MATHEMATICAL MODELLING OF ENVIRONMENTAL PROBLEMS[1]

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1. What is a mathematical model?

A model is an intellectual construct which represents reality and which can be manipulated to predict the consequences of future actions. Most of engineering work deals with the application of mathematical models to predict problems. Even the simple formula $f = ma$ (Newton) is a mathematical model of the relation between force, mass and acceleration. Using this formula engineers have been spectacularly successful in predicting the behaviour of real physical system Agborofo [1]

Much more complex mathematical models are regularly used as the size and power of our computers have grown, the size and complexity of the model we can use also have grown ([1]). However we shall concentrate largely on environmental problems. By an environmental problem, we shall mean problems concerning the environment.

(a) **Fluid mechanics**

Three main equations govern the flow of fluids namely

(i) Continuity equation,
(ii) Momentum equation and
(iii) Energy equation.

Continuity equation

The continuity equation results from the mass conservation law

$$\begin{array}{ccc|c|cc} & & \to & & \to & \\ \textit{fluid} & \textit{in} & \to & \textit{fluid inside} & \to & \textit{fluid out} \\ & & \to & & \to & \\ & & A & B. & & \end{array}$$

The law says that fluid that passes through A equals fluid inside + fluid outside. The law, translated into mathematical equation, becomes

$$\frac{\partial}{\partial t}(\rho A) + div\left(\rho A \underline{q}\right) = 0, \qquad (1)$$

where ρ = density of fluid
A = cross – sectional

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$\underline{q}$ = velocity vector

if the area through the fluid passes is constant, then equation
(1) reduces to

$$\frac{\partial \rho}{\partial t} + div\left(\rho \underline{q}\right) = 0. \qquad (2)$$

In some fluid, under certain conditions ρ may be taken as a constant.

In general

$$\rho = \rho(T) \qquad (3)$$

Momentum Equation

The momentum equation results from momentum conservation law

$$\rho \frac{D\underline{q}}{Dt} = -\nabla \rho + \rho \underline{f} + \mu \nabla^2 \underline{q} \ , \qquad (4)$$

where $\underline{q}$ is defined above, ρ is pressure $\underline{f}$ is body force per unit volume, μ is the dynamic viscosity. It is important to note here that we have assumed that the cross-sectional area is constant.

Energy equation

In the case of non-isothermal systems, the energy equation is written in terms of the temperature change. Put simply, the equation is

$$\rho c \frac{DT}{Dt} = k \nabla^2 T + \mu \phi, \qquad (6)$$

where

c is the specific heat, k is the heat dissipate, on due to viscosity.

In Cartesian coordinates

$$\phi = 2\left\{ \begin{array}{l} \left\{\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right)^2 \right. \\ \qquad + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 - \frac{2}{3}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)^2 \end{array} \right\} \qquad (7)$$

The above equations are only relevant for laminar flow.

Turbulent flows

Instability of a fluid flow may merely signal a change from one ordered state to another on the other hand, the flow may become random and this type of flow is called a turbulent flow.

Vorticity plays a key role in turbulence. In fact, its presence is a necessary feature. The vorticity equation is

$$\frac{\partial \underline{w}}{\partial t} = \underline{w}.\ \nabla \underline{q} + \upsilon \nabla^2 \underline{w} \tag{8}$$

The first term on the right is due to stretching and rotation of vortex lines, while the second represents viscons diffusion. The rate of change of vorticity squared is

$$\frac{D}{Dt} w_i w_i = \frac{D}{Dt} w^2$$

$$= w_i w_j \frac{\partial u_i}{\partial x_j} + w_i \nabla^2 w_i \tag{9}$$

Integrating

$$\frac{d}{dt}\int_v w^2\, d t = \int_s \left[w_i w_j \frac{\partial u_i}{\partial x_j} \right.$$

$$\left. - \upsilon \frac{\partial w_i}{\partial x_j} \frac{\partial w_i}{\partial x_j} \right] dt$$

$$+ \frac{1}{2} \upsilon \int_s n.\ \nabla w^2 \ d\sigma \tag{10}$$

Even if the viscosity is small, the total vorticity can grow to large values provided flows take place in three dimensions. The rate of growth of $\int_V w^2 \ dt$ decreases, if it is less than zero.

