CHAPTER 2. MORE APPLICATIONS OF ODEs

2.1. THE HARMONIC OSCILLATOR

Consider the pendulum shown.

The small object, mass m,

at the end of the pendulum,

is moving on a circle of radius

L, so the component of its velocity

tangential to the circle is $L\dot{\theta}$

Hence its tangential acceleration is

$L\ddot{\theta}$ and so by $\overrightarrow{F} = M\overrightarrow{a}$ we have

$$mL\ddot{\theta} = -mg\sin\theta.$$

An obvious solution is $\theta = 0$. This is called an EQUILIBRIUM solution, meaning that θ is a CONSTANT function. This means that if you set $\theta = 0$ initially, then θ will remain at 0 and the pendulum will not move — which of course we know is correct. There is ANOTHER equilibrium solution, $\theta = \pi$. Again, IN THEORY, if you set the pendulum EXACTLY at $\theta = \pi$, then it will remain in that position forever. IN REALITY, of course, it won't! Because the slightest puff of air will knock it over! So this equilibrium is very different from the one at $\theta = 0$. This is a very important distinction!

Equilibrium is said to be STABLE if a SMALL push away from equilibrium REMAINS small. If the small push tends to grow large, then the equilibrium is UNSTABLE. Obviously this is important for engineers! Especially you want vibrations of structures, engines, etc to remain small.

Let's look at $\theta = \pi$. By Taylor's theorem, near $\theta = \pi$, we have

$$f(\theta) = f(\pi) + f'(\pi)(\theta - \pi) + \frac{1}{2}f''(\pi)(\theta - \pi)^2 + ...$$

Now $\sin(\pi) = 0$, $\sin'(\pi) = \cos(\pi) = -1$, $\sin''(\pi) = -\sin(\pi) = 0$ etc so

$$\sin(\theta) = 0 - (\theta - \pi) - 0 + \frac{1}{6}(\theta - \pi)^3 \;\; \text{etc}$$

For small deviations away from π, $\theta - \pi$ is small, $(\theta-\pi)^3$ is much smaller, etc, so we can approximate

$$\sin(\theta) \approx -(\theta - \pi)$$

so our equation is approximately

$$ML\ddot{\theta} = -mg\sin\theta = mg(\theta - \pi).$$

Let $\phi = \theta - \pi$, so $\ddot{\phi} = \ddot{\theta}$, and now

$$\ddot{\phi} = \frac{g}{L}\phi.$$

The general solution is

$$\phi = Ae^{(\sqrt{g/L})t} + Be^{-(\sqrt{g/L})t}$$

so $\theta = \phi + \pi = Ae^{(\sqrt{g/L})t} + Be^{-(\sqrt{g/L})t} + \pi$.

As you know, the exponential function grows very quickly; so even if θ is close to π initially, it won't stay near to it very long! Very soon, θ will arrive either at $\theta = 0$ or 2π, far away from $\theta = \pi$. The equilibrium is UNSTABLE! How long does it take for things to get out of control? That is determined by $\sqrt{g/L}$ or rather $\sqrt{L/g}$, which has units of TIME. Note that it takes longer to fall over if L is large.

EXAMPLE:

An eccentric professor likes to balance pendula near their unstable equilibrium point. In a given performance, the pendulum is initially slightly away from that point, and is initially at rest. The prof's skill is such that he can stop the pendulum from falling provided that the angular deviation from the vertical angle does not double. If the shortest pendulum for which he can perform this trick is 9.8 centimetres long, estimate the speed of his reflexes.

