proportional to  $\sqrt{\epsilon}$  will exist adjacent to  $y = 0$  which must also be excluded. On the upper boundary  $y = L$ , however, the specified boundary condition is not in conflict with  $X_2^2 - X_1 = O(\epsilon)$ . Thus the above reduced chemistry PDEs are expected to be valid all the way to  $y = L$ .

Roughly speaking, the time it takes for diffusion to spread across a distance  $L$  is  $O(L^2/D_*)$  where  $D_*$  is the relevant diffusion coefficient. We see that for our PDEs,  $D_{11}$  and

$D_{22}$  have no independent say. For the reduced chemistry PDE, the relevant  $D_*$  is  $(4X_2D_{11} + D_{22})/(1 + 4X_2)$ . If  $t$  is small in comparison to  $L^2/D_*$ , then in its region of validity  $X_1$  and  $X_2$  are nearly constants (determined by initial conditions) after the initial transient. A “boundary layer” with thickness  $\sqrt{D_*t}$  grows along the sidewall ( $y = 0$ ) to exert the influence of wall boundary conditions (at  $y = 0$ ) on the solution.

- b** Find the initial conditions for this reduced chemistry PDE.

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We non-dimensionalize our independent variables and parameters as follows:

$$\xi = \frac{y}{L}, \quad (18)$$

$$\eta = \frac{t}{\epsilon}, \quad (19)$$

$$\sigma = \frac{D_{11}\epsilon}{L^2}, \quad (20)$$

$$\alpha = \frac{D_{22}}{D_{11}}. \quad (21)$$

and assume that  $D_{11} \geq D_{22}$ . We shall make the simplifying assumption that  $D_{11}$  and  $D_{22}$  are constants. The original PDE becomes (without approximation):

$$\frac{\partial X_1}{\partial \eta} = (X_2^2 - X_1) + \sigma \frac{\partial^2 X_1}{\partial \xi^2}, \quad (22)$$

$$\frac{\partial X_2}{\partial \eta} = -2(X_2^2 - X_1) + \alpha \sigma \frac{\partial^2 X_2}{\partial \xi^2}. \quad (23)$$

We confine our attention to the region  $\xi = O(1)$  and  $\eta = O(1)$ —this is the initial rapid transient period. In the small  $\epsilon$  limit,  $\sigma$  is negligibly small. Neglecting the small diffusion terms, we have two ODEs to solve to deal with the initial conditions. These are no longer stiff ODEs (with respect to  $t$ ) no matter how small  $\epsilon$  is.

For this toy problem, however, there is a short cut (which is NOT always available in the general case). When diffusion is neglected,  $2X_1 + X_2$  is approximately a conserved scalar which can be evaluated at  $t = 0$ :

$$2X_1 + X_2 = 2c_1(y) + c_2(y) \quad (24)$$

which is valid for  $\eta = O(1)$ . At the tail end of this transient, we expect  $X_1 \rightarrow X_2^2$ . Solving the quadratic equation for the tail end value of  $X_2$  (and denote it by  $X_2(t \approx \epsilon)$ ), we obtain:

$$X_2(y, t \approx \epsilon) = \frac{\sqrt{1 + 8(2c_1(y) + c_2(y))} - 1}{2}. \quad (25)$$

This will serve as the initial condition for the reduced chemistry PDE.

Repeat: this short cut is NOT generally available. In general, you need to get a computer involved.

- c Find the boundary condition at  $x \approx 0$  for this reduced chemistry PDE. Find the ODE governing the structure of the thin later in which  $X_1$  is not approximately equal to  $X_2^2$  (remember, in the slow subspace, the decay of the fast modes provide  $M$  algebraic equation; similarly, in the fast subspace, the slow modes provides  $N - M$  approximate conserved scalars). How does the thickness of this thin layer scale with  $\epsilon$ ?

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We shall use our non-dimensionalized Eq.(22) and Eq.(23). In the small  $\epsilon$  limit, we have a small  $\sigma$ . But side wall boundary conditions can be respected only if the diffusion term is kept. So the issue is to make sure the diffusion terms stay in the game in the small  $\sigma$  limit.

