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Numerical Methods for Problems with Moving Fronts

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6.5. Orthogonal Collocation on Finite Elements

The method of orthogonal collocation on finite elements provides a collocation method that is high order. It is applied here to the convective diffusion equation to illustrate its success. When the Peclet number is large, the orthognal collocation method will not provide good results since the number N must be so large to approximate the solution. In that case we are better off using the method of orthogonal collocation on finite elements, as developed by Carey and Finlayson [1975]. The domain is divided into elements and the method of orthogonal collocation is applied within each element. The numbering scheme is shown in Figure 6E.1. There are three types of nodes: those at which a boundary condition is applied (2 of these), those at which the residual is set to zero (NCOL x NE of these), and those at which the first derivative is made continuous across element boundaries (NE – 1 of these). The total number of points is then NT = (NCOL+1) NE +1. Within an element we transform the domain using

$$\xi = \frac{x - x_k}{\Delta x_k}, \qquad \Delta x_k = x_{k+1} - x_k \tag{m20}$$

so that the variable ξ goes from 0 to 1 within an element (rather than -1 to 1 as we have used for the Galerkin methods). The differential equation can be transformed to give

$$\frac{\partial c}{\partial t} + Pe \frac{1}{\Delta x_k} \frac{\partial c}{\partial \xi} = \frac{1}{\Delta x_k^2} \frac{\partial^2 c}{\partial \xi^2} \tag{m21}$$

and the boundary conditions are

$$\begin{aligned} c(0,t) &= 1 \\ \frac{1}{\Delta x_{NE}} \frac{\partial c}{\partial \xi}(1,t) &= 0 \\ c(x,0) &= f(x) \end{aligned} \tag{m22}$$

Now we are going to use four different numbering systems depending on what we are solving for. The local numbering systems within an element is shown in Figure 6E.1 and the global number system is shown in Figure 6E.2. The index i represents a global number and the index I represents a local number; in the later case the element must also be identified. Thus we have the correspondence

$$\begin{aligned} i &= (k-1)\,(NCOL + 1) + I \\ x_i &= x_{(k)} + \xi_I \Delta x_k \end{aligned} \tag{m23}$$

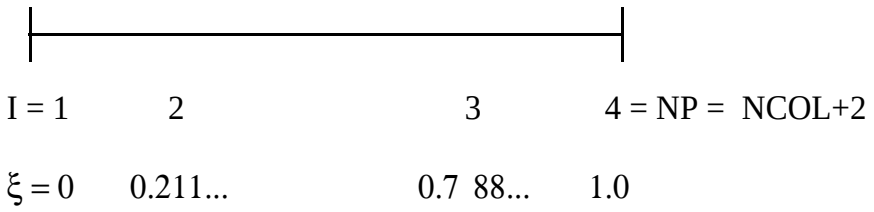


Figure 6E.1. Local numbering

On an element we set the residuals to zero.

$$\frac{\partial c}{\partial t}(\xi_I, t) + Pe \frac{1}{\Delta x_k} \frac{\partial c}{\partial \xi}(\xi_I, t) = \frac{1}{\Delta x_k^2} \frac{\partial^2 c}{\partial \xi^2}(\xi_I, t), \; I = 1,\ldots, NCOL \qquad \text{m24}$$

We also apply the boundary conditions

$$c_{i=1} = 1 \text{ or } c_{I=1}^{(1)} = 1$$

$$\frac{1}{\Delta x_{NE}} \sum_{I=1}^{NCOL+2} A_{NCOL+2,I}\, c_I^{(NE)} = 0 \qquad \text{m25}$$

$$c_I^{(k)}(0) = f(x_i)$$

Next we make the first derivatives continuous between the elements by taking

$$\frac{dc}{dx}(x_{NCOL+2}^{(k-1)}) = \frac{dc}{dx}(x_1^{(k)}) \qquad \text{m26}$$

Evaluated in the collocation method this is

$$\frac{1}{\Delta x_{k-1}} \sum_{I=1}^{NCOL+2} A_{NCOL+2,I}\, c_I^{(k-1)} = \frac{1}{\Delta x_k} \sum_{I=1}^{NCOL+2} A_{1,I}\, c_I^{(k)} \qquad \text{m27}$$

The method of solution is to use an explicit method to step forward in time.

$$\frac{c_J^{(k),n+1} - c_J^{(k),n}}{\Delta t} + \frac{Pe}{\Delta x_k} \sum_{I=1}^{N+2} A_{JI}\, c_I^{(k),n} = = \frac{1}{\Delta x_k^2} \sum_{I=1}^{N+2} B_{JI}\, c_I^{(k),n}, \; J = 2,\ldots,NCOL+1, k=1,NE \qquad \text{m28}$$

If we know the solution at time level n, c_i^n we can find $c_I^{(k),n}$. Thus we can obtain the value of c_i^{n+1} for

