An accurate numerical method for systems of differentio-integral equations associated with multiphase flow

Shu, Jian Jun; Wilks, Graham

1995

Shu, J. J., & Wilks, G. (1995). An accurate numerical method for systems of
differentio-integral equations associated with multiphase flow. *Computers & Fluids*, 24(6),
625-652.

<https://hdl.handle.net/10356/94033>

[https://doi.org/10.1016/0045-7930\(95\)00012-2](https://doi.org/10.1016/0045-7930(95)00012-2)

© 1995 Elsevier. This is the author created version of a work that has been peer reviewed
and accepted for publication by *Computers & Fluids*, Elsevier. It incorporates referee' s
comments but changes resulting from the publishing process, such as copyediting,
structural formatting, may not be reflected in this document. The published version is
available at: [DOI: [http://dx.doi.org/10.1016/0045-7930\(95\)00012-2](http://dx.doi.org/10.1016/0045-7930(95)00012-2)].

Downloaded on 26 Apr 2023 19:35:06 SGT

AN ACCURATE NUMERICAL METHOD FOR SYSTEMS OF DIFFERENTIO-INTEGRAL EQUATIONS ASSOCIATED WITH MULTIPHASE FLOW

JIAN-JUN SHU[†] and GRAHAM WILKS[‡]

University of Keele, Keele, Staffordshire ST5 5BG, England, U.K.

Abstract—An accurate numerical method which is applicable to systems of differentio-integral equations with quite general boundary conditions has been developed. The method is a useful extension of the Keller box scheme designed to facilitate the solution of differential systems involving integral operators which naturally arise in multiphase flows. A combination of merging and reduction procedures is introduced to handle the multilayer and integral operator features of such problems. The development of the method is demonstrated in the context of laminar film condensation in the presence of both external forcing and body forces.

1. INTRODUCTION

The Keller box scheme [1–3] for the solution of parabolic boundary layer equations is both accurate and robust. As a consequence it has been used extensively in solving a broad class of problems including convection flows [4], jet flows [5, 6], turbulent boundary layers [3, 7] as well as separating flows [8]. These problems have typically involved a single shear layer, each described only by governing differential equations and differential boundary conditions. The method has been particularly useful in tackling that class of problem, which although non-similar, may be formulated as a progression between known limiting similarity states which are inherent in the physical configuration under examination. Mixed convection about a heated, vertical, semi-infinite plate is just such an example when it may be argued physically that the flow will be predominantly Blasius flow at the leading edge but that downstream the flow will increasingly be dominated by free convection effects, see [9, 10]. The underlying growth rates of fundamental variables may be incorporated in the associated similarity transformation and by judicious combination or continuous transformation, [11, 12], the overall non-similarity may be incorporated in a differential system which remains $O(1)$ throughout the computational domain. Lin and co-workers e.g. [13, 14] particularly have exploited this form of solution.

In the work that follows it is demonstrated that the Keller box method can successfully be adapted to multilayer problems which, typically in a multi-phase setting, are more naturally described by differentio-integral systems. The simultaneous presence of condensate films and vapour shear layers in laminar film condensation is an example of such a multilayer parabolic system. Here there are special circumstances in which self-similarity prevails namely the cases of pure forced convection condensation or pure body force laminar condensation. In each of these separate cases the similarity system has been solved successfully using a guessing strategy based upon a specified location of the phase interface. Coupled with an iterative process based on single layer methods it has then been possible to converge onto a solution satisfying the interfacial boundary conditions for an associated set of physical parameter values e.g. [15]. However in other general circumstances for which a similarity simplification is not available the difficulties associated with the presence of a variable film thickness and the mass transfer at the phase transition have precluded detailed solutions. To obviate such difficulties authors have resorted to momentum integral and perturbation techniques as in [16–20]. These are currently the only solutions available. In the work that follows a comprehensive numerical scheme is outlined which successfully

[†]Present address: Department of Applied Mathematical Studies, University of Leeds, Leeds LS2 9JT, U.K.

[‡]Author for correspondence.

accommodates these difficulties and accordingly deals with the respective features of an unknown film thickness, multiphase and non-similarity.

It is natural, in the first instance, to envisage a non-similar multiphase, multilayer configuration which is an extension of the class of non-similar single layer problems typified by the mixed convection flow mentioned earlier. Further the configuration should provide the framework for the possible exploitation of the powerful Keller box scheme. The setting chosen is that involving combined gravity body force and forced convection laminar film condensation accompanying the flow of a saturated vapour along a cooled semi-infinite vertical wall. This configuration accordingly can be examined as a transition between well-established limiting similarity states. Moreover detailed solutions for each limiting situation are available for comparison and over the non-similar range comparisons can be made with the only available results of Jacobs [19] and Fujii and Uehara [18] who each used momentum integral methods and thin film approximations.

Although the numerical scheme is developed in this particular context the problem is regarded as a prototype of a general class of problems and it is understood that the essential numerical features of the formulation and solution algorithm may readily be adapted by any alternative example.

2. MODEL CONFIGURATION AND GOVERNING EQUATIONS

The prototype physical configuration is illustrated in Fig. 1. A steady stream of pure, saturated vapour aligned with the background gravitational field, flows with uniform velocity U_∞ over a semi-infinite plate. The surface of the plate is maintained at a uniform temperature T_w which is below the saturation temperature T^* of the external vapour stream. A thin film flow of condensate within a vapour shear layer will result. The overall flow is modelled as two dimensional and incompressible.

The velocity components (u, v) are associated with increasing x and y measured along and normal to the plate respectively. T is used to denote the temperature of the condensate and $y = \delta(x)$ denotes the interface separating the condensate and vapour phases of the flow. For the vapour phase a set of intrinsic coordinates (x^*, y^*) attached to the interface are chosen. x^* measures the distance along the interface, y^* the distance normal to it and (u^*, v^*) are the velocity components in the directions of increasing (x^*, y^*) .

If it is assumed that the thickness of the condensate film is small compared with a typical dimension of the surface then $x = x^*$ is a valid approximation. Furthermore, on the assumption

Fig. 1. Prototype physical configuration and co-ordinate system.

that all changes in physical quantities normal to the surface or the interface are large compared with changes in the x -direction, it is appropriate to invoke the boundary layer approximation. The governing boundary layer equations describing conservation of mass and momentum in both phases and thermal energy in the condensate phase are, in the usual notation, as follows

Condensate phase ($x \geq 0, 0 \leq y \leq \delta(x)$)

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (1)$$

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = g(\rho - \rho^*) + \mu \frac{\partial^2 u}{\partial y^2} \quad (2)$$

$$\rho C_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = k \frac{\partial^2 T}{\partial y^2}. \quad (3)$$

Vapour phase ($x \geq 0, y^* \geq 0, T = T^*$)

$$\frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y^*} = 0 \quad (4)$$

$$\rho^* u^* \frac{\partial u^*}{\partial x} + \rho^* v^* \frac{\partial u^*}{\partial y^*} = \mu^* \frac{\partial^2 u^*}{\partial y^{*2}} \quad (5)$$

Boundary conditions:

For $x \geq 0, y = 0$,

$$u = 0, \quad v = 0, \quad T = T_w \quad (6)$$

and at the interface,

$$x \geq 0, \quad y = \delta(x), \quad y^* = 0, \quad T = T^* \quad (7)$$

Continuity in the interface mass flow requires

$$\rho^* \left(v^* - u^* \frac{d\delta}{dx} \right) = \rho \left(v - u \frac{d\delta}{dx} \right) = -\frac{d}{dx} \left(\int_0^{\delta(x)} \rho u \, dy \right) \quad (8)$$

and for continuity in the tangential component of the interfacial velocity

$$u^* = u. \quad (9)$$

The continuity in interface shear stress components is assured if

$$\mu^* \frac{\partial u^*}{\partial y^*} = \mu \frac{\partial u}{\partial y}, \quad p = p^*. \quad (10)$$

In the vapour phase $x \geq 0, y^* \rightarrow +\infty$, the velocity must approach that of the external stream i.e.

$$u^* \rightarrow U_\infty. \quad (11)$$

The overall energy balance is given by

$$-\int_0^x k \left(\frac{\partial T}{\partial y} \right)_{y=0} dx + \int_0^{\delta(x)} \rho u h_{fg} dy + \int_0^{\delta(x)} \rho u C_p (T^* - T) dy = 0. \quad (12)$$

Here ρ , μ , C_p , k , h_{fg} and $v = \mu/\rho$ denote density, dynamic viscosity, specific heat, thermal conductivity, latent heat and kinematic viscosity respectively and an asterisk $*$ is employed to signify a vapour quantity.