One – dimensional unsteady gas flows

$$\rho_t + u\rho_x + \rho u_x = 0 \tag{11}$$

$$u_t + u u_x + {}^1\!/_e \ p_x = 0 \tag{12}$$

$$s_t + u s_x = 0 \left(= \frac{Ds}{Dt} \right) \tag{13}$$

We now go into specifics.

Example 1

Atmospheric diffusion and pollution

In recent years, mathematical models associated with transport of pollutants in the atmosphere have appeared in literature (Ayeni and Olanrewaju [4]) these models include the transport of light pollutant particles from industrial sources elevated over the ground (Berlyand [3]) and the turbulent diffusion of heavy pollutants (dust) in the atmosphere (Alli et al. [2]). Let us consider a strip of ground

$$0 < x < L,\ -\infty < y < \infty \text{ and } z \geq 0$$

The pollutant model is

$$u\frac{\partial q}{\partial x} - u\frac{\partial q}{\partial z} = \frac{\partial}{\partial z}\left(K_Z \frac{\partial q}{\partial z}\right) \tag{14}$$

Where q = q (x, $_z$) denotes the pollutant concentration in the atmosphere, u is the speed of wind, w is the settling velocity of pollutant particles and K_z is the component of the turbulent exchange co efficient. The x – axis points in the direction of the wind and the z - axis points vertically upwards with $z \geq 0$ the boundary conditions are

$$q(0, z) = 0,\ q(x, t) \to 0 \text{ as } z \to \infty$$
$$Kz\frac{\partial q}{\partial z} + wq\,\Big|_{x=0} = \phi(x),\ 0 \leq x \leq l \tag{15}$$

Previous work

$$K_z = k_, Z^r ,\ u = \mu, \quad z^\mu,\ k_,\ r,\ \mu \in R \ (Ayeni \quad and \quad Olanrewaju)[4] \tag{16}$$

$$K_z = k_1\ q^m,\ k_1, u \ \ \varepsilon R. \tag{17}$$

Method of solution

$$x^1 = \frac{x}{L}\ ,\ z^1 = \frac{z}{L}\ ,\ q^1 = \frac{q}{q_L} \tag{18}$$

$$a\frac{\partial q}{\partial x} - \frac{\partial q}{\partial z} = G\frac{\partial}{\partial z}\left(q^m \frac{\partial q}{\partial z}\right) \tag{19}$$

$$G = \frac{k_1 \quad q_L^m}{wL} = pollu\tan t \tag{20}$$

$$and \qquad a = \frac{u}{w} \tag{21}$$

$$G\,q^m \frac{\partial q}{\partial z} + q \,\Big|_{\,z=0} = g\,(x),\ 0 < x < 1 \tag{22}$$

$$q\,(0\,,z) = 0,\ q\,(x_,\,z) \to 0 \qquad as \qquad Z \to \infty \qquad g\,(x) = \frac{f\,(x)}{w\,q_L} \tag{23}$$

$$G \gg 1\ and\ a = 0\,(1)$$

$$Outer\ solution\ :\ a\frac{\partial q}{\partial x} - \frac{\partial q}{z} = 0$$

$$q \to 0 \quad as \quad z \to 0.$$

$$q\ (x_,\ z) = h\,(x + az)\ ,\ h \equiv 0$$

$$u\sin g\ \ b\,c's$$

Inner solution

$$for\ g(x) \equiv Cons\tan t$$

$$a\frac{\partial q}{\partial x} = \frac{\partial}{\partial z}\left(q^m\frac{\partial q}{\partial z}\right) q(x_,\ y) = F\,(\eta),\quad \eta = \frac{z}{x}\,,\ m \neq\ 0$$

$$q\,(x_,\ 0) = g\,(x) \qquad m\ F\ F^i + (F^i)^2 + \frac{1}{2}m\eta\ F^1 = 0 \tag{24}$$