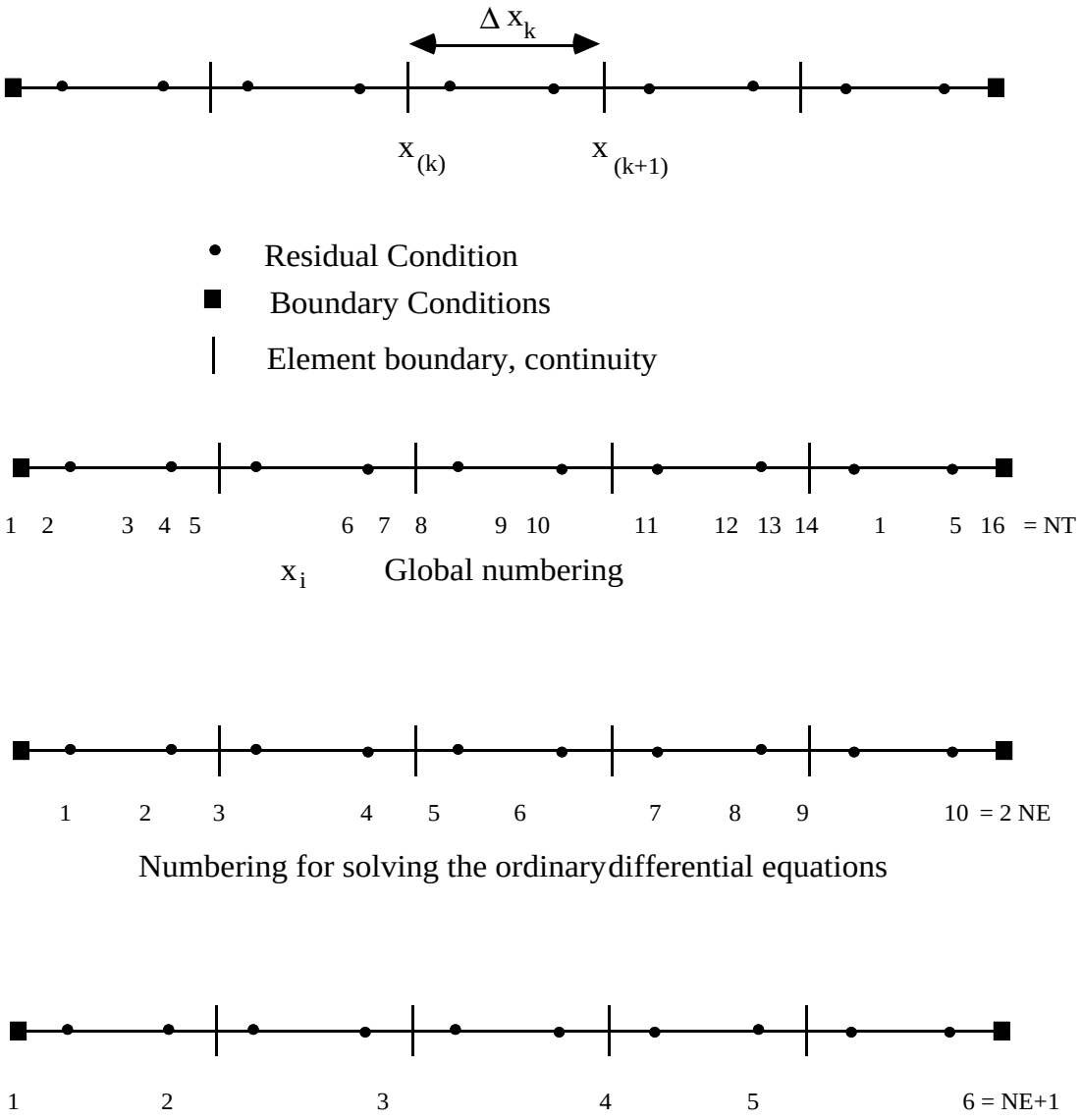


Figure 6E.2. Nodal numbering system

each of the points interior to the element, marked by • in Figure 6E.2. Implicit methods are also possible, and the linear algebra is discussed by Finlayson [1980, p. 116]. Suppose we have made the calculation Eq.(m28) for all of the collocation points interior to each element. We still need the values of c_i^{n+1} for each of the points between elements and the two end points. Rearrange the equations Eq.(m25) and Eq.(m27) to have the unknowns on the left-hand side.

$$\frac{1}{\Delta x_{k-1}} A_{NP,1} c_{I=1}^{(k-1),n+1} + \frac{1}{\Delta x_{k-1}} A_{NP,NP}\, c_{NP}^{(k-1),n+1} - \frac{1}{\Delta x_k} A_{1,1} c_{I=1}^{(k),n+1} - \frac{1}{\Delta x_k} A_{1,NP}\, c_{NP}^{(k),n+1} =$$

$$= -\frac{1}{\Delta x_{k-1}} \sum_{I=2}^{NP-1} A_{Np,I}\, c_I^{(k-1),n+1} + \frac{1}{\Delta x_k} \sum_{I=2}^{NP-1} A_{1J}\, c_I^{(k),n+1} \qquad \text{m29}$$

$$c_{I=1}^{(1),n+1} = 1$$

$$\frac{1}{\Delta x_{NE}} A_{NP,1}\, c_1^{(NE),n+1} + \frac{1}{\Delta x_{NE}} A_{NP,NP}\, c_{NP}^{(NE),n+1} = -\frac{1}{\Delta x_{NE}} \sum_{I=2}^{NP-1} A_{NP,I}\, c_1^{(NE),n+1} \qquad \text{m30}$$

We make the function continuous by taking

$$c_{NP}^{(k-1),n+1} = c_1^{(k),n+1} \qquad \text{m31}$$

This system of equations can be represented as a tri-diagonal form (see Eq. 2.51). The values of x_i in Eq. 2.51 are the values of c_i^{n+1} at the two end points and the points between the elements, using the third numbering system shown in Figure 6E.2. This tri-diagonal system can be solved and the results rearranged to provide the solution for each and every collocation point shown in Figure 6E.2, first numbering system, at the n+1-th time level.

Results are given for the method, but using the implicit method (which was readily available). For the convective diffusion equation the collocation results for 25 elements and 2 interior points are shown in Figure 6.33a. There are small oscillations. Jensen and Finlayson [1980] have shown that oscillations do not occur in the steady state problem provided

$$\frac{Pe\Delta x}{3.464} \leq 1 \qquad \text{m35}$$

This is the number that is comparable with $Pe\Delta x/2$ in the Galerkin method. For this calcualtion the quantity in Eq. (m35) takes the value 11.5. The Galerkin method with $Pe\Delta x/2 = 10$ gives the results shown in Figure 5.8a; the Taylor-Galerkin method with $Pe\Delta x/2 = 10$ gives the results shown in Figure 5.8e. There are small oscilllations in those solutions, too. When more elements are used, 50 elements and 2 interior collocation points, the method of orthogonal collocation on finite elements gives the results shown in Figure 6.33b. In this case there are no oscillations. All of these methods provide good solutions. The collocation method can also be applied with higher degree polynomials. A solution with 25 elements and 5 interior collocation points (a sixth degree polynomial within each element) gives a solution with oscillations that are very small. Here the key value is

$$\frac{Pe\Delta x}{2} \frac{1}{5} \approx\leq 1 \qquad \text{m36}$$

and it takes the value 4.

The method of orthogonal collocation on finite elements can also be applied to non-linear prob-

lems as well. If Burger's equation is solved in the form

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \qquad \text{m37}$$

we just replace Eq.(m24) with

$$\frac{\partial u}{\partial t}(\xi_I, t) + \frac{u(\xi_I, t)}{\Delta x_k} \frac{\partial u}{\partial \xi}(\xi_I, t) = \frac{\nu}{\Delta x_k^2} \frac{\partial^2 u}{\partial \xi^2}(\xi_I, t) \, , \; I = 1, \ldots, \text{NCOL} \qquad \text{m38}$$

An explicit method can be used with this set, as well. Solutions for such a method are not shown here.

