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SECOND WORKSHOP ON MATHEMATICS IN INDUSTRY

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"DISTRIBUTED PARAMETER OPTIMAL CONTROL WITH PARTICULAR REFERENCE TO THE GLASS INDUSTRY."

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1. INTRODUCTION

1.1 The forehearth problem

In the manufacture of many types of glassware one of the most critical phases is the heat conditioning of the glass after it has been melted and prior to its forming. For many products such as containers, tubing, lenses, light bulbs and tableware this conditioning starts in a refining zone and is completed in a forehearth. If such heat conditioning is not performed correctly then the glass product may be defective in many ways. For glass containers Green[1] lists possible defects caused by poorly conditioned glass as

"1. Hot glass can cause bent and choked necks, light shoulders, mould sticking and heavy bottoms.

2. Cold glass contributes to checks, breakage, thin bottoms and streaks.

3. Uneven temperature distribution causes light sides, heel taps and blisters."

The avoidance of such defects together with mounting fuel costs and the desire for increased throughput indicate that the correct design and operation of the refiner and forehearth is of extreme importance.

The number of forehearths feeding from a single refiner may range from two to eight, a typical arrangement with five such forehearths being shown in Fig. 1. A forehearth which is heat conditioning glass flowing to a gob feeder is illustrated in Fig. 2. This "short forehearth" is made up of two sections each of which is fired by a number of burners. The first section is known as the cooling zone and is additionally equipped with a wind cooling system. The burners of the second section, known as the heating or conditioning zone, are operated in such a manner as to equalise the temperature of the glass as it reaches the spout. Temperatures of the surface glass are measured at two points along the length of the forehearth with control of the outlet temperature being

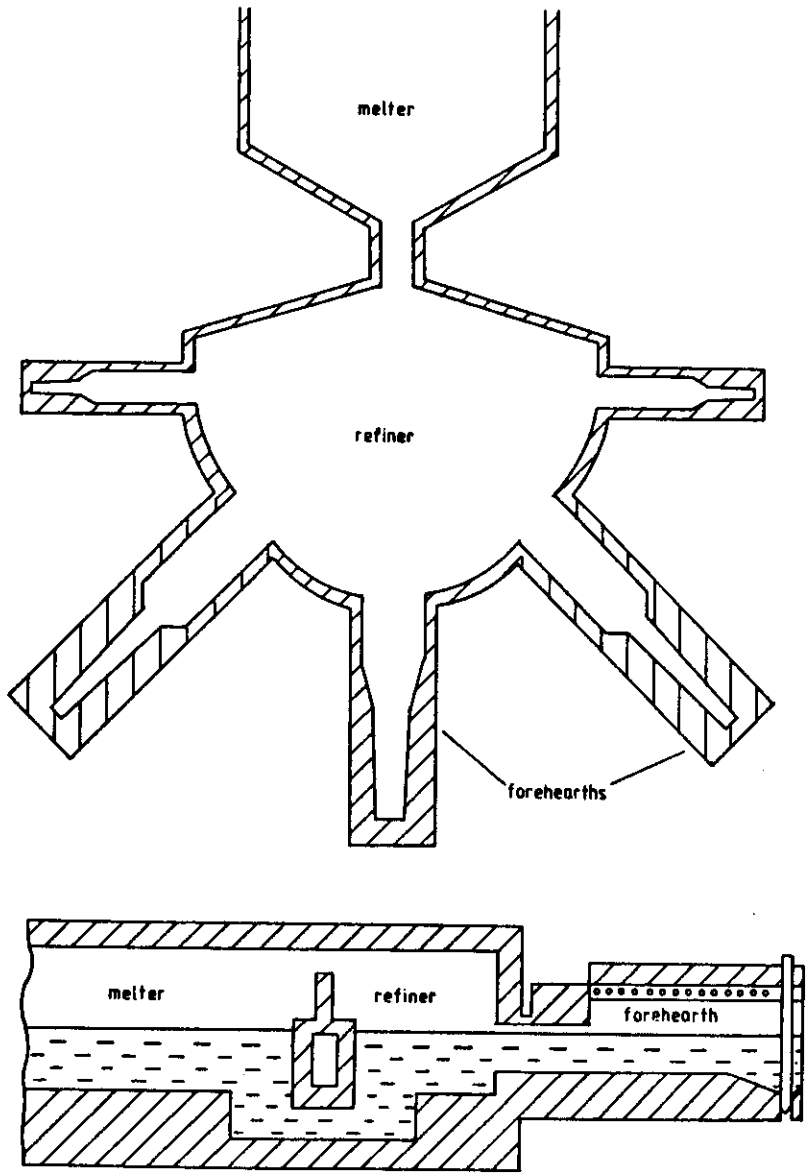


Fig. 1 - A general furnace configuration.

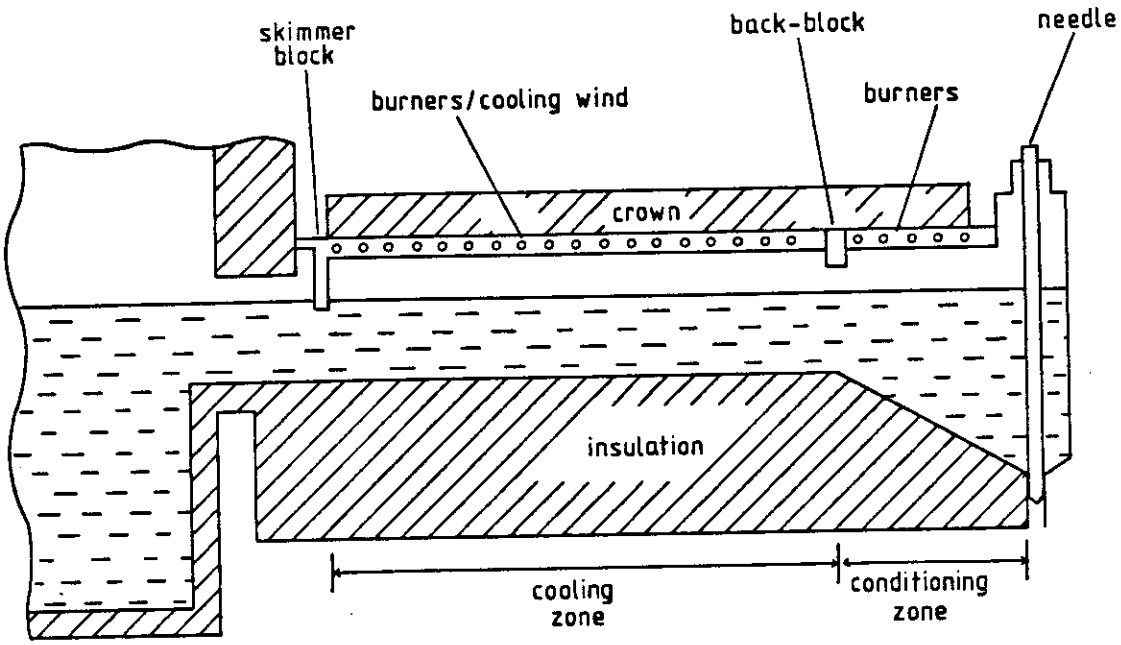


Fig. 2 - Schematic diagram of a general forehearth.

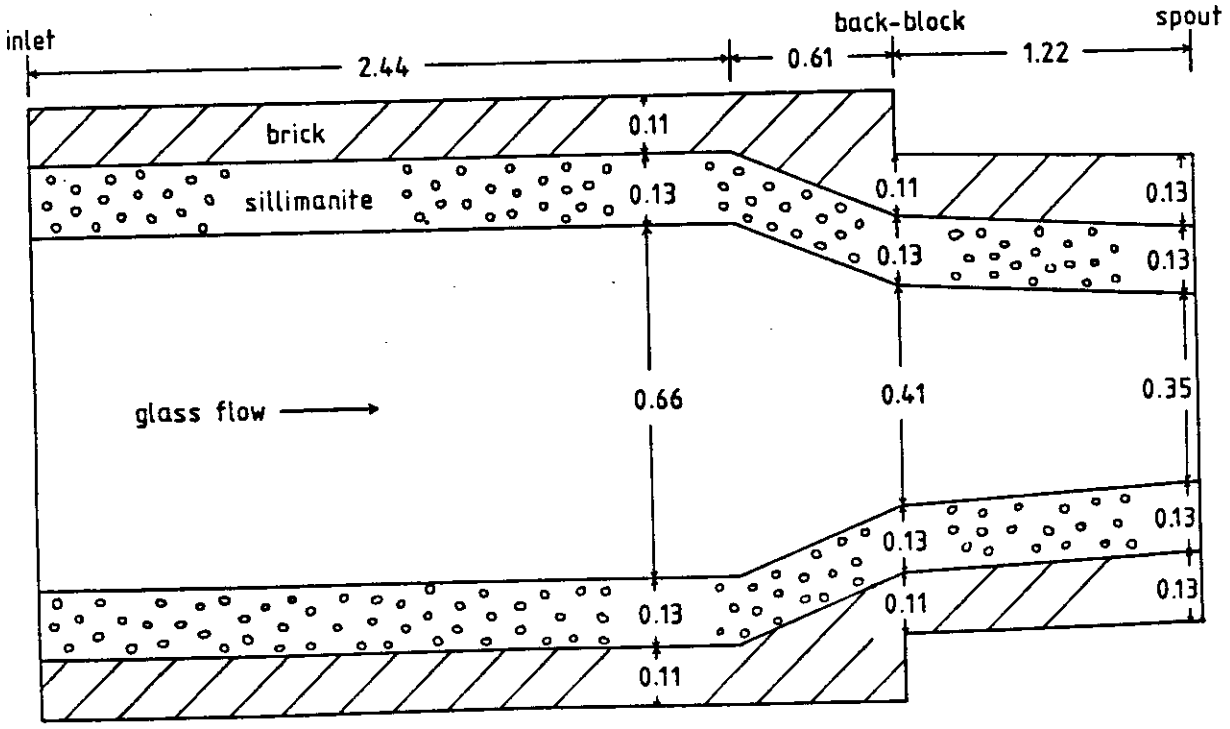


Fig. 3 - Plan of a specific short forehearth.

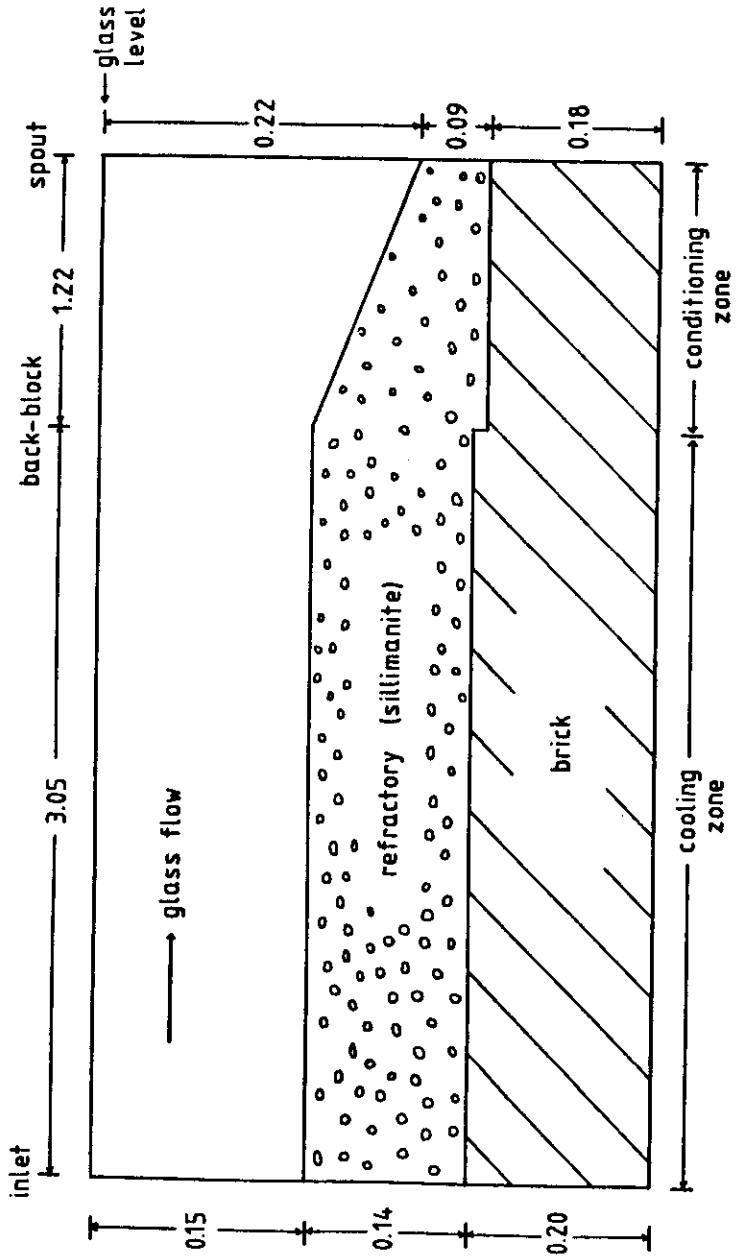


Fig. 4 - View of a specific short forehearth.

achieved by controlling the burners of the cooling and conditioning zones so that the two measured temperatures agree with two prescribed temperatures. The control of the two temperatures is currently rapid and accurate with two- and three-term control usually proving adequate. However the two set points, which ultimately determine the glass quality, are set and adjusted manually and in consequence the overall control of such a forehearth could be improved. Indeed the statement[2]

> "over a period of decades of experience, there have grown up the best-known layouts for conditioning the glass"

indicates that the basic design of forehearths is also heuristic and confirmation that such layouts are the "best" is required.

In an effort to eleviate such problems, several mathematical models of the process of heat and mass transfer within a forehearth have been developed. The flow of glass in an open channel was considered by Hearn and Booth[3] who show that the assumption that the flow of glass is laminar is not unreasonable. Henry[4] suggests that such laminar flow, which implies a lack of mixing, is one of the basic difficulties in balancing forehearth temperatures. Duffin and Johnson[5] were early workers in the development of suitable heat transfer equations and produced relatively complicated models which, when solved by finite difference techniques, gave reasonable agreement with measured temperature profiles. Carling[6] has produced further heat and mass transfer equations and while giving good agreement with measured temperatures, they are also extremely complicated. Hamilton[7] has used the simplest 2DL model of Carling to predict approximately the optimum temperature profile of the glass as it enters a particular short forehearth. This forehearth is pictured in Figs. 3 and 4 and is used as a standard reference for model verification throughout this work. Even this simpler 2DL model demands quite extensive computing facilities and can therefore only be used in

selective design studies and the need for a rapidly computable model which may be used in an on-line control scheme is clear. One such model, which also includes heat and mass balances in both melter and refiner, has been reported by McConnell and Goodson[8]. The extent of this model is such that all the individual partial differential equations are descretized to give a lumped parameter model with this discretization being particularly coarse in the forehearth.

While control of the glass surface temperature profile is at present considered to be adequate, the same is not true of the overall refiner/forehearth operation. Even in the more recent control scheme[4,9] which include extensive instrumentation to aid the forehearth operator, the operating set points must still be set manually.

Thus a simple, though reliable, distributed parameter model is required to verify the basic forehearth design and also to give effective instrumentation of forehearths with a view to controlling the overall heat conditioning process.

The structure of the distributed parameter model is crucial for its potential use as the basis for an on-line control strategy. We shall concentrate on a simple two-dimensional steady-state model. This model will be used as a basis for the development of an on-line feedforward control strategy which computes the glass surface temperature required to minimise (with respect to the simple model) the deviation of glass temperature at the spout from a prescribed value for any given set of operating conditions. The strategy has to be implementable on a microprocessor based controller whose size and speed of operation will require the development of a novel PDE solution technique.

2. THE EQUATIONS OF A SIMPLE 2D MODEL

2.1 The equation of internal heat transfer

The construction of a typical short forehearth is illustrated in Fig. 2 and the process of steady-state heat transfer in glass which is being heat conditioned in such a forehearth is to be considered. The variation of forehearth width and depth with longitudinal direction X will be accounted for and hence the model developed within this section will be referred to as the two-dimensional variable boundary (2DVB) model.

The conduction of heat in the longitudinal and lateral directions, X and Z respectively, is to be neglected since temperature gradients in these directions are small when compared to the temperature gradient in the vertical direction. An "effective conductivity", which includes both a conduction and a radiation component[11], is used and is considered to be temperature independent. Such an assumption is not unreasonable for opaque, i.e. coloured, glasses.

The flow of molten glass through open channels of rectangular cross-section has been previously studied[3] and the assumption of laminar flow is extended to this model in which the width and depth of the forehearth vary piecewise linearly with distance along the forehearth. Therefore, extending the results for laminar flow in the rectangular channel to the 2DVB model, the velocity profile is given as

$$\bar{U}(X,Y) = \frac{3\,M_f}{2\rho\bar{D}(X)\bar{W}(X)}\left[1 - \frac{Y^2}{\bar{D}^2(X)}\right] \tag{1}$$

With the assumptions outlined above, steady-state heat transfer in the glass is described by the partial differential equation[12]

$$\kappa\frac{\partial^2 T}{\partial Y^2} - U(X,Y)\frac{\partial T}{\partial X} = 0 \tag{2}$$

The temperature variable is made dimensionless by the substitution

$$\theta(X,Y) = \frac{T(X,Y) - T_r}{T_a - T_r} \tag{3}$$

where T_a and T_r are constant reference temperatures, an advantageous choice of T_r being the desired outlet temperature. Dimensionless length and depth, x and y respectively, are introduced using

$$x = \frac{X}{L} \quad \text{and} \quad y = \frac{Y}{D_{max}} \tag{4}$$

where L is the length of the forehearth and D_{max} is the maximum depth of glass in the forehearth. Equation (2) is then reformulated in dimensionless form as

$$\frac{\partial^2\theta}{\partial y^2} - U(x,y)\,\frac{\partial\theta}{\partial x} = 0 \tag{5}$$

where
$$U(x,y) = \frac{3\,c\,M_f\,D_{max}}{2K_g L\,D(x)\,W(x)\,W_{max}}\left[1 - \frac{Y^2}{D^2(x)}\right] \tag{6}$$

c = glass specific heat

K_g = glass conductivity

M_f = mass flow rate of glass

$$D(x) = \frac{\bar{D}(x)}{D_{max}}, \quad W(x) = \frac{\bar{W}(x)}{W_{max}} \tag{7}$$

2.2 Boundary conditions

The three boundary conditions which are required for the solution of the heat transfer equation (5) are provided by

(i) the inlet temperature profile

$$T(0,Y) = \bar{\mu}(Y)$$

or $$\theta(0,y) = \mu(y) \tag{8}$$

(ii) the temperature profile along the glass surface

$$T(X,0) = \bar{\gamma}_1(X)$$

or $$\theta(x,0) = \gamma_1(x) \tag{9}$$

(iii) the heat loss through the bottom of the forehearth.

This latter boundary condition will now be considered in some detail.

