TR/7 February 1972.

A METHOD FOR SOLVING MOVING BOUNDARY PROBLEMS IN HEAT FLOW
PART II: USING CUBIC POLYNOMIALS.

by

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ABSTRACT

A moving grid system has been used to get the solution of the moving boundary problem discussed earlier in Part I, but basing the necessary interpolations on ordinary cubic polynomials rather than splines. The computations are much more economical and the results obtained are also found to he more satiafactory.

A Method for Solving Moving Boundary Problems in Heat Flow : Part II Using Cubic Polynomials.

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1. Introduction.

The present authors [1] discussed a moving boundary problem arising from the diffusion of oxygen in an absorbing medium and made use of finite difference formulae for unequal intervals in the region of the moving boundary together with a Taylor's series expansion. An early finite difference method [2] proposed the use of the variable time step chosen so that the boundary always moves from one line of the space grid to the neighbouring one in a single time step. Another method [3] maintained a fixed number of equal space intervals between the surface of the medium and the moving boundary, the size of the interval being correspondingly adjusted. The present authors [4] suggested the use of a moving grid system which moves with the velocity of the moving boundary. The method made use of cubic splines to interpolate between the grid points.

In the present paper same idea of a moving grid system is employed to solve the problem discussed in [1] or [4] but the necessary interpolations are performed by using ordinary cubic polynomials rather than splines. This avoids solving the tridiagonal set of equations in Part I and the results thus obtained also show a superiority over the results obtained in [4].

For the sake of completeness of the paper we repeat sections 2 and 3 of [4].

2. An Example,

We shall introduce the new method by referring to a practical problem which the authors described in detail in the earlier paper [1]. Expressed in non-dimensional terms we require the solution of the equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - 1 \quad , \; 0 \leq x \leq \delta \; , \quad t \geq 0 \; . \tag{1}$$

with the boundary conditions

$$\frac{\partial u}{\partial x} = 0, \quad x = 0, t \geq 0 \; , \tag{2}$$

$$u = \frac{\partial u}{\partial x} - = 0, \; x = \delta(t), \quad t \geq 0, \tag{3}$$

and the initial condition

$$u = \frac{1}{2}(1\text{-}x), \quad 0 < x < 1 \; , \quad t = 0, \tag{4}$$

where δ(t) denotes the position of the moving boundary at time t.

3. A Moving Grid System.

Traditionally, we divide the region $0 \leq x \leq 1$ into n intervals each of width Δx such that $x_{i,,} = i\Delta x$, i = 0,1, . n and nΔx = 1. By some numerical procedure we advance the solution in finite time steps Δt, starting from the known solution at t = 0, given by (4) •