7.4. Special Petrov-Galerkin Weighting Functions

Because S is an even function and satisfies Eq. (7.144) we have

$$\int_0^1 \frac{dS}{ds}\, ds = -1 \qquad \text{h11}$$

Since S(1) = 0 this also says S(0) = 1. The integral

$$\int_0^1 s\, \frac{dS}{ds}\, ds \qquad \text{h12}$$

can be evaluated by regarding s as the derivative of $s^2/2$ and then integrating by parts.

$$\int_0^1 s\, \frac{dS}{ds}\, ds = \int_0^1 \frac{d}{ds}\,(s\, S\,)\, ds - \int_0^1 1\, S\, ds = -\int_0^1 S\, ds \qquad \text{h13}$$

Since S is an even function we have

$$\int_0^1 S\, ds = \frac{1}{2}\int_{-1}^1 S\, ds = \frac{1}{2} \qquad \text{h14}$$

and hence

$$\int_0^1 s\, \frac{dS}{ds}\, ds = -\frac{1}{2} \qquad \text{h15}$$

The following relation can be obtained by integrating by parts the left-hand side.

$$\int_0^1 s^2\, \frac{dS}{ds}\, ds = -2\int_0^1 s\, S\, ds \qquad \text{h16}$$

With similar manipulations, (and using the fact that T is an odd function), we obtain

$$\int_0^1 \frac{dT}{ds}\, ds = 0, \quad \int_0^1 s\, \frac{dT}{ds}\, ds = -\int_0^1 T\, ds, \quad \int_0^1 s^2\, \frac{dT}{ds}\, ds = -2\int_0^1 s\, T\, ds \qquad \text{h17}$$

In the Petrov-Galerkin method the weighted residual is set to zero, Eq. (7.141). Integrate this by parts to obtain

$$\nu \int_0^1 \frac{dW_j}{dx}\, \frac{du}{dx}\, dx - \int_0^1 \frac{dW_j}{dx}\, V(u)\, dx = 0 \qquad \text{h18}$$

The first term is

$$\nu \int_0^1 \frac{dW_j}{dx}\frac{du}{dx}\,dx = \nu \int_0^1 \frac{dS_j}{dx}\frac{du}{dx}\,dx + \nu \int_0^1 \frac{dT_j}{dx}\frac{du}{dx}\,dx \qquad \text{h19}$$

Consider each part in turn.

$$\int_0^1 \frac{dS_j}{dx}\frac{du}{dx}\,dx = \sum_{i=1}^{NT} u_i \int_0^1 \frac{dS_j}{dx}\frac{dN_i}{dx}\,dx \qquad \text{h20}$$

But the derivative of the trial function N_j is constant within an element so that we get

$$\begin{aligned}
\int_0^1 \frac{dS_j}{dx}\frac{dN_{j-1}}{dx}\,dx &= \int_{-1}^0 \left(-\frac{1}{h}\right)\frac{dS_j}{ds}\,ds \\
\int_0^1 \frac{dS_j}{dx}\frac{dN_j}{dx}\,dx &= \int_{-1}^0 \left(\frac{1}{h}\right)\frac{dS_j}{ds}\,ds + \int_0^1 \left(-\frac{1}{h}\right)\frac{dS_j}{ds}\,ds \\
\int_0^1 \frac{dS_j}{dx}\frac{dN_{j+1}}{dx}\,dx &= \int_0^1 \left(\frac{1}{h}\right)\frac{dS_j}{ds}\,ds
\end{aligned} \qquad \text{h21}$$

Combining all results gives

$$\int_0^1 \frac{dS_j}{dx}\frac{du}{dx}\,dx = -\frac{u_{j-1}}{h}\int_{-1}^0 \frac{dS_j}{ds}\,ds + \frac{u_j}{h}\left[\int_{-1}^0 \frac{dS_j}{ds}\,ds - \int_0^1 \frac{dS_j}{ds}\,ds\right] + \frac{u_{j+1}}{h}\int_0^1 \frac{dS_j}{ds}\,ds \qquad \text{h22}$$

The terms are evaluated using Eq. (7.142) and (7.144).

$$\int_0^1 \frac{dS_j}{dx}\frac{du}{dx}\,dx = \frac{1}{h}\left(-u_{j-1} + 2u_j - u_{j+1}\right) = \frac{u_j - u_{j-1}}{h} - \frac{u_{j+1} - u_j}{h} = m_j - m_{j+1} \qquad \text{h23}$$

Similarily for the second part of Eq. (h19).

$$\int_0^1 \frac{dT_j}{dx}\frac{du}{dx}\,dx = -\frac{u_{j-1}}{h}\int_{-1}^0 \frac{dT_j}{ds}\,ds + \frac{u_j}{h}\left[\int_{-1}^0 \frac{dT_j}{ds}\,ds - \int_0^1 \frac{dT_j}{ds}\,ds\right] + \frac{u_{j+1}}{h}\int_0^1 \frac{dT_j}{ds}\,ds \qquad \text{h24}$$

By Eq. (7.142) we have

$$\int_{-1}^{0} \frac{dT_j}{ds}\, ds = \int_{0}^{1} \frac{dT_j}{ds}\, ds \qquad \text{h25}$$

and by Eq. (7.144) both terms are zero. Thus there is not contribution due to the T_j function. The first term of the weighted residual is then

$$\nu \int_{0}^{1} \frac{dW_j}{dx} \frac{du}{dx}\, dx = \nu\, (m_j - m_{j+1}) \qquad \text{h26}$$

The second term of the weighted residual is

$$\begin{aligned} \int_{0}^{1} \frac{dW_j}{dx}\, V(u)\, dx &= \int_{0}^{1} \frac{dS_j}{dx}\, V(u)\, dx + \int_{0}^{1} \frac{dT_j}{dx}\, V(u)\, dx \\ &= \int_{-1}^{0} \frac{dS_j}{ds}\, V(u)\, ds + \int_{0}^{1} \frac{dS_j}{ds}\, V(u)\, ds + \int_{-1}^{0} \frac{dT_j}{ds}\, V(u)\, ds + \int_{0}^{1} \frac{dT_j}{ds}\, V(u)\, ds \end{aligned} \qquad \text{h27}$$

In the left integral (s = -1 to 0) we use

$$\begin{aligned} u &= u_{j-1} + (u_j - u_{j-1})(s + 1) \\ &= u_j + m_j\, h\, s \end{aligned} \qquad \text{h28}$$