The process of heat transfer in the refractory and brick is strictly three dimensional and is therefore described by a partial

differential equation itself. With the assumption that longitudinal and lateral heat conductions are negligible in comparison to that in the vertical direction then the above three dimensional equation reduces to one dimension and acts as the third boundary condition of the 2DVB model. The heat loss per unit area from the bottom of the glass to the refractory is given by the Fourier conduction law[33] as

$$-K_g\,\frac{\partial T}{\partial Y}\,(X,\bar{D}(X))$$

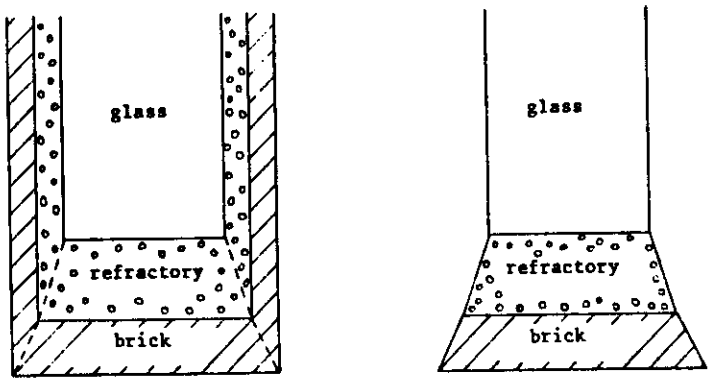
and is assumed to be constant over the width of glass at some point $X = X_1$. Thus in equilibrium

$$-K_g\,\frac{\partial T}{\partial Y}\,(X_1,\bar{D}(X_1)) = K_{eff}(X_1)\,\left[T(X_1,\bar{D}(X_1)) - T_{ba}(X_1)\right] \tag{10}$$

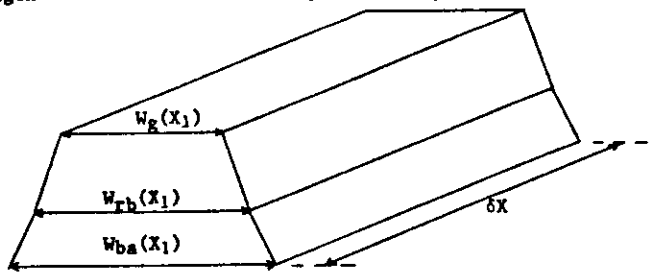
where $T_{ba}(X_1)$ is the temperature at the brick/air interface and $K_{eff}(X_1)$ is an effective conductance of the refractory and brick. The specific form of $K_{eff}(X)$ will now be developed as a piecewise function which varies as with both the width and depth of the refractory and the brick.

The process of heat transfer in the refractory and brick at the bottom of the forehearth is simplified by neglecting both longitudinal and lateral heat transfer. The equations of heat transfer are then two coupled one-dimensional Laplace equations from which the boundary condition as posed in equation (10) is easily derived. However although the lateral heat conduction is explicitly neglected certain side-effects of the overall structure may be accounted for. A cross-section of the forehearth at $X = X_1$ and an approximation to such a cross-section are illustrated on page 11.

If the structure is approximated as shown then the equations of heat transfer will still give the type of boundary condition required by equation (10) while including some side-effects.



Consider then an elemental slice of the above approximation which is of length δX and is taken at the point $X = X_1$.



If $W_g(X)$, $W_{rb}(X)$ and $W_{ba}(X)$ denote the widths of the glass/refractory interface, the refractory/brick interface and the brick/air interface respectively, then $W_g(X_1)$, $W_{rb}(X_1)$ and $W_{ba}(X_1)$ are assumed not to vary over the elemental distance δX. The following notation will now be adopted

Y_g is the distance from $Y = 0$ to the glass/refractory interface

Y_{rb} is the distance from $Y = 0$ to the refractory/brick interface

Y_{ba} is the distance from $Y = 0$ to the brick/air interface.

The thermal resistance of the refractory $R_r(X_1)$ is[13]

$$R_r(X_1) = \frac{1}{K_r}\int_{Y_g}^{Y_{rb}} \frac{dY}{A_r(Y)}$$

where K_r and $A_r(Y)$ are respectively the conductivity and the cross-

sectional area of the refractory. Now all widths vary piecewise linearly with the distance, X, along the forehearth i.e.

$$W_g(X) = w_g^0 + w_g^1 X$$
$$W_{rb}(X) = w_{rb}^0 + w_{rb}^1 X$$
$$W_{ba}(X) = w_{ba}^0 + w_{ba}^1 X$$

In addition, for this approximation, the widths of both the refractory $W_r(X,Y)$, and the brick $W_b(X,Y)$ vary linearly with depth Y. Therefore

$$W_r(X_1,Y) = w_r^0 + w_r^1 Y$$
$$W_b(X_1,Y) = w_b^0 + w_b^1 Y$$

and

$$A_r(Y) = W_r(X_1,Y)\,\delta X$$
$$= (w_r^0 + w_r^1 Y)\,\delta X$$

$$\therefore R_r(X_1) = \frac{1}{K_r}\int_{Y_g}^{Y_{rb}} \frac{dY}{(w_r^0 + w_r^1 Y)\delta X}$$

$$= \frac{1}{K_r w_r^1 \delta X}\left[\log_e(w_r^0 + w_r^1 Y)\right]_{Y_g}^{Y_{rb}}$$

and since $w_r^1 = \frac{W_g(X_1) - W_{rb}(X_1)}{Y_g - Y_{rb}}$

$$R_r(X_1) = \frac{1}{K_r \delta X}\cdot\frac{Y_g - Y_{rb}}{W_g(X_1) - W_{rb}(X_1)}\log_e\left[\frac{W_{rb}(X_1)}{W_g(X_1)}\right]$$

Similarly

$$R_b(X_1) = \frac{1}{K_b \delta X}\cdot\frac{Y_{rb} - Y_{ba}}{W_{rb}(X_1) - W_{ba}(X_1)}\log_e\left[\frac{W_{ba}(X_1)}{W_{rb}(X_1)}\right]$$

and the effective thermal conductance $K_{eff}(X_1)$ at $X = X_1$ is

$$K_{eff}(X_1) = \left[R_r(X_1) + R_b(X_1)\right]^{-1}\left[W_g(X_1)\delta X\right]^{-1}$$

where

$$R_r(X_1)+R_b(X_1) = \frac{-1}{W_g(X_1)\delta X}\left\{\frac{d_r(X_1)}{K_r}\left(\frac{W_g(X_1)}{W_g(X_1) - W_{rb}(X_1)}\right.\right.$$
$$\left.\times \log_e\left[\frac{W_{rb}(X_1)}{W_g(X_1)}\right]\right) + \frac{d_b(X_1)}{K_b}\left(\frac{W_g(X_1)}{W_{rb}(X_1) - W_{ba}(X_1)}\right.$$
$$\left.\left.\times \log_e\left[\frac{W_{ba}(X_1)}{W_{rb}(X_1)}\right]\right)\right\}$$

where $d_r(X_1)$ = refractory depth at $X = X_1$

$d_b(X_1)$ = brick depth at $X = X_1$

Therefore, the third boundary condition for the 2DVB model is

$$- K_g \frac{\partial T}{\partial Y}(X,\bar{D}(X)) = K_{eff}(X)\left[T(X,\bar{D}(X)) - T_{ba}(X)\right]$$

where

$$K_{eff}(X) = -\left\{\frac{d_r(X)}{K_r}\frac{W_g(X)}{W_g(X)-W_{rb}(X)}\log_e\left[\frac{W_{rb}(X)}{W_g(X)}\right] + \frac{d_b(X)}{K_b}\frac{W_g(X)}{W_{rb}(X)-W_{ba}(X)}\log_e\left[\frac{W_{ba}(X)}{W_{rb}(X)}\right]\right\}^{-1} \quad (11)$$

In the non-dimensional system the third boundary condition is

$$K_g \frac{\partial \theta}{\partial y}(x,D(x)) = \gamma_2(x)\left[\theta(x,D(x)) - \theta_{ba}(x)\right] \quad (12)$$

where

$$\gamma_2(x) = - K_{eff}(x) \quad (13)$$

2.3 The determination of the brick/air interface temperature

The definition of the third boundary condition by equation (12) implicitly assumes that the non-dimensional temperature $\theta_{ba}(x)$ is known at all values of x. The equivalent dimensional temperature $T_{ba}(X)$ is not readily accessible and therefore some means is sought to calculate $T_{ba}(X)$ from variables which may be measured. The development of a suitable formula will then show the effect of such variables on not only $T_{ba}(X)$ but also all other temperature profiles within the glass.

Heat is lost from the outer brick surface to the air principally by a combination of the non-linear processes of convection and radiation. We therefore seek to equate this heat loss to the heat arriving at the brick/air interface by conduction through the refractory and brick, and thereby produce an expression for $T_{ba}(X)$. The heat gained per unit area by the brick/air interface from conduction is

$$K_{out}(X)\left[T(X,\bar{D}(X)) - T_{ba}(X)\right] \quad (14)$$

where $K_{out}(X)$ is deduced as

$$K_{out}(X) = -\left\{\frac{d_r(X)}{K_r}\frac{W_{ba}(X)}{W_g(X)-W_{rb}(X)}\log_e\left[\frac{W_{rb}(X)}{W_g(X)}\right] + \frac{d_b(X)}{K_b}\frac{W_{ba}(X)}{W_{rb}(X)-W_{ba}(X)}\log_e\left[\frac{W_{ba}(X)}{W_{rb}(X)}\right]\right\}^{-1}$$

The heat lost to the air by convection and radiation is denoted by $Q_{c+r}(X)$ and is given by

$$Q_{c+r}(X) = C(T_{ba}(X)-T_\infty)^{5/4} + \sigma\varepsilon\left[(T_{ba}(X)+273)^4 - (T_\infty+273)^4\right] \quad (15)$$

where C, a convection coefficient, and ε the emissivity of the brick surface are known constants[14] and σ is Stefan-Boltzmann's constant. T_∞ is the ambient air temperature and is assumed to be independent of the X space dimension. Thus equating (14) to (15) and rearranging gives

$$T_{ba}(X) - T(X,\bar{D}(X)) + \left[K_{out}(X)\right]^{-1}\left\{C(T_{ba}(X)-T_\infty)^{5/4} + \sigma\varepsilon\left[(T_{ba}(X)+273)^4-(T_\infty+273)^4\right]\right\} = 0 \quad (16)$$

Therefore provided $T(X,\bar{D}(X))$ and T_∞ are supplied then equation (16) is a non-linear equation in $T_{ba}(X)$. Typical operating temperatures $T(X,\bar{D}(X))$ have been previously calculated[6], probable values for T_∞ are readily estimated and therefore equation (16), which is rapidly solved by a Newton-Raphson technique, provides values of $T_{ba}(X)$ at distinct X values along the length of the forehearth. The nature of the above approximation and the shape of the refractory and brick will in fact give a non-feasible $T_{ba}(X)$ i.e. it will be non-differentiable. However, the values for $T_{ba}(X)$ will still be useful in that they provide extreme values for the brick/air interface temperatures with the conduction in X direction actually causing a smoothing and averaging effect.

2.4 Summary of the 2DVB model

If $\theta(x,y)$ is the dimensionless temperature of glass in the forehearth then

$$\frac{\partial^2\theta}{\partial y^2} - U(x,y)\,\frac{\partial\theta}{\partial x} = 0 \tag{17}$$

where

$$U(x,y) = \frac{3\,c\,M_f\,D_{max}}{2\,K_g\,L\,D(x)\,W(x)\,W_{max}}\left[1 - \frac{y^2}{D^2(x)}\right] \tag{18}$$

and boundary conditions governing the process are

$$\theta(0,y) = \mu(y) \tag{19}$$

$$\theta(x,0) = \gamma_1(x) \tag{20}$$

$$K_g\,\frac{\partial\theta}{\partial y}\,(x,D(x)) = \gamma_2(x)\left[\theta(x,D(x)) - \theta_{ba}(x)\right] \tag{21}$$

where $\mu(y)$, $\gamma_1(x)$, $\theta_{ba}(x)$ are supplied temperature profiles and $\gamma_2(x)$ is a piecewise function which represents the effective conductance of bottom of the forehearth.

2.5 The optimal control problem

The optimal control problem can be broadly phrased as follows: choose the surface temperature profile (i.e. $\theta(x,0) = \gamma_1(x)$) and possibly the inlet temperature profile (i.e. $\theta(0,y) = \mu(y)$) so as to minimise the temperature deviation throughout the depth at the spout from some required value.

Firstly we consider two criteria which measure the temperature deviation from its required value (T_r). Since $\theta(x,y)$ is dimensionless temperature defined by

$$\theta(x,y) = \frac{T(x,y) - T_r}{T_a - T_r}$$

we seek to keep $\theta(1,y)$ close to zero. One criterion which immediately springs to mind is

$$E_1 = \int_0^1 [\theta(1,y)]^2\,dy$$

Thus given that $\gamma_1(x)$ (which is accurately described by a quadratic in x) and $\mu(y)$ (which is reasonably approximated by a linear function y) are parameterised we have a parametric optimisation problem:

> minimise E_1 with respect to the parameters which define $\gamma_1(x)$ and $\mu(y)$.

Unfortunately E_1 can only be evaluated from a specified parameter set following solution of the 2DVB model PDE. Thus if $\underline{\alpha}$ denotes the set of optimisable parameters and $E(\underline{\alpha})$ denotes the cost function to be minimised then for any fixed value of $\underline{\alpha}$, $\underline{\alpha}'$ say, $E(\underline{\alpha}')$ is evaluated by the following scheme.

1. $\underline{\alpha}'$ defines b.c.'s $\gamma_1(x)$, $\mu(y)$
2. Solve PDE for these b.c.'s
3. Manipulate pointwise description of $\theta(1,y)$ to create $E(\underline{\alpha}')$.

The embedding of a PDE solution within an optimisation procedure clearly prohibits this approach from on-line implementation on the grounds of both microprocessor speed and memory requirements.

Hence we are forced to look at an entirely different approach for the development of an optimal feedforward control strategy. Specifically we shall develop a PDE solution technique in which the optimisable parameters appear explicitly in an approximation to $\theta(1,y)$, and hence explicitly in the error function.

3. SOLUTION OF BOUNDARY VALUE PROBLEMS BY POLYNOMIAL APPROXIMATION METHODS

We have previously outlined the requirement that it is desirable to produce an approximate solution to the PDE (17) and associated boundary conditions (19), (20) and (21) which explicitly contains the optimisable parameters defining the inlet temperature profile (19) and the surface temperature profile (20). We shall briefly illustrate a class of boundary value problem solution techniques which may yield such a solution. In the first instance we shall use an ODE BVP to simplify algebraic considerations and shall then turn our attention to the 2DVB problem.

3.1 A 1-D heat conduction problem

Consider a thin rod whose temperature at one end ($x = 0$) is T_0 and at the other end ($x = 1$) is T_1. If the thermal conductivity of the rod k depends linearly on temperature T e.g.

$$k(T) = k_1 + k_2(T - T_0) \tag{22}$$

then the steady-state heat conduction equation is non-linear:

$$\frac{d}{dx}\left[k(T)\,\frac{dT}{dx}\right] = 0 \tag{23}$$

Introducing the dimensionless temperature variable

$$\theta(x) = \frac{T(x) - T_0}{T_1 - T_0} \tag{24}$$

gives an equivalent problem

$$\frac{d}{dx}\left[(1 + a\theta)\frac{d\theta}{dx}\right] = 0 \qquad (25)$$

or

$$(1 + a\theta)\frac{d^2\theta}{dx^2} + a\left[\frac{d\theta}{dx}\right]^2 = 0 \qquad (26)$$

subject to boundary conditions

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

This non-linear problem possesses an analytic solution:

$$\theta(x) = [-1 + \{1 + a(2 + a)x\}^{\frac{1}{2}}]/a \qquad (27)$$

which shall be used later for comparison of approximate solutions.

3.2 Weighted residual methods

The central feature of the polynomial approximation methods is the development of an approximate solution of the form

$$\bar{\theta}(x) = \sum_{j=0}^{M} \alpha_j \psi_j(x) \qquad (28)$$

where $\psi_j(x)$ is a polynomial in x, e.g. a monomial x^j, a Legendre polynomial $P_j(x)$ etc. Given that $\bar{\theta}(x)$ satisfies all boundary conditions then application of the ODE differential operator to $\bar{\theta}(x)$ will yield some function $R(\underline{\alpha},x)$. The unknown parameters $\{\alpha_j : j = 0,1,\ldots,M\}$ are then chosen to force $R(\underline{\alpha},x)$ to be "close" to zero over the domain of definition: the manner in which this is done is dictated by the choice of solution method. The function $R(\underline{\alpha},x)$ is known as the residual

(function). Thus if $x \in \Omega$ we generally force some integral of $R(\underline{\alpha},x)$ over Ω to zero. If $w_i(x)$ is some weighting function we solve the set of equations

$$\int_\Omega w_i(x)\, R(\underline{\alpha},x)\, dx = 0 \qquad i = 0,1,\ldots,M$$

for the unknowns $\{\alpha_j : j = 0,1,\ldots,M\}$.

Collocation: $w_i(x) = \delta(x - x_i)$ $\qquad (x_i \in \Omega)$

Galerkin: $w_i(x) = \psi_i(x)$

Least squares: $w_i(x) = \frac{\partial R}{\partial \alpha_i}(\underline{\alpha},x)$

(note: if R is not linear in $\underline{\alpha}$ then in this case W_i is also a function of $\underline{\alpha}$)

Method of moments: $w_i(x) = x^i$

The above methods are generally called "Weighted Residual" methods. In all methods an increasingly accurate solution is sought by incrementing M, i.e. the number of terms in the approximate solution expansion.

3.3 MWR solution of 1-D problem

We firstly consider imposition of the boundary conditions on the approximate solution. We therefore require $\bar{\theta}(x)$ to satisfy

$$\bar{\theta}(0) = 0\,, \qquad \bar{\theta}(1) = 1$$

One obvious candidate is

$$\bar{\theta}(x) = x + \sum_{j=0}^{M} \alpha_j (x^{j+2} - x) \qquad (29)$$

while a more general expression is

$$\bar{\theta}(x) = x + x(x-1) \sum_{j=0}^{M} a_j \psi_j(x) \qquad (30)$$

where $\psi_j(x)$ is a j^{th} degree polynomial in x. For simplicity we shall use the first form so that a first order approximate solution is simply

$$\bar{\theta}(x) = x + a_0(x^2 - x) \qquad (31)$$

while a second order approximation is

$$\bar{\theta}(x) = x + a_0(x^2 - x) + a_1(x^3 - x) \qquad (32)$$

etc.

In general the residual $R(\underline{a},x)$ is given by

$$R(\underline{a},x) = (1 + a\bar{\theta}) \frac{d^2\bar{\theta}}{dx^2} + a\left[\frac{d\bar{\theta}}{dx}\right]^2$$

and for numerical purposes we shall from hereon assume the constant a to be 1. Some algebra then gives:

first order approximation:

$$R(\underline{a},x) = \left[1 + a_0^2\right] + x\left[6a_0 - 6a_0^2\right] + x^2\left[6a_0^2\right]$$

second order approximation:

$$R(\underline{a},x) = \left[2a_0 + (1 - a_0 - a_1)^2\right] + x\left[6a_0(1 - a_0 - a_1) + 6a_1\right]$$
$$+ x^2\left[6a_0^2 + 12a_1(1 - a_0 - a_1)\right] + x^3\left[20a_0a_1\right] + x^4\left[15a_1^2\right]$$

Collocation:

Equations are generated by

$$\int_0^1 \delta(x - x_i)\, R(\underline{a},x)\, dx = 0 \qquad i = 1,2,\ldots,M$$

For the first order approximation we collocate at $x_0 = \frac{1}{2}$ and generate:

$$1 + 3a_0 - a_0^2/2 = 0$$

i.e. $a_0 = -0.3166$ (the other root giving incorrect flux direction at $x = 1$).

