The method of weighted residuals provides approximate solutions to the differential equations of change governing transfer of heat, mass and momentum. The problems of linear and nonlinear heat transfer, entry-length problems, and mass transfer with concentration-dependent diffusivity, illustrate the application of the method. The results provide analytical – though approximate – solutions for these problems, some of which cannot be solved by classical techniques. The discussion includes the choice of trial functions, the need for successive approximations, and comparison of different methods. The author concludes this part of the article by introducing variational methods.

by B. A. FINLAYSON

Applications of the method of weighted residuals and variational methods. I

THE method of weighted residuals and variational methods are used to solve differential equations governing the transfer of heat, mass, and momentum. The general approach is to expand the unknown solution in a series whose functional dependence on position is chosen, but which includes several adjustable parameters. These are chosen by requiring the differential equation and boundary conditions to be satisfied in some specified approximate sense. The methods are applicable to problems for which classical techniques, such as separation of variables or Laplace transform, are inapplicable. The analytical form of the result is often more convenient than solutions generated by numerical integration, and successive approximations usually require less computation time to generate. While variational methods are restricted to a small class of problems – usually linear ones – the method of weighted residuals is applicable to non-linear problems – one of its most attractive features.

We will illustrate the methods by finding approximate solutions to the equations of change governing the transfer of heat, mass, and momentum. The steady-state Navier-Stokes equation with constant physical properties and a conservative body force absorbed into the pressure gradient is (1, 2)

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial x}+\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) \quad (1)$$

with similar equations for v and w.

The unsteady-state transport equation governing diffusion in a solid with concentration-dependent diffusivity is (2)

$$\frac{\partial c}{\partial t}=\frac{\partial}{\partial x}\left[D(c)\frac{\partial c}{\partial x}\right]+\frac{\partial}{\partial y}\left[D(c)\frac{\partial c}{\partial y}\right]+\frac{\partial}{\partial z}\left[D(c)\frac{\partial c}{\partial z}\right] \quad \ldots (2)$$

while steady-state diffusion in a dilute binary liquid with constant density and diffusivity is (2)

$$u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}+w\frac{\partial c}{\partial z}=D\left[\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}+\frac{\partial^2 c}{\partial z^2}\right] \quad \ldots (3)$$

Equations 2 and 3 also apply to heat conduction, which for steady-state is governed by

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)=0 \quad \ldots (4)$$

and when the thermal conductivity is constant

$$\nabla^2 T=\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}=0 \quad \ldots (5)$$

where ∇^2 is the Laplacian operator. Of course, the method of weighted residuals is applicable to other differential equations as well. In fact, these methods have found widespread use in calculations governing nuclear reactors, and variational principles are closely related to optimisation theory applied to lumped-parameter chemical reactors. These subjects are covered elsewhere (3–7).

The examples are organised into *boundary-value problems* governing the steady-state distribution of temperature, concentration or velocity (Equations 1, 3, 4, and 5), *initial-value problems* predicting the evolution of the system from prescribed initial conditions (Equation 2), and *eigenvalue problems* which predict the value of a physical parameter for which multiple solutions exist (arising in stability theory or in the technique of separation of variables applied to initial value problems). In each case we will simply state the differential equation as a special case of Equations 1 to 5 and emphasise the techniques of solution.

Method of weighted residuals (M.W.R.)

Consider the boundary-value problem posed by Equation 5 with prescribed boundary values:

$$\nabla^2 T=0$$
$$T=T_o \quad \text{on boundary}$$

To solve this problem using the method of weighted residuals, henceforth abbreviated M.W.R., we first choose a trial solution of the form

$$T=T_o+\sum_{i=1}^{N}c_i u_i \quad \ldots (6)$$

where the functions u_i are chosen to satisfy the boundary condition $u_i=0$ and any symmetry exhibited by the problem. The trial solution then satisfies the boundary conditions for all values of the unknown constants, c_i. We substitute this trial solution into the differential equation to define the residual

$$R(c_i,x,y,z)=\nabla^2 T_o+\sum_{i=1}^{N}c_i\nabla^2 u_i \quad \ldots (7)$$

which is a known function of position for any given set of constants c_i. If the trial solution T were the exact solution, this residual would be zero for all positions. In M.W.R. we choose the constants c_i in such a way that the residual is forced to be approximately zero in some weighted-average sense. The weighted integrals of the residual are set equal to zero

$$(w_j, R)=0 \qquad j=1,2,\ldots,N \quad \ldots (8)$$

where

$$(w_j, R)=\int_v w_j R\,dx\,dy\,dz \quad \ldots (9)$$

represents an inner product or spatial average over the domain V.

Combining Equations 7 and 8 gives

$$\sum_{i=1}^{N} c_i\,(w_j,\ \nabla^2 u_i) = -\,(w_j,\ \nabla^2 T_o)$$

or simply

$$\sum_{i=1}^{N} B_{ji}\,c_i = d_j \text{ where } B_{ji} = (w_j,\ \nabla^2 u_i),\ d_j = -\,(w_j,\ \nabla^2 T_o).$$

The solution is

$$c_i = \sum_{i=1}^{N} B_{ij}^{-1}\,d_j$$

where B^{-1} is the inverse of the matrix B. These constants, substituted into (6), give the approximate solution.

The weighting functions can be chosen in several ways and each way corresponds to a different criterion in M.W.R. We could divide up the domain V into N smaller domains V_j and choose

$$w_j = \begin{cases} 1 & x \text{ in } V_j \\ 0 & x \text{ not in } V_j \end{cases}$$

The differential equation would then be satisfied on the average in each of these subdomains, hence the name *subdomain method.* As we take more and more terms (increasing N) the residual would be zero on the average in smaller and smaller subdomains – which more closely approximates the conditions fulfilled by the exact solution – and we hope that the approximate solution becomes better, too. The subdomains can be chosen at will and can even overlap if we want to emphasise some part of the domain. If we have only one subdomain, the method is usually called the integral method, or the von Karman-Pohlhousen method arising in boundary layer theory, and the differential equation is satisfied on the average in the domain.

In the *collocation method* we set the residual equal to zero at the collocation points (x_j, y_j, z_j)

$$R(c_i, x,y,z)\ |_{x=x_j,\ y=y_j,\ z=z_j} = 0 \qquad j = 1,2, \ldots, N$$

and solve for the c_i. As N increases in successive approximations, the differential equation is satisfied at more and more points, thus approaching the condition fulfilled by the exact solution. The choice of the collocation points is made with some freedom, using a simple pattern or symmetry of the problem, for example. This method is encompassed by Equation 8 provided we take the weighting function to be the Dirac delta function,

$$w_j = \delta(x-x_j,\ y-y_j,\ z-z_j).$$

In the *method of moments* the weighting functions are members of a complete set of functions, which has the property, for example, that any continuous function can be expanded in terms of the complete set. Examples of complete sets are

$$1,\ x,\ x^2,\ x^3, \ldots$$

$$\sin \pi x,\ \sin 2\pi x, \ldots$$

or orthogonal polynomials in x, such as Legendre polynomials (8). A mathematical property of complete sets of functions is that any continuous function which is orthogonal to each member of the set is necessarily zero. A function f is orthogonal to w_k if

$$\int_v f w_k dx dy dz = (f,\ w_k) = 0 \qquad \ldots . \quad (10)$$

and if $\{w_k\}$ represents a complete set of functions and Equation 10 holds for all $k = 1, 2, \ldots$ then $f \equiv 0$. Since we make the residual orthogonal to each member of a complete set in the method of moments, we expect that as N approaches infinity the residual approaches zero. We might choose weighting functions to emphasise some region of space or the convergence of our expansion may be speeded up by judicious choice of weighting function (9).