In the right integral (s = 0 to 1) we use

$$\begin{aligned} u &= u_j + (u_{j+1} - u_j)\, s \\ &= u_j + m_{j+1}\, h\, s \end{aligned} \qquad \text{h29}$$

Examine each of the terms in Eq. (h27).

$$\int_{0}^{1} \frac{dS_j}{dx}\, V(u)\, dx = \int_{-1}^{0} \frac{dS_j}{ds}\, V(u_j + m_j\, h\, s)\, ds + \int_{0}^{1} \frac{dS_j}{ds}\, V(u_j + m_{j+1}\, h\, s)\, ds \qquad \text{h30}$$

Since dS_j/ds is an odd function

$$\int_{-1}^{0} \frac{dS_j}{ds}\, V(u_j + m_j\, h\, s)\, ds = \int_{\xi=1}^{\xi=0} \frac{dS_j}{d\xi}\, V(u_j - m_j\, h\, \xi)\, d\xi = -\int_{0}^{1} \frac{dS_j}{ds}\, V(u_j - m_j\, h\, s)\, ds \qquad \text{h31}$$

and we get

$$\int_0^1 \frac{dS_j}{dx}\, V(u)\, dx = -\int_0^1 \frac{dS_j}{ds}\, V(u_j - m_j\, h\, s)\, ds + \int_0^1 \frac{dS_j}{ds}\, V(u_j + m_{j+1}\, h\, s)\, ds \qquad \text{h32}$$

The same steps applied to the term involving dT_j/ds, which is an even function, gives

$$\int_0^1 \frac{dT_j}{dx}\, V(u)\, dx = \int_0^1 \frac{dT_j}{ds}\, V(u_j - m_j\, h\, s)\, ds + \int_0^1 \frac{dT_j}{ds}\, V(u_j + m_{j+1}\, h\, s)\, ds \qquad \text{h33}$$

Thus the weighted residual becomes

$$\begin{aligned} &\nu\,(m_{j+1}\, m_j) - \int_0^1 \frac{dS_j}{ds}\, V(u_j - m_j\, h\, s)\, ds + \int_0^1 \frac{dS_j}{ds}\, V(u_j + m_{j+1}\, h\, s)\, ds + \\ &\qquad + \int_0^1 \frac{dT_j}{ds}\, V(u_j - m_j\, h\, s)\, ds + \int_0^1 \frac{dT_j}{ds}\, V(u_j + m_{j+1}\, h\, s)\, ds = 0 \end{aligned} \qquad \text{h34}$$

Now for this application we have

$$\begin{aligned} V(u_j - m_j\, h\, s) &= \frac{1}{2}u_j^2 - m_j\, u_j\, h\, s + \frac{1}{2}\, m_j^2\, h^2\, s^2 \\ V(u_j + m_{j+1}\, h\, s) &= \frac{1}{2}u_j^2 + m_{j+1}\, u_j\, h\, s + \frac{1}{2}\, m_{j+1}^2\, h^2\, s^2 \end{aligned} \qquad \text{h35}$$

Substitution into Eq. (h34) gives

$$\begin{aligned} &\nu\left(1 + \frac{u_j\, h\, \alpha}{2\nu}\right)(m_{j+1} - m_j) - \frac{u_j}{2}\,(u_{j+1} - u_{j-1}) = \\ &\quad = h^2\,(m_{j+1}^2 - m_j^2)\int_0^1 s\, S(s)\, ds + h^2\,(m_{j+1}^2 + m_j^2)\int_0^1 s\, T(s)\, ds \end{aligned} \qquad \text{h36}$$

In this equation we have let

$$\alpha = -2\int_0^1 T(s)\, ds \qquad \text{h37}$$

The parameter α thus determines the amount of upstream weighting; if both α and u_j have the same sign then the inclusion of the function T_j increases the coefficient of the diffusion term. The presence of the function T_j also decreases the truncation error. This development shows how to get an upstream method using the weighting function (7.139).

10.3. Combustion in Flames

The equations governing the propagation of flames in one dimension are given by Ramos [1987]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho\, u) = 0$$

$$\rho\left[\frac{\partial Y_i}{\partial t} + u\,\frac{\partial Y_i}{\partial x}\right] = R_i - \frac{\partial}{\partial x}(\rho\, Y_i\, V_i) \qquad \text{b1}$$

$$\rho C_p\left[\frac{\partial T}{\partial t} + u\,\frac{\partial T}{\partial x}\right] = \frac{\partial p}{\partial t} - \sum_{i=1}^{N} h_i\, R_i - \frac{\partial q_1}{\partial x} - \sum_{i=1}^{N} \rho\, Y_i\, V_i\, C_{pi}\,\frac{\partial T}{\partial x} \qquad \text{b2}$$

$$Y_N = 1 - \sum_{i=1}^{N-1} Y_i$$

$$p = \rho\,\tilde{R}\,T \sum_{i=1}^{N} \frac{Y_i}{\hat{M}_i}, \qquad C_p = \sum_{i=1}^{N} Y_i\, C_{pi} \qquad \text{b3}$$

$$h_i = h_i^0 + \int_{T_0}^{T} C_{pi}\, dT, \qquad q = -\lambda\,\frac{\partial T}{\partial x}$$

These are the continuity equation, conservation of mass, the energy equation, an equation saying the mass fractions add to one, the ideal gas law, the equation for heat capacity of a mixture, the equation for enthalpy of a species in an ideal gas, and q is the heat flux. The variables are ρ the density, u the velocity, t the time, x the distance, Y_i the mole fraction of the i-th species, w_i dot the reaction rate for the i-th species, V_i the diffusion velocity of the i-th species, p the pressure, T the absolute temperature, R squiggle the gas constant, C_p the heat capacity of the mixture, h_i the enthalpy of the i-th species, and λ the thermal conductivity. In these equations we have assumed that the flame speed is slow enough that the Mach number is low; in that case the pressure is constant in space. We have also neglected the Soret and Dufour effects (or thermal diffusion).