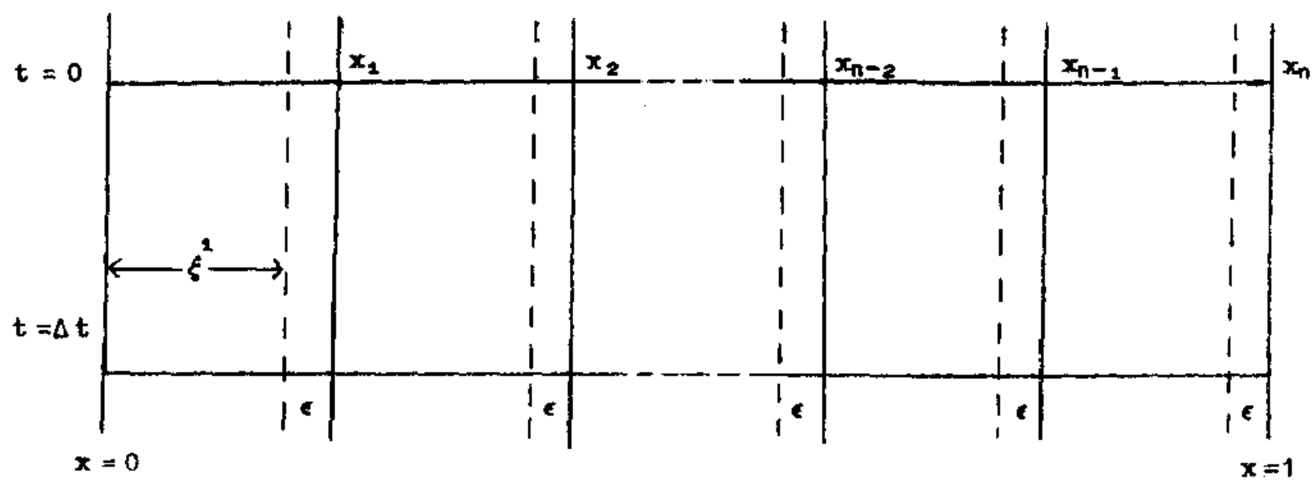

Fig.1 Moving Grid

We denote by U_i^J the values of u at (iΔx, JΔt), j-0, 1, 2 ...., so that in the first interval Δt we evaluate U_{n_1} and also the new position of the boundary which has moved from x=1 to x=1 -ε, say, as in Figure 1. We now move the whole grid a distance ε to the left as indicated by the broken lines, and we wish to evaluate values of U^0 and the second space derivatives at each of the points $x_1 - \varepsilon$, $x_2 - \varepsilon$, .., $x_{n-1} - \varepsilon$, 1 - ε. We describe another method for doing this, using ordinary cubic polynomials for interpolation between the points x_o, x_1, X_2 • • • Xn-i, 1 at t = 0. We can then proceed in similar fashion to 2Δt and in general to jΔt (j= 3,4, •••) provided we include a modification to allow for the unequal interval ξ^j at the jth time step near the surface x = 0.

4. Forward Difference Polynomial (F.D.P.) Method.

In this method we retain the same idea of a moving grid system but avoid solving the tridiagonal set of equations of FDS method [4]. Instead, the second space derivatives are calculated from the values of u by using the simple 3- point finite-difference formulae. Interpolation between any two grid points is then based on a cubic polynomial which satisfies the function values and the second derivatives at the two grid points.

Thus, we represent u(x) between the two points $x_{i,}$, x_{i+i} by

$$u_{i,i+1} \;\; \alpha + \beta x + yx^2 + \mu x^3 \quad , \qquad (5)$$

where $\alpha = \alpha(i,i+1)$ etc.

We employ the usual expressions

$$U_i'' = \frac{U_{i-1} - 2U_i + U_{i+1}}{(\Delta x)^2}, \quad i = 1, 2, \ldots n, \tag{6}$$

and at the surface x = o,

$$U_o'' = \frac{2}{\xi^2}(U_o - U_1), \tag{7}$$

where $\xi = x_1 - x_0$.

At $x = x_1$ we use a formula of the same type buy generalised to allow for the unequal interval ξ, namely

$$U_i'' = 2\left\{\frac{U_o}{\xi(\xi + \Delta x)} - \frac{U_1}{\xi \Delta x} + \frac{U_2}{\Delta x(\xi + \Delta x)}\right\}. \tag{8}$$

From (5.1) we obtain

$$U_{i,1+\ell} = 6\mu x + 2y, \tag{9}$$

and thus by inserting values U_i, U_{l+1}, U_i, U_{i+1} into (5) and (9) we derive the coefficients α, β, y, μ and hence determine the polynomial for the interval x_i to x_{i+1}

For the interval near the moving boundary we make use of the conditions derived in [1] which are given by

$$\frac{\partial^2 u}{\partial x^2} = 1, \quad \frac{\partial^3 u}{\partial x^3} = -\frac{\partial \delta}{\partial t}, \quad \frac{\partial^4 u}{\partial x^4} = \left(\frac{\partial \delta}{\partial t}\right)^2 \quad \ldots\ldots \text{ etc.}, \tag{10}$$

at the moving boundary giving $U''(x_n) = 1$.

Assuming the function values to be known at any time $j\,\Delta t$ when the distance of the moving boundary from the surface $x = 0$ is $\xi^j + r\Delta x$ the method proceeds as follows.

Obtain the second derivatives $U''(x_1)$, $i = 0, 1, \ldots\ldots, (r + 1)$ from (6),(7),(8) and (10). The value of U_r^{j+1} i.e. at the point neighbouring the moving boundary, follows from the simple explicit relationship

$$\frac{U_r^{j+1} - U_r^{j}}{\Delta t} = U(\chi_r^{j}) - 1 \,,$$

(11)

where $U^*(\chi_r^j)$ denotes the value of the second derivative at x_r at $t = j\Delta t$.