A special case of the method of moments is the *Galerkin method* in which the weighting functions w_j are the same functions used to expand the solution, u_j in Equation 6. This method is especially important because of its equivalence to variational methods as described below.

The *least squares method* minimises the mean square residual

$$\frac{\partial}{\partial c_j}\int_v R^2\,dxdydz = 0 \text{ or } \int_v \frac{\partial R}{\partial c_j}\,R\,dxdydz = 0$$

in which case the weighting function is $\partial R/\partial c_j$.

The key steps are the choice of the trial solution (6) and the selection of the criterion in M.W.R. Variations are possible in which the trial solution is expanded in terms of known functions of all variables but one

$$T(x,y,z) = \sum_{i=1}^{N} A_i(z)\,T_i(x,y)$$

leaving functions $A_i(z)$ to be determined as solutions of ordinary differential equations generated using M.W.R. (see examples 2 and 3). Another possibility is to expand the solution as a series of functions which satisfy the differential equations but not the boundary condition and apply M.W.R. on the boundary. Many other variations are possible as discussed by CRANDALL (10), COLLATZ (11), AMES (12), and FINLAYSON and SCRIVEN (13), as well as the references listed by these authors. The examples below illustrate a few of the many possibilities.

Example 1. Steady-state heat conduction with temperature-dependent thermal conductivity

We consider first a very simple example to illustrate the method. Steady-state heat conduction across a slab is governed by Equation 4 for one dimension:

$$\frac{d}{dx}\left(k\,\frac{dT}{dx}\right) = 0$$

with boundary conditions $T(o) = T_o$, $T(d) = T_1$.

Consider a temperature dependent thermal conductivity

$$k = k_o + \alpha(T - T_o)$$

where k_o and α are constant. The dimensionless equation is

$$\frac{d}{dx}\left[(1 + a\theta)\,\frac{d\theta}{dx}\right] = 0$$

$$\theta(0) = 0 \quad \theta(1) = 1$$

where

$$a = \frac{\alpha(T_1 - T_o)}{k_o} \qquad \theta = \frac{T - T_o}{T_1 - T_o}$$

We first choose a trial solution in the form of a polynomial in x because of its simplicity.

$$\theta = \sum_{i=1}^{N} c_i x^i$$

satisfies $\theta(0) = 0$, and we require

$$\sum_{i=1}^{N} c_i = 1$$

in order to satisfy the boundary condition $\theta(1) = 1$.

The residual is

$$R = k\,\frac{d^2\theta}{dx^2} + a\left(\frac{d\theta}{dx}\right)^2$$

and the weighted residual becomes

$$\int_0^1 w_k\,R\,dx = 0 \qquad k = 1, 2, \ldots, N$$

Consider the first approximation, $N = 2$

$$\theta = x - c_2\,x(1 - x) \qquad \ldots . \quad (11)$$

$$\frac{d\theta}{dx} = 1 - c_2(1 - 2x) \qquad \frac{d^2\theta}{dx^2} = 2c_2$$

$$k = 1 + a[x - c_2\,x(1 - x)]$$

We first apply the collocation method. We must choose a collocation point where the residual will be zero. Take $x = \frac{1}{2}$ because it is the midpoint of the interval zero to one. For $x = \frac{1}{2}$

$$\frac{d\theta}{dx} = 1 \qquad \frac{d^2\theta}{dx^2} = 2c_2 \qquad k = 1 + \frac{a}{2} - \frac{ac_2}{4}$$

We set the residual equal to zero at $x = \frac{1}{2}$.

$$R\ |_{x=\frac{1}{2}} = 0$$

$$\left[1 + \frac{a}{2}\left(1 - \frac{c_2}{2}\right)\right](2c_2) + a = 0$$

which determines c_2. We choose to calculate numerical results only for the case $a = 1$. In that case

$$-\tfrac{1}{2}\,c_2^2 + 3c_2 + 1 = 0 \text{ or } c_2 = -0{\cdot}317$$

The other solution to the quadratic in c_2 is rejected as being physically unrealistic since it gives the heat flux in the wrong direction at $x = 1$. The approximate solution is then

$$\theta = x + 0{\cdot}317\,x(1 - x) \qquad \ldots . \quad (12)$$

We next consider the subdomain method. For the first approximation the domain is taken from zero to one. (For the M-th approximation the interval $0 \rightarrow 1$ could be split into segments of length $1/M$.) The weighted residual is thus

$$\int_0^1 R\,dx = 0$$

and the differential equation is satisfied on the average. For $a = 1$

$$\int_0^1 [1 + x - c_2 x(1-x)]\, 2c_2\, dx + \int_0^1 [1 - c_2(1-2x)]^2\, dx = 0$$

which, after some manipulation, gives $c_2 = -\frac{1}{3}$. The approximate solution is then

$$\theta = x + 0{\cdot}333\, x(1-x) \qquad \ldots . \quad (13)$$

Note that this solution differs only slightly from that derived by the collocation method. The method of moments can be applied using the weighting functions $(1,x,x^2, \ldots)$. For the first approximation the weighting function is 1 and the solution is the same as that derived by the subdomain method.

We apply the Galerkin method by using the weighting function $x(1-x)$, which is the first approximating function in (11). The weighted residual

$$\int_0^1 x(1-x)\, R(x,c_2)\, dx = 0$$

gives the approximate solution

$$\theta = x + 0{\cdot}326\, x(1-x) \qquad \ldots . \quad (14)$$

How good are the results? For the first approximation we should not expect very accurate results, but comparisons to the exact solution $\theta = -1 + \sqrt{1+3x}$ in Table I indicate the temperature is accurate to 8%. When no exact solution is available for comparison, there is no way to estimate the accuracy of the first approximation. Higher approximations must be computed and successive approximations must converge before we can say with any assurance that we have an accurate solution.

TABLE I—Temperature for nonlinear steady-state heat conduction

x	Collocation Equation 12	Gelerkin Equation 14	Method of moments		Exact solution
			Equation 13	Equation 16	
0·10	0·129	0·129	0·130	0·143	0·140
0·25	0·309	0·311	0·313	0·332	0·323
0·50	0·579	0·582	0·583	0·594	0·581
0·75	0·809	0·811	0·813	0·809	0·803
0·90	0·929	0·929	0·930	0·925	0·924

We compute the second approximation using the method of moments. The conditions on the constants are

$$\int_0^1 R\, dx = 0 \qquad \int_0^1 xR dx = 0 \qquad \ldots . \quad (15)$$

The algebra now becomes more lengthy and for more difficult problems the solution for $c_1, c_2, \ldots$ could be found using a computer. The approximate solution satisfying (15) is

$$\theta = \frac{3}{2}x - \frac{3}{4}x^2 + \frac{1}{4}x^3 \qquad \ldots . \quad (16)$$

This solution differs only slightly from the first approximation (see Table I) so that we stop with the second approximation. It is within 3% of the exact solution. Notice that use of the weighting function, x, for $N = 2$ emphasises large x, and the solution is improved near $x = 1$ but not for x near 1/2. Thus the choice of weighting function can be used to emphasise certain regions where we would like to have the residual approximated well. When the residual is small, the error in the solution may be small, too, although there is no theoretical reason why this should be true. This point illustrates the fact that applications of M.W.R. can be moulded to our particular problem or interest. In this example we used a simple polynomial for a trial solution, applied several different criteria of M.W.R. to calculate the approximate solution, and stopped with the second approximation because it differed very little from the first approximation.