One form of the equations is for an infinite premixed combustible fluid mixture. The x-position goes from $-\infty < x < \infty$ and the flame propagates from one boundary ($x = -\infty$) to the other. If the mixture is stationary, the fluid velocity ahead of the flame is zero. We transform the equations into a Lagrangian coordinate system in order to eliminate the convection term. This is possible because of the infinite extent of the physical domain. We go from

$$(t, x) \rightarrow (\tau, \psi) \qquad \text{b4}$$

where

$$\tau = t$$
$$\frac{\partial \psi}{\partial x} = \rho$$
$$\frac{\partial \psi}{\partial t} = \int_{-\infty}^{x} \frac{\partial \rho}{\partial t}\, dx = -\int_{-\infty}^{x} \frac{\partial (\rho\, u)}{\partial x}\, dx = -\rho\, u \qquad \text{b5}$$

The derivatives are then calculated using

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial \tau}\frac{\partial \tau}{\partial t} + \frac{\partial \rho}{\partial \psi}\frac{\partial \psi}{\partial t}$$
$$\frac{\partial (\rho u)}{\partial x} = \frac{\partial (\rho u)}{\partial \tau}\frac{\partial \tau}{\partial x} + \frac{\partial (\rho u)}{\partial \psi}\frac{\partial \psi}{\partial x} \qquad \text{b6}$$

Since

$$\frac{\partial \tau}{\partial t} = 1, \quad \frac{\partial \psi}{\partial t} = -\rho\, u$$
$$\frac{\partial \tau}{\partial x} = 0, \quad \frac{\partial \psi}{\partial x} = \rho \qquad \text{b7}$$

we obtain

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial \tau} - \rho u \frac{\partial \rho}{\partial \psi}$$
$$\frac{\partial (\rho u)}{\partial x} = \rho \frac{\partial (\rho u)}{\partial \psi} \qquad \text{b8}$$

The continuity equation is then

$$\frac{\partial \rho}{\partial \tau} - \rho u \frac{\partial \rho}{\partial \psi} + \rho \frac{\partial (\rho u)}{\partial \psi} = 0 \qquad \text{b9}$$

which becomes

$$\frac{\partial \rho}{\partial \tau} + \rho^2 \frac{\partial u}{\partial \psi} = 0 \qquad \text{b10}$$

Likewise the derivatives of temperature and mass fraction are given by

$$\frac{\partial T}{\partial x} = \frac{\partial T}{\partial \tau}\frac{\partial \tau}{\partial x} + \frac{\partial T}{\partial \psi}\frac{\partial \psi}{\partial x} = \rho \frac{\partial T}{\partial \psi} \qquad \text{b11}$$

Thus the convective derivatives are

$$\frac{\partial T}{\partial t} + u\,\frac{\partial T}{\partial x} = \frac{\partial T}{\partial \tau} - \rho u\,\frac{\partial T}{\partial \psi} + u\,\rho\,\frac{\partial T}{\partial \psi} = \frac{\partial T}{\partial \tau} \qquad \text{b12}$$

With these manipulations the equations become

$$\frac{\partial Y_i}{\partial \tau} = \frac{1}{\rho} R_i - \frac{\partial}{\partial \psi}(\rho\, Y_i\, V_i)$$

$$\frac{\partial T}{\partial \tau} = \frac{1}{\rho C_p}\left[- \sum_{i=1}^{N} h_i R_i - \rho \frac{\partial q_1}{\partial \psi} - \sum_{i=1}^{N} \rho^2\, Y_i\, V_i\, C_{pi}\, \frac{\partial T}{\partial \psi} \right] \qquad \text{b13}$$

The boundary conditions are

$$\frac{\partial T}{\partial \psi}(-\infty, \tau) = \frac{\partial T}{\partial \psi}(\infty, \tau) = 0$$

$$\frac{\partial Y_i}{\partial \psi}(-\infty, \tau) = \frac{\partial Y_i}{\partial \psi}(\infty, \tau) = 0 \qquad \text{b14}$$

$$T(-\infty, \tau) = T^{un},\ Y_i(-\infty, \tau) = Y_i^{un}$$

and the initial conditions are

$$T(\psi, 0) = T^{un}(\psi)$$

$$Y_i(\psi, 0) = Y_i^{un}(\psi) \qquad \text{b15}$$

where the superscript “un” represents the value in the unburned region.

The Fickian model is obtained by making further assumptions. Assume that the binary diffusion coefficients of all pairs of chemicals are the same, the specific heats of all species are the same and that

$$\rho^2 D = \beta = \text{constant} \qquad \text{b16}$$

The diffusion velocity is given by Fick’s law

$$V_i = - D \frac{\partial}{\partial x}(\ln Y_i) = D \rho \frac{\partial}{\partial \psi}(\ln Y_i) = - \frac{D\rho}{Y_i} \frac{\partial Y_i}{\partial \psi}$$

$$\rho\, Y_i\, V_i = - D \rho^2 \frac{\partial Y_i}{\partial \psi} = - \beta \frac{\partial Y_i}{\partial \psi} \qquad \text{b18}$$

The Lewis number is taken as one.

$$\mathrm{Le} = \frac{\lambda}{\rho D C_p} = 1 \qquad \text{b45}$$

The equations are then

$$\frac{\partial Y_i}{\partial \tau} = \beta \frac{\partial^2 Y_i}{\partial \psi^2} + \frac{R_i}{\rho}$$

$$\frac{\partial T}{\partial \tau} = \beta \frac{\partial^2 T}{\partial \psi^2} - \sum_{i=1}^{N} \frac{h_i}{\rho} \frac{R_i}{\rho C_p} \qquad \text{b17}$$

Another simplification of Eq.(b13) applies when a burner-stabilized flame is achieved. The premixed gas enters the burner at the flame holder at x = 0 and flows to the flame zone and on to the burned zone (see Figure 10E.3). In this case we make the same transformation in Eq. (b.5) except that we replace one equation with:

$$\frac{\partial \psi}{\partial t} = \int_0^x \frac{\partial \rho}{\partial t}\, dx = -\int_0^x \frac{\partial (\rho\, u)}{\partial x}\, dx = -\rho\, u + \dot{m}(t) \qquad \text{b19}$$