A significant step in formulating the problem for comprehensive solutions is the introduction of the characteristic non-dimensional co-ordinate $\xi = 1/\text{Fr}_x = gx/U_\infty^2$. This co-ordinate provides the basis for a unified framework within which the features of dominant forced convection condensation and dominant body force condensation may be associated with small and large ξ respectively, in other words, large and small Froude numbers respectively.

3. CONTINUOUS TRANSFORMATION FORMULATION

Hunt and Wilks [11] have demonstrated the advantages of introducing a continuous transformation in the characteristic coordinate. It is this method which is adapted to the present problem to yield a set of equations which adequately accommodate the essential features of each of the extremes of forced convection and body force condensation.

The following transformations are introduced

$$\psi = \lambda \sqrt{2\nu U_\infty x} r(\xi) f(\xi, \eta), \quad \eta = \lambda \frac{\sqrt{U_\infty}}{\sqrt{2\nu}} \frac{y}{x^{1/2}} t(\xi), \quad (13)$$

$$\psi^* = \sqrt{2\nu^* U_\infty x} r^*(\xi) f^*(\xi, \eta^*), \quad \eta^* = \frac{\sqrt{U_\infty}}{\sqrt{2\nu^*}} \frac{y^*}{x^{1/2}} t^*(\xi), \quad (14)$$

$$T - T^* = (T_w - T^*) s(\xi) \theta(\xi, \eta) \quad (15)$$

where $r(\xi)$, $t(\xi)$, $r^*(\xi)$, $t^*(\xi)$ and $s(\xi)$ are to be chosen to effect a smooth transition between the two extreme regimes. Under these transformations the governing equations (1)–(5) and boundary conditions (6)–(11) become

$$\frac{\partial^3 f}{\partial \eta^3} + \frac{(\xi r^2)'}{rt} f \frac{\partial^2 f}{\partial \eta^2} - \frac{2\xi(rt)'}{t^2} \left(\frac{\partial f}{\partial \eta} \right)^2 + \frac{2\xi}{t^3 r} + \frac{2\xi r}{t} \left(\frac{\partial f}{\partial \xi} \frac{\partial^2 f}{\partial \eta^2} - \frac{\partial f}{\partial \eta} \frac{\partial \xi}{\partial \eta} \frac{\partial^2 f}{\partial \eta} \right) = 0 \quad (16)$$

$$\frac{\partial^2 \theta}{\partial \eta^2} + P_r \left[\frac{(\xi r^2)'}{rt} f \frac{\partial \theta}{\partial \eta} - \frac{2\xi r s'}{st} \frac{\partial f}{\partial \eta} \theta + \frac{2\xi r}{t} \left(\frac{\partial f}{\partial \xi} \frac{\partial \theta}{\partial \eta} - \frac{\partial f}{\partial \eta} \frac{\partial \theta}{\partial \xi} \right) \right] = 0 \quad (17)$$

$$\frac{\partial^3 f^*}{\partial \eta^{*3}} + \frac{(\xi r^{*2})'}{r^* t^*} f^* \frac{\partial^2 f^*}{\partial \eta^{*2}} - \frac{2\xi(r^* t^*)'}{t^{*2}} \left(\frac{\partial f^*}{\partial \eta^*} \right)^2 + \frac{2\xi r^*}{t^*} \left(\frac{\partial f^*}{\partial \xi} \frac{\partial^2 f^*}{\partial \eta^{*2}} - \frac{\partial f^*}{\partial \eta^*} \frac{\partial \xi}{\partial \eta^*} \frac{\partial^2 f^*}{\partial \eta^*} \right) = 0 \quad (18)$$

where $P_r = \nu/\kappa$ and κ is the thermometric conductivity $k/\rho C_p$. The boundary conditions are:

at the wall $\eta = 0$,

$$f = 0, \quad \frac{\partial f}{\partial \eta} = 0, \quad s\theta = 1; \quad (19)$$

and at the interface $\eta = \eta_\delta(\xi)$, $\eta^* = 0$,

$$\theta = 0,$$

$$r^* f^* = \lambda \omega r f, \quad r^* t^* \frac{\partial f^*}{\partial \eta^*} = \lambda^2 r t \frac{\partial f}{\partial \eta}, \quad r^* t^{*2} \frac{\partial^2 f^*}{\partial \eta^{*2}} = \lambda^3 \omega r t^2 \frac{\partial^2 f}{\partial \eta^2} \quad (20)$$

where

$$\omega = \left(\frac{\rho \mu}{\rho^* \mu^*} \right)^{1/2} \quad \text{and} \quad \lambda = \left(\frac{\rho - \rho^*}{\rho} \right)^{1/4}$$

In the vapour as $\eta^* \rightarrow +\infty$,

$$r^* t^* \frac{\partial f^*}{\partial \eta^*} \rightarrow 1. \quad (21)$$

Equation (12) becomes

$$\begin{aligned} H_0 \left[\left(\frac{\partial \theta}{\partial \eta} \right)_{\eta=0} + P_r \left[\frac{(\xi r^2)'}{rt} + \frac{2\xi r s'}{st} \right] \int_0^{\eta_\delta(\xi)} \frac{\partial f}{\partial \eta} \theta \, d\eta + 2\xi P_r \frac{r}{t} \int_0^{\eta_\delta(\xi)} \left(\frac{\partial^2 f}{\partial \xi \partial \eta} \theta + \frac{\partial f}{\partial \eta} \frac{\partial \theta}{\partial \xi} \right) d\eta \right] \\ + \frac{(\xi r^2)'}{rst} (f)_{\eta=\eta_\delta(\xi)} + 2\xi \frac{r}{st} \left(\frac{\partial f}{\partial \xi} \right)_{\eta=\eta_\delta(\xi)} + 2\xi \frac{r}{st} \left(\frac{\partial f}{\partial \eta} \right)_{\eta=\eta_\delta(\xi)} \frac{d\eta_\delta(\xi)}{d\xi} = 0 \end{aligned} \quad (22)$$

where $H_0 = C_p \Delta T / P_r h_{fg}$ with $\Delta T = T^* - T_w$. In the (ξ, η) -plane the thickness of the condensate layer is $\eta = \eta_\delta(\xi)$ when $y = \delta(x)$. With

$$r(0) = s(0) = t(0) = r^*(0) = t^*(0) = 1 \quad (23)$$

the forced convection condensation formulation of [17] is recovered. The prescriptions of