Solution: The problem is saying that the angle ϕ [the deviation from the vertical] is initially very small, and its initial rate of change is zero. So $\phi(0) = \epsilon$ [some very small number] and $\dot{\phi}(0) = 0$. Differentiating our solution for $\phi(t)$ above and substituting we get A + B = ϵ and A - B = 0, so in fact

A = B = $\epsilon/2$ and so

$$\phi = \epsilon\ cosh((\sqrt{g/L})t) = \epsilon\ cosh(10t)$$

since from the given data g/L = 100/sec^2. Now our objective is to calculate how long it takes for ϕ to double, so we need to find t such that $2\epsilon = \epsilon\ cosh(10t)$. Clearly t = $\cosh^{-1}(2)/10 \approx 0.132$ sec.

SUMMARY: The equation $\ddot{\phi} = +\frac{g}{L}\phi$ is a symptom of INSTABILITY. The system is at equilibrium, but it will run away uncontrollably on a time scale fixed by $\sqrt{L/g}$.

Now what about $\theta = 0$? Here of course we use Taylor's theorem around zero,

$$f(\theta) = f(0) + f'(0)\theta + \frac{1}{2}f''(0)\theta^2 + ...$$
$$\sin(\theta) = 0 + \theta - 0 - \frac{1}{6}\theta^3 + ...$$

so $\sin(\theta) \approx \theta$ and we have approximately

$$mL\ddot{\theta} = -mg\theta \quad \text{or}$$

$$\ddot{\theta} = -\frac{g}{L}\theta = -\omega^2\theta$$

with $\omega^2 = g/L$. That minus sign is crucial!

General solution is $C\cos(\omega\, t) + D\sin(\omega\, t)$ where C and D are arbitrary constants.

Now using trigonometric identities you can show that ANY expression of the form $C\cos(x) + D\sin(x)$ can be written as

$$C\cos(x) + D\sin(x) = \sqrt{C^2 + D^2}\cos(x - \gamma)$$

where $\tan(\gamma) = D/C$. [You can see this easily by taking the scalar product of the vectors $\begin{bmatrix} C \\ D \end{bmatrix}$ and $\begin{bmatrix} \cos(x) \\ \sin(x) \end{bmatrix}$.]

So now we can write our general solution as

$$\theta = A\cos(\omega t - \delta)$$

[**Check**: this does satisfy $\ddot{\theta} = -\omega^2\theta$ and it does contain TWO arbitrary constants, A and δ]. In this case, θ is never larger than A, never smaller than $-A$, so IF θ WAS SMALL INITIALLY, it REMAINS

SMALL! [We call A the AMPLITUDE.] So the equilibrium in this case is STABLE. This is called SIMPLE HARMONIC MOTION. Clearly θ repeats its values every time ωt increases by 2π [since cos is periodic with period 2π]. Now

$$\omega t \rightarrow \omega t + 2\pi$$

means

$$t \rightarrow t + \frac{2\pi}{\omega}$$

So $\frac{2\pi}{\omega} = 2\pi\sqrt{L/g}$ is the time taken for θ to return to its initial value, the PERIOD. Again it takes a long time if L is large. The number ω is called the ANGULAR FREQUENCY.

SUMMARY: The equation $\ddot{\theta} = -\omega^2\theta$ is a symptom of STABILITY. The system oscillates, with a constant amplitude, around equilibrium on a time scale fixed by $\sqrt{L/g}$. The angular frequency is ω.

2.2. DAMPED, FORCED OSCILLATORS.

When an object moves fairly slowly through air, the RESISTANCE DUE TO FRICTION is approximately proportional to its speed, and of course in the OPPOSITE DIRECTION. So in the case of the pendulum, where the speed of the object is $L\dot{\theta}$, the DAMP-

ING FORCE is

$$-SL\dot{\theta}$$

where S is some positive constant. We now have

$$mL\ddot{\theta} = -mg\sin\theta - SL\dot{\theta}$$

$$\approx -mg\theta - SL\dot{\theta}$$

if θ is close to zero. Thus

$$m\ddot{\theta} + S\dot{\theta} + \frac{mg}{L}\theta = 0,$$

and this is the equation of DAMPED HARMONIC MOTION. We can also attach a motor to the pendulum, that is, an external force $F(t)$ which may depend on time. Then

$$mL\ddot{\theta} = -mg\sin\theta - SL\dot{\theta} + F(t)$$

and if θ remains small, we get

$$m\ddot{\theta} + S\dot{\theta} + \frac{mg}{L}\theta = \frac{1}{L}F(t),$$

the equation of FORCED damped harmonic motion.