The Taylor's series for U_r obtained by expanding about the moving point can be written as in [4],

$$U_r = U(\delta) - \ell\left(\frac{\partial u}{\partial x^2}\right)_{x=\delta} + \frac{1}{2}\ell^2\left(\frac{\partial^2 u}{\partial x^2}\right)_{x=\delta} - \frac{1}{6}\ell^3\left(\frac{\partial^3 u}{\partial x^3}\right)_{x=\delta} + \ldots\ldots,$$

where $\ell(0 \leq \ell \leq \Delta x)$ is the distance of the moving point from U_r.

Using (3) and (10) and assuming that the boundary is not moving too quickly, the above relation gives to a reasonable accuracy

$$\ell = \sqrt{(2U_r)} \,. \qquad (12)$$

Therefore, once U_r^{j+1} is known from (11), we can find the position of the moving boundary from (12). Hence, the movement, ε^{j+1}, of the boundary in time Δt, from $j\Delta t$ to $(j + 1)\Delta t$ is given by

$$\varepsilon^{j+1} = \Delta x - \ell^{j+1} \,. \qquad (13)$$

Having got ε from (13) we then interpolate the values of $u(x)$ at $t = j\Delta t$ at the points $x_1 - \varepsilon$, $x_2 - \varepsilon$, ...,x_r-ε",δ-ε using (5) and the corresponding second derivatives from the linear relationship

$$\frac{U^*(x^j_{i+1}) - U^*(x)}{x^j_{i+1} - x} = \frac{U^*(x^j_{i+1}) - U^*(x^j_i)}{x^j_{i+1} - x^j_i} \qquad (14)$$

where x^j_i denotes the ith mesh po int auch that $x^j_i = \xi^j + (i-1)\Delta x$ at time $j\Delta t$; $x^j_i \le x \le x^j_{i+1}$ and $i = 0,1, \ldots r$.

The values of u(x) at x_1, x_2 ,.................... x_r , at time $(j+1)\Delta t$ follow at once from

$$\frac{U^{J+i}(x^{j+i}_i) - U^j(x^j_i - \in^{j+i})}{\Delta t} = U^*(x^j_i - \in^{j+i}) - 1 , \qquad (15)$$

$$x^{j+i}_i = x^j_i - \in^{j+i} , \; i = 1,2, \ldots r ,$$

together with

$$\frac{U^{J+1}_o - U^j_o}{\Delta t} = U^*(x^j_o) - 1 \text{, at the surface } x = 0. \qquad (16)$$

We should remember that the space interval x_1 - $Xo = \xi$ is not fixed and varies from one time step to the next.

We proceed in steps Δt in this way testing ξ at each step for stability. When $\frac{\Delta t}{\xi^2} \ge \frac{1}{2}$ we replace ξ by $\Delta x + \xi$ to get values at the next time step and proceed as before. A stability analysis for this method has been appended at the end of the paper.

5. Results and Discussion.

Let us rewrite the expression for the analytical solution obtained in [1] for small times when the boundary x = 1 has not moved to the working accuracy

$$U(x,t) \tilde{-} \frac{1}{2}(1-x)^2 - 2\sqrt{(\frac{t}{w})}\ \exp\left\{-\left(-\frac{x}{2\sqrt{t}}\right)^2\right\} + \text{xerfc}\left(\frac{x}{2\sqrt{t}}\right), \quad (17)$$

$$0 \le x \le 1.$$

We start the FDP and the FGL* solutions from the values taken from (17) at t = 0.025 and give a comparison for the positions of the moving boundary and the surface concentrations in Tables I and II respectively. The figures throughout for corresponding step size show a very good agreement in both cases. The corresponding values obtained by using cubic splines in Part I are also presented for comparison in Tables I and II.

Apart from getting superior results by the FDP method the effort involved in using it, is appreciably less than for the FDS method essentially because the latter involves the solution of a tridiagonal set of equations at each time step.

Considering the important problem of roughness in the positions of the moving boundary which is produced by the FGL method near the times where the process used to calculate the concentration in the neighbourhood of the moving point is transferred one space interval towards the surface x = 0. We give in Table III

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* Fixed Grid Lagrange, the numerical method used in [1] •

the positions of the boundary at and around such times of shifting the interval in the FGL method along with the corresponding figures from the FDP method. The irregularities produced in the former method are clearly visible while their counterparts show a smooth behavior throughout.