$$\begin{aligned} r(\xi) &= (1 + 16\xi)^{1/4}, \quad s(\xi) = 1, \quad t(\xi) = (1 + \xi)^{1/4}, \\ r^*(\xi) &= (1 + 16\xi)^{1/4}, \quad t^*(\xi) = (1 + \xi)^{1/4} \end{aligned} \quad (24)$$

retain the forced convection required at small ξ but now incorporate the Koh *et al.* [15] pure body force formulation at large ξ . The resulting unified basis of computation is now the system of equations

$$\begin{aligned} \frac{\partial^3 f}{\partial \eta^3} + \frac{1 + 24\xi}{(1 + \xi)^{1/4}(1 + 16\xi)^{3/4}} f \frac{\partial^2 f}{\partial \eta^2} - \frac{\xi(17 + 32\xi)}{2(1 + \xi)^{5/4}(1 + 16\xi)^{3/4}} \left(\frac{\partial f}{\partial \eta} \right)^2 \\ + \frac{2\xi}{(1 + \xi)^{3/4}(1 + 16\xi)^{1/4}} + \frac{2\xi(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left\{ \frac{\partial f}{\partial \xi} \frac{\partial^2 f}{\partial \eta^2} - \frac{\partial f}{\partial \eta} \frac{\partial^2 f}{\partial \xi \partial \eta} \right\} = 0 \end{aligned} \quad (25)$$

$$\frac{\partial^2 \theta}{\partial \eta^2} + P_r \left[\frac{1 + 24\xi}{(1 + \xi)^{1/4}(1 + 16\xi)^{3/4}} f \frac{\partial \theta}{\partial \eta} + 2\xi \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left\{ \frac{\partial f}{\partial \xi} \frac{\partial \theta}{\partial \eta} - \frac{\partial f}{\partial \eta} \frac{\partial \theta}{\partial \xi} \right\} \right] = 0 \quad (26)$$

$$\begin{aligned} \frac{\partial^3 f^*}{\partial \eta^{*3}} + \frac{1 + 24\xi}{(1 + \xi)^{1/4}(1 + 16\xi)^{3/4}} f^* \frac{\partial^2 f^*}{\partial \eta^{*2}} - \frac{\xi(17 + 32\xi)}{2(1 + \xi)^{5/4}(1 + 16\xi)^{3/4}} \left(\frac{\partial f^*}{\partial \eta^*} \right)^2 \\ + \frac{2\xi(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left\{ \frac{\partial f^*}{\partial \xi} \frac{\partial^2 f^*}{\partial \eta^{*2}} - \frac{\partial f^*}{\partial \eta^*} \frac{\partial^2 f^*}{\partial \xi \partial \eta^*} \right\} = 0 \end{aligned} \quad (27)$$

$$\begin{aligned} H_0 \left[\left(\frac{\partial \theta}{\partial \eta} \right)_{\eta=0} + P_r \frac{1 + 24\xi}{(1 + \xi)^{1/4}(1 + 16\xi)^{3/4}} \int_0^{\eta_\delta(\xi)} \frac{\partial f}{\partial \eta} \theta \, d\eta \right. \\ \left. + 2\xi P_r \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \int_0^{\eta_\delta(\xi)} \left(\frac{\partial^2 f}{\partial \xi \partial \eta} \theta + \frac{\partial f}{\partial \eta} \frac{\partial \theta}{\partial \xi} \right) d\eta \right] \\ + \frac{1 + 24\xi}{(1 + \xi)^{1/4}(1 + 16\xi)^{3/4}} (f)_{\eta=\eta_\delta(\xi)} + 2\xi \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left(\frac{\partial f}{\partial \xi} \right)_{\eta=\eta_\delta(\xi)} \\ + 2\xi \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left(\frac{\partial f}{\partial \eta} \right)_{\eta=\eta_\delta(\xi)} \frac{d\eta_\delta(\xi)}{d\xi} = 0 \end{aligned} \quad (28)$$

to be solved subject to boundary conditions

$$f(\xi, 0) = 0, \quad \frac{\partial f(\xi, 0)}{\partial \eta} = 0, \quad \theta(\xi, 0) = 1, \quad \theta(\xi, \eta_\delta(\xi)) = 0, \quad (29)$$

$$f^*(\xi, 0) = \lambda \omega f(\xi, \eta_\delta(\xi)), \quad \frac{\partial f^*(\xi, 0)}{\partial \eta^*} = \lambda^2 \frac{\partial f(\xi, \eta_\delta(\xi))}{\partial \eta},$$

$$\frac{\partial^2 f^*(\xi, 0)}{\partial \eta^{*2}} = \lambda^3 \omega \frac{\partial^2 f(\xi, \eta_\delta(\xi))}{\partial \eta^2}, \quad (30)$$

$$\frac{\partial f^*(\xi, +\infty)}{\partial \eta^*} = \frac{1}{(1 + \xi)^{1/4}(1 + 16\xi)^{1/4}} \quad (31)$$

Equation (28) can be simplified, using equations (26) and (29), to

$$\begin{aligned}
& H_0 \left(\frac{\partial \xi}{\partial \eta} \right)_{\eta = \eta_\delta(\xi)} + \frac{1 + 24\xi}{(1 + \xi)^{1/4} (1 + 16\xi)^{3/4}} (f)_{\eta = \eta_\delta(\xi)} \\
& + 2\xi \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left(\frac{\partial f}{\partial \xi} \right)_{\eta = \eta_\delta(\xi)} \\
& + 2\xi \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}} \left(\frac{\partial f}{\partial \eta} \right)_{\eta = \eta_\delta(\xi)} \frac{d\eta_\delta(\xi)}{d\xi} = 0.
\end{aligned} \quad (32)$$

The general class of differentio-integral systems under examination may therefore be abbreviated as

$$\frac{\partial^3 f}{\partial \eta^3} + \alpha(\xi) f \frac{\partial^2 f}{\partial \eta^2} + \beta(\xi) \left[\gamma(\xi) - \left(\frac{\partial f}{\partial \eta} \right)^2 \right] = 2\xi p(\xi) \left[\frac{\partial f}{\partial \eta} \frac{\partial^2 f}{\partial \xi \partial \eta} - \frac{\partial^2 f}{\partial \eta^2} \frac{\partial f}{\partial \xi} \right] \quad < \eta < \eta_\delta(\xi) \quad (33)$$

$$\frac{1}{P_r} \frac{\partial^2 \theta}{\partial \eta^2} + \alpha(\xi) f \frac{\partial \theta}{\partial \eta} = 2\xi p(\xi) \left[\frac{\partial f}{\partial \eta} \frac{\partial \theta}{\partial \xi} - \frac{\partial \theta}{\partial \eta} \frac{\partial f}{\partial \xi} \right] \quad 0 < \eta < \eta_\delta(\xi) \quad (34)$$

$$\frac{\partial^3 f^*}{\partial \eta^{*3}} + \alpha(\xi) f^* \frac{\partial^2 f^*}{\partial \eta^{*2}} - \beta(\xi) \left(\frac{\partial f^*}{\partial \eta^*} \right)^2 = 2\xi p(\xi) \left[\frac{\partial f^*}{\partial \eta^*} \frac{\partial^2 f^*}{\partial \xi \partial \eta^*} - \frac{\partial^2 f^*}{\partial \eta^{*2}} \frac{\partial f^*}{\partial \xi} \right] \quad \eta^* > 0 \quad (35)$$