Example 2. Steady-state heat conduction in a solid

Consider another example – heat conduction in a slab which extends from zero to infinity in the y-direction and from zero to one in the x-direction. The method of weighted residuals will be applied to reduce the partial differential equation (5) involving x and y derivatives to a set of ordinary differential equations involving only y derivatives.

The heat conduction equation for this problem is

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

and consider boundary conditions

$$T(x,0) = x(1-x) \qquad T(x,\infty) = 0$$
$$T(0,y) = T(1,y) = 0$$

We wish to estimate the average heat flux along the boundary $y = 0$:

$$N \equiv -\int_0^1 \left.\frac{\partial T}{\partial y}\right|_{y=0} dx$$

The first approximation is a trial solution of the form

$$T = x(1-x)\, c_1(y)$$

where $c_1(y)$ satisfies $c_1(0) = 1$, $c_1(\infty) = 0$. Note that this function satisfies the symmetry of the problem – it is symmetric about $x = \frac{1}{2}$. The y-dependence of the solution is left unspecified. The residual is

$$R(T) = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = -2c_1 + x(1-x)\frac{d^2 c_1}{dy^2}$$

Apply the Galerkin method first

$$\int_0^1 x(1-x)\, R(T)\, dx = 0$$

to obtain

$$-2c_1 \frac{1}{6} + \frac{d^2 c_1}{dy^2}\frac{1}{30} = 0$$

which has a solution

$$c_1(y) = e^{-\sqrt{10}\, y}$$

The first approximation is thus

$$T = x(1-x)\, e^{-\sqrt{10}\, y}$$

The collocation method requires a choice of collocation points. The point $x = \frac{1}{2}$ gives

$$R(T)\,|_{x=\frac{1}{2}} = 0 \text{ or } c_1 = e^{-\sqrt{8}\, y}$$

while the point $x = \frac{3}{4}$ (and hence $x = \frac{1}{4}$, too, by symmetry) gives

$$R(T)\,|_{x=\frac{3}{4}} \text{ or } c_1 = e^{-\sqrt{32/3}\, y}$$

The subdomain method uses

$$\int_0^1 R(T)\, dx = 0 \text{ to obtain } c_1 = e^{-\sqrt{12}\, y}$$

while the least squares method requires

$$\frac{\partial}{\partial \lambda}\int_0^\infty \int_0^1 R^2\, dxdy = 0 \text{ or } c_1 = e^{-\sqrt{10{\cdot}47}\, y}$$

provided the trial solution is taken as $T = x(1-x)\, e^{-\lambda y}$. Notice that all methods give similar results with slight differences in the numerical values.

Next apply the Galerkin method to obtain a second approximation

$$T = x(1-x)\, c_1(y) + x^2(1-x)^2\, c_2(y)$$

The weighted residuals are

$$\int_0^1 x(1-x)\, R(T)\, dx = 0 \qquad \int_0^1 x^2(1-x)^2\, R(T)\, dx = 0$$

which results in the solution (10)

$$c_1 = 0{\cdot}8035e^{-3{\cdot}1416y} + 0{\cdot}1965e^{-10{\cdot}1059y}$$
$$c_2 = 0{\cdot}9105(e^{-3{\cdot}1416y} - e^{-10{\cdot}1059y})$$

The average heat flux at $y = 0$ is calculated from these results. With $T = x(1-x)e^{-\lambda y}$ for the first approximation

$$-\left.\frac{\partial T}{\partial y}\right|_{y=0} = x(1-x)\lambda$$

and $N = \int_0^1 x(1-x)\lambda dx = \frac{\lambda}{6}$.

The results for the various methods are shown in Table II. The first and second approximation for the Galerkin method differ by only 2·4%, so we stop with the second approximation. It differs from the exact value.

$$N = \frac{16}{\pi^3}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3}$$

derived by separation of variables by only 1/2%.

TABLE II—Average heat flux in example 2

Method	N
Exact	0·543
Galerkin. $N = 1$	0·527
$N = 2$	0·540
Collocation, $x = \frac{1}{2}$	0·471
$x = \frac{1}{4}, \frac{3}{4}$	0·544
Subdomain	0·577
Least squares	0·540

This problem illustrates the general technique of using M.W.R. to reduce a partial differential equation to a set of ordinary differential equations which are easier to solve. The same approach can, in principle, be applied to any partial differential equation.

Example 3. Unsteady-state diffusion with concentration-dependent diffusivity

As an application to initial value problems, consider one-dimensional, unsteady-state diffusion which is governed by

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)$$

$$D = e^{kc}$$

$$c = 1 \text{ at } x = 0$$

$$\frac{\partial c}{\partial x} = 0 \text{ at } x = 1$$

$$c = 0 \text{ at } t = 0$$

with dimensionless variables $c = c'/c_o$, $D = D'/D_o$, $x = x'/d$, $t = D_o t'/d^2$. We expect a solution for small time which is close to the error function arising in penetration theory. However, the presence of the boundary at $x = 1$ and the non-linear diffusion coefficient make the error function solution inapplicable here. We will find an approximate solution, valid for small time, using the collocation method, and compare the results to numerical integrations performed by CRANK (14).

We first outline a method applicable when the diffusivity is constant (10, 15, 16). Expand the trial solution in a series

$$c(x,t) = 1 + \sum_{i=1}^{N} A_i(t)X_i(x) \qquad \ldots . \quad (17)$$

where the X_i are any functions satisfying the boundary conditions

$$X_i(o) = 0 \quad X'_i(1) = 0$$

such as

$$X_i(x) = x^{i+1} - (i+1)x$$

Then the trial solution satisfies the boundary conditions. The residual is defined, with D = constant = 1,

$$R = \frac{\partial c}{\partial t} - \frac{\partial^2 c}{\partial x^2}$$

We apply the collocation method for the first approximation.

$$c = 1 + A_1(t)(x^2 - 2x)$$

$$\frac{\partial c}{\partial t} = \frac{dA_1}{dt}(x^2 - 2x) \qquad \frac{\partial^2 c}{\partial x^2} = 2A_1$$

The residual is then

$$R = \frac{dA_1}{dt}(x^2 - 2x) - 2A_1$$

We choose the collocation point $x = 1$ because we are going to compare values of $c(1, t)$.

$$R\,|_{x=1} = 0$$

gives

$$\frac{dA_1}{dt} = -2A_1 \text{ or } A_1 = e^{-2t}$$

We cannot satisfy the initial conditions exactly so that we define an initial residual

$$R_o = 0 - [1 + A_1(o)(x^2 - 2x)]$$

and apply collocation to it at $x = 1$.

$$A_1(o) = 1$$

The first approximation is then

$$c_1 = 1 + e^{-2t}(x^2 - 2x)$$

The second approximation has also been calculated (15)

$$c_2(1,t) = 1 - 1{\cdot}261e^{-2{\cdot}456t} + 0{\cdot}261e^{-19{\cdot}54t}$$

and these are compared in Table III to the exact solution derived by separation of variables.