For the second order approximation we collocate at $x_0 = \frac{1}{3}$ and $x_1 = \frac{2}{3}$ and generate:

$$1 + 2a_0 + \frac{4}{3}a_1 - \frac{16}{27}a_1a_0 - \frac{1}{3}a_0^2 - \frac{4}{27}a_1^2 = 0$$

$$1 + 4a_0 + \frac{22}{3}a_1 - \frac{38}{27}a_1a_0 - \frac{1}{3}a_0^2 - \frac{37}{27}a_1^2 = 0$$

which, following numerical solution, give

$$a_0 = -0.5992\,, \qquad a_1 = 0.1916$$

Galerkin

Equations are generated by

$$\int_0^1 \psi_i(x)\, R(\underline{a},x)\, dx \qquad i = 0,1,\ldots,M$$

In the first order case we use $\psi_0(x) = (x^2 - x)$ while in the second order case we use $\psi_0(x) = (x^2 - x)$ and $\psi_1(x) = (x^3 - x)$. Much algebra yields for the first order approximation

$$-\frac{1}{6}-\frac{1}{2}\alpha_0+\frac{1}{30}\alpha_0^2=0$$

$$\Rightarrow \alpha_0 = -0.3262$$

and for the second order approximation:

$$-\frac{1}{6}-\frac{1}{2}\alpha_0-\frac{23}{30}\alpha_1+\frac{1}{10}\alpha_0\alpha_1+\frac{8}{105}\alpha_1^2+\frac{1}{30}\alpha_0^2=0$$

$$-\frac{1}{4}-\frac{4}{5}\alpha_0-\frac{13}{10}\alpha_1+\frac{11}{70}\alpha_0\alpha_1+\frac{1}{20}\alpha_0^2+\frac{1}{8}\alpha_1^2=0$$

$$\Rightarrow \alpha_0 = -0.6558 \qquad \alpha_1 = 0.2152$$

Least squares

Equations are generated by

$$\int_0^1 \frac{\partial R}{\partial \alpha_i}(\underline{\alpha},x)\,R(\underline{\alpha},x)\,dx \qquad i = 0,1,\ldots,M$$

The first order approximation yields

$$18\alpha_0^3-40\alpha_0-15=0$$

$$\Rightarrow \alpha = -0.4049$$

while the second order approximation (eventually) yields

$$3+12\alpha_0+24\alpha_1+\frac{4}{5}\alpha_0\alpha_1+2\alpha_0^2+\frac{6}{5}\alpha_1^2+\frac{20}{7}\alpha_0\alpha_1^2+\frac{9}{5}\alpha_0^2\alpha_1+\frac{2}{5}\alpha_0^3+\frac{111}{70}\alpha_1^3=0$$

$$5+24\alpha_0+\frac{264}{5}\alpha_1+\frac{12}{5}\alpha_0\alpha_1+\frac{2}{5}\alpha_0^2+\frac{96}{35}\alpha_1^2+\frac{333}{70}\alpha_0\alpha_1^2+\frac{20}{7}\alpha_0^2\alpha_1+\frac{3}{5}\alpha_0^3+\frac{96}{35}\alpha_1^3=0$$

$$\Rightarrow \alpha_0 = -0.6251 \qquad \alpha_1 = 0.1905$$

Method of moments

Equations are generated by

$$\int_0^1 x^i\,R(\underline{\alpha},x)\,dx = 0 \qquad i = 0,1,\ldots,M$$

The first order approximation gives

$$2\alpha_0^2+3\alpha_0-3\alpha_0^2+1+\alpha_0^2=0$$

$$\Rightarrow 3\alpha_0+1=0$$

$$\Rightarrow \alpha_0 = -0.3333$$

while the second order approximation gives

$$1+3\alpha_0+5\alpha_1=0$$

$$\frac{1}{2}+2\alpha_0+4\alpha_1=0$$

$$\Rightarrow \alpha_0 = -0.75 \qquad \alpha_1 = 0.25$$

(Note: the linearity of equations is generated by coincidence in this problem).

3.4 Orthogonal collocation

General collocation methods involve arbitrary selection of collocation points at which the residual is forced to zero. Such points could be chosen to advantage given some a priori knowledge of the solution variation; however in general an arbitrary assignment (such as equidistant points) can be improved upon.

The idea underlying orthogonal collocation is to approximate the integral of the weighted residual by a quadrature rule. Thus

$$\int_0^1 W_k(x)\, R(\underline{\alpha},x)\, dx = \sum_{j=1}^{N} w_j\, W_k(x_j)\, R(\underline{\alpha},x_j)$$

where w_j are quadrature weights for collocation points x_j. The method then proceeds simply to force

$$R(\underline{\alpha},x_j) = 0 \qquad j = 1,2,\ldots,M+1$$

where there are (M + 1) unknowns $\underline{\alpha}$ and the x_j's have been chosen via the appropriate (M + 1)th order quadrature rule. Thus an approximate quadrature equivalent of the original integral weighted residual is forced to zero. The x_j collocation points are selected from quadrature schemes which give accurate integral approximations for very few terms in the quadrature expansion. Typically, the collocation points would be chosen from the Gauss-Legendre quadrature rule which (on [0,1]) yields points:

N	x_j
1	0.50000 00000
2	0.21132 48654
	0.78867 51346
3	0.11270 16654
	0.50000 00000
	0.88729 83346
4	0.06943 18442
	0.33000 94783
	0.66999 05218
	0.93056 81558
5	0.04691 00771
	0.23076 53450
	0.50000 00000
	0.76923 46551
	0.95308 99230

Gauss-Legendre collocation points on [0,1] ($N \leq 5$)

Advantages of this method include the fact that collocation points are prescribed; the equations to be solved by the unknown parameters $\underline{\alpha}$ are easily formed (no integration to be performed); as in all weighted residual methods, boundary conditions are often easily included.

A potentially major disadvantage is that the order of the collocation rule is determined by the unknown parameters. The accuracy of integral approximation may then be quite poor with the result than the integral weighted residual may be forced closely to zero for various $W_k(x)$

weighting functions. (This latter point is particularly pertinent when we come to application of collocation methods in two space dimensions).

We shall now apply Gauss-Legendre orthogonal collocation to our 1-D heat conduction problem. We take the approximate expansion to be equation (31) for the first order approximation and equation (32) for the second order approximation. (Note: in orthogonal collocation the "trial" or basis functions $P_i(x)$ are often chosen as orthogonal polynomials (e.g. Legendre polynomials on [0,1] could be used here)). Orthogonal polynomials recurrence relationships can then be used when derivatives are applied and terms are collected. Additionally the resultant algebraic equations for $\underline{\alpha}$ are usually better conditioned; this is particularly important for large M.

For the first order approximation we allocate at $x_0 = \frac{1}{2}$ and generate

$$1 + 3\alpha_0 - \alpha_0^2/2 = 0$$

$$\Rightarrow \alpha_0 = -0.3166$$

while for the second order approximation we collocate at $x_0 = 0.21132$, $x_1 = 0.78867$ to obtain

$$1 + 1.2679\alpha_0 - 0.1962\alpha_1 + 0.3849\alpha_0\alpha_1 + 1.685 \times 10^{-5}\alpha_0^2 + 0.4940\alpha_1^2 = 0$$

$$1 + 4.7320\alpha_0 + 10.1960\alpha_1 - 0.3849\alpha_0\alpha_1 - 1.7786 \times 10^{-5}\alpha_0^2 - 0.6607\alpha_1^2 = 0$$

$$\Rightarrow \alpha_0 = -0.7224 , \qquad \alpha_1 = 0.2344$$

We now collect a set of numerical comparisons for the various methods: point collocation, Galerkin, least squares, moments and orthogonal collocation. We note that for a = 1 the true solution is

$$\theta(x) = -1 + (1 + 3x)^{\frac{1}{2}}$$

and for various values of x we have

x	0.0	0.1	0.2	0.3	0.4	0.5
θ(x)	0.0	0.1402	0.2649	0.3784	0.4832	0.5811

x	0.6	0.7	0.8	0.9	1.0
θ(x)	0.6733	0.7607	0.8439	0.9235	1.0

1st ORDER APPROXIMATIONS									
COLLOCATION		ORTHOGONAL COLLOCATION		MOMENTS		GALERKIN		LEAST SQUARES	
α_0 = -0.3166247		α_0 = -0.3166247		α_0 = -0.3333333		α_0 = -0.3262379		α_0 = -0.40486330	
APPROX.	RESIDUAL	APPROX.	RESIDUAL	APPROX.	RESIDUAL	APPROX.	RESIDUAL	APPROX.	RESIDUAL
0.0000	1.1003	0.0000	1.1003	0.0000	1.1111	0.0000	1.1064	0.0000	1.1639
0.1285	0.8561	0.1285	0.8561	0.1300	0.8511	0.1294	0.8532	0.1364	0.8322
0.2507	0.6241	0.2507	0.6240	0.2533	0.6044	0.2522	0.6128	0.2648	0.5207
0.3665	0.4040	0.3665	0.4040	0.3700	0.3711	0.3685	0.3851	0.3850	0.2286
0.4755	0.1960	0.4755	0.1960	0.4800	0.1511	0.4782	0.1702	0.4972	-0.0438
0.5792	0.2962 E-06	0.5792	0.2962 E-06	0.5833	-0.0556	0.5816	-0.0819	0.6012	-0.2965
0.6760	-0.1840	0.6760	-0.1840	0.6800	-0.2489	0.6782	-0.2213	0.6972	-0.5296
0.7665	-0.3559	0.7665	-0.3559	0.7700	-0.4289	0.7685	-0.3979	0.7850	-0.7430
0.8507	-0.5158	0.8507	-0.5158	0.8533	-0.5956	0.8522	-0.5617	0.8648	-0.9368
0.9285	-0.6637	0.9285	-0.6637	0.9300	-0.7489	0.9294	-0.7127	0.9364	-1.1109
1.0000	-0.7995	1.0000	-0.7995	1.0000	-0.8889	1.0000	-0.8510	1.0000	-1.2653

2nd ORDER APPROXIMATIONS									
COLLOCATION		ORTHOGONAL COLLOCATION		MOMENTS		GALERKIN		LEAST SQUARES	
α_0 = -0.59920817 α_1 = 0.19162281		α_0 = -0.72243018 α_1 = 0.2343734		α_0 = -0.75 α_1 = 0.25		α_0 = -0.65575945 α_1 = 0.21517767		α_0 = -0.62513383 α_1 = 0.19045445	
APPROX.	RESIDUAL	APPROX.	RESIDUAL	APPROX.	RESIDUAL	APPROX.	RESIDUAL	APPROX.	RESIDUAL
0.0000	0.7829	0.0000	0.7695	0.0000	0.7500	0.0000	0.7638	0.0000	0.8080
0.1350	0.4435	0.1418	0.3349	0.1428	0.3001	0.1377	0.3863	0.1374	0.4381
0.2591	0.1989	0.2706	0.0276	0.2720	-0.0135	0.2636	0.1189	0.2635	0.1671
0.3735	0.0373	0.3877	-0.1700	0.3893	-0.2099	0.3790	-0.0529	0.3793	-0.0173
0.4794	-0.0518	0.4946	-0.2731	0.4960	-0.3060	0.4851	-0.1419	0.4860	-0.1260
0.5779	-0.0774	0.5927	-0.2951	0.5938	-0.3164	0.5833	-0.1591	0.5846	-0.1689
0.6702	-0.0475	0.6834	-0.2476	0.6840	-0.2535	0.6748	-0.1141	0.6769	-0.1543
0.7574	0.0314	0.7680	-0.1398	0.7683	-0.1274	0.7609	-0.0145	0.7633	-0.0894
0.8407	0.1542	0.8481	-0.0206	0.8480	-0.0540	0.8430	0.1336	0.8452	0.0201
0.9211	0.3171	0.9249	0.2283	0.9248	0.2851	0.9222	0.3257	0.9237	0.1697
1.0000	0.5174	1.0000	0.4797	1.0000	0.5625	1.0000	0.5590	1.0000	0.3561

The Galerkin and least squares perform comparably and better than the other methods. (A more global behaviour index, e.g. $\int_0^1 \bar{\theta}(x)\,dx$ may be a better indicator of this). Orthogonal collocation is considerably easier to apply than the latter two methods and also gives a reasonable approximation.

3.5 Numerical implementation

While an increase in the model order involves little overhead for the collocation methods, considerable extra analytic effort is required for the integral methods. Since a numerical equation solver will be required for more accurate (and larger order) approximations a reasonable suggestion would involve computing the integrals, which from the left hand sides of the equations, numerically. This approach allows perfectly accurate higher order approximations to be computed.

3.6 Extended orthogonal collocation

The quadrature approximation

$$\int_0^1 W_k(x)\ R(\underline{\alpha},x)dx \approx \sum_{j=1}^{N} w_j\ W_k(x_j)\ R(\underline{\alpha},x_j)$$

may only be accurate when N (the number of collocation points) $\geq$ (M + 1) (the number of parameters $\underline{\alpha}$). One method of forcing the integral of the weighted residual to zero would be to solve the problem:

$$\min_{\underline{\alpha}} \sum_{k=0}^{M} \left[\sum_{j=1}^{N} w_j\ W_k(x_j)\ R(\underline{\alpha},x_j)\right]^2$$

The clear disadvantages of this extended approach are the need to specify the quadrature weights w_j in addition to the collocation

points x_j; the need to specify the weight functions $W_k(x)$ and the potential scale of the optimisation problem. However, a reasonable solution to the original problem with relatively few unknowns $\underline{\alpha}$.

3.7 Linear differential operators

The 1-D heat conduction problem used to illustrate the previous methods was chosen deliberately to illustrate their potential application to non-linear problems and to introduce sub-problems for which optimisation procedures could provide solutions.

If, however, the original differential equation is linear then the residual $R(\underline{\alpha},x)$ will also be linear in the unknowns $\underline{\alpha}$ and all methods (except extended orthogonal collocation) yield solutions from a (usually small) set of linear algebraic equations.

3.8 Least squares orthogonal collocation

We shall now derive an alternative algorithm which derives from the least squares weighted residual method. This algorithm deals with the problems of quadrature rule order and approximation expansion order as reasonably distinct items.

The least squares weighted residual method is generally posed as

$$\min_{\underline{\alpha}} \int_0^1 R^2(\underline{\alpha},x)\,dx$$

which has, as its quadrature equivalent, the problem

$$\min_{\underline{\alpha}} \sum_{j=1}^{N} w_j\ R^2(\underline{\alpha},x_j)$$

An equivalent problem is then to solve the over-determined equation set ($N > M + 1$ in general)

$$\sqrt{w_j}\, R(\underline{\alpha}, x_j) = 0 \qquad j = 1,2,\ldots,N$$

in least squares sense for the unknowns $\underline{\alpha}$.

If $R(\underline{\alpha},x)$ is linear in $\underline{\alpha}$ then the latter over-determined equation set is itself linear in $\underline{\alpha}$ and efficient methods of solution are available (e.g. Householder transformation techniques).

If the weights w_j and collocation points x_j are chosen via a Gaussian quadrature scheme, then we shall call this latter approach least squares orthogonal collocation.

3.9 Boundary condition optimisation

An essential feature of weighted residual solution techniques is the explicit inclusion of one or more boundary conditions in the analytic approximate solution. If such boundary conditions contain optimisable parameters then this class of methods may yield approximate solutions which explicitly depend on such parameters. We shall therefore turn back to the 2DVB model which governs the glass temperature distribution and develop a weighted residual approximate solution which does explicitly depend on the surface and inlet temperature profile parameters.

4. SOLUTION OF THE 2DVB MODEL

4.1 Introduction

Observation of the equations which describe the 2DVB model and the shape of the domain over which they are defined indicates that the application of an analytic solution approach, typically separation of variables or integral transforms, is not feasible. Therefore a technique which will yield on approximate solution must be applied.

The major advantages of expressing the approximate solution as a finite summation of polynomials are rapid simulation and the potential of explicit optimisation of boundary condition parameters. Such an approximate solution is therefore sought for the 2DVB model.

4.2 The general application of polynomial approximation methods.

The basic PDE to be considered has the general form

$$\mathcal{L}[\theta] = 0 \tag{33}$$

where $\mathcal{L}$ is a linear time-invariant partial differential operator defined over some two-dimensional spatial domain S. The PDE (33) is subject to certain boundary conditions which make the problem well-posed.

An approximate solution $\bar{\theta}(x,y)$ to the equation (33), together with its associated boundary conditions, is expressed as

$$\bar{\theta}(x,y) = \gamma_0(x,y) + \sum_{j=1}^{M} \alpha_j \psi_j(x,y) \tag{34}$$

When the solution to (33) is not known an interior method is employed. The functions $\gamma_0(x,y)$ and $\psi_j(x,y)$ ($j = 1, \ldots, M$) are chosen so that $\bar{\theta}(x,y)$ satisfies all the boundary conditions and the constants α_j are determined in such a way that $\bar{\theta}(x,y)$ represents, in some sense, an approximate solution of the equation

$$\mathcal{L}[\bar{\theta}] = 0$$

The application of the linear operator $\mathcal{L}$ to $\bar{\theta}$ yields a residual $R(\underline{\alpha},x,y)$ i.e.

$$\mathcal{L}[\bar{\theta}] = R(\underline{\alpha},x,y) \tag{35}$$

Many of the methods of polynomial approximation are contained within the method of weighted residuals (MWR). Generally, in the MWR, the α_j are chosen so that the residual is forced to be zero in some average sense by equating weighted integrals of the residual to zero. Thus the M linear equations

$$\langle w_i, R(\underline{\alpha},x,y)\rangle_2 = 0 \qquad i = 1, \ldots, M \tag{36}$$

are solved to give the M unknowns α_j, where the inner product $\langle,\rangle_2$ is defined by

$$\langle U,V\rangle_2 = \int_S U(x,y)V(x,y)dS \tag{37}$$

Since $\mathcal{L}$ is a linear operator

$$\mathcal{L}[\bar{\theta}] = \mathcal{L}[\gamma_0(x,y)] + \sum_{j=1}^{M} \alpha_j \mathcal{L}[\psi_j(x,y)] \tag{38}$$

Therefore

$$R(\underline{\alpha},x,y) = R_0(x,y) + \sum_{j=1}^{M} \alpha_j R_j(x,y) \tag{39}$$

where

$$R_0(x,y) = \mathcal{L}[\gamma_0(x,y)]$$

$$R_j(x,y) = \mathcal{L}[\psi_j(x,y)] \qquad j = 1, \ldots, M$$

The α_j (j=1, ..., M) are solutions of the matrix equation

$$\tilde{\lambda}\,\underline{\alpha} = \underline{e} \tag{40}$$

where the matrix elements are given by

$$\lambda_{ij} = \langle w_i, R_j\rangle_2$$

$$e_i = -\langle w_i, R_0\rangle_2$$

With the MWR as stated above there are three important choices to be made:

(i) the value of M,

(ii) the form of the basis functions $\psi_j(x,y)$,

(iii) the form of the weighting functions $w_i(x,y)$.

All three factors influence the ease of computation of the $\tilde{\lambda}$ matrix and $\underline{e}$ vector and ultimately the accuracy of the final approximate solution.