$$\begin{aligned}
& H_0 \left(\frac{\partial \theta}{\partial \eta} \right)_{\eta=0} + P_r \alpha(\xi) \int_0^{\eta_\delta(\xi)} \frac{\partial f}{\partial \eta} \theta \, d\eta + 2\xi P_r p(\xi) \int_0^{\eta_\delta(\xi)} \left(\frac{\partial^2 f}{\partial \eta \partial \xi} \theta + \frac{\partial f}{\partial \eta} \frac{\partial \theta}{\partial \xi} \right) d\eta \\
& + \alpha(\xi) (f)_{\eta = \eta_\delta(\xi)} + 2\xi p(\xi) \left(\frac{\partial f}{\partial \xi} \right)_{\eta = \eta_\delta(\xi)} + 2\xi p(\xi) \left(\frac{\partial f}{\partial \eta} \right)_{\eta = \eta_\delta(\xi)} \frac{d\eta_\delta(\xi)}{d\xi} = 0
\end{aligned} \quad (36)$$

where $\alpha(\xi)$, $\beta(\xi)$, $\gamma(\xi)$ and $p(\xi)$ may be particular to a given physical configuration. The most general boundary conditions are of the forms

$$\begin{aligned}
& f(\xi, 0) = 0, \quad \frac{\partial f(\xi, 0)}{\partial \eta} = 0, \quad \theta(\xi, 0) = 1, \quad \theta(\xi, \eta_\delta(\xi)) = 0, \\
& C_0 f^*(\xi, 0) = f(\xi, \eta_\delta(\xi)), \quad C_1 \frac{\partial f^*(\xi, 0)}{\partial \eta^*} = \frac{\partial f(\xi, \eta_\delta(\xi))}{\partial \eta}, \\
& C_2 \frac{\partial^2 f^*(\xi, 0)}{\partial \eta^{*2}} = \frac{\partial^2 f(\xi, \eta_\delta(\xi))}{\partial \eta^2}, \\
& \frac{\partial f^*(\xi, +\infty)}{\partial \eta^*} = U_e(\xi)
\end{aligned} \quad (37)$$

where C_0 , C_1 and C_2 are physical constants and $U_e(\xi)$ is the external velocity field. The last boundary conditions which ensure unique solutions of the equations are

$$\frac{\partial^2 f^*(\xi, +\infty)}{\partial \eta^{*2}} = 0 \quad \text{and} \quad \frac{\partial^3 f^*(\xi, +\infty)}{\partial \eta^{*3}} = 0. \quad (38)$$

Using these, it is easily shown from the equations that

$$-\beta(\xi) U_e^2(\xi) = 2\xi p(\xi) U_e(\xi) \frac{dU_e(\xi)}{d\xi}. \quad (39)$$

Therefore $U_e(\xi)$ is a solution of the above first order equation within at most an arbitrary constant of integration. This constant may be determined by the value $U_e(0)$. When $\xi > 0$, $U_e(\xi)$ is a function determined by both the coefficients of the equations and the value of $U_e(0)$ rather than an arbitrary function. For this reason, we may rewrite the last boundary condition as

$$\frac{\partial f^*(0, +\infty)}{\partial \eta^*} = U_e(0) \quad \text{and} \quad \frac{\partial^2 f^*(\xi, +\infty)}{\partial \eta^{*2}} = 0 \quad \xi > 0. \quad (40)$$

Notice that the first, second and third of the governing equations are differential equations, whilst the fourth equation is a differentio-integral equation. We shall examine separately the differencing scheme for the purely differential systems before examining a scheme for the differentio-integral system.

4. MERGING, AND A DIFFERENCE SCHEME FOR DIFFERENTIAL EQUATIONS AND DIFFERENTIAL BOUNDARY CONDITIONS

In designing a solution algorithm it is important to recognise that for a fixed physical configuration, in particular for a specified H_0 , $\eta_\delta(\xi)$ is an evolving element of the solution. In earlier self-similar solution strategies $\eta_\delta(0)$ and $\eta_\delta(+\infty)$ have been prescribed and an associated value of H_0 identified from correlations involving simultaneously stream function and temperature boundary data obtained by imposing matching conditions at the liquid-vapour interface. This approach is not feasible in a non-similar setting where a prescribed, common H_0 has to apply over $0 < \xi < +\infty$. This consideration is fundamental to the subsequent formulation of the solution algorithm. In particular the equations are recast in terms of a coordinate normalised with respect to the local film thickness $\eta_\delta(\xi)$. As a consequence, in the algorithm, $\eta_\delta(\xi)$ can be identified as the solution of an independent unknown at each ξ station of a marching scheme. Specifically we define the new variables

$$F(\xi, \phi) = f(\xi, \eta), \quad \Theta(\xi, \phi) = \theta(\xi, \eta), \quad \phi = \eta/\eta_\delta(\xi), \\ F^*(\xi, \phi^*) = f^*(\xi, \eta^*), \quad \phi^* = 1 + \eta^*/\eta_\delta(\xi). \quad (41)$$

The differential equations and all boundary conditions transform to the following systems of equations

$$\frac{\partial^3 F}{\partial \phi^3} + \alpha(\xi)\eta_\delta(\phi)F \frac{\partial^2 F}{\partial \phi^2} + \beta(\xi)\eta_\delta(\xi) \left[\gamma(\xi)\eta_\delta^2(\xi) - \left(\frac{\partial F}{\partial \phi} \right)^2 \right] \\ = 2\xi p(\xi) \left[\eta_\delta(\xi) \frac{\partial F}{\partial \phi} \frac{\partial^2 F}{\partial \xi \partial \phi} - \frac{d\eta_\delta(\xi)}{d\xi} \left(\frac{\partial F}{\partial \phi} \right)^2 - \eta_\delta(\xi) \frac{\partial^2 F}{\partial \phi^2} \frac{\partial F}{\partial \xi} \right] \quad 0 < \phi < 1 \quad (42)$$

$$\frac{1}{P_r} \frac{\partial^2 \Theta}{\partial \phi^2} + \alpha(\xi)\eta_\delta(\xi)F \frac{\partial \Theta}{\partial \phi} = 2\xi p(\xi)\eta_\delta(\xi) \left[\frac{\partial F}{\partial \phi} \frac{\partial \Theta}{\partial \xi} - \frac{\partial \Theta}{\partial \phi} \frac{\partial F}{\partial \xi} \right] \quad 0 < \phi < 1 \quad (43)$$

$$\frac{\partial^3 F^*}{\partial \phi^{*3}} + \alpha(\xi)\eta_\delta(\xi)F^* \frac{\partial^2 F^*}{\partial \phi^{*2}} - \beta(\xi)\eta_\delta(\xi) \left(\frac{\partial F^*}{\partial \phi^*} \right)^2 \\ = 2\xi p(\xi) \left[\eta_\delta(\xi) \frac{\partial F^*}{\partial \phi^*} \frac{\partial^2 F^*}{\partial \xi \partial \phi^*} - \frac{d\eta_\delta(\xi)}{d\phi} \left(\frac{\partial F^*}{\partial \phi^*} \right)^2 - \eta_\delta(\xi) \frac{\partial^2 F^*}{\partial \phi^{*2}} \frac{\partial F^*}{\partial \xi} \right] \quad \phi^* > 1 \quad (44)$$

with boundary conditions

$$F(\xi, 0) = 0, \quad \frac{\partial F(\xi, 0)}{\partial \phi} = 0, \quad \Theta(\xi, 0) = 1, \quad \Theta(\xi, 1) = 0,$$

$$C_0 F^*(\xi, 1) = F(\xi, 1), \quad C_1 \frac{\partial F^*(\xi, 1)}{\partial \phi^*} = \frac{\partial F(\xi, 1)}{\partial \phi}$$

$$C_2 \frac{\partial^2 F^*(\xi, 1)}{\partial \phi^{*2}} = \frac{\partial^2 F(\xi, 1)}{\partial \phi^2},$$

$$\frac{\partial F^*(0, +\infty)}{\partial \phi^*} = U_e(0)\eta_\delta(0) \quad \text{and} \quad \frac{\partial^2 F^*(\xi, +\infty)}{\partial \phi^{*2}} = 0 \quad \xi > 0. \quad (45)$$