TABLE III—Concentration for unsteady-state diffusion

t	$c_1(1, t)$	$c_2(1, t)$	Exact $c(1, t)$
0·1	0·181	0·050	—
0·2	0·330	0·234	0·228
0·4	0·551	0·528	0·526
0·6	0·699	0·711	0·710
1·0	0·865	0·892	0·892
2·0	0·982	0·991	0·991
∞	1·000	1·000	1·000

Next we treat the non-linear problem. For small times, the concentration changes in a region near the boundary $x = 0$ in the manner suggested by Fig. 1. As time increases this region grows until the boundary at $x = 1$ is reached. Consider a penetration depth, $q(t)$ which characterises this region. For $x < q$ the concentration has a smooth profile going from $c = 1$ at $x = 0$ to $c = 0$ at $x = q$. For $x > q$ the concentration is very close to zero and we set it equal to zero in the approximation. We represent the concentration, $c(x,t)$, by a 'similar' profile

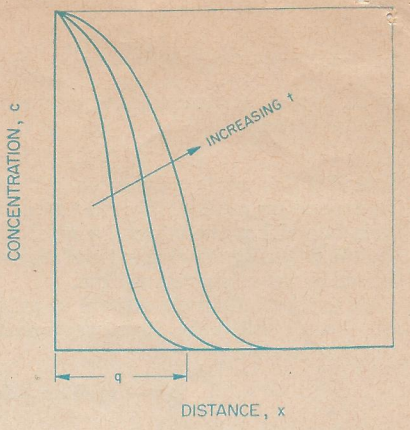


Fig. 1 Expected Concentration Profile for Diffusion with Concentration-dependent Diffusivity.

$$c = \phi(\eta) \quad \eta = x/q(t)$$

and use the collocation method to determine ϕ and q. The boundary conditions are

$$\phi(o) = 1 \qquad \phi(1) = 0 \qquad \phi'(1) = 0 \qquad \ldots . \quad (18)$$

$$q(o) = 0$$

and the solution is valid until $q(t) = 1$. First we calculate the residual

$$R = \frac{\partial c}{\partial t} - \frac{dD}{dc}\left(\frac{\partial c}{\partial x}\right)^2 - D\frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial c}{\partial t} = -\phi'\eta\frac{\dot{q}}{q} \qquad \frac{\partial c}{\partial x} = \phi'/q \qquad \frac{\partial^2 c}{\partial x^2} = \phi''/q^2$$

$$q^2R = -\phi'\eta q\dot{q} - e^{k\phi}[\phi'' + k(\phi')^2]$$

We apply the collocation method and choose $\eta = \frac{1}{2}$ as the collocation point. This point is the midpoint of the variable interval $0 < x < q(t)$ and is chosen mostly by convention. The collocation method gives

$$q^2R\,|_{\eta=\frac{1}{2}} = 0$$

$$2q\dot{q} = -4\{e^{k\phi}[\phi'' + k(\phi')^2]/\phi'\}_{\eta=\frac{1}{2}} \equiv A \qquad \ldots . \quad (19)$$

The differential equation for q can be solved to give

$$q(t) = \sqrt{A}\,t^{\frac{1}{2}}$$

where the value of A depends on the trial function chosen for ϕ.

It is convenient to choose ϕ as a power series in η

$$\phi = \sum_{i=0}^{N} a_i\eta^i \qquad \ldots . \quad (20)$$

with the restrictions $a_o = 1$

$$\sum_{i=0}^{N} a_i = 0 \qquad \sum_{i=1}^{N} ia_i = 0 \qquad \ldots . \quad (21)$$

to satisfy the boundary conditions (18). The first approximation ($N = 2$) yields

$$a_1 + a_2 = -1 \qquad a_1 + 2a_2 = 0$$

or $a_1 = -2$, $a_2 = 1$. The function ϕ is then

$$\phi = (1 - \eta)^2$$

We recognise immediately that this function will be a rough approximation at best because it does not allow an inflection point, as is required by the exact solution (14). We calculate the derivatives needed to evaluate A

$$\phi' = -2(1 - \eta) \qquad \phi'(\tfrac{1}{2}) = -1$$

$$\phi'' = 2$$

$$A = 4e^{k/4}[2 + k]$$

For the case $k = 2{\cdot}303$ we obtain $A = 30{\cdot}6$, $A^{\frac{1}{2}} = 5{\cdot}53$. The approximate solution is then

$$\phi = (1 - \eta)^2 \qquad \eta = \frac{x}{q(t)} \qquad q = 5{\cdot}53t^{\frac{1}{2}}$$

provided $5{\cdot}53t^{\frac{1}{2}} \leqslant 1$. A quantity of interest is the total amount of species absorbed in time t, which is just

$$M = \int_0^1 c(x,t)dx = 1{\cdot}84t^{\frac{1}{2}}$$

We next calculate a second approximation. For $N = 3$ we need another condition to completely specify the terms a_o through a_3 in

the power series (20). Collocation can again be applied, and we choose the point $\eta = 0$ as the added collocation point. This choice simplifies the computations and also tends to weight most heavily the boundary in which we are most interested.

$$q^2R\,|_{\eta=0} = 0 \text{ requires } \phi''(o) + k[\phi'(o)]^2 = 0$$

Since $\phi''(o) = 2a_2$, $\phi'(o) = a_1$ we have the condition

$$2a_2 + ka_1^2 = 0$$

in addition to (21). The solution is

$$a_1 = \frac{2 \pm \sqrt{4 + 6k}}{k}$$

which, for $k = 2{\cdot}303$, gives

$$a_1 = -0{\cdot}964 \qquad a_2 = -1{\cdot}071 \qquad a_3 = 1{\cdot}036$$

The constant A is now 35·1 and the approximate solution becomes

$$\phi = 1 - 0{\cdot}964\eta - 1{\cdot}071\eta^2 + 1{\cdot}036\eta^3$$

$$\eta = x/q(t) \qquad q = 5{\cdot}93t^{\frac{1}{2}} \leqslant 1$$

We expect this solution to be a better approximation, since it contains an inflection point and indeed the value

$$M = 2{\cdot}49t^{\frac{1}{2}}$$

is very close to the value obtained by CRANK (14) using an iterative numerical technique

$$M = 2{\cdot}45t^{\frac{1}{2}}$$

The first and second approximations yield concentration profiles which are compared to CRANK's solution in Fig. 2. It is apparent that global properties of the solution, such as M, are approximated more accurately than are detailed values of the concentration. This feature is often true of approximate solutions but is acceptable

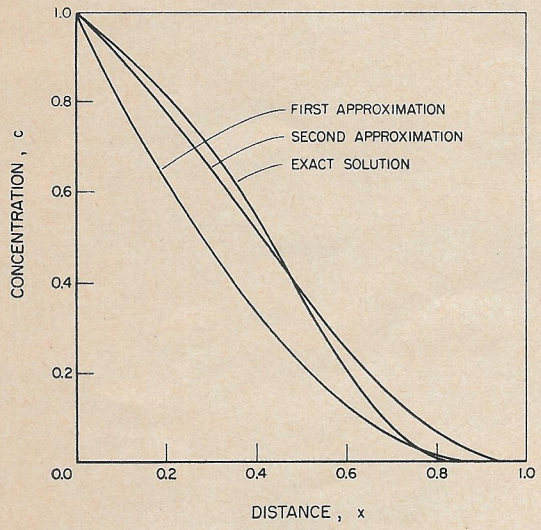


Fig. 2 Concentration Profile at t = 0·0285 for Sorption with $D = e^{2{\cdot}303c}$.

since the global properties are the ones usually desired anyway. The poor first approximation suggests that we must be cautious about accepting a one-term approximation in difficult non-linear problems.