where

$$\dot{m}(t) = \rho(0,t)\, u(0,t) \qquad \text{b20}$$

is the mass flux at the flame holder. Eq. (b13) are then

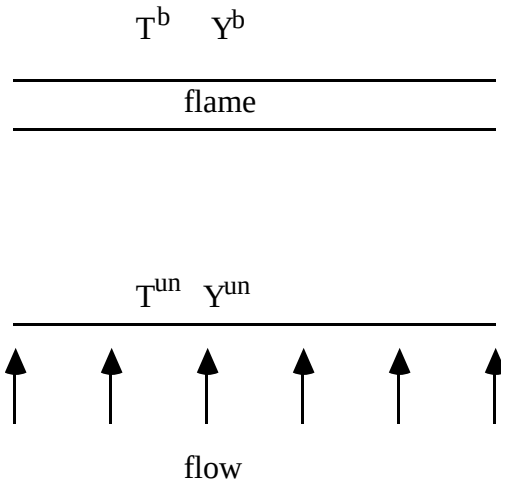


Figure 10E.3. Burner-stabilized Flame Geometry

$$\frac{\partial Y_i}{\partial \tau} + \dot{m}\frac{\partial Y_i}{\partial \psi} = \frac{1}{\rho} R_i - \frac{\partial}{\partial \psi}(\rho\, Y_i\, V_i)$$

$$\frac{\partial T}{\partial \tau} + \dot{m}\frac{\partial T}{\partial \psi} = \frac{1}{\rho C_p}\left[-\sum_{i=1}^{N} h_i\, R_i + \rho\frac{\partial q_1}{\partial \psi} - \sum_{i=1}^{N} \rho^2\, Y_i\, V_i\, C_{pi}\frac{\partial T}{\partial \psi} \right] \qquad \text{b21}$$

We consider only steady-state solutions of these equations

$$\dot{m}\frac{dY_i}{d\psi} = R_i - \frac{d}{d\psi}(\rho\, Y_i\, V_i)$$

$$\dot{m}\frac{dT}{d\psi} = \frac{1}{C_p}\left[-\sum_{i=1}^{N} h_i\, R_i - \frac{dq_1}{d\psi} - \sum_{i=1}^{N} \rho\, Y_i\, V_i\, C_{pi}\frac{dT}{d\psi} \right] \qquad \text{b22}$$

together with boundary conditions

$$T(0) = T^{un}, \quad Y_i(0) = Y_i^{un}$$

$$\frac{dT}{dx}(0) = \frac{dT}{dx}(\infty) = 0$$

$$\frac{dY_i}{dx}(0) = \frac{dY_i}{dx}(\infty) = 0 \qquad \text{b23}$$

We must solve these equations for the distribution of mole fractions, Y_i, and temperature, T; we must also solve for the mass flux, m dot.

10.4. Transient Catalytic Muffler

The unsteady problem uses the full equations Eq. (10.150)-(10.151). A finite difference formulation of this equation would give

$$\alpha_5 \left[\alpha_3 \frac{dT_i^s}{dt} - \left(\frac{r_{hs}}{L} \right)^2 \frac{T_{i+1}^s - T_i^s + T_{i-1}^s}{\Delta z^2} \right] + \frac{1}{2} Nu \left(T_i^s - T_i \right) + \beta_5 < r_i > = 0 \qquad c11$$

which is to be solved subject to the steady equations Eq. (10.135)-(10.136) and Eq. (10.138). Young and Finlayson [1976] did this using orthogonal collocation on finite elements for the solid temperature and solving the integro-differential equations, Eq. (10.150)-(10.151). Here we consider several other options. If we evaluate the integral in Eq. Eq. (10.148)-(10.149) from one grid point to the next we get

$$T_{i+1} = e^{-2 \alpha_1 Nu \Delta z} T_i + 2 \alpha_1 Nu \int_{z_i}^{z_{i+1}} e^{-2 \alpha_1 Nu (z_{i+1} - z')} T^s(z') \, dz', \quad z_{i+1} = z_i + \Delta z \qquad c12$$

If the integral is evaluated using the trapezoid rule, the result is

$$T_{i+1} = e^{-2 \alpha_1 Nu \Delta z} \left[T_i + \frac{2 \alpha_1 Nu \Delta z}{2} T_i^s \right] + \frac{2 \alpha_1 Nu \Delta z}{2} T_{i+1}^s \qquad c13$$

This equation is of the form

$$T_{i+1} = \gamma_1 T_i + \gamma_2 T_{i+1}^s + \gamma_3 T_i^s \qquad c14$$

If the Euler method is applied to Eq. (10.135)-(10.136) we get

$$\frac{T_{i+1} - T_i}{\Delta z} + 2 \alpha_1 Nu T_i = 2 \alpha_1 Nu \, T_i^s \qquad c15$$

or if a second-order Runge-Kutta method is applied we get instead

$$\frac{T_{i+1} - T_i}{\Delta z} + \frac{2 \alpha_1 Nu}{2} \left(T_i + T_{i+1} \right) = \frac{2 \alpha_1 Nu}{2} \left(T_i^s + T_{i+1}^s \right) \qquad c16$$

Both Eq. (c15-16) can be rearranged to give

$$T_{i+1} = T_i \left(1 - 2 \alpha_1 Nu \Delta z \right) + 2 \alpha_1 Nu \Delta z \, T_i^s \qquad c17$$

or

$$T_{i+1} = \left(\frac{1 - \alpha_1 Nu \Delta z}{1 + \alpha_1 Nu \Delta z} \right) T_i + \frac{\Delta z}{2} \frac{2 \alpha_1 Nu}{1 + \alpha_1 Nu \Delta z} \left(T_i^s + T_{i+1}^s \right)$$

Notice that these are appoximations in various degrees to Eq. (c13). They can also be put into the form of Eq. (c14). Thus the temperature equations are Eq. (c11) and Eq. (c14). The equations are similar for the mole fraction Y and Y^S. The equation (10.147) or Eq. (10.149) can be written in finite difference form as

$$Y_{i+1} = \delta_1 \, Y_i + \delta_2 \, Y^s_{i+1} + \delta_3 \, Y^s_i \qquad \text{c18}$$

where the Euler method uses

$$\delta_1 = 1 - 2 \, \alpha_2 \, Sh \, \Delta z, \quad \delta_2 = 0, \quad \delta_3 = 2 \, \alpha_2 \, Sh \, \Delta z \qquad \text{c19}$$

and the Runge-Kutta method uses

$$\delta_1 = \frac{1 - \alpha_2 \, Sh \, \Delta z}{1 + \alpha_2 \, Sh \, \Delta z}, \quad \delta_2 = \frac{\alpha_2 \, Sh \, \Delta z}{1 + \alpha_2 \, Sh \, \Delta z}, \quad \delta_3 = \frac{\alpha_2 \, Sh \, \Delta z}{1 + \alpha_2 \, Sh \, \Delta z} \qquad \text{c20}$$