A direct approach to the solution of equations (42)–(45) would involve separate solution schemes for the condensate and vapour phase elements of the problem. Iterating backward and forward between the two schemes would be necessitated in order to reconcile the boundary conditions at the interface. As an alternative, in the present formulation, the stream function and temperature distribution in both phases, or across both layers, are amalgamated into unified functions incorporating possible discontinuities which accommodate the interfacial boundary conditions. A single coupled momentum and energy system results to which a Keller box methodology can be readily applied. The result is a single scheme in which iterations to satisfy the boundary conditions are inherently imbedded and for which the rate of convergence will mirror that of the overall scheme. We merge $F(\xi, \phi)$ and $F^*(\xi, \phi^*)$ into a unitary function and introduce a continuation of the definition domain of $\Theta(\xi, \phi)$ to the infinite region as follows

$$\begin{aligned} g(\xi, \phi) &= \begin{cases} F(\xi, \phi) & 0 \leq \phi \leq 1-0 \\ F^*(\xi, \phi^*) & \phi = \phi^* \geq 1+0 \end{cases} \\ \varphi(\xi, \phi) &= \begin{cases} \Theta(\xi, \phi) & 0 \leq \phi \leq 1-0 \\ 0 & \phi \geq 1+0 \end{cases} \end{aligned} \quad (46)$$

It is obvious that $g(\xi, \phi)$ and $\varphi(\xi, \phi)$ are not defined at $\phi = 1$, but there are left and right limits at $\phi = 1$, providing the values for each of the functions at $\phi = 1$. In other words, they may be thought to be multivalued functions at $\phi = 1$. $-$ and $+$ mean the left limit and the right limit respectively. In terms of the new variables the transformed equations in the domain $\xi \geq 0, \phi \geq 0$ are

$$\begin{aligned} \frac{\partial^3 g}{\partial \phi^3} + \alpha(\xi) \eta_\delta(\xi) g \frac{\partial^2 g}{\partial \phi^2} + \beta(\xi) \eta_\delta(\xi) \left[\gamma(\xi) \eta_\delta^2(\xi) H(1-\phi) - \left(\frac{\partial g}{\partial \phi} \right)^2 \right] \\ = 2\xi p(\xi) \left[\eta_\delta(\xi) \frac{\partial g}{\partial \phi} \frac{\partial^2 g}{\partial \xi \partial \phi} - \frac{d\eta_\delta(\xi)}{d\xi} \left(\frac{\partial g}{\partial \phi} \right)^2 - \eta_\delta(\xi) \frac{\partial^2 g}{\partial \phi^2} \frac{\partial g}{\partial \xi} \right] \end{aligned} \quad (47)$$

$$\frac{1}{P_r} \frac{\partial^2 \varphi}{\partial \phi^2} + \alpha(\xi) \eta_\delta(\xi) g \frac{\partial \varphi}{\partial \phi} = 2\xi p(\xi) \eta_\delta(\xi) \left[\frac{\partial g}{\partial \phi} \frac{\partial \varphi}{\partial \xi} - \frac{\partial \varphi}{\partial \phi} \frac{\partial g}{\partial \xi} \right] \quad (48)$$

with boundary conditions

$$g(\xi, 0) = 0, \quad \frac{\partial g(\xi, 0)}{\partial \phi} = 0, \quad \varphi(\xi, 0) = 1, \quad \varphi(\xi, 1-0) = 0, \quad \varphi(\xi, 1+0) = 0, \quad (49)$$

$$\begin{aligned} C_0 g(\xi, 1+0) &= g(\xi, 1-0), \quad C_1 \frac{\partial g(\xi, 1+0)}{\partial \phi} = \frac{\partial g(\xi, 1-0)}{\partial \phi}, \\ C_2 \frac{\partial^2 g(\xi, 1+0)}{\partial \phi^2} &= \frac{\partial^2 g(\xi, 1-0)}{\partial \phi^2}, \end{aligned} \quad (50)$$

$$\begin{aligned} \frac{\partial g(0, +\infty)}{\partial \phi} &= U_e(0) \eta_\delta(0) \quad \text{and} \quad \frac{\partial^2 g(\xi, +\infty)}{\partial \phi^2} = 0 \quad \xi > 0, \\ \varphi(\xi, +\infty) &= 0 \end{aligned} \quad (51)$$

where two new conditions for $\varphi(\xi, \phi)$ are added to maintain consistency between the unknown functions and conditions and $H(x)$ is the unit-step function, also known as the Heaviside function or Heaviside's step function, which is usually defined by

$$H(x) = \begin{cases} 0 & x < 0 \\ 1/2 & x = 0 \\ 1 & x > 0 \end{cases}$$

Using the same idea, one may also merge the three functions, $F(\xi, \phi)$, $F^*(\xi, \phi^*)$ and $\Theta(\xi, \phi)$, into a unitary function, but it is not helpful in solving the resulting difference equations hereafter because the differential equation for $\Theta(\xi, \phi)$ involves the unknown function $F(\xi, \phi)$.

The above is the main preparatory stage for introducing a merging procedure for the differential equations and conditions. Its principal requirements are based on the five following points:

(i) all unknown functions appear explicitly in both the equations and the boundary conditions;
(ii) unknown functions which represent the same physical property and are independent of each other in their differential equations are merged. These may only include one which is defined over a finite domain;

(iii) all unknown functions with finite domain—those newly merged and the unmerged remainder—are continued into new unknown functions over an infinite domain. In a broad case, that a function with finite domain is continued into another new function with infinite domain is the same as having the function with finite domain merge with a known solution of an auxiliary equation over an infinite domain;

(iv) the necessary and appropriate conditions to maintain consistency are added;

(v) boundary conditions at $+\infty$ may be replaced by asymptotic representations or alternatively a sufficiently large finite domain may be chosen, at the outer edge of which, the boundary conditions are understood to be satisfied. For simplicity we have adopted the latter approach in the present work.