This same problem has been treated by FUJITA using the method of moments (14). In the present notation, FUJITA assumes trial functions of the form

$$c(x,t) = B(t)(x_o - x)^2 + E(t)(x_o - x)^3 \qquad \ldots\ (22)$$

where $B(t)$, $E(t)$, $x_o(t)$ are functions to be determined subject to the boundary condition

$$1 = B(t)\,x_o^2 + E(t)\,x_o^3 \qquad \ldots\ (23)$$

The function x_o is again a penetration depth. FUJITA applies the method of moments and sets

$$\int_0^1 R\,dx = 0 \qquad \int_0^1 xR\,dx = 0$$

The approximation derived by him gives, for $D = e^{2{\cdot}303\,c}$,

$$M = 2{\cdot}46t^{\frac{1}{2}}$$

which is close to the exact solution. We can rearrange the trial function (22) to give

$$c(x,t) = B(t)\,x_o^2\left(1 - \frac{x}{x_o}\right)^2 + E(t)x_o^3\left(1 - \frac{x}{x_o}\right)^3$$

or, using (23)

$$c(x,t) = \left(1 - \frac{x}{x_o}\right)^2 - E(t)x_o^3\left(1 - \frac{x}{x_o}\right)^2\frac{x}{x_o}$$

which is similar to the trial function we used with the collocation method except that $E(t)\,x_o^3$ is a function of time rather than constant. This comparison illustrates the point that M.W.R. can be applied in many ways to suit the preference or convenience of the engineer or scientist.

The approximations discussed so far are limited to small time. After the penetration depth becomes equal to one, another form similar to Equation 17, must be assumed for the trial solution. This procedure is identical, except in complexity, with that used in Example 2. FUJITA has derived a solution in this manner (14).

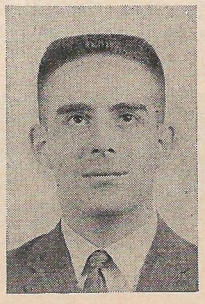
General comments

These applications illustrate the key points in M.W.R. The first step is to choose a trial function. The boundary conditions and symmetry of the problem are usually employed to restrict the list of possible functions. If several candidates remain, each set is probably equally suitable and the choice can be made on a basis of convenience in performing the remaining computations. The second step is to choose a criterion in M.W.R. The different criteria give slightly different results but the difference usually decreases with successive approximations. The collocation method is easiest to apply because the residual is easily evaluated at the collocation points whereas the other methods require the calculation of certain integrals. However, for the first approximation the results depend greatly on the choice of collocation points. The least squares method is usually unwieldy and for that reason has been applied here in only one example. The Galerkin method appears to give consistently better results, although the theoretical grounds for preferring it apply only to linear, self-adjoint problems which have a variational principle (see below). The last step in the analysis requires calculation of successive approximations. The first approximation is easy to calculate but seldom closer than 10%. Higher approximations must be calculated until two successive approximations differ by an amount less than the desired accuracy. Even in that case no theoretical grounds exist for saying the approximate solution is a good one, but we usually accept it as a good approximation in the absence of information on error bounds.

In the examples we solved non-linear boundary and initial-value problems by reducing the partial differential equation (involving derivatives in two or more variables) to sets of ordinary differential equations, which were solved exactly, or to sets of algebraic equations, which were even easier to solve. The same technique can be used to simplify any problem, provided an approximate solution is acceptable. For initial-value problems we used two approaches – penetration length concept and separation of variables – to achieve similar results. The method of weighted residuals thus provides a convenient tool for solving the equations of change governing the transfer of heat, mass, and momentum as well as equations arising in other fields. Whereas M.W.R. can be applied to all problems, more powerful results are sometimes provided by variational principles, which are not as generally applicable and which are discussed in Part II.

References for this paper appear at the end of Part II.

CONTRIBUTOR



Dr FINLAYSON graduated from Rice University with a B.A. and M.S. in Chemical Engineering. He received the Ph.D. degree in 1965 from the University of Minnesota, doing work in convective instability and variational and approximate methods of solving differential equations. The next two years were spent as Lt., U.S.N.R. in the Office of Naval Research doing contract supervision of infrared research. In 1967 he accepted his present position as Assistant Professor, Department of Chemical Engineering, University of Washington.

Variational methods, which are applicable to fewer problems, are illustrated for problems of rectilinear flow in ducts and eigen-value problems arising in the penetration theory of mass transfer. Both methods yield convenient analytic solutions, easily derived, and successive approximations can oftentimes be calculated on a computer in less time than is necessary to find a numerical solution.

by B. A. FINLAYSON

Applications of the method of weighted residuals and variational methods

IN Part I* we applied the Method of Weighted Residuals (M.W.R.) to heat and mass transfer problems which were complicated by a temperature or concentration dependence of the thermal conductivity or diffusivity. Next we consider the complication caused by convection and apply M.W.R. to a mass transfer problem with known fluid motion. Variational methods are also applied to the same problem as well as to the rectilinear flow of the fluid through a rectangular duct.

Example 4. Mass transfer to moving fluid

Consider the problems illustrated in Fig. 3. A liquid film is flowing down an inclined plane with a parabolic velocity profile as shown. At $z = 0$ the fluid surface is exposed to a stagnant gas containing a component which diffuses into the fluid. The governing equation is (3) with axial diffusion neglected.

$$(1 - x^2)\frac{\partial c}{\partial z} = \frac{\partial^2 c}{\partial x^2} \qquad \ldots . (24)$$

The dimensionless variables are: $x = x'/d$, $c = c'/c_o$, $z = z'D/w_o d^2$ $w' = w_o[1 - (x/d)^2]$. The initial and boundary conditions are

$$c = 1 \quad \text{at} \quad x = 0$$

$$\frac{\partial c}{\partial x} = 0 \quad \text{at} \quad x = 1$$

$$c = 0 \quad \text{at} \quad z = 0$$

We will apply the method of weighted residuals in two different ways. The first method uses the concept of a penetration depth while the second method employs separation of variables and then uses M.W.R. to solve the resulting eigenvalue problem.

Consider the concentration profile as z increases from zero. Near $z = 0$ the concentration differs from zero only near the interface. The distance from the interface to the point where the concentration is essentially zero defines a penetration depth, which increases with z (see the dotted line in Fig. 3). Approximate the concentration within the penetration depth by

$$c = \phi(\eta) \qquad \eta = x/\delta(z)$$

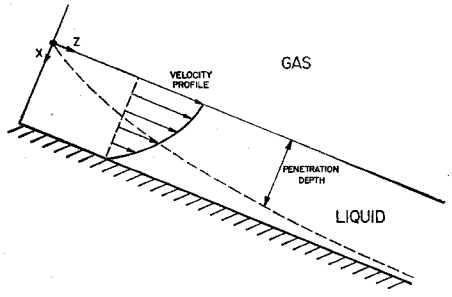


Fig. 3 Diffusion into a falling liquid film.

where

$$\phi(0) = 1 \qquad \phi(1) = 0 \qquad \phi'(1) = 0$$

and the approximation is valid until $\delta(z) = 1$. A profile

$$\phi = (1 - \eta)^2(1 + b\eta)$$

satisfies these conditions with b undetermined. The residual is

$$R = (1 - x^2)\frac{\partial c}{\partial z} - \frac{\partial^2 c}{\partial x^2}$$

with the derivatives given by

$$\frac{\partial c}{\partial z} = -\phi'\eta\frac{\dot{\delta}}{\delta} \qquad \frac{\partial^2 c}{\partial x^2} = \phi''/\delta^2$$

The residual is then

$$\delta^2 R = -(1 - \eta^2\delta^2)\eta\phi'\delta\dot{\delta} - \phi''$$

Apply the collocation method at $\eta = \frac{1}{2}, 1$.