Table IV gives a comparison of the surface concentrations obtained by the FDP and the FGL methods at and around times when the first space interval ξ in the former is increased to $\xi+\Delta x$ for the succeeding compulations. It is interesting to note that the differences in the concentrations show no sign of irregularities.

TABLE I

Comparison of $10^4\delta$ at different times. All solutions start from the analytical solution at t = 0.025.

Time / Method		0.040	0.060	0.100	0.120	0.140	0.160	0.180	0.185
FGL	Δx=0.05	9992	9918	9346	8781	7966	6799	4942	4178
FDP	Δx =0.10	9988	9904	9308	8734	7912	6725	4830	4114
	Δx = 0.05	9992	9918	9344	8780	7968	6798	4948	4258
FDS	Δx= 0.10	9993	9920	9327	8739	7892	6664	4680	3917

TABLE II

Comparison of 10^4U at the surface x=0, at different times. All solutions start from the analytical solution at t = 0.025.

Time / Method		0.040	0.060	1 0.100	0.120	0.140	0.160	0.180	0.185
FGL	Δx = 0.05	2742	2234	1430	1089	777	486	216	151
FDP	Δx = 0.10	2745	2238	1434	1093	780	490	219	155
	Δx = 0. 05	2742	2234	1429	1089	776	486	216	151
FDS	Δx= 0.10	2736	2277	1424	1083	771	481	210	145

TABLE III

Table showing the irregularities in the position of the moving boundary, calculated by the FGL method. Comparatively smooth figures are shown for the FDP method ($\Delta x = 0.10$),

Time	FG-L Method			FDP Method		
	$10^4\delta$	$-\Delta$	$-\Delta^2$	$10^4\delta$	$-\Delta$	$-\Delta^2$
	9099	29		9104		
	9070	30	1	9076	28	0
0.110	9040	30	0	9048	28	1
	9010	26	-4	9019	29	0
	8984			8990	29	
	8141	52		8145		
	8089	55	3	8100	45	1
0.137	8034	40	15	8054	46	0
	7994		0	8008	46	2
	7954			7960		
	7277			7256	61	
	7204	73		7195		
0.154	7124	80	7	7132	63	2
	7037	87	-35	7068	64	1
	6985	52		7002	66	2
	6396			6343	82	
	6306	90	13	6261		
0.167	6203	103	55	6177	84	2
	6045	158	-92	6090	87	1
	5979	66		6002	88	
	5499			5520		
	5393	106	19	5415	105	4
0.176	5268	125	123	5306	109	4
	5020	248	-165	5193	113	
	4937	83		5077	116	3
	4652	114		4563		
	4538	132	18	4421	142	
0.184	4406	392	260	4271	150	8
	4014	102	-290	4114	157	7
	3912			3948	166	9

NOTE : The data are tabulated at an interval of time $\Delta t = 0.001$. The underlined values correspond to the times when the interpolation process near the moving boundary is transferred one step to the left.

TABLE IV

Table showing the smoothness of the surface concentrations calculated by the FDP method at times when the first interval is increased by Δx, Corresponding figures for the FGL method are given for comparison (Δx = 0· 10).

Time	FDP Method		FGL Method	
	10^4U_o	-Δ	10^4U_0	-Δ
0·093	1599		1598	
	1580	19	1580	18
	1562	18	1561	19
	1543	17	1543	18
	1525	18	1524	19
0·127	1013		1013	
	997	16	997	16
	321	16	981	16
	965	16	965	16
	950	15	950	15
0·148	691		691	
	676	15	677	14
	662	14	662	15
	647	15	647	15
	633	14	633	14
0·163	476		476	
	462	14	462	14
	448	14	448	14
	434	14	435	13
	420	14	421	14
0·174	325		326	
	312	13	312	14
	298	14	299	13
	285	13	286	13
	272	13	272	14
0·182	219		220	
	206	13	207	13
	193	13	194	13
	180	13	181	13
	168	12	168	13

NOTE: The data are tabulated at an interval of time Δt = 0.001. The underlined values correspond to the times when the first space interval is increased by Δx.

6, Generalisation.