Let's look at the unforced but damped case first. The ODE will always have the form

$$m\ddot{x} + b\dot{x} + kx = 0.$$

With the usual trick, $x = e^{\lambda t}$, we get

$$m\lambda^2 + b\lambda + k = 0.$$

Quadratic in λ, so 3 cases: both roots real, both complex, both equal.

[a] BOTH REAL : OVERDAMPING

Example, $\ddot{x} + 3\dot{x} + 2x = 0$

$$\lambda^2 + 3\lambda + 2 = 0 \rightarrow \lambda = -1, -2,$$

general solution $B_1 e^{-t} + B_2 e^{-2t}$. The motion very rapidly dies away to zero. Obviously we have too much friction.

[b] BOTH COMPLEX: UNDERDAMPING

Example, $\ddot{x} + 4\dot{x} + 13x = 0$

$$\lambda^2 + 4\lambda + 13 = 0 \rightarrow \lambda = -2 \pm 3i$$

general solution $B_1 e^{-2t}\cos(3t) + B_2 e^{-2t}\sin(3t)$, which can be written as

$$x = Ae^{-2t}\cos(3t - \delta).$$

The graph is obtained by "multiplying together" the graphs of e^{-2t} and $A\cos(3t-\delta)$:

This is like a simple harmonic oscillator such that the amplitude is a function of time.

In general if we have an equation for an unforced, damped harmonic oscillator, such that

$$m\ddot{x} + b\dot{x} + kx = 0,$$

$$m\lambda^2 + b\lambda + k = 0,$$

then if the solutions for λ are COMPLEX, we say that the system is UNDERDAMPED. We get

$$x(t) = Ae^{\frac{-bt}{2m}} \cos(\beta t - \delta)$$

where $\beta = \frac{1}{2m}\sqrt{4mk - b^2}$. You can think of this as "SHM with frequency β and amplitude $Ae^{\frac{-bt}{2m}}$." Here β is often called the QUASI-FREQUENCY and $\frac{2\pi}{\beta}$ is the QUASI-PERIOD. Notice that in this problem, UNLIKE in true SHM, there are actually TWO independent time scales: $\frac{2\pi}{\beta}$ has units of time but so does $\frac{2m}{b}$. This second time scale tells you how quickly the amplitude dies out. [They are INDEPENDENT because given m and b you can work out $\frac{2m}{b}$ but not $\frac{2\pi}{\beta}$ [since you have not been given

k.]

2.3. FORCED OSCILLATIONS

Suppose you have a mass m which can move in a horizontal line. It is attached to the end of a spring which exerts a force

$$F_{\text{spring}} = -kx$$

where x is the extension of the spring and k is a constant (called the spring constant). This is Hooke's Law. Now we attach an external MOTOR to the mass m. This motor exerts a force $F_0 \cos(\alpha t)$, where F_0 is the amplitude of the external force and α is the frequency. If $F_0 = 0$ we just have, from Newton,

$$m\ddot{x} = -kx,$$

so we get $\ddot{x} = -\omega^2 x, \ \ \omega = \sqrt{k/m}$. Here ω is the frequency that the system has if we leave it alone that is, it is the NATURAL frequency. It has NOTHING TO DO with α of course $-$ we can choose α to suit ourselves.