$$F\,(0) = c\,,\ F(\infty) = 0$$

$F\,(\infty)$ is obtained by matching outer and inner solutions

When c >0 , then $F^1(0) = -\gamma$, $\gamma>0$
Special case m = 0
F = 1 – e r f(η)
When m ≠ 0, the fundamental solution of (24) is

$$F = \left[\frac{mz^2}{2(4+2m))\, x} \right]^{1/m}$$

The General case : In general, a solution of (24) which satisfies the boundary condition is obtained numerically. Using shooting technique, we let

$$F_1 = \eta\,, \quad F_2 = F\,, \quad F_3 = F^1$$

We obtain

$$\begin{pmatrix} F_1^1 \\ \\ F_2^1 \\ \\ F_3^1 \end{pmatrix} = \begin{pmatrix} 1 \\ \\ F_3 \\ \\ -F_3^2 - \frac{1}{2} m\, F_1\, F_2 \,/\, m\, F_2 \end{pmatrix}$$

$$\begin{pmatrix} F_1(0) \\ \\ F_2(0) \\ \\ F_3(0) \end{pmatrix} = \begin{pmatrix} 0 \\ \\ 1 \\ \\ -\eta \end{pmatrix}$$

Theorem 1: There exists a unique solution of the equation, which satisfies the boundary conditions

Theorem 2: Let u (x, z, m) be a solution then $u(x, z, m)^m = u(x, z, -m)^{-m}$ as $m \to \infty$.

Example 2: **Filtration of Impurities**

Mathematical model for filtration is the process of separating solid particles suspended in a liquid solution by pouring the mixture through a filter. This process is accomplished by passing liquid through a porous medium. Filtration of solid/liquid separation has found practical uses in the chemical food, brewing and agro allied industries for many years and up to now (Agborofo [1]). Johansen and Anderson [9] formulated a mathematical model for large-scale filtration of aluminum Dewan and Chenevert [8] formulated a mathematical model for filtration of water – base mud during drilling. The relevant equations for filtration of impurities are:

$$\rho_t + v(t)\; c_x = 0$$
$$\rho_t = \beta\, c - a(t)\, \rho,$$

where

$$v(t) = \frac{v_0}{1+\gamma t}\ ,\ a\ (t) = a_0\ v(t) \quad = \frac{a_0\, v_0}{1+\gamma t}$$

$$v_0\ ,\ \gamma,\ a_0\ \text{are constants}$$

$$\rho(0) = 0,\ c\ (o,t) = c_0,\ \ c_0\ = \text{constant},$$

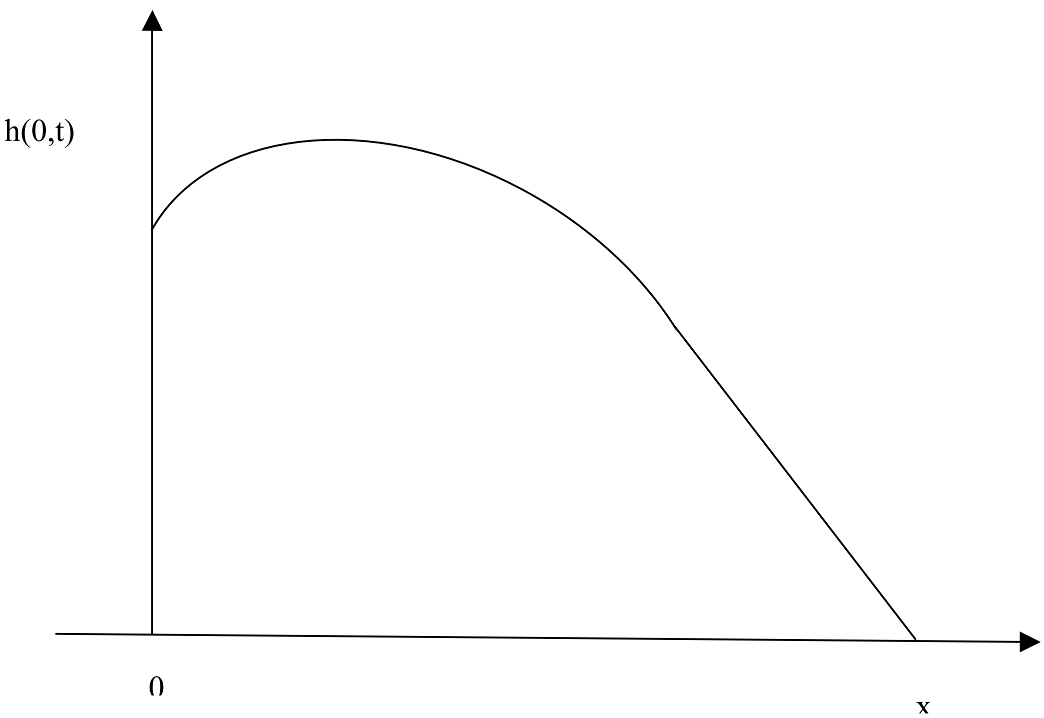
where x is the coordinate along the thickness of the filter.