The Eq. (10.138) is then

$$-\alpha_6 \, \beta_4 < r >_i + \frac{1}{2} \, Sh \, (Y^s_i - Y_i) = 0 \qquad \text{c21}$$

Consider the case when the variables T_i, Y_i, T^s_i, Y^s_i are known at some time t. Then Eq. (c11) can be used to step forward to determine T^s_i at time $t + \Delta t$ for all i. Eq. (c14) can then be used to step forward to determine T_i at time $t + \Delta t$ for all i. Next look at the concentration equation for the first node.

$$-\alpha_6 \, \beta_4 < r >_1 + \frac{1}{2} \, Sh \, (Y^s_1 - Y_1) = 0 \qquad \text{c22}$$

The value of Y_1 would be known from the boundary condtions at every time t, including time $t + \Delta t$. Thus we must evaluate the reaction rate. Use $y = Y_1$ in Eq. (10.139), then $y_0 = Y_1$ in Eq. (10.142), and then calculate $< r >_1$ from Eq. (10.143). Then Eq. (c22) gives Y^s_1.

At this point in the calculations we have the value of T_i and T^s_i at time $t + \Delta t$ for all i, and we know Y_1, Y^s_1 at time $t + \Delta t$. We then solve Eq. (c18) and (c21) for Y_2, Y^s_2 at time $t + \Delta t$. These are written in terms of the unknowns Y^{n+1}_{i+1}, $Y^{s,n+1}_{i+1}$ and the known quantities Y^{n+1}_i, $Y^{s,n+1}_i$.

$$Y^{n+1}_{i+1} - \delta_2 \, Y^{s,n+1}_{i+1} = \delta_1 \, Y^{n+1}_i + \; + \delta_3 \, Y^{s,n+1}_i \qquad \text{c23}$$

$$-\alpha_6 \, \beta_4 < r >^{n+1}_{i+1} + \frac{1}{2} \, Sh \, (Y^{s,n+1}_{i+1} - Y^{n+1}_{i+1}) = 0 \qquad \text{c24}$$

This set of two equations must be solved simultaneously for i=1. Then we can increase i and repeat until we reach an i representing the end of the reactor. Then we know T_i, Y_i, T^s_i, Y^s_i at time $t + \Delta t$ for all i. We then repeat the process. Of course, all the techniques discussed in the book can be applied. In particular the nodes can be moved as the front moves and concentrated near the reaction zone. Travelling waves could also be evaluated.

12.3. Compressibility Method

The first method originated with Chorin [1967] and is called the artificial compressibility method because the incompressible fluid is allowed to have a small compressibility. The chief problem with the Navier-Stokes equations and the continuity equation is that the Navier-Stokes equations are equations for velocities, and they include the pressure gradient. The continuity equation is a constraint on the velocity but is in essence the equation for pressure. The continuity equation for an incompressible fluid does not have a time derivative in it, so in the artificial compressibility method a time derivative is added. The continuity equation is expanded to be

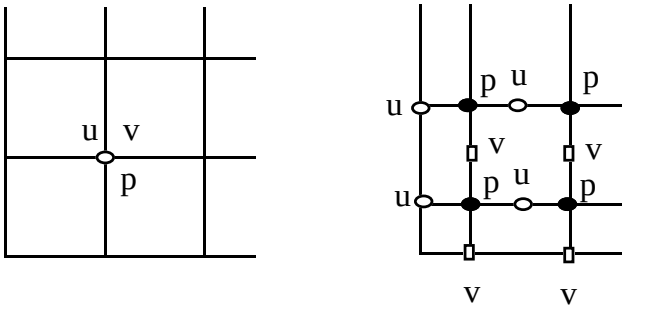
$$\frac{\partial p}{\partial t} + c^2 \nabla \cdot \mathbf{u} = 0 \qquad \text{u1}$$

The constant parameter c^2 is chosen to aid in convergence and the transient itself does not have any physical significance. The method is termed artificial compressibility because Eq. (u1) is the continuity equation for a compressible fluid with an equation of state

$$p = c^2 \rho \qquad \text{u2}$$

The method itself is listed in Table 12.2. Now we have three (or four) parabolic equations in time for the pressure and the two (or three) velocity components. Standard algorithms for parabolic equations can be applied.

When the algorithm is applied each variable can be identified with the same node, as shown in Figure 12.E1(a), or different grids can be used for different variables, as in Figure 12.E1(b).



(a) regular mesh (b) staggered mesh

Figure 12.E1. Finite difference meshes

The first grid, Figure 12.E1(a) is not a preferred one because the boundary conditions for pressure are inconvenient to derive. We discuss here the equations involving boundary terms for the staggered grid, Figure 12.E1(b), which is known as the MAC mesh. Consider the problem shown in Figure 12.E2, an entry flow problem with a solid boundary, a line of symmetry, an entry condition and an exit condition.

For side A the u nodes occur on the boundaries, so that we set the u velocity there. The same thing is true for the v velocity on B and C. However, the v velocity nodes are not on the boundary A, nor are the u velocity nodes on the boundary B. On A we force the boundary condition by taking the v-

value Δx/2 outside the mesh to equal minus the v-value Δx/2 inside the mesh. Then the average value is zero, and the average value represents the v-value on A.

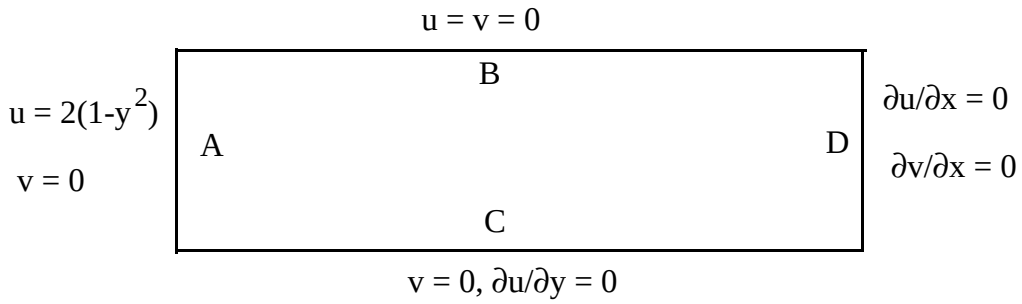


Figure 12.E2. Entry-length problem

$$v_{0,j+1/2} = - v_{1,j+1/2}$$

In an analogous fashion we use

$$u_{i+1/2,M+1} = -u_{i+1/2,M}$$

for the u-boundary conditions on surface B. To force the first derivative of u to zero on boundary C we use

$$u_{i+1/2,M+1} = -u_{i+1/2,M}$$

This represents the value of the first derivative centered on y=0. On the exit boundary D the v derivative is centered on the exit.