If $F_0 \neq 0$, then we have

$$m\ddot{x} + kx = F_0 \cos \alpha t.$$

Let z be a complex function satisfying

$$m\ddot{z} + kz = F_0 \ e^{i\alpha t}.$$

Clearly the real part, $Re\ z$, satisfies the above equation, so we can solve for z and them take the real part. We try

$$z = C\ e^{i\alpha t}$$

and get

$$mC(i\alpha)^2 e^{i\alpha t} + C\ k\ e^{i\alpha t} = F_0 e^{i\alpha t}$$

$$\Rightarrow C = \frac{F_0}{k - m\alpha^2} = \frac{F_0/m}{\omega^2 - \alpha^2}$$

So $$Re\ z = \tfrac{F_0/m}{\omega^2-\alpha^2} \cos(\alpha t)$$

and the general solution is

$$x = A\cos(\omega t - \delta) + \frac{F_0/m}{\omega^2 - \alpha^2} \cos(\alpha t).$$

Note that

$$\dot{x} = -A\omega \sin(\omega t - \delta) - \frac{\alpha F_0/m}{\omega^2 - \alpha^2} \sin(\alpha t).$$

The arbitrary constants A and δ are fixed by giving $x(0)$ and $\dot{x}(0)$ as usual. For example, suppose $x(0) = \dot{x}(0) = 0$, then

$$0 = A\cos(\delta) + \frac{F_0/m}{\omega^2 - \alpha^2}$$

$$0 = A\omega\sin(\delta).$$

Assuming $F_0 \neq 0$, we cannot have $A = 0, \Rightarrow \delta = 0$. So $A = -\frac{F_0/m}{\omega^2-\alpha^2}$,

$$x = \frac{F_0/m}{\omega^2 - \alpha^2}\left[\cos(\alpha t) - \cos(\omega t)\right].$$

Using the trigonometric identity

$$\cos A - \cos B = -2\sin\left(\frac{A-B}{2}\right)\sin\left(\frac{A+B}{2}\right)$$

we find

$$x = \frac{2F_0/m}{\alpha^2 - \omega^2} \sin\left[\left(\frac{\alpha - \omega}{2}\right) t\right] \sin\left[\left(\frac{\alpha + \omega}{2}\right) t\right]$$

Now remember that α is under our control, ω is not. Suppose we adjust α to be very close to ω, but not equal to it. Then we can think of this solution in the following way:

$$x = \left\{\frac{2F_0/m}{\alpha^2 - \omega^2} \sin\left[\left(\frac{\alpha - \omega}{2}\right) t\right]\right\} \times \sin\left[\left(\frac{\alpha + \omega}{2}\right) t\right]$$

The reason for splitting it like this is that $\frac{\alpha-\omega}{2}$ will be very SMALL, so LOW-FREQUENCY, while $\frac{\alpha+\omega}{2}$ is much larger, high frequency. So if we write

$$x = A(t) \sin\left[\left(\frac{\alpha + \omega}{2}\right) t\right]$$

then we have a sine function with an amplitude which is a (MUCH LOWER-FREQUENCY) sine function! We say that the system has a BEAT, and $\frac{\alpha-\omega}{2}$ is called the BEAT FREQUENCY.

Notice that the amplitude function

$$A(t) = \frac{2F_0/m}{\alpha^2 - \omega^2} \sin\left[\left(\frac{\alpha - \omega}{2}\right) t\right]$$

has a maximum value $\left|\frac{2F_0/m}{\alpha^2-\omega^2}\right|$ which becomes very large when α is very close to ω.

What happens if we let $\alpha \to \omega$? We have

$$A(t) = \frac{2F_0/m}{\alpha+\omega} \times \frac{\sin\left[\frac{\alpha-\omega}{2}t\right]}{\alpha-\omega}$$
$$\to \frac{F_0}{m\omega} \times \frac{t}{2} = \frac{F_0 t}{2m\omega}$$

by L'Hopital's rule. So in this limit

$$x = \frac{F_0 t}{2m\omega}\sin(\omega t)$$

and we see that the oscillations

go completely out of control.