v(t) is the filtration rate c(x, t) is the concentration of impurities suspended in the liquid, ρ(x, t) is the concentration of impurities in the sediment B, is the kinetic coefficient assumed to be a constant .
c_0 is the impurity concentration in the liquid at the filter inlet.

Example 3: Flow in a porous media

Baremblatt and Vazquez [6] developed a mathematical model for filtration through a horizontal porous medium under the condition of gentle shopping

$$\frac{\partial h}{\partial t} = k \quad \frac{\partial^2 h^2}{\partial x^2}$$



Darcy's law

$$m\frac{\partial h}{\partial t} + div\,(hu) = 0 \qquad (concervation\,law)$$

$$u = -\frac{k}{\mu}\frac{\partial p}{\gamma x} \qquad (Darcy's\,law)$$

$$p = \rho\, g\, h$$

$$\mu = -\frac{k\rho g\, hx}{\mu}$$

So

$$\frac{\partial h}{\partial t} = \left(\frac{kpg}{2\mu m}\right)^{1/2} \frac{\partial^2}{\partial x^2}\left(h^2\right)$$

h = height
ρ = fluid density
g = acceleration due to gravity
μ = fluid viscosity
k = permeability of the medium
m = porosity.

In general,

$$\frac{\partial h}{\partial t} = k\,\frac{\partial^2 h^n}{\partial x^2}$$

$$h(x,t) = Bt^{-\alpha} f(\eta)$$

$$n = \frac{x}{At^B}$$

$$x_f = At^B, \; x_0 = \lambda\; At^B$$

Example 4:

Tracking in – situ – combustion front using the thin flame technique
Def: In – situ combustion is an oil recovery in which oxygen enriched air is injected into a reservoir in order to displace the oil. Under suitable conditions the oxygen will burn with part of the oil raising the temperature of the reservoir and reducing the viscosity of the oil, hence allowing it to flow more easily [7]

$$\rho v \frac{du}{dx} = -\frac{\partial \rho}{\partial x} + \mu \frac{d^2 u}{dx^2}$$

$$Take \quad \frac{\partial \rho}{\partial x} = 0, \quad v = const.$$

$$\frac{du}{dx} - \frac{\mu}{\rho v} \frac{d^2 u}{dx^2} = 0$$

$$let \ u = e^{mx} \qquad m - \frac{\mu}{\rho v} m^2 = 0$$

$$\Rightarrow m = 0 \ \ or \ \ m = \frac{\rho v}{\mu}$$

$$u = a + b \ e^{\left(\frac{\rho v}{\mu} x\right)}.$$

$$Take \ u(0) = 0, \ u^1(0) = 1$$

$$We\,obtain \quad a + b = 0, \ b \frac{\rho v}{\mu} = 1, \ b = \frac{\mu}{\rho v}$$

$$u = \frac{\mu}{\rho v} \left(e^{\left(\frac{\rho v}{\mu} x\right)} - 1 \right)$$

The chemical reaction scheme consists of a single heavy oil burning reaction, which occurs for oil in the liquid phase only.