Now we write the equations as a first order system by introducing the new dependent variables $u(\xi, \phi)$, $v(\xi, \phi)$ and $w(\xi, \phi)$ as follows:

$$\frac{\partial g}{\partial \phi} = u \quad (52)$$

$$\frac{\partial u}{\partial \phi} = v \quad (53)$$

$$\begin{aligned} \frac{\partial v}{\partial \phi} + \alpha(\xi)\eta_\delta(\xi)gv + \beta(\xi)\eta_\delta(\xi)[\gamma(\xi)\eta_\delta^2(\xi)H(1-\phi) - u^2] \\ = 2\xi p(\xi) \left[\eta_\delta(\xi)u \frac{\partial u}{\partial \xi} - \frac{d\eta_\delta(\xi)}{d\xi} u^2 - \eta_\delta(\xi)v \frac{\partial g}{\partial \xi} \right] \end{aligned} \quad (54)$$

$$\frac{\partial \phi}{\partial \phi} = w \quad (55)$$

$$\frac{1}{P_r} \frac{\partial w}{\partial \phi} + \alpha(\xi)\eta_\delta(\xi)gw = 2\xi p(\xi)\eta_\delta(\xi) \left[u \frac{\partial \phi}{\partial \xi} - w \frac{\partial g}{\partial \xi} \right]. \quad (56)$$

The boundary conditions now become

$$g(\xi, 0) = 0, \quad u(\xi, 0) = 0, \quad \phi(\xi, 0) = 1, \quad \phi(\xi, 1-0) = 0, \quad \phi(\xi, 1+0) = 0, \quad (57)$$

$$C_0 g(\xi, 1+0) = g(\xi, 1-0), \quad C_1 u(\xi, 1+0) = u(\xi, 1-0), \quad C_2 v(\xi, 1+0) = v(\xi, 1-0), \quad (58)$$

$$u(0, \phi_\infty) = U_\infty(0)\eta_\delta(0) \quad \text{and} \quad v(\xi, \phi_\infty) = 0 \quad \xi > 0, \quad \phi(\xi, \phi_\infty) = 0. \quad (59)$$

We place an arbitrary rectangular net of points (ξ_n, ϕ_j) on $\xi \geq 0$, $0 \leq \phi \leq \phi_\infty$ and use the notation:

$$\begin{aligned} \xi_0 = 0, \quad \xi_n = \xi_{n-1} + k_n, \quad n = 1, 2, \dots; \\ \phi_0 = 0, \quad \phi_j = \phi_{j-1} + h_j, \quad j = 1, 2, \dots, J_1, \dots, J_2; \end{aligned} \quad (60)$$

where $\phi_{J_1} = 1$, $\phi_{J_2} = \phi_\infty$. As a result of the discontinuity for $g(\xi, \phi)$ and non-differentiability of $\phi(\xi, \phi)$ at $\phi = 1$, the point $\phi = 1$ must be included as a mesh-point. No additional restrictions need be placed on the meshwidths h_j and k_n except this requirement. Because $g(\xi, \phi)$ and $\phi(\xi, \phi)$ have two values at $\phi = 1$, there are two ways to construct the scheme. One is that the function has two values at the same point $\phi = 1$, that is, the left limit and the right limit. The other is that the point $\phi = 1$ is thought to be two points with zero distance between them, that is, $h_{J_1+1} = 0$, and the function values at the left point and the right point are the left limit and the right limit respectively. Here we implement the former. Note that, for any function $z(\xi, \phi)$, z''_{j_1} represents the left limit or the right limit hereafter.

If $(g_j^n, u_j^n, v_j^n, \phi_j^n, w_j^n)$ are to approximate (g, u, v, ϕ, w) at (ξ_n, ϕ_j) , the difference approximations are defined, for $1 \leq j \leq J_2$, by

$$\frac{g_j^n - g_{j-1}^n}{h_j} = u_{j-1/2}^n \quad (61)$$

$$\frac{u_j^n - u_{j-1}^n}{h_j} = v_{j-1/2}^n \quad (62)$$

$$\begin{aligned} & \frac{v_j^{n-1/2} - v_{j-1}^{n-1/2}}{h_j} + \alpha_{n-1/2}(\eta_\delta(\xi)gv)_{j-1/2}^{n-1/2} \\ & + \beta_{n-1/2}\gamma_{n-1/2}H(J_1 - j + 1/2)(\eta_\delta^3(\xi))_{j-1/2}^{n-1/2} - \beta_{n-1/2}(\eta_\delta(\xi)u^2)_{j-1/2}^{n-1/2} \\ & = 2\xi_{n-1/2}p_{n-1/2} \left[(\eta_\delta(\xi)u_{j-1/2}^{n-1/2}) \frac{u_{j-1/2}^n - u_{j-1/2}^{n-1}}{k_n} \right. \\ & \left. - (u^2)_{j-1/2}^{n-1/2} \frac{\eta_\delta(\xi_n) - \eta_\delta(\xi_{n-1})}{k_n} - (\eta_\delta(\xi)v)_{j-1/2}^{n-1/2} \frac{g_{j-1/2}^n - g_{j-1/2}^{n-1}}{k_n} \right] \end{aligned} \quad (63)$$

$$\frac{\phi_j^n - \phi_{j-1}^n}{h_j} = w_{j-1/2}^n \quad (64)$$

$$\begin{aligned} & \frac{1}{P_r} \frac{w_j^{n-1/2} - w_{j-1}^{n-1/2}}{h_j} + \alpha_{n-1/2}(\eta_\delta(\xi)gw)_{j-1/2}^{n-1/2} = 2\xi_{n-1/2}p_{n-1/2} \left[(\eta_\delta(\xi)u)_{j-1/2}^{n-1/2} \frac{\phi_{j-1/2}^n - \phi_{j-1/2}^{n-1}}{k_n} \right. \\ & \left. - (\eta_\delta(\xi)w)_{j-1/2}^{n-1/2} \frac{g_{j-1/2}^n - g_{j-1/2}^{n-1}}{k_n} \right] \end{aligned} \quad (65)$$

where $\xi_{n-1/2} = (\xi_n + \xi_{n-1})/2$, $\alpha_{n-1/2}$, $\beta_{n-1/2}$, $\gamma_{n-1/2}$ and $p_{n-1/2}$ are the values of $\alpha(\xi)$, $\beta(\xi)$, $\gamma(\xi)$ and $p(\xi)$ at $\xi_{n-1/2}$ respectively and for any function $z(\xi, \phi)$ we have introduced a notation for averages and intermediate values as

$$\begin{aligned} z_{j-1/2}^n &= (z_j^n + z_{j-1}^n)/2 \\ z_j^{n-1/2} &= (z_j^n + z_{j-1}^{n-1})/2 \\ z_{j-1/2}^{n-1/2} &= (z_j^n + z_{j-1}^n + z_{j-1}^{n-1} + z_{j-1/2}^{n-1})/4. \end{aligned} \quad (66)$$

Note that equations (61), (62), (64) are centered at $(\xi_n, \phi_{j-1/2})$ while equations (63), (65) are centered at $(\xi_{n-1/2}, \phi_{j-1/2})$, i.e. when a ξ derivative is absent equations can be differenced about the point $(\xi_n, \phi_{j-1/2})$. It was found in practice that this damps high frequency Fourier error components better than differencing about $(\xi_{n-1/2}, \phi_{j-1/2})$.

The boundary conditions become simply

$$\begin{aligned} g_0^n &= 0, \quad u_0^n = 0, \quad \phi_0^n = 1, \quad \phi_{J_1-0}^n = 0, \quad \phi_{J_1+0}^n = 0, \\ C_0 g_{J_1+0}^n &= g_{J_1-0}^n, \quad C_1 u_{J_1+0}^n = u_{J_1-0}^n, \quad C_2 v_{J_1+0}^n = v_{J_1-0}^n, \\ u_{J_2}^0 &= U_e(0)\eta_\delta(0) \quad \text{and} \quad v_{J_2}^n = 0 \quad n = 1, 2, \dots, \quad \phi_{J_2}^n = 0. \end{aligned} \quad (67)$$