This situation is called

RESONANCE. We see that IF A

SYSTEM IS FORCED IN A WAY

THAT AGREES WITH ITS OWN

NATURAL FREQUENCY, IT CAN OSCILLATE UNCONTROLLABLY.

This can be very dangerous! In reality resonance does not get completely out of control, because we cannot really ignore friction [or RESISTANCE in the case of an electrical circuit]. So we should really solve

$$m\ddot{x} + b\dot{x} + kx = F_0 \cos \alpha t$$

$$m\ddot{z} + b\dot{z} + kz = F_0 e^{i\alpha t}$$

Set $z = ce^{i\alpha t}$ and take the real part at the end.

$$\rightarrow c = \frac{F_0}{k - m\alpha^2 + ib\alpha} = \frac{F_0[k - m\alpha^2 - ib\alpha]}{(k - m\alpha^2)^2 + b^2\alpha^2}$$

(Using the identity $\frac{1}{A+iB} = \frac{A-iB}{(A+iB)(A-iB)} = \frac{A-iB}{A^2+B^2}$.)

So we need the real part of this complex number times $e^{i\alpha t} = \cos(\alpha t) + i\sin(\alpha t)$. Now in general we have

$$(C + iD)(E + iF) = CE - DF + i[CF + DE]$$

Similarly here

$$\frac{F_0[k - m\alpha^2 - ib\alpha]}{(k - m\alpha^2)^2 + b^2\alpha^2} \times [\cos(\alpha t) + i\sin(\alpha t)]$$

has real part

$$x(t) = \frac{F_0(k - m\alpha^2)\cos(\alpha t) + F_0 b\alpha\sin(\alpha t)}{(k - m\alpha^2)^2 + b^2\alpha^2}.$$

To this we should add the general solution of $m\ddot{x} + bx + kx = 0$. But we know already what that looks like – whether overdamped or underdamped, the solution rapidly (exponentially) TENDS TO ZERO. We call that part of the solution the TRANSIENT. So after the transient dies off, we are left with this expression.

We saw earlier that ANY expression of the form $C\cos(x) + D\sin(x)$ can be written as

$$C\cos(x) + D\sin(x) = \sqrt{C^2 + D^2}\cos(x - \gamma)$$

where $\tan(\gamma) = D/C$.

So here we have

$$x(t) = \frac{\frac{1}{m}F_0\cos(\alpha t - \gamma)}{\sqrt{(\omega^2 - \alpha^2)^2 + \frac{b^2}{m^2}\alpha^2}}$$

So the system eventually settles down into a steady oscillation, BUT AT FREQUENCY α, NOT ω! Also, the AMPLITUDE of this oscillation is a FUNCTION OF α,

$$A(\alpha) = \frac{F_0/m}{\sqrt{(\omega^2 - \alpha^2)^2 + \frac{b^2}{m^2}\alpha^2}}$$

The graph of this is called the AMPLITUDE RESPONSE CURVE. Depending on the values of the parameters, this curve might have a SHARP MAXIMUM, meaning that the system will suddenly respond strongly if α is chosen to be the value that gives that maximum. This is something to be avoided in some cases [things might break] but welcomed in others [you want your mobile phone to ignore all frequencies but one].

2.4. CONSERVATION.

Newton's 2nd law involves TIME derivatives, but sometimes it can be expressed in terms of SPATIAL derivatives, by means of the following trick:

$$\frac{d}{dx}\left(\frac{1}{2}\dot{x}^2\right) = \dot{x}\frac{d\dot{x}}{dx} = \frac{dx}{dt}\,\frac{d\dot{x}}{dx} = \ddot{x} \quad \text{(chain rule).}$$

For SHM we have

$$m\ddot{x} = -kx$$

so

$$m\frac{d}{dx}(\frac{1}{2}\dot{x}^2) = -kx.$$

But now we can integrate both sides:

$$\frac{1}{2}m\dot{x}^2 = -\frac{1}{2}kx^2 + E$$

where E is a constant of integration. So we have

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2.$$

As you know, $\frac{1}{2}m\dot{x}^2$ is called the KINETIC ENERGY of the oscillator, and $\frac{1}{2}kx^2$ is called the POTENTIAL ENERGY. We call E the TOTAL ENERGY. The fact that E is CONSTANT is called the conservation of energy.