Obviously the upper limit of summation M instrinsically affects the accuracy of the final approximation. Small values of M are unlikely to yield an approximation of suitable accuracy, regardless of the choice of ψ_j and w_i. Alternatively, a large value of M leads to a great deal of computation for the $\tilde{\lambda}$ matrix, the $\underline{e}$ vector and the subsequent inversion of the $\tilde{\lambda}$ matrix. Convergence bounds do exist for certain classes of but many are extremely conservative, leading to an unneccesarily large value of M. Thus, a suitable value of M is usually determined by numerical testing.

The basis functions $\psi_j(x,y)$ involve terms which impose the boundary conditions exactly on the approximate solution and are usually subject to the restrictions that they are linearly independent and form a complete set. Apart from these requirements the choice of $\psi_j(x,y)$ is free. Therefore the basis functions are often chosen to simplify the computation of the $\tilde{\lambda}$ matrix and the $\underline{e}$ vector. Monomials give particularly easy evaluation of the inner product integrals but they are generally not favoured since the corresponding $\tilde{\lambda}$ matrix tends to be ill-conditioned[15,16]. Orthogonal polynomials, however, yield a well conditioned $\tilde{\lambda}$ matrix and are therefore used in the majority of applications of the MWR.

The particular method of the MWR to be applied is determined by the choice of weighting functions $w_i(x,y)$. Two of the most common forms of $w_i(x,y)$ are $w_i(x,y) = \frac{\partial R}{\partial \alpha_i} = R_i(x,y)$ and $w_i(x,y) = \psi_i(x,y)$ which correspond to the method of least squares and Galerkin's method

respectively.

Once the value M, and the form of the functions $\psi_j(x,y)$ and $w_i(x,y)$ have been selected, the problem reduces to one of evaluating the inner product integrals and solving the set of simultaneous equations (40). If the linear operator $\mathcal{L}$ has an elementary form e.g. constants or simple polynomials multiply the differentials, and the spatial domain S is trivial e.g. $[0,1] \times [0,1]$, then the inner product integrals can be generated by recurrence relations. Therefore, if the original problem does not satisfy either of these conditions, an attempt is usually made to reformulate another equivalent problem which does. The spatial domain S may be transformed typically by a change of variables or alternatively by conformal mapping in two dimensions. Unfortunately, however, either transformation will invariably complicate the linear operator $\mathcal{L}$ or the boundary conditions. The linear operator itself may be restructured but this should only be done by a change of variables and not by spatially multiplicative factors. This point will be illustrated by reference to the PDE governing the 2DVB model. At first sight, it is tempting to multiply equation (45) by the non-zero factor $D^3(x)W(x)$ to give a new equation to be solved

$$\hat{\mathcal{L}}[\theta] = D^3(x)W(x)\frac{\partial^2\theta}{\partial y^2} - \beta\left[D^2(x) - y^2\right]\frac{\partial\theta}{\partial x} = 0 \qquad (41)$$

However, this equation still cannot be solved analytically, and thus on substituting the approximate solution $\bar{\theta}(x,y)$ into equation (41) a new residual $\hat{R}(\underline{a},x,y)$ is formed and

$$\hat{R}(\underline{a},x,y) = D^3(x)W(x)R(\underline{a},x,y)$$

Thus the residual from the original 2DVB model equation has been weighted by a factor $D^3(x)W(x)$ and this may yield erroneous results (c.f. Levy's method[17,18]). In practice many PDE's have neither a convenient operator $\mathcal{L}$ or spatial domain S and transformations may not alter this situation, the 2DVB model being one such PDE. Suitable recurrence relations may

then be difficult, perhaps impossible, to generate and it becomes necessary to evaluate the inner product integrals numerically by a quadrature algorithm.

All the inner product integrals involve the integration of a function multiplied by at least one basis function and thus any given quadrature algorithm will require the value of such basis functions at specified points. The advantage of using orthogonal polynomials rather than monomials as basis functions has already been noted and thus the evaluation of such polynomials must now be considered. The most obvious method of polynomial evaluation is to simply multiply the corresponding powers and coefficients together exactly as they are written. Unfortunately such a method is both inefficient and may in certain circumstances yield erroneous results. Typically the evaluation of a Legendre polynomial on $[0,1]$ of high order requires the multiplication and addition of terms of greatly varying magnitude and the accumulation of error is significant. A second method which is both stable and more efficient than the latter involves bracketing the polynomial and is known as Horner's scheme[19]. However, such a scheme does not employ any special structure which the MWR formulation may possess. In particular the fact that each basis function, i.e. orthogonal polynomial, is involved in several integrals may be further exploited. Thus, since an orthogonal polynomial value at a given point is rapidly computable from lower order orthogonal polynomial values at the same point, and the same is true of their derivatives, then an even more efficient scheme could be based on the utilisation of such values. The adaption of any quadrature algorithm to accomodate such features would become extremely cumbersome and thus for problems in which the inner product integrals have to be evaluated numerically it is advantageous to seek a method which is equivalent to MWR and is computationally more efficient. Orthogonal collocation is one such method.

The method of orthogonal collocation is derived by expressing the inner product integral as a quadrature formula:

$$\langle w_i, R(\underline{\alpha},x,y)\rangle_2 = \int_S w_i(x,y)R(\underline{\alpha},x,y)dS$$

$$= \sum_{k=1}^{N_q} W_k\, w_i(x_k,y_k)R(\underline{\alpha},x_k,y_k) \qquad (42)$$

In the standard application of the method, N_q is chosen equal to M and a solution of the equations

$$\langle w_i, R(\underline{\alpha},x,y)\rangle_2 = 0 \qquad i = 1, \ldots, M$$

is provided by the solution of the equations

$$R(\underline{\alpha},x_k,y_k) = 0 \qquad k = 1, \ldots, N_q\ (=M)$$

The questions of the positioning of the collocation points (x_k,y_k), the number of such points N_q and the choice of the weighting factors W_k are all interrelated. These factors together with the structure of the residual $R(\underline{\alpha},x,y)$ and the shape of the domain S determine the accuracy of the quadrature formula (42) and ultimately the error in the approximate polynomial solution. In certain circumstances, similar to those for which the inner product integrals can be evaluated by recurrence relations, the choice of N_q equal to M implies that the quadrature scheme (42) is exact and hence the results from orthogonal collocation and those from the MWR would be identical. When the quadrature formula is only an approximation, as would be the case for the 2DVB model, the choice $N_q = M$ may still yield reasonable results if M is large. However, it is desirable to have a minimal number of terms in the final approximation and for small N_q (=M) the error in the quadrature approximation may be quite large; leading to the possibility of inaccurate results.

Thus, to accomodate both an accurate quadrature formula and the desire to have a low order polynomial approximation, the value of N_q must be greater than M. This will lead to a least squares problem as

demonstrated in the next section.

4.3 Least squares collocation

It is now convenient to specify the particular form of MWR for which an equivalent collocation technique is sought. The choice of weighting function

$$w_i(x,y) = \frac{\partial R}{\partial \alpha_i}(\underline{\alpha},x,y) \qquad (42)$$

gives the least squares method in the MWR. The argument against such a weighting function is that it often leads to cumbersome equations[40]. However, it will be shown in the subsequent development that the least squares method has an equivalent collocation scheme which is extremely versatile and efficient.

With $w_i(x,y)$ as given in equation (43) the basic problem to be solved is

$$\min_{\underline{\alpha}} \int_S R^2(\underline{\alpha},x,y)\, dS \qquad (44)$$

Applying the general quadrature formula (42) an approximately equivalent problem is

$$\min_{\underline{\alpha}} \sum_{k=1}^{N_q} W_k R^2(\underline{\alpha},x_k,y_k) \qquad (45)$$

Clearly, the least squares solution of the N_q equations

$$\sqrt{W_k}\, R(\underline{\alpha},x_k,y_k) = 0$$

i.e.

$$\sqrt{W_k} \sum_{j=1}^{M} \alpha_j R_j(x_k,y_k) = -\sqrt{W_k}\, R_0(x_k,y_k) \qquad (46)$$
$$k = 1, \ldots, N_q$$

will also be a solution of (45) and hence an approximate solution of (44).

Thus the original least squares integral problem is now repored as a least squares collocation problem which will be shown to be useful in determining values for N_q and M and will ultimately provide the

approximate solution of the PDE.

4.4 Least squares collocation using Patterson quadrature

Consider the basic approximate solution

$$\bar{\theta}(x,y) = \gamma_o(x,y) + \sum_{j=1}^{M} \alpha_j \psi_j(x,y) \qquad (47)$$

in which the upper limit of summation, M, is fixed. An efficient quadrature scheme is required such that

(i) N_q is small, yet the quadrature formula is accurate

and

(ii) the computation involved in the scheme is minimal.

It is well known that the Gaussian quadrature formulae satisfy the first requirement and within this class the Gauss-Legendre formula is particularly easy to apply since, in one dimension, the collocation points x_k are the zeroes of Legendre polynomials. Indeed it is these points which often form the basis of orthogonal collocation. Explicitly this quadrature formula is expressed as

$$\int_o^1 f(x)\,dx \approx \sum_{k=1}^{n} W_k f(x_k) = I_n \qquad (48)$$

where x_k (k=1,2, ..., n) are the zeroes of the n-th order Legendre polynomial $P_n(x)$, on $[0,1]$ and W_k(k=1,2, ..., n) are known constants. If the n-th order approximation I_n is not considered to be accurate, then a higher order approximation I_{n_1} ($n_1 > n$) will have to be evaluated. However, the zeroes of the Legendre polynomials of orders n and n_1 are all different and hence f(x) has to be evaluated at n_1 new points. Patterson[20,21] proposed a new quadrature formula in which all the quadrature points are retained and used in any higher order approximation. This quadrature formula is only slightly less accurate than the comparable Gauss-Legendre scheme and it has obvious computational advantages. In practice, when determining the convergence of the

quadrature formula, n is usually chosen to follow the sequence

{1,3,7,15,31, ...}

i.e.

$$\text{number of quadrature points at r-th iteration} = \sum_{\ell=1}^{r} 2^{\ell-1}$$

Thus the standard Gauss-Legendre scheme requires $\sum_{\ell=1}^{r} 2^{\ell-1}$ additional function evaluations at the r-th iteration, while Patterson quadrature requires only 2^{r-1} similar evaluations at the same iteration. For integrals in higher dimensions the difference in the number of additional function evaluations is even more significant. In two dimensions, for example, over the square domain $[0,1] \times [0,1]$ the difference at the r-th (r > 1) iteration is equal to the number of points at the (r-1)th iteration i.e. $\left[\sum_{\ell=1}^{r-1} 2^{\ell-1}\right]^2$.

Patterson quadrature points and weights therefore satisfy both requirements (i) and (ii) and will now be used as the basis of the collocation procedure. The points and weights are readily generated by extending Patterson's one dimensional integration routine once the domain S has been transformed to the square $[0,1] \times [0,1]$.

Assume that the domain S has been transformed to $[0,1] \times [0,1]$ and that the residual defined over $[0,1] \times [0,1]$ is $\mathcal{R}(\underline{\alpha},x,y)$. This assumption is not restrictive, as will be shown later. With the order of approximate solution M and the collocation points and weights specified, the number of collocation points is determined as follows. The parameters in the boundary conditions are initially assigned numerical values. Then the right hand sides of equations (46) are known and this set of equations is readily solved by recursive least squares. Hence, for a given value of $N_q = N_{q1}$, the values α_i(i=1, ..., M) are evaluated without the need of an explicit matrix inversion. The values of the residuals $\mathcal{R}_j(x_k,y_k)$ (j=1, ..., M), $\mathcal{R}_o(x_k,y_k)$ are stored during the process of the recursive least squares

algorithm and the summation

$$I_M(N_{q1}) = \sum_{k=1}^{N_{q1}} W_k \mathcal{R}^2(\underline{\alpha}, x_k, y_k) \tag{49}$$

is evaluated on termination of the algorithm. N_{q1} is then increased to N_{q2} and the resulting $\alpha_i (i=1, \ldots, M)$ are re-evaluated, again using recursive least squares. Since Patterson collocation points are employed, the residuals $\mathcal{R}_j(x_k,y_k)$ $(j=1, \ldots, M)$ and $\mathcal{R}_o(x_k,y_k)$ need only be evaluated at a few new points with the previously stored values being recalled within the algorithm. The relative error between $I_M(N_{q1})$ and $I_M(N_{q2})$ is then used as a convergence criterion for N_q. Thus, if ε_c is a given constant and

$$\left| \frac{I_M(N_{q1}) - I_M(N_{q2})}{I_M(N_{q2})} \right| < \varepsilon_c \tag{50}$$

then N_q is set equal to N_{q2} and the process is terminated. The final value of N_q is dependent upon M, a suitable value of which will now be determined. M is initially chosen to be m_1 and the corresponding N_q is evaluated by the scheme outlined above. M itself may be incremented to a new value m_2 and the whole process of determining a suitable N_q will be recommenced. The incrementation of M is then terminated when

$$\left| I_{m_2}(N_q(m_2)) - I_{m_1}(N_q(m_1)) \right| < \varepsilon_p \tag{51}$$

and the final value of M is chosen to be m_2. Thus, there now exists a rational method for calculating appropriate values of the constants N_q and M.

The method outlined above utilises a recursive least squares algorithm which in turn requires that the boundary condition parameters have been assigned specific numerical values. When a simulation of a PDE is required then all parameters will have values and thus the above method will give an accurate solution without the

need to perform any direct matrix inversion. However, the real power of the general polynomial approximation method is that boundary conditions may be explicitly contained in the final expansion and any subsequent optimisation of boundary condition parameters may often be performed analytically. The above discussion is still useful in this more general context since if the unspecified parameters are given realistic values then M and N_q together with corresponding collocation and weights are generated. The over determined system that has been solved by recursive least squares is of the form

$$c_A \underline{\alpha} = c_{\underline{b}} \tag{52}$$

where

$$c_{A_{ij}} = \sqrt{W_i}\,\mathcal{R}_j(x_i,y_i)$$

$$c_{b_i} = \sqrt{W_i}\,\mathcal{R}_o(x_i,y_i)$$

$$i = 1, \ldots, N_q$$

$$j = 1, \ldots, M$$

and throughout the recursive algorithm the values of $\mathcal{R}_j(x_i,y_i)$ and hence $c_{A_{ij}}$ have been stored. Thus the pseudo-inverse $(c_A{}^T c_A)^{-1} c_A{}^T$ can be calculated and the vector of unknowns $\underline{\alpha}$ is then expressed as a function of the boundary condition parameters by

$$\underline{\alpha} = (c_A{}^T c_A)^{-1} c_A{}^T \, c_{\underline{b}} \tag{53}$$

This evaluation is further simplified if the boundary condition parameters, $\underline{\tilde{Y}} = (\tilde{Y}_1, \ldots, \tilde{Y}_{N_c})$ say, enter into the boundary conditions only as multiplicative and additive constants. Then the residual due to the imposed boundary conditions may be expressed as

$$\mathcal{R}_o(x,y) = \sum_{\ell=1}^{N_b} f_\ell(\underline{\tilde{Y}})\, g_\ell\,(x,y) \tag{54}$$

and hence

$$\underline{\alpha} = (c_A{}^T c_A)^{-1}\, c_A{}^T B\, \underline{f} \tag{55}$$

where

$$B_{i\ell} = \sqrt{W_i}\, g_\ell(x_i,y_i)$$

$$f_\ell = f_\ell(\underset{\sim}{Y})$$

$$i = 1, \ldots, N_q$$

$$\ell = 1, \ldots, N_b$$

The final approximate solution is thus determined as an explicit function of the parameters in the boundary conditions.

4.5 The treatment of non-imposed boundary conditions

For many models described by PDE's it may be difficult or even impossible to simultaneously impose all the given boundary conditions on to the approximate solution. The effect of the non-imposed boundary conditions must still be included and should clearly influence the final approximate solution. Two situations are likely to lead to such a non-imposition

(i) there are a large number of boundary conditions,

(ii) one or more of the boundary conditions is defined over a complicated domain.

Consider firstly that only one boundary condition cannot be exactly imposed on the approximate solution. Let this boundary condition be of the form

$$\mathcal{L}_b[\theta] = f \tag{56}$$

where $\mathcal{L}_b$ is a time-invariant linear differential operator and f is some function, both defined over a given boundary Γ. The boundary residual $R_b(\underset{\sim}{\alpha},x,y)$, $(x,y)\varepsilon\Gamma$, may then be defined as

$$R_b(\underset{\sim}{\alpha},x,y) = \mathcal{L}_b[\hat{\theta}] - f \tag{57}$$

The vector $\underset{\sim}{\alpha}$ must be found such that both the interior and boundary residuals are simultaneously forced to zero. One obvious and convenient formulation which would achieve this is

$$\min_{\underset{\sim}{\alpha}} \int_S R^2(\underset{\sim}{\alpha},x,y)\, dS + \int_\Gamma R_b^2(\underset{\sim}{\alpha},x,y)d\Gamma \tag{58}$$

Once again, the equivalent collocation problem is sought and therefore

(58) is reposed as

$$\min_{\underset{\sim}{\alpha}} \sum_{k=1}^{N_q} W_k \mathcal{R}^2(\underset{\sim}{\alpha},x_k,y_k) + \sum_{\ell=1}^{N_{q1}} W_{\ell 1} \mathcal{R}_b^2(\underset{\sim}{\alpha},x_\ell,y_\ell) \tag{59}$$

where the interior residual $\mathcal{R}$ and the boundary residual $\mathcal{R}_b$ are defined over $[0,1] \times [0,1]$ and $[0,1]$ respectively. Clearly, the least squares solution of the over determined system

$$\sqrt{W_k}\,\mathcal{R}(\underset{\sim}{\alpha},x_k,y_k) = 0$$

$$k = 1, \ldots, N_q \quad (x_k,y_k)\varepsilon[0,1]\times[0,1] \tag{60}$$

$$\sqrt{W_{\ell 1}}\,\mathcal{R}_b(\underset{\sim}{\alpha},x_\ell,y_\ell) = 0$$

$$\ell = 1, \ldots, N_{q1} \quad x_\ell \text{ or } y_\ell \varepsilon [0,1] \tag{61}$$

The three constants M, N_q and N_{q1} and the associated collocation points and weights must now be determined. As before, M is given an initial value m_1 and $N_q(m_1)$ is evaluated by the procedure described in section 4.4. At the end of this process $\underset{\sim}{\alpha}$ will have a fixed value, $\underset{\sim}{\alpha}_1$ say. The same procedure is then repeated to determine $N_{q1}(m_1)$, the initial value of $\underset{\sim}{\alpha}$ being taken as $\underset{\sim}{\alpha}_1$ with the residual $\mathcal{R}_b$ being evaluated at various collocation points on $[0,1]$. When N_{q1} is judged to have converged $\underset{\sim}{\alpha}$ will have a new value, $\underset{\sim}{\alpha}_2$ say, which is a solution of (59) for the given M. M is then incremented and this whole process is repeated. The convergence criterion for M is taken as the error between two successive evaluations of the sum of the two total residuals i.e. the function being minimised in (59). The method of obtaining $\underset{\sim}{\alpha}$ as an explicit combination of imposed boundary condition parameters is then also as previously discussed and will yield expressions comparable to (53) and (55). Indeed, if any parameters in the non-imposed boundary conditions do not multiply any function of θ then it is also possible to express $\underset{\sim}{\alpha}$ in terms of such parameters.