$R(\phi)|_{\eta=1} = 0$ implies $\phi''(1) = 0$ or $b = -1$

$R(\phi)|_{\eta=\frac{1}{2}} = 0$ requires

$$\left(1 - \frac{\delta^2}{4}\right)\delta\frac{d\delta}{dz} = -2\phi''(\tfrac{1}{2})/\phi^1(\tfrac{1}{2}) = 8 \qquad \ldots . (25)$$

The solution to this differential equation gives

$$\delta^2/2 - \delta^4/16 = 8z$$

or

$$\delta^2 = 4 - 4\sqrt{1 - 8z}$$

This equation, together with $\phi = (1 - \eta)^3$ constitutes the approximate solution to this problem, valid until $\delta = 1$ or $z = 7/128$. The mixing-cup concentration is

$$\langle c \rangle = \frac{\int_0^1 (1 - x^2)\, c(x,z)dx}{\int_0^1 (1 - x^2)dx} = \frac{3\delta}{8}\left[1 - \frac{\delta^2}{15}\right]$$

A common assumption in this kind of problem is to assume a flat velocity profile, which leads to a similar approximate solution. Replacing $(1 - x^2)$ by 2/3 in Equation 24 (to maintain equivalent average velocities) we get

$$\frac{2}{3}\delta\frac{d\delta}{dz} = 8 \quad \text{or} \quad \delta = 4{\cdot}90z^{\frac{1}{2}}$$

in place of Equation 25. The mixing-cup concentration is now

$$\langle c \rangle = \frac{\int_0^1 \frac{2}{3}\, c(x,z)dx}{\int_0^1 \frac{2}{3}\, dx} = \delta/4$$

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Both solutions are listed in Table IV to illustrate the effect of the parabolic velocity profile.

TABLE IV—Mixing-cup concentration along flat plate

z	$\langle c \rangle$ Uniform velocity	$\langle c \rangle$ Parabolic velocity
0	0	0
0·01	0·122	0·150
0·02	0·173	0·212
0·03	0·212	0·259
0·04	0·245	0·299
0·05	—	0·335

The second approach, separation of variables, requires homogeneous boundary conditions at $x = 0, 1$. Consider the variable $y = c - 1$, which satisfies the same differential equation as c but homogeneous boundary conditions:

$$y = 0 \quad \text{at} \quad x = 0$$

$$\frac{\partial y}{\partial x} = 0 \quad \text{at} \quad x = 1$$

$$y = -1 \quad \text{at} \quad z = 0$$

Substitute

$$y(x,z) = X(x)\,Z(z)$$

into the Equation 24, and divide by $(1 - x^2)XZ$ to obtain

$$\frac{1}{Z}\frac{dZ}{dz} = \frac{1}{(1-x^2)X}\frac{d^2X}{dx^2} = -\lambda$$

Since a function of z alone is equal to a function of x alone, they both must be constant. Then

$$Z = Z(o)e^{-\lambda z}$$

while X satisfies

$$\ddot{X} + \lambda(1 - x^2)X = 0$$

$$X(o) = 0 \qquad \dot{X}(1) = 0 \qquad \ldots\ (26)$$

This is an eigenvalue problem, which has solutions only for certain λ, and is complicated by the factor $(1 - x^2)$. The exact solution was derived by PIGFORD (17), but we will obtain an approximate solution to illustrate the application of M.W.R. to eigenvalue problems.

A trial solution is chosen to satisfy the boundary conditions. The set of functions

$$\{\sin(n\pi x/2)\} \quad n = 1, 3, 5, \ldots$$

fulfils this criterion. In fact these are the exact eigenfunctions if the complicating factor $(1 - x^2)$ is replaced by 1. Although not used here, the trial functions $\{\eta^i - i\eta\}$ would be equally suitable. For the first approximation

$$y = c_1 \sin(\pi x/2)$$

The residual is then

$$R(y) = -\left(\frac{\pi}{2}\right)^2 c_1 \sin(\pi x/2) + \lambda(1 - x^2)\,c_1 \sin(\pi x/2)$$

Apply the Galerkin method to obtain

$$\int_0^1 \sin(\pi x/2)\,R(y) = 0$$

which gives a value of λ

$$\lambda = \frac{\left(\frac{\pi}{2}\right)^2 \int_0^1 \sin^2(\pi x/2)dx}{\int_0^1 (1 - x^2)\sin^2(\pi x/2)dx} \qquad \ldots\ (27)$$

If the integrals are evaluated we find $\lambda = 5{\cdot}317$. The other criteria could be used as well, although we will see below that the Galerkin method has certain advantages for this problem. The collocation method provides

$$R(y)\,|_{x=x_1} = 0 \quad \text{or} \quad \lambda = \frac{(\pi/2)^2}{(1 - x_1^2)}$$

We can see that this method gives an approximation anywhere from $(\pi/2)^2$ to ∞ depending on the collocation point. The value $x_1 = 1/2$ gives $\lambda = 3{\cdot}29$. The subdomain method requires

$$\int_0^1 R(y)dx = 0$$

$$\lambda = \frac{\left(\frac{\pi}{2}\right)^2 \int_0^1 \sin(\pi x/2)dx}{\int_0^1 (1 - x^2)\sin(\pi x/2)dx} = 4{\cdot}59$$

To assess the accuracy we find a second approximation using the Galerkin method. Take

$$y = c_1 \sin(\pi x/2) + c_2 \sin(3\pi x/2)$$

The Galerkin method requires

$$\int_0^1 \sin(\pi x/2)\,R(y)dx = 0 \qquad \int_0^1 \sin(3\pi x/2)\,R(y)dx = 0$$

and these equations will be of the form

$$\sum_{j=1}^{2} (B_{ij} - \lambda C_{ij})\,c_j = 0 \qquad i = 1, 2 \quad \ldots\ (28)$$

This set of algebraic equations has a nontrivial solution if and only if the determinant of coefficients vanishes, i.e.

$$|B_{ij} - \lambda C_{ij}| = 0$$

which has, in this case, two roots for λ. These values are approximations to the first and second eigenvalues: $\lambda_1 = 5{\cdot}126$, $\lambda_2 = 45{\cdot}54$. Since the approximation for λ changed only $\frac{1}{2}\%$ we conclude without theoretical justification that it is a good approximation. The exact values are $\lambda_1 = 5{\cdot}121$, $\lambda_2 = 39{\cdot}31$. To obtain a better result for λ_2 we would have to calculate a third approximation, of course. Higher approximations are easily calculated by a computer. The eigenfunctions corresponding to each eigenvalue are found by solving Equation 28 for c_1 and c_2 for each λ, but we will not make those computations. The remaining calculations follow the usual separation of variables approach with the approximate eigenfunctions replacing the exact eigenfunctions. As is usually the case in a solution derived by separation of variables, the series converges slowly for small z. However, we also derived a solution which is especially suited for small z. Combination of both solutions gives meaningful results for all z.