2.5. EULER's EQUATION.

A BEAM is a long, thin object used in buildings etc, which bends when subjected to loads. Suppose you have a beam which is only supported at one end, which we take to be the origin (x, y) = (0, 0); this is called a CANTILEVER We assume that there is a LOAD on the beam — this might just be the weight of the beam itself, but it could be things we put on top of the beam, or it could be other forces pushing upward. Then of course the beam must bend. We want to know the shape of the beam; that is, we want to find y [the distance through which the beam bends down] as a function of x [the horizontal position].

We measure the load as FORCE PER UNIT LENGTH, $w(x)$. Note the units of w(x): newtons per metre. Our convention is that w(x) is positive in the UPWARD direction.

Now of course the amount of bending of the beam depends on several things. It will of course depend on the load, but it will also depend on what the beam is made of — you would expect aluminium to bend differently from steel, even if the load is the same. This stiffness is measured by a constant E called YOUNG'S MODULUS, which has units of pressure [force per unit area, newtons per square metre]. It could be a function of x.

The amount of bending also depends on the SHAPE of the cross-section of the beam, measured by a constant I is called the SECOND MOMENT OF AREA of the beam. This has units of $[\text{length}]^4$. It turns out that the deflection of the beam, y = y(x), is governed by the FOURTH-ORDER ODE, EULER'S EQUATION,

$$\frac{d^2}{dx^2}\left[EI\frac{d^2y}{dx^2}\right] = w(x)$$

[Please check that the left side has the right units, newtons per metre!] Let's suppose that E and I are both constant, and that w(x) is only due to the weight of the beam itself; we assume

$w(x) = \text{constant} = -\alpha$. (Remember that w is positive in the UPWARD direction.)

QUESTION: What is Δ, the maximum deflection, in terms of L, the horizontal length of the beam?

Answer:

$$\frac{d^4y}{dx^4} = \frac{w}{EI} = -\frac{\alpha}{EI} \;\rightarrow$$

$$\frac{d^3y}{dx^3} = -\frac{\alpha x}{EI} + A$$

by integration. Now for physics reasons $\frac{d^3y}{dx^3} = 0$

when evaluated at x = L [basically because there is no force there]. Thus

$$0 = \frac{d^3y}{dx^3}(L) = -\frac{\alpha L}{EI} + A.$$

Hence we have

$$\boxed{A = \tfrac{\alpha L}{EI}} \quad .$$

So

$$\begin{aligned} \frac{d^3y}{dx^3} &= -\frac{\alpha x}{EI} + \frac{\alpha L}{EI} \quad \rightarrow \\ \frac{d^2y}{dx^2} &= -\frac{\alpha x^2}{2EI} + \frac{\alpha L x}{EI} + B, \end{aligned}$$

where we have integrated again. But $\frac{d^2y}{dx^2} = 0$ when evaluated at x = L [basically because there is no "twisting" at the end]. So

$$0 = \frac{d^2y}{dx^2}(L) \;=\; -\frac{\alpha L^2}{2EI} + \frac{\alpha L^2}{EI} + B$$

$$\Rightarrow \boxed{B = \tfrac{\alpha L^2}{2EI} - \tfrac{\alpha L^2}{EI} = -\tfrac{\alpha L^2}{2EI}}$$

$$\Rightarrow \frac{d^2y}{dx^2} = -\frac{\alpha x^2}{2EI} + \frac{\alpha L x}{EI} - \frac{\alpha L^2}{2EI}$$

$$\Rightarrow \frac{dy}{dx} = -\frac{\alpha x^3}{6EI} + \frac{\alpha L x^2}{2EI} - \frac{\alpha L^2 x}{2EI} + C.$$