Heavy oil + Oxygen $\longrightarrow$ light oil + inert gas + water

Oxygen mass balance

$$\phi \frac{\partial}{\partial t}\left(s_g \rho_g y_5\right) + \frac{\partial}{\partial x}\left(v_g \rho_g y_s\right) = -s_5 r$$

Oil mass balance

$$\phi \frac{\partial}{\partial t}\left(s_g \rho_g y_2\right) + \frac{\partial}{\partial x}\left(v_0 \rho_0 x_2 + v_g \rho_g y_2\right) = -s_2 r$$

Energy balance

$$\frac{\partial}{\partial t}\left(\rho c_p T\right) + \left(v_g \rho_g c_{pg} + v_0 \rho_0 c_{p0}\right)\frac{\partial T}{\partial x}$$

$$= \lambda \frac{\partial^2 T}{\partial x^2} + r \Delta H$$

$$r = A e^{-E/RT} f\left(s, p, y, x\right),$$

where

A	=	frequency coefficient in reaction rate
C_p	=	heat capacity
E	=	activation energy
P	=	pressure
R	=	Gas constant
r	=	reaction rate
s	=	stoictriometric rate
S	=	Saturation
T	=	Temperature
t	=	time
V	=	Velocity
v	=	flame velocity
x	=	oil phase mole fraction
y	=	Gas phase mole faction
DH	=	Heat Reaction
λ	=	thermal conducvity
ρ	=	density
ϕ	=	porosity
0	=	oil phase
g	=	gas phase
2	=	heavy oil component
5	=	oxygen component

Example 5 The Pre – mixed flame (one dimension)
$A \rightarrow B$

The governing equations are:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0 \ \textit{contiunity equation}$$

$$\rho \frac{Du}{Dt} = - \nabla \rho + \mu \nabla^2 u \ \textit{momentum equation}$$

$$\rho \frac{DY}{Dt} = D \nabla^2 Y - A Y^a \ Exp\left(-E/_{RT} \right) \textit{Species equation}$$

$$\rho c \frac{DT}{Dt} = K \nabla^2 T + QAY^a \exp\left(-E/_{RT} \right) E \ \textit{energy equation}$$

where

p = density of reactants
u = velocity
ρ = pressure
Q = heat release per unit mass.

When reactant consumption is small and we let $\theta = \frac{E}{RT_0^2}(T - T_0)$ where T_0 is the initial temperature, we obtain the energy equation.

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x_2} + \delta \ \exp \ \theta / (1 + \in \theta) \quad (1)$$

This problem may be solved with initial and boundary conditions

$$\theta(x,0) = \theta(-1,t) = \theta(1,t) = 0. \quad (2)$$

A steady solution when $(\in \to 0)$ is

$$\theta = 2 \ln \left(\exp \frac{1}{2} \theta_n \sec h X \right), \quad (3)$$

where

$$c^2 = \frac{1}{2} \delta \exp(\theta_m)$$

equation (3) shows that a steady solution does not exists for all $\delta > 0$.

New Research Problems:

1. ***Example 1.***
   (a) Discuss conditions for existence and uniqueness of solution
   (b) Solve the problem when

$(i) \qquad K_Z = k_1 Z^r + k_2 q^m$

$(ii) \qquad K_Z = k_1 Z^r q^m$

Example 3

(a) Discuss the existence and uniqueness of solution when n = 3, 4, 5
(b) Solve the problem n = 4 numerically or using series solution technique

Example 4

(a) Solve the problem using the thin flame technique
(b) Solve the problem when $\varepsilon \to 0$ and

$$r = A\, y_2^a \; y_5^b \; \exp\left(-E \big/ RT\right)$$

when

(i) a = b = 1
(ii) a = 1, b = 2

Example 5

Solve the problem for a three – step reaction

$$A \to B \to C \to D$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} + \delta_1 \, e^{\theta} + \delta_2 \, e^{a\theta} + \delta_3 \, e^{b\theta}$$

$$\theta(x,0) = \theta(-1,t) = \theta\,(1,t) = 0$$

(i) Unsteady problem numerically
(ii) Steady problem numerically
for various values of *a* and *b*.

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