Variational principles

Variational principles exist for special cases of the equations of change and provide a basis for the variational method to derive approximate solutions. Again, a trial solution is assumed whose functional dependence on position is chosen but which includes several undetermined parameters. The prescription for finding these parameters employs the variational principle, but applications are otherwise similar to applications of M.W.R. In fact, variational methods give the same approximate solution as applications of the Galerkin method. Even so, the variational principles give powerful results which are not suggested by M.W.R., in the few problems for which variational principles exist. The variational methods are illustrated by application to two problems. More complete engineering treatments of the calculus of variations are contained in books by HILDEBRAND (18), and CRANDALL (10) and the mathematical aspects are discussed by COURANT and HILBERT (19), KANTOROVICH and KRYLOV (20), and MIKHLIN (21).

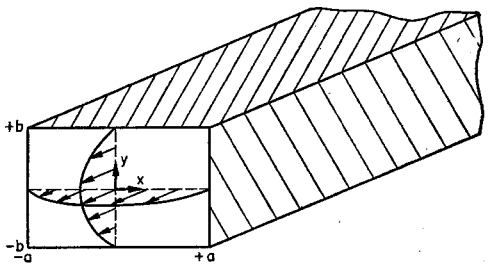

Fig. 4 Laminar flow in rectangular duct.

Example 5. Laminar flow in rectangular duct

We consider rectilinear flow in a duct with rectangu ar cross section, as shown in Fig. 4. Equation 1 reduces to

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = -\lambda \qquad \ldots\ (29)$$

with boundary conditions $w = 0$ at $x = \pm a$, $y = \pm b$, where $\lambda = (p_o - p_L)/\mu L$ is the applied pressure gradient divided by viscosity.

In the variational method we expand the unknown solution in a series

$$w(x,y) = \sum_{i=1}^{N} c_i w_i(x,y) \qquad \ldots\ (30)$$

where the functions w_i satisfy the boundary conditions and are twice differentiable and the constants c_i are arbitrary. This expansion is substituted into a variational integral

$$\phi(w) = \int_A \left\{ w\lambda - \frac{1}{2}\left[\left(\frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial y}\right)^2\right]\right\} dxdy \quad \ldots . (31)$$

to obtain

$$\phi(w) = \sum_{i=1}^{N} c_i \lambda \int_A w_i dxdy - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j \int_A \left[\frac{\partial w_i}{\partial x}\frac{\partial w_j}{\partial x} + \frac{\partial w_i}{\partial y}\frac{\partial w_j}{\partial y}\right] dxdy$$

It can be shown (22, 23) that the exact solution to Equation 29 maximises the integral (31) and this provides the basis for the variational method. We maximise the integral with respect to variations in the c_i.

$$\frac{\partial \phi}{\partial c_k} = 0 = \lambda \int_A w_k dxdy - \sum_{i=1}^{N} c_i \int_A \left[\frac{\partial w_i}{\partial x}\frac{\partial w_k}{\partial x} + \frac{\partial w_i}{\partial y}\frac{\partial w_k}{\partial y}\right] dxdy \quad \ldots . (32)$$

$$k = 1, 2, \ldots, N$$

This set of equations is of the form

$$\sum_{i=1}^{N} A_{ki} c_i = b_k \quad \ldots . (33)$$

which can be solved for the constants c_i. The expansion (30) then is an approximate solution to the problem. Since the variational integral is a maximum for the exact solution, the approximate solution must give a lower value of ϕ than does the exact solution. The approximation thus provides a lower bound on the exact solution. Furthermore because of Equation 32 the integral is stationary with respect to changes in c_i – i.e., insensitive to changes in c_i – so that we expect a good answer. It can be shown that the variational integral is $\lambda/2$ times the flow rate, Q, for the exact solution (22, 23). Hence the approximate solution provides a lower bound on the exact flow rate.

$$\phi(w) \leqq \frac{\lambda}{2} Q$$

This feature of the variational principle allows us to calculate a lower bound on the flow rate even if we cannot integrate the differential equation for some unusual shape of duct.

As a simple example of the variational method, we calculate a lower bound for the flow rate through the rectangular duct shown in Fig. 4. The velocity must vanish at $x = \pm a$, $y = \pm b$ and is symmetric about $x = 0$ and $y = 0$. Admissible functions which satisfy these conditions are

$$w_i = [1 - (x/a)^2]^i \, [1 - (y/b)^2]^i$$

$$w_i = \cos\frac{(2i-1)\pi x}{2a} \cos\frac{(2i-1)\pi y}{2b}$$

Either set of functions could be used, but we will use the polynomials in the trial solution (30). Equations 32 and 33 must be solved for the c_i. In this case, for example,

$$A_{11} = \int_{-b}^{+b}\int_{-a}^{+a}\left[\left(\frac{\partial w_1}{\partial x}\right)^2 + \left(\frac{\partial w_1}{\partial y}\right)^2\right] dxdy$$

and

$$\frac{\partial w_1}{\partial x} = -\frac{2}{a}\frac{x}{a}\left(1 - \frac{y^2}{b^2}\right), \quad \frac{\partial w_1}{\partial y} = -\frac{2}{b}\frac{y}{b}\left(1 - \frac{x^2}{a^2}\right)$$

which gives $A_{11} = 128(a^2 + b^2)/45ab$. The other integrals are similar, and for $N = 2$:

$$A_{ij} = \begin{bmatrix} 128/45 & (32)^2/(15 \times 35) \\ (32)^2/(15 \times 35) & (256/105)^2/3 \end{bmatrix} \left(\frac{a^2 + b^2}{ab}\right) \quad \ldots . (34)$$

with $b_1 = 16ab\lambda/9$ and $b_2 = 256ab\lambda/225$.

The first approximation is then $A_{11}c_1 = b_1$ or

$$\frac{128}{45}\frac{a^2 + b^2}{ab} c_1 = \lambda \frac{16ab}{9}$$

$$c_1 = \frac{5}{8}\lambda \frac{a^2b^2}{a^2 + b^2}$$

The approximate velocity profile is

$$w(x,y) = \frac{5}{8}\lambda \frac{a^2b^2}{a^2 + b^2}\left[1 - \left(\frac{x}{a}\right)^2\right]\left[1 - \left(\frac{y}{b}\right)^2\right]$$

and the lower bound on flow rate is

$$Q(w) = \int_{-b}^{+b}\int_{-a}^{+a} w(x,y)\, dxdy = \frac{10}{9}\lambda \frac{a^3b^3}{a^2 + b^2}$$

The flow rate and velocity at the centre are compared to the exact solution in Table V for the special case $a = b$. The flow rate is 1% low while the centreline velocity is 6% high. This illustrates a general feature of variational methods: an integral, such as Q, is approximated closely by the variational method but the solution itself may not be approximated as well.

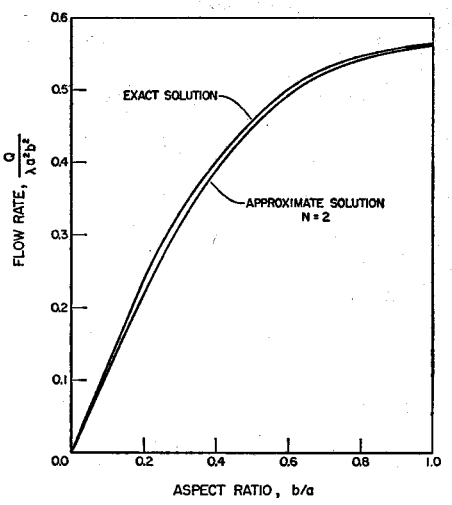

Fig. 5 Flow rate in rectangular duct.