Extension of this method to incorporate more than one non-imposed boundary condition is trivial and a more general situation may also be solved. Consider a total of q non-imposed boundary conditions with residuals ${}_jR_b(\underline{\alpha},x,y)$ where $(x,y) \in \Gamma_j$ $(j=1, \ldots, q)$. Consider also that

(i) the domain S is not readily transformable to $[0,1]\times[0,1]$ but that subdomains $S_1, \ldots, S_{p1}$ are individually transformable

and

(ii) the parameters which are involved in the basic PDE vary within S but are constant within each of the subdomains

$$S_{p1+1}, \ldots, S_p$$

Then, an approximate solution is provided by

$$\min_{\underline{\alpha}} \sum_{i=1}^{p} \int_{S_i} {}_iR^2(\underline{\alpha},x,y)dS_i + \sum_{j=1}^{q} \int_{\Gamma_j} {}_jR_b^2(\underline{\alpha},x,y)d\Gamma_j \qquad (62)$$

which is readily solved by extending the process outlined for one non-imposed boundary condition. The general outline of the procedure is shown by the flow diagrams of Figs. 5 and 6.

4.6 The application of least squares Patterson collocation to the 2DVB model.

The 2DVB model provides a useful illustration of the power and application of the theory developed in Section 4.5. Both the PDE (45) and its associated third boundary condition (16) are defined over non-regular domains. Moreover, the parameters involved in the terms W(x) and D(x) vary over the spatial domain S, but are constant within each subdomain S_1, S_2, S_3, the domains being shown diagramatically in Fig. 7. Therefore least squares Patterson collocation is immediately applicable to the 2DVB model while other standard forms of MWR or orthogonal collocation would not be.

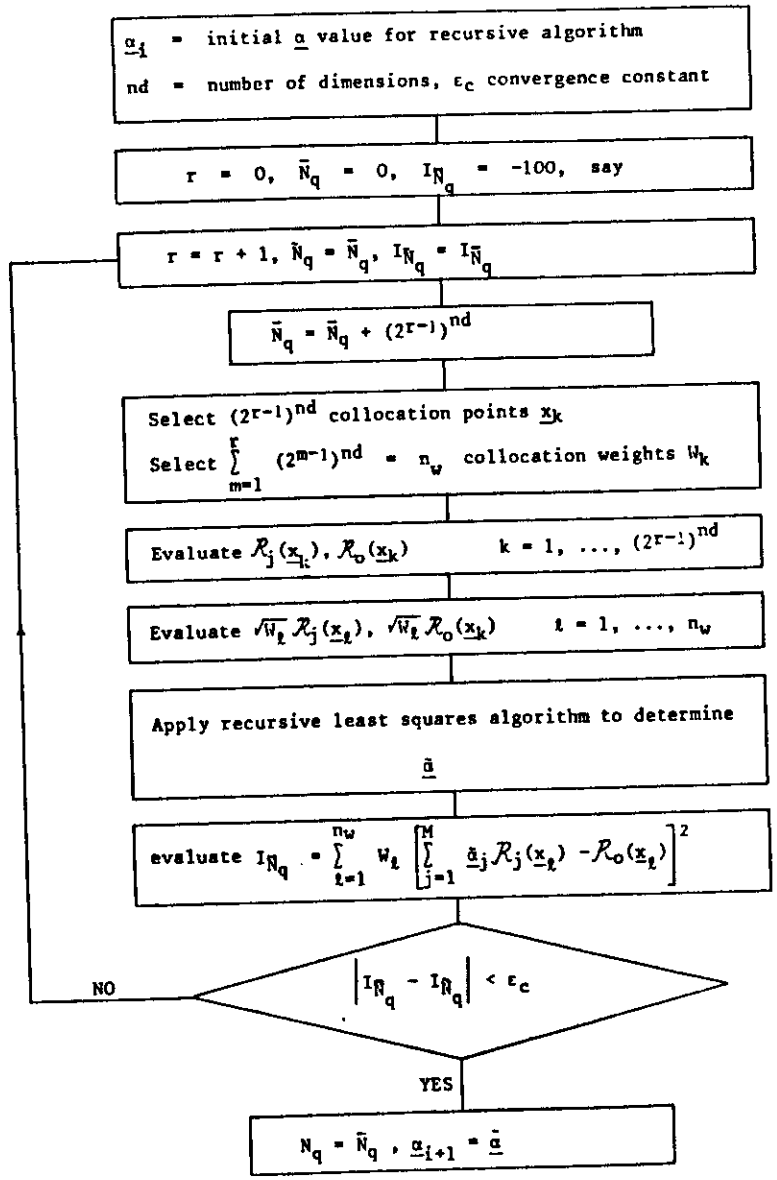


Fig. 5 - Recursive loop 1 - the determination of a suitable N_q value.

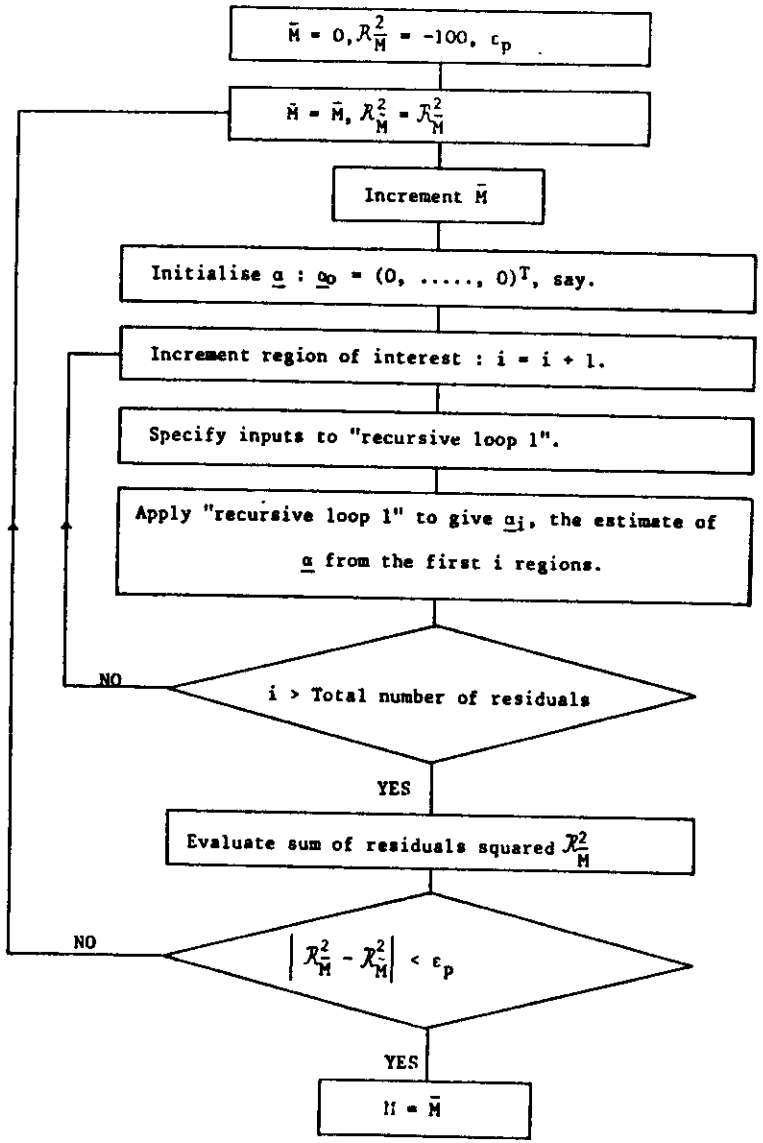


Fig. 6 - Recursive loop 2 - the determination of a suitable M value.

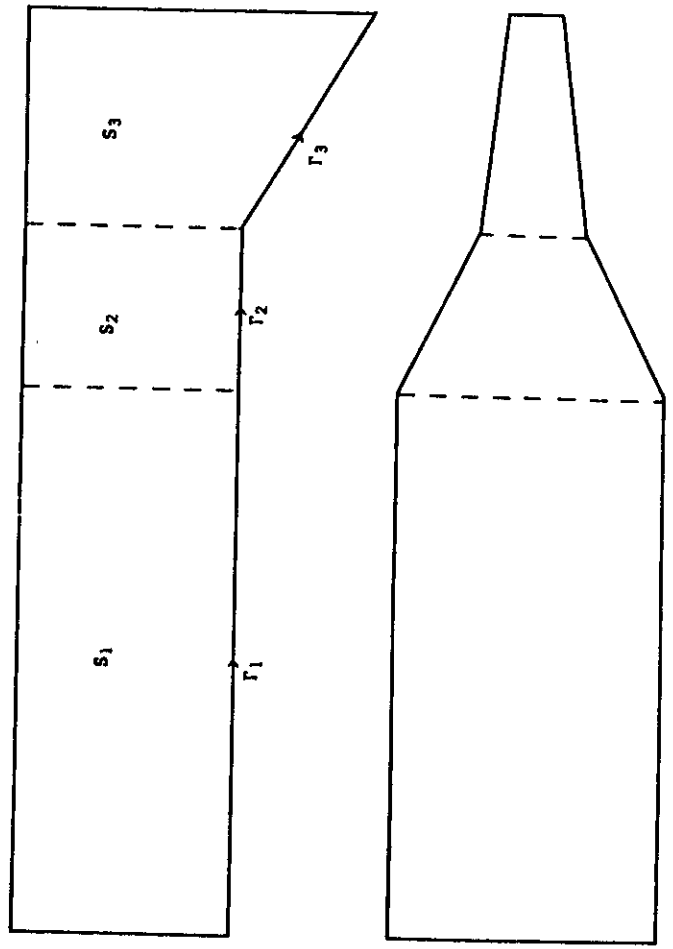


Fig. 7 - Domain definitions for the short forehearth.

It is easy to impose the first two boundary conditions

$$\theta(o,y) = \mu(y)$$

$$\theta(x,o) = \gamma_1(x)$$

onto an approximate solution. Thus, one convenient form of $\bar{\theta}(x,y)$ which satisfies both of these equations simultaneously is

$$\bar{\theta}(x,y) = \gamma_1(x) + \mu(y) - \mu(o) + xy \sum_{k=1}^{M} \alpha_k \psi_k(x,y) \qquad (63)$$

As discussed previously, the choice of Legendre polynomials as basis functions in one space dimension yields well conditioned equations and therefore a natural choice for $\psi_k(x,y)$ is a product of Legendre polynomials. Therefore (88) is assumed to take the form

$$\bar{\theta}(x,y) = \gamma_1(x) + \mu(y) - \mu(o) + xy \sum_{\substack{i,j=0 \\ i+j=k}}^{N} \alpha_k \bar{P}_i(x)\bar{P}_j(y) \qquad (64)$$

where $\bar{P}_i(x)$, $\bar{P}_j(y)$ are non-normalised Legendre polynomials which are orthogonal on $[0,1]$.

The interior residual is given by

$$R(\underline{\alpha},x,y) = \frac{\partial^2\bar{\theta}}{\partial y^2} - U(x,y)\frac{\partial\bar{\theta}}{\partial x} \qquad (65)$$

where

$$U(x,y) = \frac{\beta_1}{W(x)D(x)}\left[1 - \frac{y^2}{D^2(x)}\right]$$

and

$$\beta_1 = \frac{3\,M_f\,c\,D_{max}}{2\,K_g\,L\,W_{max}}$$

in the nomenclature of section 1. The residual $R_o(x,y)$ due to the imposed boundary conditions is

$$^{\ell}R_o(x,y) = \frac{\partial^2\mu}{\partial y^2} - U_{\ell}(x,y)\frac{\partial\gamma_1}{\partial x}$$

$$= \mu''(y) - U_{\ell}(x,y)\dot{\gamma}_1(x) \qquad (66)$$

where

$$' = \frac{d}{dy}, \quad '' = \frac{d^2}{dy^2}, \quad \cdot = \frac{d}{dx}$$

and $U_{\ell}(x,y) = U(x,y)$ in zone ℓ (ℓ=1,2,3).

The contribution to the interior residual from a basis function $xy\psi_k(x,y) = xy\,\bar{P}_i(x)\bar{P}_j(y)$ is

$$^{\ell}R_k(x,y) = \frac{\partial^2}{\partial y^2}\left[xy\bar{P}_i(x)\bar{P}_j(y)\right] - U_{\ell}(x,y)\frac{\partial}{\partial x}\left[xy\bar{P}_i(x)\bar{P}_j(y)\right]$$

$$= 2x\bar{P}_i(x)\bar{P}_j'(y) + xy\,\bar{P}_i(x)\bar{P}_j''(y)$$

$$-U_{\ell}(x,y)\left[y\bar{P}_i(x)\bar{P}_j(y) + xy\dot{\bar{P}}_i(x)\bar{P}_j(y)\right] \qquad (67)$$

where the connection between i, j and k is inferred from the summation (64).

Since the interior residual has different parameters in each of the three zones S_1, S_2, S_3 it is necessary to transform the integral of residual squared over each zone into the equivalent integral over $[0,1] \times [0,1]$. The most general integral is that over S_3, the integrals over S_1 and S_2 being simplifications of it. Therefore the determinant, $J_3(\bar{x},\bar{y})$, $(\bar{x},\bar{y})\in[0,1]\times[0,1]$, of the Jacobian matrix is sought such that

$$\int_{S_3} {}^3R^2(\underline{\alpha},x,y)dy\,dx = \int_{x_2}^{x_3}\int_{o}^{a+bx} {}^3R^2(\underline{\alpha},x,y).dydx$$

$$= \int_0^1\int_0^1 J_3(\bar{x},\bar{y})\,{}^3R^2(\underline{\alpha},\bar{x},\bar{y})d\bar{y}d\bar{x}$$

$$= \int_0^1\int_0^1 {}^3\bar{R}^2(\underline{\alpha},\bar{x},\bar{y})d\bar{y}d\bar{x} \qquad (68)$$

Two simple transformations from S_3 to $[0,1] \times [0,1]$ are

$$\bar{x} = \frac{x-x_3}{x_3-x_2}$$

$$\bar{y} = \frac{y}{a+bx}$$

i.e.

$$x = (x_3-x_2)\bar{x} + x_2 \qquad (69)$$

$$y = (a+bx)\bar{y} \qquad (70)$$

$$\therefore J_3(\bar{x},\bar{y}) = \det \begin{bmatrix} \frac{\partial y}{\partial \bar{y}} & \frac{\partial y}{\partial \bar{x}} \\ \frac{\partial x}{\partial \bar{y}} & \frac{\partial x}{\partial \bar{x}} \end{bmatrix}$$

$$= \det \begin{bmatrix} a+b\{x_2+\bar{x}(x_3-x_2)\} & b(x_3-x_2)y \\ 0 & (x_3-x_2) \end{bmatrix}$$

$$\therefore J_3(\bar{x},\bar{y}) = (a+bx)\,(x_3-x_2) \tag{71}$$

where x is related to $\bar{x}$ by the linear transformation (69). The corresponding transformations in zones S_1 and S_2 have an identical form to (71) with

$x_3 \to x_2$			$x_3 \to x_1$		
$x_2 \to x_1$			$x_2 \to x_0$		
$b \to 0$			$b \to 0$		
$a \to d_1$	in S_2		$a \to d_1$	in S_1	(72)

$$\therefore J_2(\bar{x},\bar{y}) = d_1(x_2-x_1) \tag{73}$$

$$J_1(\bar{x},\bar{y}) = d_1(x_1-x_0) \tag{74}$$

The third boundary condition, which is defined by

$$K_g \left.\frac{\partial \theta}{\partial y}\right|_{y=D(x)} = \gamma_2(x)\left[\theta-\theta_{ba}\right]_{y=D(x)}$$

where the parameters in $\gamma_2(x)$ vary over $\Gamma_2(y=D(x))$, but are constant within each subsection $\Gamma_1,\Gamma_2,\Gamma_3$, must now be accounted for. The boundary residual due to the imposed boundary conditions is

$${}^{m}R_{bo}(x) = K_g\mu'(y) - {}^{m}\gamma_2(x)\left[\gamma_1(x)+\mu(y)-\mu(o)-\theta_{ba}\right]_{y=D_m(x)} \tag{75}$$

while the boundary residual arising from the basis function $xy\,\psi_k(x,y) = xy\bar{P}_i(x)\bar{P}_j(y)$ is

$${}^{m}R_{bk}(x) = K_g\left[x\bar{P}_i(x)\bar{P}_j(y) + xy\bar{P}_i(x)\bar{P}_j'(y)\right]_{y=D_m(x)} - {}^{m}\gamma_2(x)\left[xy\bar{P}_i(x)\bar{P}_j(y)\right]_{y=D_m(x)} \tag{76}$$

where ${}^{m}\gamma_2(x)$ and $D_m(x)$ denote the functions $\gamma_2(x)$ and $D(x)$ in zone

$\Gamma_m(m=1,2,3)$. Each line integral is now redefined over $[0,1]$ by means of a simple linear transformation. Thus

$$\int_{\Gamma_3} {}^{3}R_b^2(x,y)d\Gamma_3 = \int_{x_2}^{x_3} {}^{3}R_b^2(x)dx$$

$$= \int_0^1 (x_3-x_2)^2\ {}^{3}R_b^2(\bar{x})d\bar{x}$$

$$= \int_0^1 {}^{3}\mathcal{R}^2(\bar{x})d\bar{x} \tag{77}$$

where

$$x = (x_3-x_2)\bar{x} + x_2$$

Identical transformations with the substitutions (72) also redefine the integrals over Γ_2 and Γ_1.

The approximate solution of the 2DVB model is therefore given by

$$\min_{\underline{\alpha}} \sum_{\ell=1}^{3}\int_0^1\int_0^1 {}^{\ell}\mathcal{R}^2(\underline{\alpha},\bar{x},\bar{y})d\bar{y}d\bar{x} + \sum_{m=1}^{3}\int_0^1 {}^{m}\mathcal{R}_b^2(\underline{\alpha},\bar{x}) \tag{78}$$

where

$${}^{\ell}\mathcal{R} = \sqrt{J_{\ell}(\bar{x},\bar{y})}\left[\sum_{\substack{i,j=0\\ i+j=k}}^{N} \alpha_k\,{}^{\ell}\mathcal{R}_k(\bar{x},\bar{y}) - {}^{\ell}\mathcal{R}_o(\bar{x},\bar{y})\right] \tag{79}$$

$${}^{m}\mathcal{R}_b = \sqrt{(x_m-x_{m-1})}\left[\sum_{\substack{i,j=0\\ i+j=k}}^{N} \alpha_k\,{}^{m}\mathcal{R}_{bk}(\bar{x}) - {}^{m}\mathcal{R}_{bo}(\bar{x})\right] \tag{80}$$

$$\ell = 1,2,3 \qquad m = 1,2,3$$

and the Jacobians, residuals and transformations $x \to \bar{x}$, $y \to \bar{y}$ have all been defined. Thus the 2DVB model can now be solved by least squares Patterson collocation.

4.7 Results.

Before considering the optimisation of boundary condition parameters the validity of the whole Patterson collocation technique must be demonstrated. This will be done by showing that when all the boundary condition and PDE parameters are specified that

i) the solution converges for increasing M

and

ii) the convergent solution is correct.

Since the 2DVB model does not possess an analytic solution, the accuracy of the convergent polynomial approximation can only be demonstrated by a direct comparison with a solution provided by a conventional numerical technique. A suitable finite difference scheme has been produced by Whitfield for this comparison.