We consider the same latent heat type problem as discussed in [4]. In non-dimensional form the relevant equations are ,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad , \qquad 0 \le x \le \delta(t) \quad ; \qquad (18)$$

$$\frac{\partial u}{\partial x} = -1 \; , \qquad x = 0 \, , \; t \ge o \quad ; \qquad (19)$$

$$u = 0, \quad x = \delta(t), \qquad t \ge 0 \quad ; \qquad (20)$$

$$\frac{\partial u}{\partial x} = -\frac{\partial \delta}{\partial t} = -\delta' \; , \qquad x = \delta(t) \; ; \qquad (21)$$

$$\delta = 0, \qquad t = 0. \qquad (22)$$

Let us assume that the values of U_0, U_1 .... U_r , U_{r+1} are known at the jth time level and the position of the moving boundary is also known at that time which is given by $\delta^j = \xi^j + r\,\Delta x$. The width of all the meshes is Δx except the first one which is ξ^j •

The second derivatives at the surface and the first mesh points, at the jth time level, can be computed by (7) and (8) respectively while at the intermediate points they can be obtained by (6).

To get second derivative at the last mesh point i.e. the moving boundary we differentiate (20) with respect to t and use (18) and (21) such that

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{x=\delta} = \left(\frac{\partial \delta}{\partial t}\right)^2 = \delta'^2 \; , \qquad (23)$$

giving $U''(x_{r+1}) = \dot{\delta}^2$ where δ is a function of t.

But the Taylor's expansion for U_r about the moving boundary, after making the appropriate substitutions, gives as in [4] ,

$$\dot{\delta} = -1+\sqrt{(1+2U_r)}, \tag{24}$$

which in turn, using (23) gives

$$U''(x_{r+1}) = \{-1+\sqrt{\{1+2U_r)}\}^2 . \tag{25}$$

The new position of the moving boundary at the $(j+1)^{th}$ time level is determined from (24) after replacing δ by a forward finite difference i.e.

$$\frac{\delta^{J+1} - \delta^{J}}{\Delta t} = 1 + \sqrt{(1+2U_r^j)} . \tag{26}$$

The interpolations for the value of u and its second derivative for $x_i, \leq x \leq x_{i+1}$, $i = 0, 1,... (r - 1)$ can be performed by using (5) and (14.) respectively.. But for the interval next to the moving boundary the relations (20) and (25) are to be used for the desired interpolations.

It should again be remembered that as the boundary $\delta(t)$ is moving forward the first interval ξ becomes larger and larger with time. As soon as it becomes greater than Δx we should break it into two intervals making the second to be of width Δx and the interval nearest to the surface $x = 0$ to be of width $\xi - \Delta x$. The value of u, at the new mesh point, has to be interpolated using (5).

Acknowledgment.

This work has been supported by a research studentship awarded to R. S. Gupta by the Science Research Council.

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APPENDIX

Stability Analysis for F.P.P.Method.

Following the same argument as in the previous paper [1], it is easy to show that for stability, we require the largest modulus of the eigenvalues of the square matrix A to be less than unity where A is given by

$$\underline{A} = \begin{bmatrix} \left(1-\frac{2\Delta t}{\xi 2}\right) & \frac{2\Delta t}{\xi 2} & & & & \\ \frac{2\Delta t}{\xi(\xi+\Delta x)} & \left(1-\frac{2\Delta t}{\xi\Delta x}\right) & \frac{2\Delta t}{\Delta x(\xi+\Delta x)} & & & \\ 0 & r & (1-2r) & r & & \\ & & . & . & . & . \\ & & & & & r(1-2r) \end{bmatrix}$$

Applying Brauer's theorem as in [1] to the first and second rows of $\underline{\delta}$ we get

(i) $\left|\left|\lambda - \left(1 - \frac{2\Delta t}{\xi^2}\right)\right|\right| \leq \frac{2\Delta t}{\xi^2}$ giving $\frac{\Delta t}{\xi^2} \leq \frac{1}{2}$ and

(ii) $$\lambda - \left(1 - \frac{2\Delta t}{\xi \Delta x}\right) \le \frac{2\Delta t}{\Delta x\,\xi} \quad \frac{\Delta t}{\xi \Delta x} \le \frac{1}{2} \quad ,$$

respectively.

When $\xi < \Delta x$, the stability condition clearly is $\frac{\Delta t}{\xi^2} \le \frac{1}{2}$ However, when $\xi \ge \Delta x$ the conditions (i) and (ii) are automatically satisfied since we have $\frac{\Delta t}{\Delta x^2} \le \frac{1}{2}$ for the explicit scheme at the intermediate points.