5. REDUCTION, AND A DIFFERENCE SCHEME FOR DIFFERENTIO-INTEGRAL EQUATIONS

Using the same transformation as in the merging procedure for the differential equations and the differential boundary conditions, the differentio-integral equation transforms to the following equation

$$H_0 \left[\left(\frac{\partial \Theta}{\partial \phi} \right)_{\phi=0} + P, \alpha(\xi) \eta_\delta(\xi) \int_0^1 \frac{\partial F}{\partial \phi} \Theta \, d\phi + 2\xi P, p(\xi) \eta_\delta(\xi) \int_0^1 \left(\frac{\partial^2 F}{\partial \phi \partial \xi} \Theta + \frac{\partial F}{\partial \phi} \frac{\partial \Theta}{\partial \xi} \right) d\phi \right] + \alpha(\xi) \eta_\delta(\xi) (F)_{\phi=1} + 2\xi p(\xi) \eta_\delta(\xi) \left(\frac{\partial F}{\partial \xi} \right)_{\phi=1} = 0 \quad (68)$$

or

$$H_0 \left[(w)_{\phi=0} + P, \alpha(\xi) \eta_\delta(\xi) \int_0^1 u \varphi \, d\phi + 2\xi P, p(\xi) \eta_0(\xi) \int_0^1 \left(\frac{\partial u}{\partial \xi} \varphi + u \frac{\partial \varphi}{\partial \phi} \right) d\phi \right] + \alpha(\xi) \eta_\delta(\xi) (g)_{\phi=1} + 2\xi p(\xi) \eta_\delta(\xi) \left(\frac{\partial g}{\partial \xi} \right)_{\phi=1} = 0. \quad (69)$$

The main preparatory stage for developing a difference scheme for the differentio-integral equation is a reduction procedure. Its principal requirements are based on the two following points:

- (i) the transformations used for the differentio-integral equations are the same as those for the differential equations and conditions;
- (ii) the formulation should always ensure that all limits of integration are constants. The differences approximations are defined by

$$\begin{aligned} H_0 \left\{ w_0^{n-1/2} + P, \alpha_{n-1/2} \sum_{j=1}^{J_1} (\eta_\delta(\xi) u \phi)_{j-1/2}^{n-1/2} h_j \right. \\ \left. + 2\xi_{n-1/2} P, p_{n-1/2} \sum_{j=1}^{J_1} \left[(\eta_\delta(\xi) \varphi)_{j-1/2}^{n-1/2} \frac{u_{j-1/2}^n - u_{j-1/2}^{n-1}}{k_n} \right. \right. \\ \left. \left. + (\eta_\delta(\xi) u)_{j-1/2}^{n-1/2} \frac{\varphi_{j-1/2}^n - \varphi_{j-1/2}^{n-1}}{k_n} \right] h_j \right\} + \alpha_{n-1/2} (\eta_\delta(\xi) g)_{J_1}^{n-1/2} \\ + \xi_{n-1/2} p_{n-1/2} [\eta_\delta(\xi_n) + \eta_\delta(\xi_{n-1})] \frac{g_{J_1}^n - g_{J_1}^{n-1}}{k_n} = 0. \end{aligned} \quad (70)$$

Note that the equation is centered at the line $\xi = \xi_{n-1/2}$.

6. SOLUTION OF THE DIFFERENCE EQUATIONS

The nonlinear difference equations may now be solved recursively starting with $n = 0$ (on $\xi = \xi_0 = 0$). In the case of $n = 0$ we retain equations (61), (62) and (64) with $n = 0$ and simply alter equations (63), (65) and (70) by setting $\xi_{n-1/2} = 0$ and using superscripts $n = 0$ rather than $n - 1/2$ in the remaining terms. The resulting difference equations, are then solved by the scheme below and accurate approximations to the solution of the systems of the ordinary differential equations are obtained.

In general when the solution is known on $\xi = \xi_{n-1}$ the solution on the line $\xi = \xi_n$ can be obtained. In detail suppose $\{g_j^{n-1}, u_j^{n-1}, v_j^{n-1}, \varphi_j^{n-1}, w_j^{n-1}\}_{j=0}^{J_2}$ are known. To simplify notation we now write: $\{g_j^n, u_j^n, v_j^n, \varphi_j^n, w_j^n\} \equiv \{g_j, u_j, v_j, \varphi_j, w_j\}$. With this notation we multiply equations (61), (62) and (64) by h_j , equation (63) by $2h_j$, (65) by $2P, h_j$ and (70) by 2 to get $1 \leq j \leq J_2$:

$$\begin{aligned} g_j - g_{j-1} - h_j u_{j-1/2} &= 0 \\ u_j - u_{j-1} - h_j v_{j-1/2} &= 0 \\ v_j - v_{j-1} + \alpha_{n-1/2} h_j \eta_\delta(\xi_n) (g v)_{j-1/2} \\ &+ \beta_{n-1/2} h_j \eta_\delta(\xi_n) [\gamma_{n-1/2} \eta_\delta^2(\xi_n) H(J_1 - j + 1/2) - (u^2)_{j-1/2}] \\ &- \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [\eta_\delta(\xi_n) (u_{j-1/2})^2 - (\eta_\delta(\xi_n) - \eta_\delta(\xi_{n-1})) (u_{j-1/2}^{n-1} u_{j-1/2} + (u^2)_{j-1/2}) \\ &- \eta_\delta(\xi_n) (u^2)_{j-1/2}^{n-1} - \eta_\delta(\xi_n) (\xi_n) (g_{j-1/2} - g_{j-1/2}^{n-1}) v_{j-1/2} - \eta_\delta(\xi_{n-1}) v_{j-1/2}^{n-1} g_{j-1/2}] = S_{j-1/2}^{n-1} \\ \varphi_j - \varphi_{j-1} - h_j w_{j-1/2} &= 0 \end{aligned} \quad (71)$$

$$\begin{aligned}
& w_j - w_{j-1} + P_r \alpha_{n-1/2} h_j \eta_\delta(\xi_n) (g w)_{j-1/2} - \frac{2\xi_{n-1/2}}{k_n} P_r p_{n-1/2} h_j [\eta_\delta(\xi_n) (\varphi_{j-1/2} - \varphi_{j-1/2}^{n-1}) u_{j-1/2} \\
& + \eta_\delta(\xi_{n-1}) u_{j-1/2}^{n-1} \varphi_{j-1/2} - \eta_\delta(\xi_n) (g_{j-1/2} - g_{j-1/2}^{n-1}) w_{j-1/2} - \eta_\delta(\xi_{n-1}) w_{j-1/2}^{n-1} g_{j-1/2} = T_{j-1/2}^{n-1} \\
& H_0 \left\{ w_0 + P_r \alpha_{n-1/2} \eta_\delta(\xi_n) \sum_{j=1}^{J_1} (u \varphi)_{j-1/2} h_j + \frac{2\xi_{n-1/2}}{k_n} P_r p_{n-1/2} \sum_{j=1}^{J_1} [2\eta_j(\xi_n) \varphi_{j-1/2} u_{j-1/2} \right. \\
& \left. - (\eta_\delta(\xi_n) - \eta_\delta(\xi_{n-1})) (u_{j-1/2}^{n-1} \varphi_{j-1/2} + \varphi_{j-1/2}^{n-1} u_{j-1/2})] h_j \right\} + \alpha_{n-1/2} \eta_\delta(\xi_n) g_{J_1} \\
& + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} [\eta_\delta(\xi_n) (g_{J_1} - g_{J_1}^{n-1}) + \eta_\delta(\xi_{n-1}) g_{J_1}] = R_\delta^{n-1}
\end{aligned}$$

Abbreviations $S_{j-1/2}^{n-1}$, $T_{j-1/2}^{n-1}$, R_δ^{n-1} , together with a number of subsequent abbreviations introduced for clarity, appear in expanded form in the Appendix.