$$v_{N+1,j+1/2} = v_{N-1,j+1/2}$$

The u-velocity is expressed at nodes that are on the boundary. To set the first derivative to zero we take the value –Δx from the exit to equal to the value +Δx from the exit.

$$u_{N+3/2,j} = u_{N-1/2,j}$$

Following these rules, and using an explicit method for integrating in time, gives the following algorithm for this case.

$$\frac{u^{n+1}_{i+1/2,j} - u^{n}_{i+1/2,j}}{\Delta t} = - \frac{p^{n}_{i+1,j} - p^{n}_{i,j}}{\Delta x} - u^{n}_{i+1/2,j}\frac{u^{n}_{i+3/2,j} - u^{n}_{i-1/2,j}}{2\Delta x} +$$
$$- \frac{1}{4}\left(v^{n}_{i+1,j+1/2} + v^{n}_{i,j+1/2} + v^{n}_{i,j-1/2} + v^{n}_{i+1,j-1/2}\right)\frac{u^{n}_{i+1/2,j+1} - u^{n}_{i+1/2,j-1}}{2\Delta y} +$$
$$+ \frac{1}{Re}\left(\frac{u^{n}_{i+3/2,j} - 2u^{n}_{i+1/2,j} + u^{n}_{i-1/2,j}}{\Delta x^2} + \frac{u^{n}_{i+1/2,j+1} - 2u^{n}_{i+1/2,j} + u^{n}_{i+1/2,j-1}}{\Delta y^2}\right) \qquad \text{u5}$$

$$i = 1, \ldots, N; \; j=1, \ldots, M$$

$$\frac{v^{n+1}_{i,j+1/2} - v^{n}_{i,j+1/2}}{\Delta t} = - \frac{p^{n}_{i,j+1} - p^{n}_{i,j}}{\Delta y} - v^{n}_{i,j+1/2}\left(\frac{v^{n}_{i,j+3/2} - v^{n}_{i,j-1/2}}{2\Delta y} \right)$$

$$- \frac{1}{4}\left(u^{n}_{i+1/2,j} + u^{n}_{i+1/2,j+1} + u^{n}_{i-1/2,j} + u^{n}_{i-1/2,j+1}\right) \frac{v^{n}_{i+1,j+1/2} - v^{n}_{i-1,j+1/2}}{2\Delta x} +$$

$$+ \frac{1}{\mathrm{Re}} \left(\frac{v^{n}_{i+1,j+1/2} - 2v^{n}_{i,j+1/2} + v^{n}_{i-1,j+1/2}}{\Delta x^2} + \frac{v^{n}_{i,j+3/2} - v^{n}_{i,j+1/2} + v^{n}_{i,j-1/2}}{\Delta y^2} \right)$$

$$i = 1, \ldots, N;\ j=1, \ldots, M\text{-}1$$

$$\frac{p^{n+1}_{i,j} - p^{n}_{i,j}}{\Delta t} = -c^2 \left[\frac{u^{n+1}_{i+1/2,j} - u^{n+1}_{i-1/1,j}}{\Delta x} + \frac{v^{n+1}_{i,j+1/2} - v^{n+1}_{i,j-1/2}}{\Delta y} \right]$$

$$i = 1, \ldots, N;\ j=1, \ldots, M$$

surface A: $u_{1/2,j} = 2\left(1 - y_j^2\right)$, $v_{0,j+1/2} = - v_{1,j+1/2}$

surface B: $u_{i+1/2,M+1} = -u_{i+1/2,M}$, $v_{i,M+1/2} = 0$

surface C: $u_{i+1/2,0} = u_{i+1/2,1}$, $v_{i,1/2} = 0$

surface D: $u_{N+3/2,j} = u_{N-1/2,j}$, $v_{N+1,j+1/2} = v_{N-1,j+1/2}$

13.4. u-v Formulation

Another way to solve this problem is to tackle the second-order problem, Eq. (13.91), but with the new variable

$$v = \frac{\partial u}{\partial t} \qquad \text{f3}$$

Then Eq. (13.91) is

$$\frac{\partial v}{\partial t} = -\frac{v}{E} + \frac{1}{E}\frac{\partial^2 u}{\partial y^2} \qquad \text{f4}$$

coupled with

$$\frac{\partial u}{\partial t} = v \qquad \text{f2}$$

We now have a system of two equations to solve for u(y,t) and v(y,t). Note that the two equations look like a diffusion Eq.(f4) with a source term and an equation with only a source term, Eq. (f2). The convective nature of the problem is not apparent with this formulation. Only a centered finite difference method is suitable here, since upstream derivatives cannot be used on the non-existent convection terms.

$$\begin{aligned} \frac{dv_i}{dt} &= -\frac{v_i}{E} + \frac{u_{i+1} - 2\,u_i + u_{i-1}}{E\Delta y^2} \qquad i = 2,\ldots,\ N-1 \\ \frac{du_i}{dt} &= v_i \end{aligned} \qquad \text{f5}$$

This set is applied at the points i = 2,..., N-1. The two end points must be handled with boundary conditions.

$$\begin{aligned} u(0,t) &= 1 \quad \text{or } u_1(t) = 1 \\ u(1,t) &= 0 \quad \text{or } u_N(t) = 0 \end{aligned} \qquad \text{f6}$$

Thus we know the value of u_1 and u_N that are needed in the first of Eq. (f5) when i = 2 or i = N-1. We do not know the corresponding values of v_1 and v_N, but fortunately *we do not need them*.. Thus we have enough equations for the solution. The initial conditions are

$$\begin{aligned} u(y,0) &= 0 \ \text{ or } u_i(0) = 0, \ \ i = 1,\ldots N \\ \frac{\partial u}{\partial t}(y,0) &= 0 \ \text{ or } v_i(0) = 0, \ i=2,\ldots,N-1 \end{aligned} \qquad \text{f7}$$

We then integrate the 2(N-2) equations, Eq.(f5), together with the boundary conditions, Eq.(f6), beginning with the initial conditions, Eq.(f7).

The stability of this set of equations can be derived using the Fourier analysis, which gives

$$\Delta t \leq \frac{\Delta y^2}{4} \qquad \text{f12}$$

or a time step four times smaller than for the other set of equations.