The second approximation can be calculated using Equations 33 and 34. The results are

$$c_1 = 0{\cdot}711548\ \lambda a^2b^2/(a^2 + b^2)$$

$$c_2 = -0{\cdot}126208\ \lambda a^2b^2/(a^2 + b^2)$$

which gives

$$Q = 1{\cdot}1214\ \lambda a^3b^3/(a^2 + b^2).$$

This approximation is so close to the first one that we stop with the second approximation. In Fig. 5 the flow rate is compared to the exact solution, which is derived by separation of variables as an infinite series of cosines and hyperbolic cosines (24, 25).

TABLE V—Flow rate and velocity for square duct

Method	$Q/\lambda a^4$	$u(o, o)/\lambda a^2$
Exact solution	0·5622	0·2945
Variational solution		
$N = 1$	0·5556	0·3125
$N = 2$	0·5607	0·2927

There is a close relationship between the variational method and the Galerkin method. The Galerkin method applied to the same flow problem would yield for the weighted residual

$$\int_A w_k \left[\lambda + \sum_{i=1}^{N} c_i \nabla^2 w_i\right] dxdy = 0$$

This equation can be rearranged using the divergence theorem to give

$$\lambda \int_A w_k dxdy - \sum_{i=1}^{N} c_i \int_A \left[\frac{\partial w_i}{\partial x}\frac{\partial w_j}{\partial x} + \frac{\partial w_i}{\partial y}\frac{\partial w_j}{\partial y}\right] dxdy$$

which are the same as Equations 32 to find c_i in the variational method. The solutions are thus identical. The advantage of the variational formulation is that we know the approximation provides a lower bound on flow rate, which is a quantity of interest. The Galerkin method, on the other hand, provides the same approximation to the flow rate, but we do not know *a priori* whether it is above or below the true value.

Upper bounds on the flow rate can also be derived (22, 23) using variational principles, although we will not do so here. Calculation of both upper and lower bounds enables us to estimate the flow rate, with known error limits, in situations for which we cannot find an exact solution. Thus the variational method provides powerful results. Unfortunately it is not applicable to very many equations, particularly non-linear ones, that we want to solve. The basis of the method relies on finding a variational integral (31) which corresponds to the differential equation. Without going into the details of how this correspondence is established or when it can be done, suffice it to say that a variational integral cannot be found corresponding to every problem. For example, the steady-state Navier-Stokes equation (1) has no variational principle unless the inertial terms on the left-hand side are identically zero, as in example 5. The unsteady-state transport equation (2) does not have a variational principle and the linear transport equation (3) has a variational

Symbols used

a = one-half the width of rectangular duct; dimensionless value of dk/dT;
b = one-half the height of rectangular duct;
c = concentration;
d = thickness of solid slab or fluid layer;
D = diffusivity;
k = thermal conductivity; parameter in $D = e^{kc}$;
M = total amount of species absorbed;
$M.W.R.$ = Method of Weighted Residuals;
N = average heat flux at boundary;
p = pressure;
Q = flow rate;
R = residual;
t = time;
T = temperature;
u, v, w = velocity components;
V = spatial domain;
x, y, z = position components.

Greek letters

α = coefficient of change of thermal conductivity with temperature;
δ = penetration depth;
λ = related to pressure drop $= (p_o - p_L)/\mu L$;
ρ = density;
ν = kinematic viscosity μ/ρ;
μ = viscosity;
θ = dimensionless temperature;
∇^2 = Laplacian differential operator $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$.

principle only for an inviscid fluid. The heat conduction equation (4) has a variational principle in the special case of constant thermal conductivity (5). For those problems without variational integrals we can still apply M.W.R. since it does not rely on a variational integral. See references (26–27) for examples of variational principles for steady-state flow problems.

By using a broadened definition of variational principles, it is possible to devise variational methods for some of the equations (1–5) but the methods do not provide upper and lower bounds and are no more useful than the Galerkin method or another criterion in M.W.R. In fact, in some cases the methods are identical to the Galerkin method. See references (28–30) for examples as well as (31) for further discussion of the methods. Since we can apply M.W.R. to any problem without hunting for a variational integral, we usually employ variational methods only when they provide upper and lower bounds, or other useful information, as in examples 5 and 6.

Example 6. Eigenvalue problems

Consider the mass transfer problem treated above by M.W.R. (26).

$$y'' + \lambda(1 - x^2)y = 0$$
$$y(o) = 0 \qquad y'(1) = 0$$

The variational functional is in this case (10)

$$\lambda = \frac{-(y,y'')}{((1 - x^2)y,y)} = \frac{(y,y')}{((1 - x^2)y,y)}$$

We choose for trial functions

$$y(x) = \sum_{i=1}^{N} c_i \sin [(2i - 1)\pi x/2]$$

which satisfy the boundary conditions. The variational method, sometimes called the Rayleigh-Ritz method, requires that we minimise this ratio among all c_i. For $N = 1$

$$y = c_1 \sin \frac{\pi x}{2}$$

and

$$y'' = -\left(\frac{\pi}{2}\right)^2 c_1 \sin \frac{\pi x}{2}$$

Then

$$\lambda = \frac{\left(\frac{\pi}{2}\right)^2 \int_0^1 \sin^2 \frac{\pi x}{2}\, dx}{\int_0^1 (1 - x^2) \sin^2 \frac{\pi x}{2}\, dx}$$

and the approximation must be an upper bound since the exact solution minimises the ratio. Notice that this equation is identical to that derived using the Galerkin method (27). By using the variational principle we obtain the additional information that the answer is an upper bound on the exact value and the eigenvalue is stationary to changes in the constants $c_k(\partial\lambda/\partial c_k = 0)$. However, the Rayleigh-Ritz and Galerkin computations are identical. The other criteria in M.W.R., such as collocation or moments, do not make the eigenvalue stationary and for this reason are usually not applied to eigenvalue problems. For $N = 2$ the upper bound must decrease or remain the same as the value for $N = 1$, as is the case in Table VI for the variational or Galerkin methods. The other criteria in M.W.R. yield values which can be above or below the true value, as shown.

TABLE VI—Approximate eigenvalues

Method		λ_1	λ_2
Galerkin or Variational	$N = 1$	5·317	
	$N = 2$	5·126	45·54
Exact		5·121	39·31
Collocation	$N = 1$	3·29	
Subdomain	$N = 1$	4·59	

In summary, special cases of the transport equations have variational principles. In the few cases where variational methods are feasible they yield powerful results, such as error bounds, and the variational methods should be employed. Even so, the Galerkin method gives the same approximate solution. In more general cases the Galerkin method or another criterion in M.W.R. must be used because the variational methods are not applicable.

Conclusion

The method of weighted residuals can be used to solve the non-linear, unsteady-state problems arising from the transport equations. The method reduces the differential equation to a set of algebraic or ordinary differential equations which are solved to provide the approximate solution in analytic form. If we need only a rough answer a one-term approximation is usually adequate. Otherwise successive approximations are calculated to give confidence in the results. The variational method is only applicable to a few situations, but it sometimes yields upper and lower bounds on macroscopic quantities of interest. In those cases it is more powerful than the Galerkin method, which yields identical approximate solutions. The method of weighted residuals provides an attractive method of approximating solutions to the non-linear equations confronting the chemical engineer.

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