But if the beam is horizontal where it is supported,

$\frac{dy}{dx}(0) = 0$ so

$$0 = -0 + 0 - 0 + C$$

$$\rightarrow \boxed{C = 0}$$

$$\rightarrow y = -\frac{\alpha x^4}{24EI} + \frac{\alpha L x^3}{6EI} - \frac{\alpha L^2 x^2}{4EI} + D,$$

where we have integrated yet again! Finally the point of support is the origin, so $y(0) = 0$, so

$$\boxed{D = 0}$$

Thus

$$y = \frac{\alpha L^4}{2EI}\left[-\frac{1}{12}\left(\frac{x}{L}\right)^4 + \frac{1}{3}\left(\frac{x}{L}\right)^3 - \frac{1}{2}\left(\frac{x}{L}\right)^2\right]$$

So now finally we can work out the maximum deflection of the beam: you can easily show that this maximum occurs at the end [x = L] in agreement with common sense, so all we have to do is to substitute x = L into y and get

$$\Delta = y(L) = \frac{\alpha L^4}{2EI}\left[-\frac{1}{12} + \frac{1}{3} - \frac{1}{2}\right]$$

and so we obtain the famous CANTILEVER DEFLECTION FORMULA

$$\Delta = -\frac{\alpha L^4}{8EI}.$$

The negative answer of course reflects the fact that the cantilever always bends DOWNWARDS. Check that the answer MAKES SENSE: the deflection is larger for larger loads α, of course that makes sense. The deflection is smaller if EI is large, that is, if the beam is very stiff: that too makes sense. Finally, the deflection is greater if the beam is very long [large L], which also makes sense. [Are you in the habit of checking that your answers MAKE SENSE??]

There is still a surprise here though: notice that if you make your cantilever twice as long, the downwards deflection does not double $---$ it increases by a factor of SIXTEEN! So watch out if you want to build balconies etc. [The power of 4 here is a relic of the fact that we solved a FOURTH-order ODE.]

2.6. THE PLUG FLOW REACTOR.

In chemical engineering, a PLUG FLOW REACTOR is like a long tube into which you push some mixture of chemicals which move through the tube while they react with each other. These devices can be very complicated objects, and we are not going to pretend to describe how they really work. But we can set up a very simple MATHEMATICAL MODEL of such a gadget, with the understanding that a REALISTIC model would be very much more complicated!

For example, you push in hydrogen and oxygen at

one end, and get water coming out the other end. Since Oxygen is cheap and Hydrogen is expensive, we assume that we pump in a lot of Oxygen compared to the Hydrogen, so there is plenty of Oxygen all the way along the PFR. The question we want to answer is: what happens to the concentration of Hydrogen as a function of position in the PFR? Of course it will decrease, but how rapidly? Assume

[a] That everything flows through the PFR at constant speed u, and the cross-sectional area is A, a constant.

[b] That there is no mixing upstream or downstream $\rightarrow$ everything that happens in a small region of the PFR is controlled by chemical reactions IN that re-

gion and by flows in and out from the neighbouring regions.

[c] All temperatures are constant in time.

Now at a point x along the PFR, how many molecules of H_2 are passing by per second? Let $C_{H_2}(x)$ be the CONCENTRATION of hydrogen (molecules per cubic metre) at x. Then in a time δt, let δN_{H_2} be the number that pass by. Then δN_{H_2} is the number of H_2 molecules in the cylinder shown in the diagram.