So we introduce the following new independent variables:

$$\xi_* = \frac{\xi}{\sqrt{\sigma}}, \quad (26)$$

$$\eta_* = \epsilon \eta = t. \quad (27)$$

Note:  $\eta_*$  is the original independent time variable. Our original PDEs in terms of these independent variables ( $\xi_*$  and  $t$ ) are then:

$$\epsilon \frac{\partial X_1}{\partial t} = (X_2^2 - X_1) + \frac{\partial^2 X_1}{\partial \xi_*^2}, \quad (28)$$

$$\epsilon \frac{\partial X_2}{\partial t} = -2(X_2^2 - X_1) + \alpha \frac{\partial^2 X_2}{\partial \xi_*^2}. \quad (29)$$

In the small  $\epsilon$  limit, the time derivative terms on the left hand sides can be neglected to yield two second order ODEs

which can honor the wall boundary conditions ( $X_1(0, t) = b_1(t)$ , and  $X_2(0, t) = b_2(t)$ ). The second boundary condition to be applied for “large”  $\xi_*$  is that  $X_1$  should approach  $X_2^2$  at the edge of this thin boundary layer.

Again, for this toy problem, there is a short cut—which is not generally available. Once the time derivatives are neglected, we immediately see that  $2X_1 + \alpha X_2$  is independent of  $\xi_*$  (a conserved scalar with respect to  $\xi_*$ ), and can be evaluated at  $\xi_* = 0$ :

$$2X_1 + \alpha X_2 = 2b_1(t) + \alpha b_2(t). \quad (30)$$

At the outer edge of this layer  $\xi_* \gg 1$ , we expect  $X_1 \approx X_2^2$ . So solving the quadratic equation, we obtain:

$$X_2(\xi = O(\epsilon), t) = \frac{\sqrt{\alpha^2 + 8(2b_1(t) + \alpha b_2(t))} - \alpha}{2}, \quad (31)$$

which will serve as the boundary condition for the reduced chemistry PDE for  $X_2$ . Again, I emphasize that this short cut is not always available. Without such shortcuts, computers must be involved. We have a two-point boundary value problem, and some work needs to be done to come up with a good computational algorithm to handle this.

- d** Find the boundary condition at  $y \approx L$  for this reduced chemistry PDE.

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We can deal with the situation for  $y \approx L$  using the equations above—provided we interpret  $\xi$  to be  $1 - y/L$ . So the upper boundary remains at  $\xi = 0$ .

So the boundary conditions for the ODEs Eq.(28) and Eq.(29) are:

$$\frac{\partial X_1}{\partial \xi_*}(\xi_* = 0, t) = 0, \quad (32)$$

$$\frac{\partial X_2}{\partial \xi_*}(\xi_* = 0, t) = 0, \quad (33)$$

$$X_1(\xi_* \gg 1, t) = X_2^2(\xi_* \gg 1, t). \quad (34)$$

By inspection, we can conclude that  $X_1 = X_2^2 = \text{constant}$  is our solution. In other words, the reduced chemistry approximation  $X_1 = X_2^2$  is valid throughout the inside of this

boundary layer. So, for the reduced chemistry PDE, the correct boundary conditions is:

$$\frac{\partial X_2}{\partial y}(L, t) = 0. \quad (35)$$

Note that if the fluxes specified at the  $y = L$  boundaries were finite numbers, then there will be a non-trivial boundary layer which must be solved to determine the boundary condition for the reduce chemistry PDE.

A number of you analyzed this problem by taking advantage of Eq.(30). Differentiating it with respect to  $\xi_*$ , some suggested that the appropriate boundary condition for the reduced chemistry PDE is  $X_2 = -D_{22}/(4D_{11})$  (to make this equation happy). This choice is made by rejecting the “trivial” solution—that  $\partial X_2/\partial \xi_* = 0$ .

For this problem, it turns out that the trivial solution is the correct solution. Think about it and I am sure you will agree.

- e This is *not* required. But if you have in your toolbox a diffusion PDE solver that can handle the reduced chemistry PDE, I would appreciate getting some numerical solutions from some volunteers. Pick for yourselves  $c_1(t)$ ,  $c_2(t)$ ,  $b_1(y)$  and  $b_2(y)$  (constants are fine), the values of  $L$ ,  $D_{11}$  and  $D_{22}$ , and the range of  $t$  the numerical simulations would cover. Remember, the reduced chemistry model is valid for any “asymptotically small” values of  $\epsilon$ .

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No takers so far.