The dimensions of a specific forehearth, which is heat-conditioning green glass, are illustrated in Figs. 3 and 4, while all other physical constants are listed below:

$K_g = 6$ W m^{-1} $°C^{-1}$

$c = 840.12$ J kg^{-1} $°C^{-1}$

$\rho = 2350.0$ kg m^{-3}

$K_r = 1.54$ W m^{-1} $°C^{-1}$

$K_b = 0.34$ W m^{-1} $°C^{-1}$

throughput = 23 Tonne/day

i.e, $M_f = 0.2662$ kg sec^{-1} .

Equations (11) and (13), which express the effective conductance of the refractory at the bottom of the forehearth as a function of the conductivities K_r and K_b and the corresponding dimensions, are extremely cumbersome and therefore, with all the constants as supplied above, an approximation to $K_{eff}(x)$ was sought which could rapidly be evaluated.

Quadratic polynomials ${}^{i-}\gamma_2(x)$ were derived for each zone i (i = 1,2,3) via quadratic interpolation as

$$ {}^{1-}\gamma_1(X) = (-2.198)L \tag{81} $$

$$ {}^{2-}\gamma_2(X) = (-0.7399 + 2.900X - 4.870Z^2)L \tag{82} $$

$$ {}^{3-}\gamma_3(X) = (-0.08059 + 0.1009X - 2.331X^2)L \ . \tag{83} $$

A further simplification of the third boundary condition was achieved by assuming that the temperature at the brick/air interface, T_{ba}, was constant and equal to 130°C.

It has already been shown that the inlet and surface temperature profiles, which describe the first two boundary conditions may be well approximated by a linear and a quadratic polynomial respectively. Therefore $\mu(y)$ and $\gamma_1(x)$ are taken to be

$$ \mu(y) = \mu_0 + \mu_1 y \tag{84} $$

$$ \gamma_1(x) = \gamma_{10} + \gamma_{11}x + \gamma_{12}x^2 \tag{85} $$

the back-block and spout being convenient points at which to compare both measured, finite difference and Patterson collocation results.

For the inlet and surface boundary conditions as shown in Fig. 8, the collocation procedure described in section 4.6 was

followed with the convergence constant ε_c set equal to 0.02, yielding a relatively accurate quadrature formula. The number of collocation points was found to be

$$N_q = 49, \quad N_{q1} = 7 \text{ in each zone for } N = 2$$

$$N_q = 255, \quad N_{q1} = 15 \text{ in each zone for } 3 \leq N \leq 7 \ .$$

Convergence of the Patterson collocation technique is clearly shown in Fig. 7 by the monotonically decreasing sum of squared residuals. Figs. 8 and 9 show that the approximate polynomial solution does in fact converge to the finite difference solution and that N = 6 provides an accurate solution of the 2DVB model.

With the value of N determined, a comparison of the temperature profiles predicted by the 2DVB model with measured profiles is now possible. On the short forehearth under consideration there are two temperature sensors at distances 2.76m and 4.04m along the forehearth. The quadratic polynomial approximation to the surface temperature is determined by interpolation between the temperatures at the two sensors and the projected surface temperature at the inlet. Fig. 10 shows the agreement between profiles measured by Hamilton and the 2DVB model when solved by finite difference and by Patterson collocation with N = 6. Clearly the 2DVB model compares favourably with the measured values and also with other analytic models e.g., the model of Abbott and Whitfield[22] or the 2DL model of Carling.

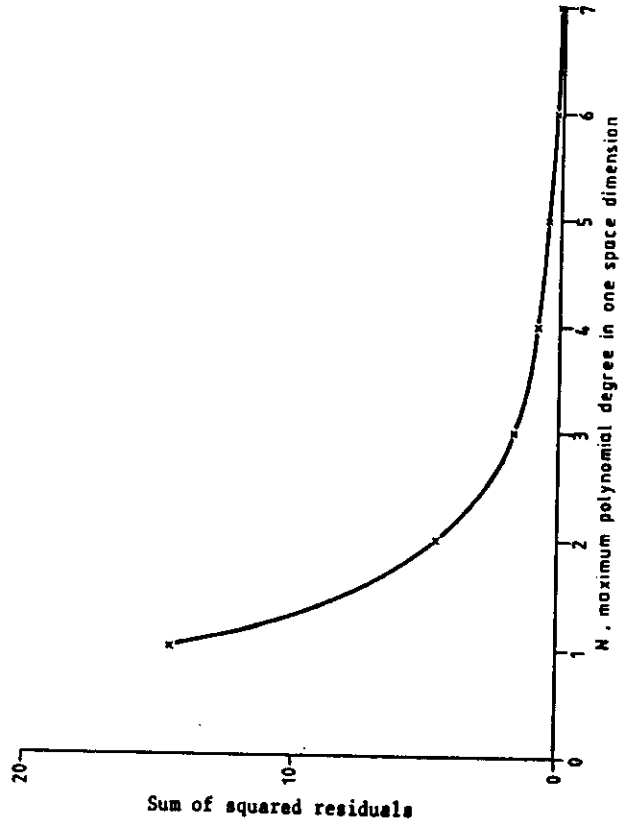


Fig. 7 - Convergence of the sum of squared residuals to zero with increasing order of approximation.

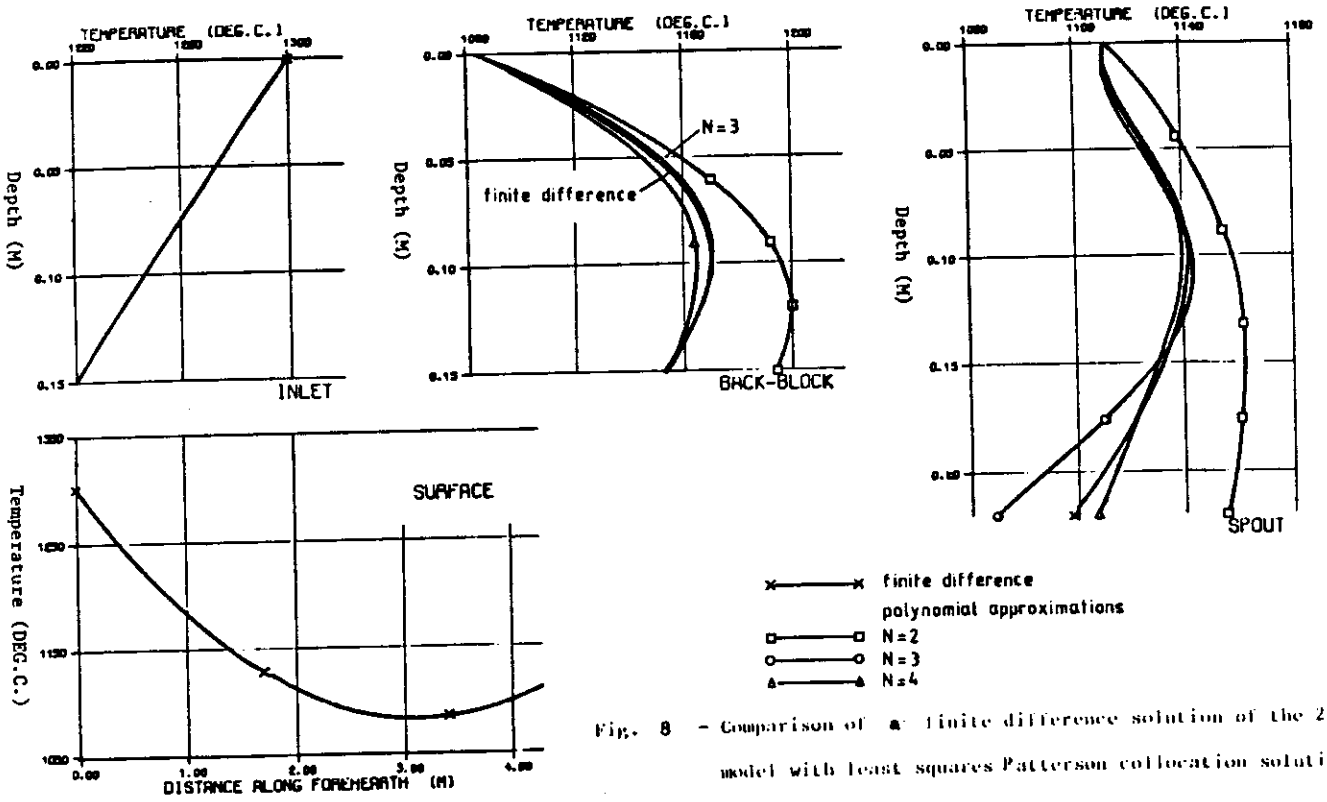


Fig. 8 - Comparison of a finite difference solution of the 2DVB model with least squares Patterson collocation solutions for N = 2,3,4.

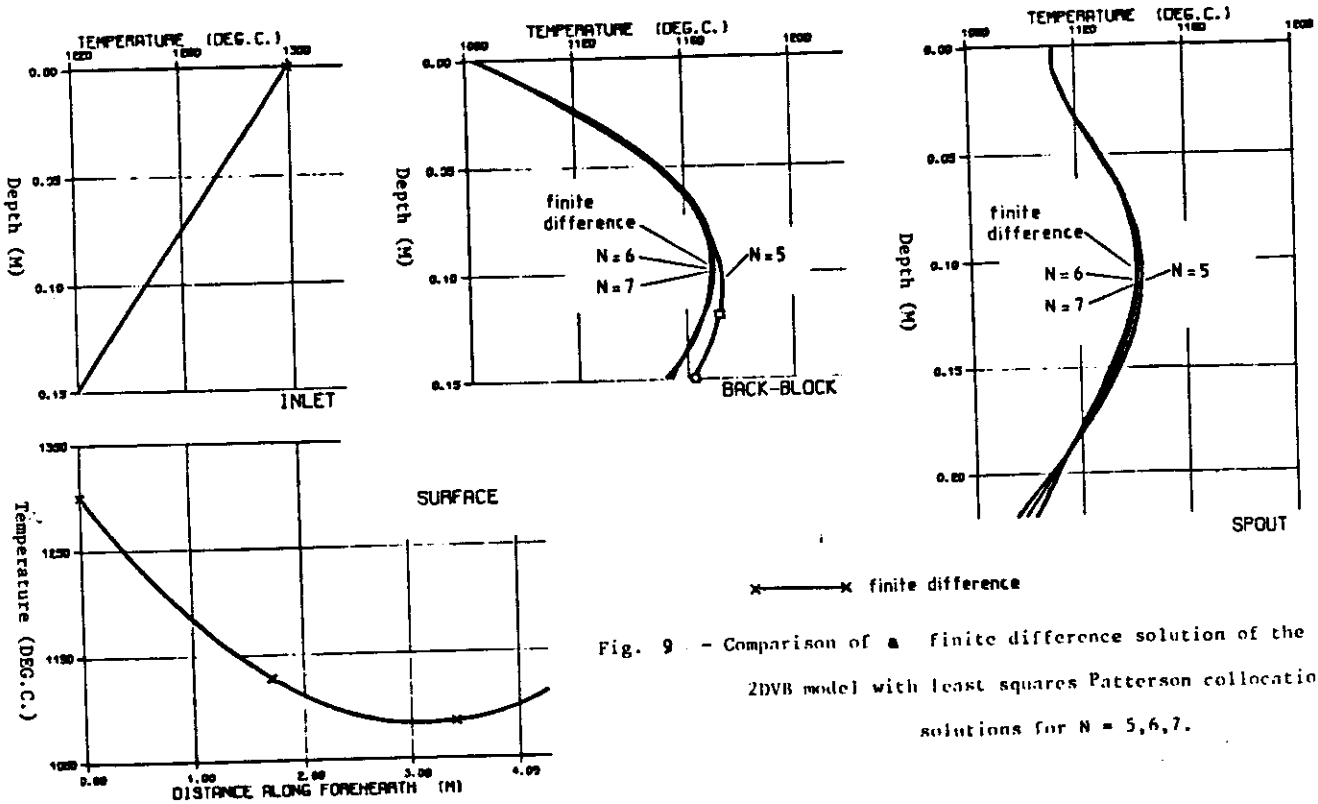


Fig. 9 - Comparison of a finite difference solution of the 2DVB model with least squares Patterson collocation solutions for N = 5,6,7.

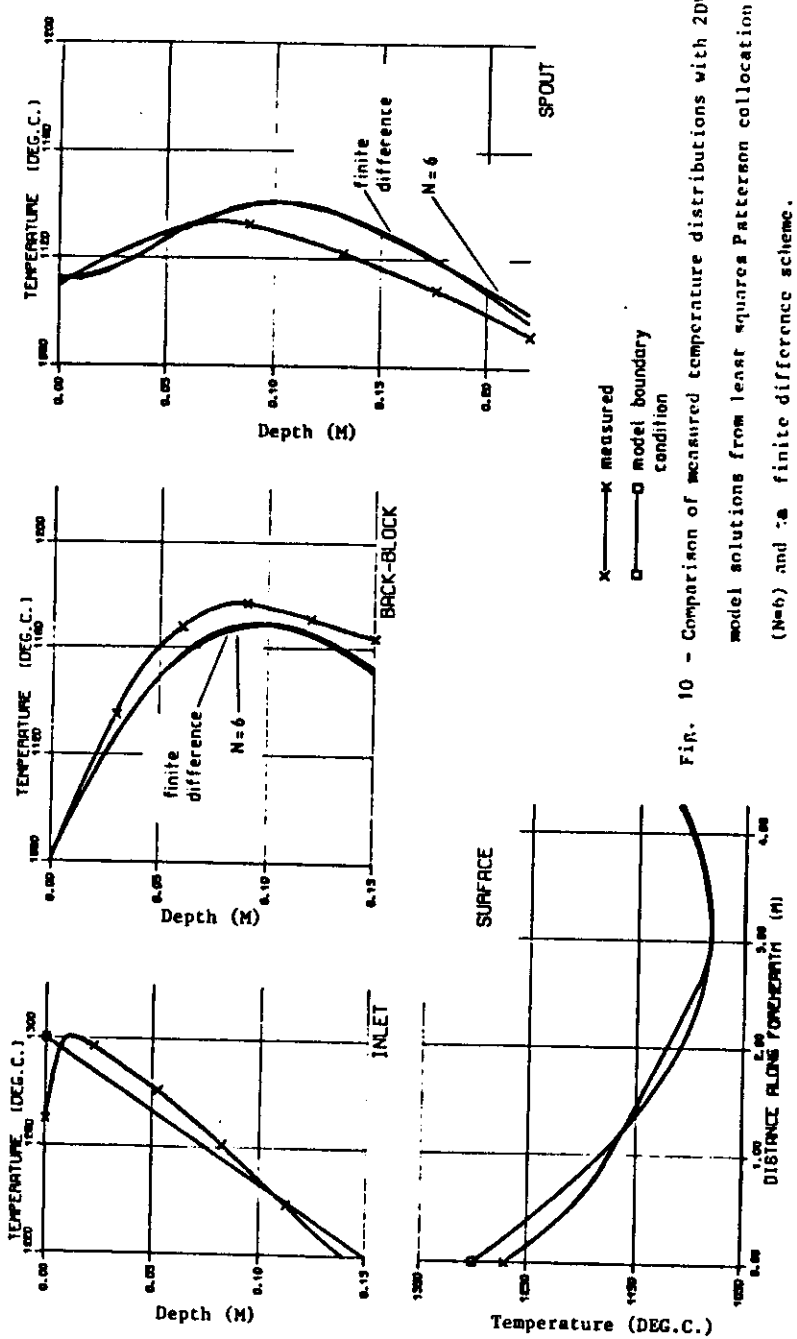


Fig. 10 - Comparison of measured temperature distributions with 2DVB model solutions from least squares Patterson collocation (N=6) and a finite difference scheme.

5. OPTIMISATION OF STEADY-STATE FOREHEARTH OPERATING CONDITIONS.

5.1 The Identification of Control Parameters.

The purpose of the forehearth is to heat-condition glass which has been melted down in a furnace so that the glass leaves the forehearth with a uniform desired temperature and is then suitable for moulding. Thus the temperature of the glass at the spout is required to be a given constant throughout its depth. For a specific forehearth and a fixed throughput of glass only the inlet and surface temperature profiles may be varied to control the outlet temperature. Indeed, the inlet temperature may also be predetermined by the operating conditions within the furnace, leaving only the surface profile as variable and this will itself be constrained by the geometry of the cooling and conditioning zones. Under the assumption that the inlet and surface temperature profiles may be adequately approximated by a linear and a quadratic polynomial respectively then in the most general operating situation there are four parameters μ_1, γ_{10}, γ_{11}, γ_{12} which may be available to control the outlet temperature. This follows since the further assumption that the inlet and surface profiles concur at (X, Y) = (0, 0) implies that $\mu_0 = \gamma_{10}$. If the inlet temperature is controllable at all, it is only to the extent that its mean value may be varied while the shape of its profile is fixed. Thus the difference in the temperature of the glass between its surface and the bottom of the forehearth is assumed to be a prescribed constant T_e and this in turn determines μ_1

$$\mu_1 = \frac{(0, 0) - (0, 0)}{d} \tag{86}$$

$$\therefore \mu_1 = \frac{T_e}{d(T_a - T_r)} \tag{87}$$

and in general only the three parameters γ_{10}, γ_{11}, γ_{12} will be controllable.

5.2 The Development of Suitable Performance Criteria.

It is now required to consider performance criteria which indicate the deviation of the predicted temperature distribution at the spout from the desired value. Since the polynomial approximation method yielded an expression for the inlet temperature as an explicit combination of the control parameters a general analytic performance criterion is sought. Thus, in the non-dimensional co-ordinate system a suitable "cost function" is

$$C = \int_0^1 \omega(y) \left[T(1, y) - T_d\right]^2 dy \qquad (88)$$

and if the reference temperature in the non-dimensional temperature variable is chosen as $T_r = T_d$ then C is simply expressed as

$$C = \left(T_a - T_r\right)^2 \int_0^1 \omega(y) \left[\theta(1, y)\right]^2 dy \quad . \qquad (89)$$

Two specific forms of the weighting function $\omega(y)$ will be applied. The first is $\omega(y) = 1$, which is a Lengendre weighting on [0, 1] and gives a strict least squares cost function. The minimisation of such a cost function is known to yield an optimum profile with an uneven error distribution over the non-dimensional depth y. In particular, the errors tends to be larger at both ends of the interval [0, 1] and this could lead to an undesirable outlet temperature distribution. Therefore a second cost function which weights both ends of the interval [0, 1] more heavily than the remainder of [0, 1] is also considered. This cost function has

$$\omega(y) = \frac{1}{\sqrt{y(1 - y)}}$$

which is a Chebyshev weighting on [0, 1] and is known to yield a smoother optimum error distribution. Thus the following two cost functions will be used

$$\text{cost function 1} = (T_a - T_r)^2 \int_0^1 \theta^2(1, y)\, dy \qquad (90)$$

$$\text{cost function 2} = (T_a - T_r)^2 \int_0^1 \frac{\theta^2(1, y)\, dy}{[y(1 - y)]^{\frac{1}{2}}} \quad . \qquad (91)$$

5.3 The Imposition of Constraints on the Surface Temperature Profile.

A range of operating conditions were investigated and it proved necessary to impose one hard constraint on the surface temperature profile. Specifically, if the temperature of the glass at its surface falls below 1080°C then a "freezing" effect, which is to be avoided, ensues. The short forehearth under consideration has a cooling zone which starts at the inlet and extends to the back-block, non-dimensional distance x_2 along the forehearth, followed by a conditioning zone from that point to the end of the forehearth. It is therefore reasonable to assume that the minimum temperature along the length of the glass surface will occur at the back-block. In non-dimensional terms, the above constraint is then expressed as

$$\theta(x, 0) \geq \theta_m \qquad (92)$$

where

$$\theta_m = \frac{1080 - T_r}{T_a - T_r} \qquad (93)$$

and under the further assumption of a quadratically distributed surface temperature, the constraint becomes

$$\gamma_{10} + \gamma_{11}x + \gamma_{12}x^2 \geq \theta_m \quad . \tag{94}$$

Now, since the minimum of the quadratic polynomial

$$\gamma_{10} + \gamma_{11}x + \gamma_{12}x^2$$

occurs at

$$x_m = -\frac{\gamma_{11}}{2\gamma_{12}} \tag{95}$$

and such a minimum is assumed to occur at the back-block, non-dimensional distance x_2, along the forehearth, then (95) simplifies to

$$\gamma_{11} = -2\gamma_{12}x_2 \tag{96}$$

and (94) reduces to

$$\gamma_{10} - \gamma_{12}x_2^2 \geq \theta_m \tag{97}$$

which is clearly linear in γ_{10} and γ_{12}.