Since $\begin{pmatrix} Number\ of \\ molecules \end{pmatrix} = \left(\frac{molecules}{volume}\right) \times (volume)$ we have

$$\delta N = C_{H_2}(x) \times Au\delta t$$

because $A =$ area of base and $u\delta t$ is the height. So

$$\frac{dN}{dt} = \lim_{\delta t \to 0} \frac{\delta N}{\delta t} = C_{H_2}(x)Au$$

Now of course we are LOSING H_2 molecules as the gases move down the PFR, because of the reaction. Consider a small piece of

the tube, of length δx.

Then this PLUG satisfies

(1) H_2 molecules are flowing IN

at x, at a rate $C_{H_2}(x)Au$.

(2) H_2 molecules are flowing OUT at $x + \delta x$ at a rate $C_{H_2}(x + \delta x)Au$.

(3) H_2 molecules are being DESTROYED inside the small piece of tube, at a rate

$$-2rA\delta x.$$

Here r is RATE PER UNIT VOLUME at which the reaction

$$2H_2 + O_2 \rightarrow 2H_2O$$

happens in each unit of volume inside the PFR [so units of r are $\frac{1}{\sec \times m^3}$]. Note the MINUS because we are losing H_2, and the 2 because each reaction costs 2 molecules of H_2.

Since the total matter content cannot increase or decrease,

$$C_{H_2}(x)Au - C_{H_2}(x+\delta x)Au - 2rA\delta x = 0$$

or, since $\delta C_{H_2} \equiv C_{H_2}(x+\delta x) - C_{H_2}(x)$,

$$- \delta C_{H_2} Au - 2rA\delta x = 0$$

$$\Rightarrow \quad u\frac{dC_{H_2}}{dx} = u \lim_{\delta x \to 0} \frac{\delta C_{H_2}}{\delta x} = -2r.$$

Now r depends on many things, for example the concentration of H_2, the temperature, etc etc etc. Let's construct a simple MODEL of this situation. It's pretty clear that the main thing that controls the rate of a reaction is the concentration, and it's also clear that the higher the concentration, the faster the reaction will go — so the rate should be an increasing function of the concentration, and of course it should be zero when the concentration is zero. So the SIMPLEST POSSIBLE model we can think of is given by the equation

$$r = kC_{H_2}(x),$$

where k [units 1/sec — check this!] is a positive constant [because we always assume here that the temperature is constant — in general k will depend on the temperature of course]. That is, we assume that the rate is [approximately!] proportional to the concentration. Then

$$u\frac{dC_{H_2}}{dx} = -2kC_{H_2}$$

$$\rightarrow \frac{dC_{H_2}}{C_{H_2}} = -\frac{2k}{u}$$

$$\rightarrow \ell n|C_{H_2}| = \ell n\ C_{H_2} = -\frac{2kx}{u} + \text{ constant}$$

$$\rightarrow C_{H_2} = C_{H_2}(0)e^{\frac{-2kx}{u}},$$

where x = 0 at the top [or "beginning"] of the PFR.

Check the units — remember that it does not make sense to take the exponential of something that has units, so kx/u should have no units [we say it is DIMENSIONLESS]. Check that our answer MAKES SENSE. For example, our result says that the concentration decreases more rapidly when u is small and k is large — is that sensible, based on your knowledge of chemistry [or common sense!]?

If T is the time from the reagents entering the PFR to their exit, $u = \frac{X}{T}$ where X is the full length of the PFR, and we have

$$C_{H_2}(\text{exit}) = C_{H_2}(\text{entrance})e^{-2kT}.$$

What this relation is really telling us is that Plug Flow Reactors are a good idea, because they are very efficient. As you know, the exponential function decreases very rapidly, so the Hydrogen is being turned into water very efficiently — almost none of it is left by the time you come to the end of the PFR. Notice too that the important parameter here is the TIME the mixture spends inside the PFR. Finally, remember where that 2 came from — it came from the chemical formula for the reaction. So you have to know your Chemistry to use one of these things.

So PFRs are good, unless they blow up of course..... remember that we deliberately left out temperature. We need a more complicated model....