5.4 Optimisation via Polynomial Approximation.

It is now shown that the boundary condition control parameters enter linearly into the approximate polynomial solution $\bar{\theta}(x, y)$ and quadratically into the general cost function (89). Hence the unconstrained optimisation of the general cost function eventually yields a set of linear equations which are solved to give optimum parameter values.

The basic approximate solution of the 2DVB model is given by least squares Patterson collocation as

$$\bar{\theta}(x, y) = \gamma_1(x) + \mu(y) - \mu(0) + xy \sum_{i,j=0}^{N}{}' \alpha_k \bar{P}_i(x)\, \bar{P}_j(y)$$

where $\sum_{i,j=0}^{N}{}'$ denotes that the index k within the summation sign is chosen by

$$k = \frac{n(n+1)}{2} + (i+1) \quad \text{for } i, j = 0,1,\ldots,N;\ i + j = n;$$

$$n = 0,1,\ldots,N$$

$\underline{\alpha}$ is the solution of the linear equations

$$\left[A_1 + A_2\beta_1 + A_3\beta_1^2\right] \underline{\alpha} = \left[A_4 + A_5\beta_1\right] \underline{c}$$

where A_1, A_2, A_3, A_4, A_5 are matrices generated by the collocation procedure and

$$\underline{c} = \left[\beta_1\gamma_{11},\ \beta_1\gamma_{12},\ 1,\ \mu_1,\ \gamma_{10},\ \gamma_{11},\ \gamma_{12}\right]^T \quad .$$

Consider optimisation of the general cost function (89) with respect to μ_1, γ_{10}, γ_{11}, γ_{12} i.e., both the inlet and surface profiles are unconstrained. If ζ_i denotes any one of these parameters then the optimum with respect to ζ_i is given by the solution of

$$\frac{\partial}{\partial\zeta_i}\left[(T_a - T_r)^2 \int_0^1 \omega(y)\, \bar{\theta}^2(1, y)dy\right] = 0 \quad .$$

Thus if T_a is chosen as a constant independent of μ_1, γ_{10}, γ_{11}, γ_{12} then the required solution is that of

$$\int_0^1 \omega(y)\, \bar{\theta}(1, y)\, \frac{\partial\bar{\theta}}{\partial\zeta_i}(1, y)dy = 0 \quad . \tag{98}$$

The following definitions simplify the notation

$$\xi_1(y) = \frac{\partial\bar{\theta}}{\partial\mu_1}(1, y) = y + y \sum_{i,j=0}^{N}{}' \bar{P}_i(1)\, \bar{P}_j(y)\, G_k \tag{4}$$

$$\xi_2(y) = \frac{\partial\bar{\theta}}{\partial\gamma_{10}}(1, y) = 1 + y \sum_{i,j=0}^{N}{}' \bar{P}_i(1)\, \bar{P}_j(y)\, G_k \tag{5}$$

$$\xi_3(y) = \frac{\partial \bar{\theta}}{\partial \gamma_{11}}(1, y) = 1 + y \sum_{i,j=0}^{N'} \bar{P}_i(1)\, \bar{P}_j(y)\left\{G_k^{(6)} + \beta_1 G_k^{(1)}\right\}$$

$$\xi_4(y) = \frac{\partial \theta}{\partial \gamma_{12}}(1, y) = 1 + y \sum_{i,j=0}^{N'} \bar{P}_i(1)\, \bar{P}_j(y)\left\{G_k^{(7)} + \beta_1 G_k^{(2)}\right\}$$

$$\xi_5(y) = y \sum_{i,j=0}^{N'} \bar{P}_i(1)\, \bar{P}_j(y)\, G_k^{(3)}$$

where

$$G_k^{(m)} = \sum_{\ell=1}^{M} \left[A_1 + A_2\beta_1 + A_3\beta_1^2\right]^{-1}_{k\ell} \left[A_4 + A_5\beta_1\right]_{\ell m}$$

$$M = (N + 1)(N + 2)/2$$

and

$$\left[A_1 + A_2\beta_1 + A_3\beta_1^2\right]^{-1}_{k\ell}$$

denotes the element in the k-th row and the ℓ-th column of

$$\left[A_1 + A_2\beta_1 + A_3\beta_1^2\right]^{-1}$$

and a similar notation holds for $\left[A_4 + A_5\beta_1\right]$.

Then (98) has the general form

$$\sum_{j=1}^{4} \zeta_j \int_0^1 \omega(y)\, \xi_j(y)\, \xi_i(y)\, dy = -\int_0^1 \omega(y)\, \xi_5(y)\, \xi_i(y) dy \qquad (99)$$

and optimisation with respect to any combination of the ζ_i is attained by solving the corresponding set of linear equations provided by (99). The Hessian matrix should also be proved positive definite to guarantee a minimum of cost function.

The restriction on the surface temperature given by the constraint of section 5.3 is applied by first performing unconstrained optimisation of the parameters γ_{10}, γ_{11}, γ_{12} if the inlet temperature T(0, 0) is not specified, or similar optimisation of γ_{11}, γ_{12} if T(0, 0) is specified. If the resulting optimum parameters violate the inequality constraint (97) then the equality constraint

$$\gamma_{10} - \gamma_{12}x_2^2 = \theta_m \qquad (100)$$

must certainly be satisfied. Thus (98) yields the substitution

$$\gamma_{12} = \frac{1}{x_2^2}\left[\gamma_{10} - \theta_m\right] \qquad (101)$$

and the problem becomes unconstrained optimisation of a quadratic cost function and hence the optimum parameters subject to the inequality constraint (92) are also found from the solution of a set of linear equations.

5.5 Results.

The theory outlined above has been applied to the forehearth shown in Figs. 3 and 4 with green glass constants as previously specified. Following section 4, the highest order of Lengendre polynomial in the basis functions was chosen to be N = 6, the difference between the inlet temperatures at the glass surface and the bottom of the forehearth fixed at T_e = 80°C and the required temperature at the spout was taken to be T_d = 1100°C.

For the standard throughput of 23 tonne/day the unconstrained surface and inlet profiles predicted by the analytic formulae were found to be physically unfeasible. Thus, for a throughput of

23 tonne/day the inequality constraint (92) which guarantees a realisable profile, must be imposed. The resultant optimum surface and inlet profiles, together with the predicted back-block and spout temperature distributions, are shown graphically in Fig. 11 for both cost functions. Both sets of profiles compare favourably with those Hamilton obtained by numerical experimentation .

The optimum distributions at the spout also illustrate the applicability of the Chebyshev weighting which defines cost function 2; the large error at the bottom of the forehearth with the Legendre weighting producing an undesirable deviation from the required temperature at this point.

The most feasible range of inlet surface temperatures is 1200°C - 1300°C and the effect of constraining T(0, 0) to lie within this range was investigated for throughputs ranging from 15 tonne/day to 35 tonne/day. With the inequality constraint (92) imposed on the optimisation of the surface profile, the variations of cost function 2 with inlet temperature T(0, 0) are shown in Fig. 12. The graphs clearly demonstrate the importance of maintaining T(0, 0) at the optimum value. This is particularly true of the higher throughputs for which the large curvature of both cost functions indicates that a small step away from the optimum T(0, 0) will lead to a considerably poorer outlet profile. The approximately constant level of optimum cost function values in Fig. 12 illustrates another, less obvious, fact, i.e. an increase of throughput from 15 tonne/day to 35 tonne/day will yield the same quality of glass output provided that the respective T(0, 0) optima are maintained.

A numerical optimisation of the boundary conditions based on

the finite difference scheme has also been performed to verify the results produced by the polynomial approximation and to illustrate typical computational requirements. This technique involved the optimisation of the cost functions with respect to the boundary condition parameters, such parameters being adjusted by the Powell method . Each update of the parameters requires a re-evaluation of the cost function by a new finite difference simulation and, as Table 1 shows, computation time increases rapidly with the number of optimisable parameters.

With reference to Table 1, all off-line computation is performed in simulation 1 and for a specified structure such a simulation is only required once. Optimisations 4, 5 and 6 are a little misleading in that they appear to indicate an increase in computation time for a decreasing number of optimisable parameters when applying the polynomial approximation; this is simply due to the functioning of the computer program which requires more input/output for an increasing number of constraints.

In several situations, e.g. the overall refiner/forehearth operation, many more than three parameters may need to be optimised and the classical approach of coupling a finite difference with numerical optimisation would be impracticable while the polynomial approximation obtained by least squares Patterson collocation remains entirely feasible.

Table 2, showing storage requirements, provides a further illustration of the applicability of polynomial approximation once a single least squares Patterson collocation solution has been performed.

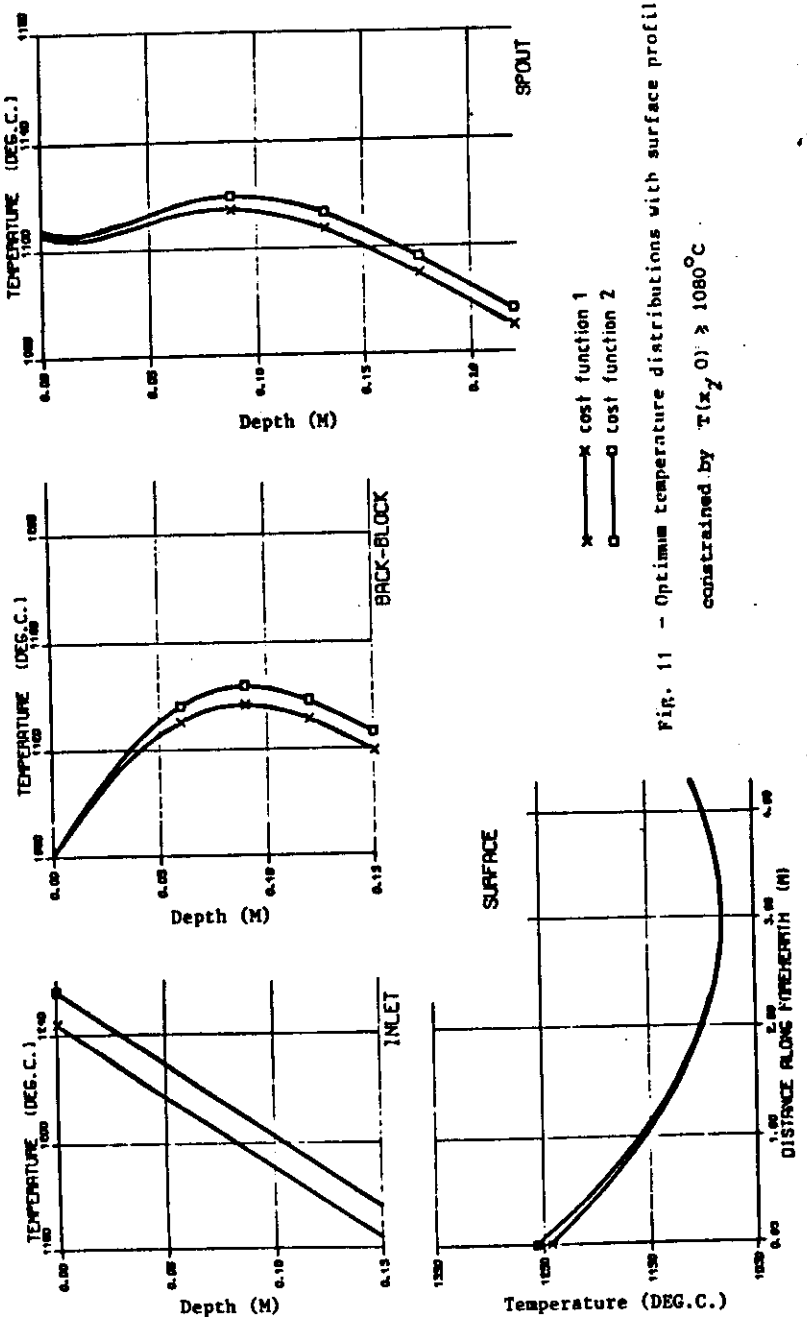


Fig. 11 - Optimum temperature distributions with surface profile constrained by $T(x_2, 0) \geq 1080^{\circ}C$

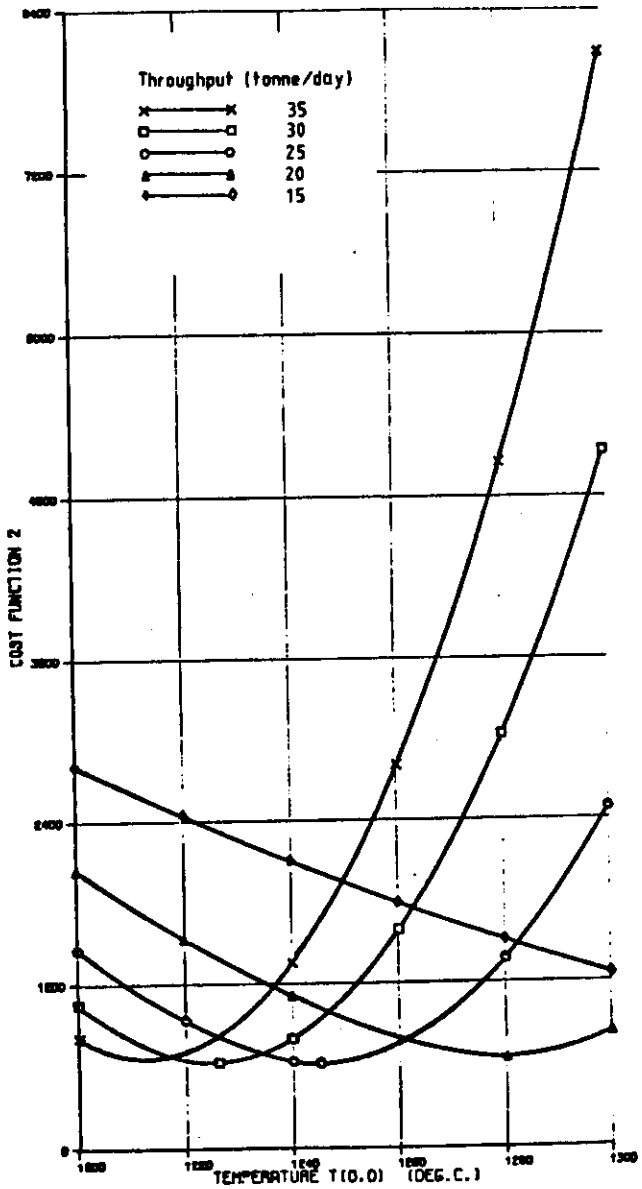


Fig. 12 - Variation of cost function 2 with inlet temperature T(0,0) with surface profile constrained by $T(x_2, 0) \geq 1080^{\circ}C$

Table 1

A comparison of CPU times (secs) for various simulations of the 2DVB model and optimisations of boundary temperature profiles.

Simulation/ optimisation	Least squares Patterson collocation	Finite difference
1	299.041	1.033
2	3.415	1.033
3	1.127	1.033
4	1.528	1.630
5	1.500	21.156
6	1.429	93.076

Simulation/ optimisation	Description
1	Simulation, with output, for specified forehearth structure, glass constants, T_{ba} and boundary temperature parameters. Patterson collocation procedure has N = 6.
2	Assuming simulation 1 has been performed once, this is a simulation, with output, for a change in the parameter β_1.
3	Assuming simulation 1 has been performed once, this is a simulation, with output, for a change in any of the boundary temperature profile constants μ_o, μ_1, γ_{10}, γ_{11}, γ_{12}.
4	Optimisation with surface profile constrained, inlet temperature profile specified: a 1 parameter optimisation.
5	Optimisation with surface profile constrained, T_e specified: a 2 parameter optimisation.
6	Optimisation with only T_e specified: a 3 parameter optimisation.

Table 2

Computer storage requirements (K bytes) for least squares Patterson collocation and finite difference solution of the 2DVB model with boundary profile optimisation.

	Least squares Patterson collocation	Finite difference
Overall simulation and optimisation	68K	12K
Simulation and optimisation for a specified forehearth	8K	10K

5.6 Conclusions.

We have presented a technique to solve a specified type of PDE by producing a closed form approximation with explicit boundary condition parameter dependence. The general application of this collocation technique is based on the use of Patterson quadrature points and weights and is therefore more efficient than other collocation schemes which would typically use Gauss-Legendre points and weights. This additional efficiency is produced by the retention and re-use of previously calculated collocation function values if collocation at a certain number of points is not considered to be sufficiently accurate.

With the determination of collocation points and approximation order complete, the Patterson collocation technique provides a closed form approximate solution to a given partial differential equation. Therefore simulation of the system governed by the PDE is particularly easy, requiring little computer time or storage and optimisation of imposed boundary condition parameters may be performed analytically. Thus, even for complicated DPS's defined over non-regular domains, feedforward control parameters may be predicted with a relatively small computing effort.

A practical application of the method to the heat-conditioning of glass in a forehearth has been illustrated. The 2DVB model of this process was not amenable to solution by standard MWR techniques. However, the least squares Patterson collocation approach was successful, the convergence to the correct solution with increasing order of approximation being demonstrated by comparison with a finite difference solution.

Several optimisation studies have been performed. One such study confirmed optimal profiles Hamilton [7] obtained by numerical experimentation while another showed that a greatly increased throughput was feasible without imparing the quality of the glass.

The computation times and storage shown in Tables 1 and 2 indicate that the approximate solution of the 2DVB model obtained by least squares Patterson collocation can be readily incorporated into an overall forehearth control scheme as feedforward action.

6. THE DISTRIBUTED PARAMETER SYSTEM MAXIMUM PRINCIPLE: AN INTRODUCTION.

Many engineering systems are distributed in nature and are only accurately described by one or more partial differential equations. Thus the state variables which characterise such systems are not only functions of time but are also functions of one or more spatial co-ordinates. We shall now consider optimal control of such systems. Recollection of the structure of the optimal control solution for lumped parameter systems indicates that optimal control of distributed parameter systems is far from trivial. Indeed in most physical situations we must question whether or not the input/output problem is truly distributed or whether it is in practice multi-input/multi-output. If this were the case the additional complexity of an internally distributed model may not be of any real additional benefit and a lumped (though potentially large order) model may be more appropriate.

Butkovskii[24-29], Butkovskii and Lerner[23] were early workers in the formulation of optimal control solutions for distributed parameter systems. Several other problems have also been considered by various authors though there are few reports of practical implementation.

6.1 Optimal control problem formulation.

We shall consider a spatial domain Ω with boundary $\partial\Omega$ and any point within the domain being represented by an m-dimensional spatial co-ordinate vector

$$\underline{z}^T = [z_1, z_2, \ldots, z_m] \quad .$$

At any point in time t the state of the system is denoted as a vector function

$$\underline{x}(\underline{z}, t) = \begin{bmatrix} x_1(z_1, \ldots, z_m, t) \\ x_2(z_1, \ldots, z_m, t) \\ \vdots \\ x_N(z_1, \ldots, z_m, t) \end{bmatrix}$$

while a distributed control vector is denoted

$$\underline{u}(\underline{z}, t) = \begin{bmatrix} u_1(z_1, \ldots, z_m, t) \\ u_2(z_1, \ldots, z_m, t) \\ \vdots \\ u_r(z_1, \ldots, z_m, t) \end{bmatrix}$$

where $\underline{z} \in \Omega$ in general, though the domain of the control vector is often the boundary $\partial\Omega$ or some subregion thereof. We shall only consider distributed parameter systems of the form:

$$\frac{\partial \underline{x}}{\partial t} = \underline{f}\left[\underline{z}, t, \underline{x}(z,t), \frac{\partial \underline{x}}{\partial z_1}, \ldots, \frac{\partial \underline{x}}{\partial z_m}, \ldots, \frac{\partial^K \underline{x}}{\partial z_1^{k_1} \partial z_2^{k_2} \ldots \partial z_m^{k_m}}, \ldots, \underline{u}(\underline{z}, t)\right]$$

with $K = \sum_{i=1}^{m} k_i$, being subject to appropriate initial and boundary conditions. From this point we use the notation

$$\frac{\partial^K \underline{x}(\underline{z},t)}{\partial \underline{z}^K} \triangleq \frac{\partial^{k_1+k_2+\ldots+k_m} \underline{x}(\underline{z},t)}{\partial z_1^{k_1} \partial z_2^{k_2} \ldots \partial z_m^{k_m}}$$

for all $k_1, k_2, \ldots, k_m$ such that $\sum_{i=1}^{m} k_i = K$. We therefore have system equations:

$$\frac{\partial \underline{x}(\underline{z},t)}{\partial t} = \underline{f}\left[\underline{z}, t, \underline{x}(\underline{z},t), \frac{\partial^K \underline{x}(\underline{z},t)}{\partial \underline{z}^K}, \underline{u}(\underline{z},t)\right]$$

subject to initial conditions $\underline{x}(\underline{z},t_o) = \underline{x}_o(\underline{z})$ and conditions on

$$\frac{\partial^{K-1} \underline{x}}{\partial \underline{z}^{K-1}}, \quad \frac{\partial^{K-2} \underline{x}}{\partial \underline{z}^{K-2}}, \ldots, \frac{\partial \underline{x}}{\partial \underline{z}}, \underline{x}$$

at t_o and $\partial\Omega$.

We wish to find an admissible control vector $\underline{u}(\underline{z},t)$ which minimises the following cost function for fixed initial time t_o and terminal time t_f:

$$J = \int_\Omega g\left[\underline{x}(\underline{z}, t_f), t_f\right] d\Omega + \int_{t_o}^{t_f} \int_\Omega f_o\left[\underline{z}, t, \underline{x}(\underline{z},t), \frac{\partial^K \underline{x}(\underline{z},t)}{\partial \underline{z}^K}, \underline{u}(\underline{z},t)\right] d\Omega \, dt .$$

Without proof (which is via variational calculus not dissimilar to the lumped parameter Hamiltonian development) we quote the solution as:

Define a Hamiltonian

$$\mathcal{H} = f_o + \underline{p}^T(z,t)\, \underline{f} .$$

Then the Hamiltonian (partial differential) equations are:

$$\frac{\partial \underline{x}}{\partial t} = \frac{\partial \mathcal{H}}{\partial \underline{p}} = \underline{f}$$

$$\frac{\partial \underline{p}}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \underline{x}} - (-1)^K \frac{\partial^K}{\partial \underline{z}^K}\left[\frac{\partial \mathcal{H}}{\partial\left\{\frac{\partial^K \underline{x}}{\partial \underline{z}^K}\right\}}\right]$$

and the optimal control $\underline{u}^*(\underline{z},t)$ obeys

$$[\underline{u}^*(\underline{z},t)] \leq \mathcal{H}[\underline{u}(\underline{z},t)]$$

for all admissible $\underline{u}(\underline{z},t)$. i.e. $\underline{u}^*(\underline{z},t)$ mimimises the Hamiltonian. When the set of admissible controls is unbounded the latter statement yields the requirement that

$$\frac{\partial \mathcal{H}}{\partial \underline{u}} = \underline{0} .$$

Boundary conditions for Hamilton's partial differential equations are supplied by the physical problem boundary conditions and

$$\left.\frac{\partial g}{\partial \underline{x}}\right|_{t=t_f} = \left.\underline{p}(\underline{z},t)\right|_{t=t_f}$$

and

$$\left.\frac{\partial^{K-1}}{\partial \underline{z}^{K-1}}\left[\frac{\partial \mathcal{H}}{\partial\left\{\frac{\partial^K \underline{x}}{\partial \underline{z}^K}\right\}}\right]\right|_{\underline{z}\in\partial\Omega, t=t_f} = \underline{0} .$$

Example.

Consider a one dimensional heat diffusion system:

$$\frac{\partial \tilde{x}}{\partial t}(\tilde{z},t) = \left[\frac{k}{\rho c}\right] \frac{\partial^2 \tilde{x}}{\partial \tilde{z}^2}(\tilde{z},t) + \frac{\tilde{u}(\tilde{z},t)}{\rho c}$$

where the medium has temperature $\tilde{x}(\tilde{z},t)$, conductivity k, density ρ, specific heat c and $\tilde{u}(\tilde{z},t)$ is the heat supplied per unit volume.

A normalised equivalent of this problem is then

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial z^2} + u(z,t)$$

which is subject to initial condition

$$x(z,0) = x_o(z)$$

and certain boundary conditions, here for simplicity,

$$\frac{\partial x}{\partial z}(0,t) = 0 \quad \text{and} \quad \frac{\partial x}{\partial z}(z_e,t) = 0 \ .$$

Suppose that we wish to find a control signal u(z,t) which minimises:

$$J = \frac{1}{2}\int_o^{t_f}\left[\int_o^{z_e} x^2(z,t)\,dz + r\int_o^{z_e} u^2(x,t)\,dz\right]dt$$

where t_f is fixed and r is a relative weighting parameter. The Hamiltonian for this problem is:

$$\mathcal{H} = \frac{1}{2}x^2 + \frac{1}{2}r\,u^2 + p\left[\frac{\partial^2 x}{\partial z^2} + u\right] \ .$$

Therefore Hamilton's equations are:

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial z^2} + u \qquad \text{(state)}$$

and

$$\frac{\partial p}{\partial t} = -x - (-1)^2\frac{\partial}{\partial z^2}\left[\frac{\partial \mathcal{H}}{\partial\left\{\frac{\partial^2 x}{\partial z^2}\right\}}\right] \qquad \text{(co-state)}$$

(there being no other derivatives in z)

i.e.

$$\frac{\partial p}{\partial t} = -x - \frac{\partial^2 p}{\partial z^2} \ .$$

Since the control is unbounded we have optimal control given by

$$\frac{\partial \mathcal{H}}{\partial u} = 0 \quad \text{i.e.}$$

$$ru + p = 0.$$

Hence the overall optimal control solution is given by:

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial z^2} + u$$

subject to

$$x(z,0) = x_o(z); \quad \frac{\partial x}{\partial z}(0,t) = 0; \quad \frac{\partial x}{\partial z}(z_e,t) = 0$$

$$\frac{\partial p}{\partial t} = -x - \frac{\partial^2 p}{\partial z^2}$$

subject to

$$p(z,t_f) = 0; \quad \frac{\partial p}{\partial z}(0,t) = 0; \quad \frac{\partial p}{\partial z}(z_e,t) = 0$$

where $u(z,t) = -\frac{1}{r}p(z,t)$.

Thus in contrast to the lumped parameter situation where Hamilton's equations yield coupled ordinary differential equations in the distributed situation we have coupled partial differential equations. The open-loop optimal control is now derived by linking the state, co-state and optimal control equations. Thus

$$p(z,t) = -ru(z,t)$$

and hence from the co-state equation

$$-r\frac{\partial u}{\partial t} = -x + r\frac{\partial^2 u}{\partial z^2} \ .$$

Thus

$$\frac{\partial x}{\partial t} = r\frac{\partial^2 u}{\partial t^2} + r\frac{\partial^3 u}{\partial z^2 \partial t}$$

and

$$\frac{\partial^2 x}{\partial z^2} = r\frac{\partial^3 u}{\partial z^2 \partial t} + r\frac{\partial^4 u}{\partial z^4}$$

and the state equation gives

$$r\frac{\partial^2 u}{\partial t^2} = r\frac{\partial^4 u}{\partial z^4} + u$$

or

$$r\frac{\partial^4 u}{\partial z^4} - r\frac{\partial^2 u}{\partial t^2} + u = 0$$

which is a linear PDE and may be tackled by separation of variables. The requisite initial and boundary conditions are:

$$p(z,t_f) = 0 \quad \Rightarrow \quad u(z,t_f) = 0$$

$$\frac{\partial p}{\partial z}(0,t) = 0 \quad \Rightarrow \quad \frac{\partial u}{\partial z}(0,t) = 0$$

$$\frac{\partial p}{\partial z}(z_e,t) = 0 \quad \Rightarrow \quad \frac{\partial u}{\partial z}(z_e,t) = 0$$

$$x(z,0) = x_o(z) \Rightarrow \quad r\frac{\partial u}{\partial t}(z,0) + r\frac{\partial^2 u}{\partial z^2}(z,0) = x_o(z)$$

$$\frac{\partial x}{\partial z}(0,t) = 0 \quad \Rightarrow \quad \frac{\partial^2 u}{\partial z \partial t}(0,t) + \frac{\partial^3 u}{\partial z^3}(0,t) = 0$$

$$\frac{\partial x}{\partial z}(z_e,t) = 0 \quad \Rightarrow \quad \frac{\partial^2 u}{\partial z \partial t}(z_e,t) + \frac{\partial^3 u}{\partial z^3}(z_e,t) = 0 \quad .$$

There is little to be gained in detailing the variables separable solution at this stage. We do however note that the optimal control u(z,t) is derived from a PDE which is subject to

initial conditions at $z = 0$ and $z = z_e$ and terminal conditions at $z = 0$ and $z = z_e$. We therefore have a spatially distributed two-point boundary value problem.

6.2 Spatial discretization.

An approximate finite dimensional state space problem can be produced by discretizing the spatial variation of the distributed state(s). There are several schemes to achieve this though in this exposition we shall simply choose a finite difference approach. We shall also consider a problem in which there is only one distributed state. Therefore consider optimal control of the latter one dimensional heat conduction system:

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial z^2} + u(z,t)$$

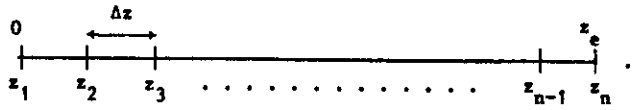
subject to

$$x(z,0) = x_o(z)$$

$$\frac{\partial x}{\partial z}(0,t) = 0$$

$$\frac{\partial x}{\partial z}(z_e,t) = 0 \quad .$$

Consider the spatial domain equally divided into n divisions:



Then

$$\Delta z = z_e/(n-1)$$

and we denote the temperature at any point z_i by

$$x(z_i,t) = x_i(t).$$

A central difference approximation to the second derivative term gives

$$\frac{\partial^2 x}{\partial z^2}(z_i,t) \simeq \frac{x_{i+1}(t) - 2x_i(t) + x_{i-1}(t)}{(\Delta z)^2}$$

and hence at each point z_i $(i = 1,2,\ldots,n)$ we have

$$\dot{x}_i(t) = \frac{x_{i+1}(t) - 2x_i(t) + x_{i-1}(t)}{(\Delta z)^2} + u_i(t) \quad .$$

The boundary conditions at $z = 0$ and $z = z_e$ give

$$\frac{\partial x}{\partial z}(0,t) \simeq \frac{x_1(t) - x_0(t)}{\Delta z} = 0 \quad \Rightarrow \quad x_0(t) = x_1(t)$$

$$\frac{\partial x}{\partial z}(z_e,t) \simeq \frac{x_{n+1}(t) - x_n(t)}{\Delta z} = 0 \Rightarrow x_{n+1}(t) = x_n(t)$$

and hence we have that the temperatures within the domain are governed by a set of n equations

$$\dot{x}_1(t) = \frac{1}{(\Delta z)^2}\left[x_2(t) - x_1(t)\right] + u_1(t)$$

$$\dot{x}_2(t) = \frac{1}{(\Delta z)^2}\left[x_3(t) - 2x_2(t) + x_1(t)\right] + u_2(t)$$

$$\vdots$$

$$\dot{x}_{n-1}(t) = \frac{1}{(\Delta z)^2}\left[x_n(t) - 2x_{n-1}(t) + x_{n-2}(t)\right] + u_{n-1}(t)$$

$$\dot{x}_n(t) = \frac{1}{(\Delta z)^2}\left[-x_n(t) + x_{n-1}(t)\right] + u_n(t) \quad .$$

We therefore have a classical constant coefficient state-space system description

$$\dot{\underline{x}} = A\,\underline{x} + B\,\underline{u}$$

where

$$A = \frac{1}{(\Delta z)^2}\begin{bmatrix} -1 & 1 & 0 & 0 & 0 \ldots\ldots 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \ldots\ldots 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \ldots\ldots 0 & 0 & 0 & 0 \\ \vdots & & & & & & & \\ 0 & 0 & 0 & 0 & 0 \ldots\ldots 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 \ldots\ldots 0 & 0 & 1 & -1 \end{bmatrix}$$

and $B = I_n$ the $(n \times n)$ identity matrix. The cost function in the distributed problem was posed as

$$J = \frac{1}{2}\int_0^{t_f}\left[\int_0^{z_e} x^2(z,t)\,dz + r\int_0^{z_e} u^2(z,t)\,dz\right]dt$$

which, replacing the spatial integrals by a quadrature rule, is adapted to

$$J = \frac{1}{2}\int_0^{t_f}\left[\sum_{i=1}^{n} q_i\, x_i^2(t) + r\sum_{i=1}^{n} r_i\, u_i^2(t)\right]dt \quad .$$

The simple trapezoid rule gives

$$q_1 = q_n = r_1 = r_n = \tfrac{1}{2}\Delta z \quad \text{and} \quad q_i = r_i = \Delta z \quad (i = 2,\ldots,n-1).$$

Hence we can express J in standard (LQP) form:

$$J = \frac{1}{2}\int_0^{t_f}\left[\underline{x}^T(t)\,Q\,\underline{x}(t) + \underline{u}^T(t)\,R\,\underline{u}(t)\right]dt$$

with

$$Q = R = \Delta z \begin{bmatrix} \frac{1}{2} & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \frac{1}{2} \end{bmatrix} .$$

6.3 The optimal distributed linear regulator problem.

We shall use the one dimensional diffusion equation to illustrate the derivation of distributed linear feedback control laws. Thus we again focus on

$$z \in [0, z_e] = \Omega$$

and

$$\frac{\partial x}{\partial t}(z,t) = \frac{\partial^2 x}{\partial z^2}(z,t) + u(z,t)$$

where

$$\left[\beta x(z,t) - \frac{\partial x}{\partial y}(z,t)\right]\Bigg|_{\substack{z=0,\\ z=z_e}} = 0$$

$$x(z,0) = x_0(z) .$$

Here we seek a control $u(z,t)$ to minimise the quadratic index of performance:

$$J = \frac{1}{2}\int_\Omega \int_\Omega x(z,t_f)\, S(z,z')\, x(z',t_f)\, dz\, dz'$$

$$+ \frac{1}{2}\int_o^{t_f} \left[\int_\Omega\int_\Omega x(z,t)\, Q(z,z')\, x(z',t)\, dz\, dz' + R\int_\Omega u^2(z,t)\, dz\right] dt$$

where $S(z,z')$ and $Q(z,z')$ are positive semi-definite for z and $z' \in \Omega$ and R is a positive constant. To obtain a symmetric Riccati type equation we form an augmented cost function:

$$J' = \frac{1}{2}\int_\Omega \int_\Omega x(z,t_f)\, S(z,z')\, x(z',t_f)\, dz\, dz'$$

$$+ \frac{1}{2}\int_o^{t_f} \left[\int_\Omega \int_\Omega x(z,t)\, Q(z,z')\, x(z',t)\, dz\, dz' + R\int_\Omega u^2(z,t)\, dz\right] dt$$

$$+ \int_\Omega p(z,t)\left[\frac{\partial^2 x}{\partial z^2}(z,t) + u(z,t) - \frac{\partial x}{\partial t}(z,t)\right] dz$$

$$+ \int_\Omega p(z',t)\left[\frac{\partial^2 x}{\partial z^2}(z',t) + u(z',t) - \frac{\partial x}{\partial t}(z',t)\right] dz'$$

which gives rise to an associated Hamiltonian

$$\mathcal{H} = \frac{1}{2}\int_\Omega \int_\Omega x(z,t)\, Q(z,z')\, x(z',t)\, dz\, dz'$$

$$+ \frac{1}{2}\int_\Omega \int_\Omega R\, u(z,t)\, u(z',t)\, dz\, dz'$$

$$+ \frac{1}{2}\int_\Omega p(z,t)\left[\frac{\partial^2 x}{\partial z^2}(z,t) + u(z,t)\right] dz$$

$$+ \frac{1}{2}\int_\Omega p(z',t)\left[\frac{\partial^2 x}{\partial z^2}(z',t) + u(z',t)\right] dz' .$$

By applying the maximum principle and then assuming that the co-states are formed by a feedback of the states, i.e.

$$p(z,t) = \int_\Omega P(z,z',t)\, x(z',t)\, dz'$$

$$p(z',t) = \int_\Omega P(z,z',t)\, x(z,t)\, dz$$

we evolve a control law:

$$u(z,t) = -R^{-1} \int_\Omega P(z,z',t)\, x(z',t)\, dz'$$

from $\partial \mathcal{H}/\partial u = 0$. Much algebra then shows that the function $P(z,z',t)$ satisfies the (Riccati) partial differential equation:

$$\frac{\partial P}{\partial t} + \frac{\partial^2 P}{\partial z^2} + \frac{\partial^2 P}{\partial z'^2} - R^{-1} \int_\Omega P(z'',z',t)\, P(z,z'',t)\, dz''$$

$$+ Q(z,z') = 0 \ .$$

The associated boundary conditions are

$$\beta\, P(z,z',t) - \frac{\partial P}{\partial z}(z,z',t)\Big|_{\substack{z=0,\\ z=z_e}} = 0$$

$$\beta\, P(z',z,t) - \frac{\partial P}{\partial z'}(z',z,t)\Big|_{\substack{z'=0,\\ z'=z_e}} = 0$$

$$P(z,z',t_f) = S(z,z') \ .$$

As in the lumped parameter situation this problem has to be solved off-line in backward time before replay in real-time. However even the off-line solution is non-trivial, with an integral term significantly complicating the Riccati partial differential equation.

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