That is if all the variables are known at location $n-1$ then the difference equations resulting from equations (71) and (67) give a set of $5J_2 + 11$ nonlinear equations for the $5J_2 + 11$ unknowns g_j^n , u_j^n , v_j^n , φ_j^n , w_j^n , $j = 0, 1, \dots, J_1 - 0, J_1 + 0, \dots, J_2$ and $\eta_\delta(\xi_n)$ which we compute by means of Newton's method. The iterates are denoted by $\{g_j^{(i)}, u_j^{(i)}, v_j^{(i)}, \varphi_j^{(i)}, w_j^{(i)}, \eta_\delta^{(i)}(\xi_n)\}$. They are determined by first writing

$$\begin{aligned}
g_j^{(i+1)} &= g_j^{(i)} + \delta g_j^{(i)}, \quad u_j^{(i+1)} = u_j^{(i)} + \delta u_j^{(i)}, \quad v_j^{(i+1)} = v_j^{(i)} + \delta v_j^{(i)}, \\
\varphi_j^{(i+1)} &= \varphi_j^{(i)} + \delta \varphi_j^{(i)}, \quad w_j^{(i+1)} = w_j^{(i)} + \delta w_j^{(i)}, \\
\eta_\delta^{(i+1)}(\xi_n) &= \eta_\delta^{(i)}(\xi_n) + \delta \eta_\delta^{(i)}(\xi_n)
\end{aligned}$$

and then inserting these expressions in place of $\{g_j, u_j, v_j, \varphi_j, w_j, \eta_\delta(\xi_n)\}$ in equation (71). Quadratic and cubic terms in $\{\delta g_j^{(i)}, \delta u_j^{(i)}, \delta v_j^{(i)}, \delta \varphi_j^{(i)}, \delta w_j^{(i)}, \delta \eta_\delta^{(i)}(\xi_n)\}$ are neglected. The resulting linear systems of equations can be written in vector-matrix form as:

$$R_j^{(i)} \delta_j^{(i)} - L_j^{(i)} \delta_{j-1}^{(i)} + H_j^{(i)} \delta \eta_\delta^{(i)}(\xi_n) = \mathbf{r}_{j-1/2}^{(i)}, \quad \text{for } j = 1, 2, \dots, J_2 \quad (72)$$

and

$$\tilde{\alpha}_\delta^{(i)} \delta g_{J_1}^{(i)} + H_0 \delta w_0^{(i)} + \tilde{h}_\delta^{(i)} \eta_\delta^{(i)} + \sum_{j=0}^{J_1} (\tilde{\beta}_j^{(i)} \delta u_j^{(i)} + \tilde{\gamma}_j^{(i)} \delta \varphi_j^{(i)}) = \gamma_\delta^{(i)}. \quad (73)$$

Here we have introduced the (column) vectors (see the Appendix)

$$\begin{aligned}
\delta_j^{(i)} &\equiv (\delta g_j^{(i)}, \delta u_j^{(i)}, \delta v_j^{(i)}, \delta \varphi_j^{(i)}, \delta w_j^{(i)})^\top, \\
\mathbf{r}_{j-1/2}^{(i)} &\equiv (\beta_{j-1/2}^{(i)}, \tau_{j-1/2}^{(i)}, \alpha_{j-1/2}^{(i)}, \gamma_{j-1/2}^{(i)} + S_{j-1/2}^{n-1}, \sigma_{j-1/2}^{(i)} + T_{j-1/2}^{n-1})^\top
\end{aligned}$$

and

$$\begin{aligned}
\gamma_\delta^{(i)} &\equiv d_\delta^{(i)} + R_\delta^{n-1} \\
d_\delta^{(i)} &= -H_0 \left\{ w_0^{(i)} + P_r \alpha_{n-1/2} \eta_\delta^{(i)}(\xi_n) \sum_{j=1}^{J_1} (u^{(i)} \varphi^{(i)})_{j-1/2} h_j \right. \\
&+ \frac{2\eta_{n-1/2}}{k_n} P_r p_{n-1/2} \sum_{j=1}^{J_1} [2\eta_\delta^{(i)}(\xi_n) u_{j-1/2}^{(i)} \varphi_{j-1/2}^{(i)} \\
&- (\eta_\delta^{(i)}(\xi_n) - \eta_\delta(\xi_{n-1})) (u_{j-1/2}^{(i)} \varphi_{j-1/2}^{(i)} + \varphi_{j-1/2}^{(i)} u_{j-1/2}^{(i)})] h_j \left. \right\} \\
&- \alpha_{n-1/2} \eta_\delta^{(i)}(\xi_n) g_{J_1}^{(i)} - \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} [\eta_\delta^{(i)}(\xi_n) (g_{J_1}^{(i)} - g_{J_1}^{(n-1)}) - \eta_\delta(\xi_{n-1}) g_{J_1}^{(i)}] \quad (74)
\end{aligned}$$

$$\tilde{\alpha}_\delta^{(i)} = \alpha_{n-1/2} \eta_\delta^{(i)}(\xi_n) + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} [\eta_\delta^{(i)}(\xi_n) + \eta_\delta(\xi_{n-1})] \quad (75)$$

$$\tilde{h}_\delta^{(i)} = H_0 P_r \left\{ \alpha_{n-1/2} \sum_{j=1}^{J_1} (u^{(i)} \varphi^{(i)})_{j-1/2} h_j + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} \sum_{j=1}^{J_1} [2u_{j-1/2}^{(i)} \varphi_{j-1/2}^{(i)} - u_{j-1/2}^{n-1} \varphi_{j-1/2}^{(i)} - \varphi_{j-1/2}^{n-1} u_{j-1/2}^{(i)}] h_j \right\} + \alpha_{n-1/2} g_{J_1}^{(i)} + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} (g_{J_1}^{(i)} - g_{J_1}^{n-1}) \quad (76)$$

$$\tilde{\beta}_j^{(i)} = 1/2 H_0 P_r \left\{ \alpha_{n-1/2} \eta_\delta^{(i)}(\xi_n) \varphi_j^{(i)} (h_j + h_{j+1}) + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} [2\eta_\delta^{(i)}(\xi_n) (\varphi_{j-1/2}^{(i)} h_j + \varphi_{j+1/2}^{(i)} h_{j+1}) - (\eta_\delta^{(i)}(\xi_n) - \eta_\delta(\xi_{n-1})) (\varphi_{j-1/2}^{n-1} h_j + \varphi_{j+1/2}^{n-1} h_{j+1})] \right\} \quad (77)$$

$$\tilde{s}_j^{(i)} = 1/2 H_0 P_r \left\{ \alpha_{n-1/2} \eta_\delta^{(i)}(\xi_n) u_j^{(i)} (h_j + h_{j+1}) + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} [2\eta_\delta^{(i)}(\xi_n) (u_{j-1/2}^{(i)} h_j + u_{j+1/2}^{(i)} h_{j+1}) - (\eta_\delta^{(i)}(\xi_n) - \eta_\delta(\xi_{n-1})) (u_{j-1/2}^{n-1} h_j + u_{j+1/2}^{n-1} h_{j+1})] \right\}. \quad (78)$$

$h_0 = h_{J_1+1} = 0$ applies only in the last two expressions for $\tilde{\beta}_j^{(i)}$ and $\tilde{s}_j^{(i)}$ rather than in others appearing in this paper. The 5×5 matrices are:

$$R_j^{(i)} = \begin{bmatrix} 0 & 1 & -h_j/2 & 0 & 0 \\ 0 & 0 & 0 & 1 & -h_j/2 \\ 1 & -h_j/2 & 0 & 0 & 0 \\ a_j^{(i)} & b_j^{(i)} & c_j^{(i)} & 0 & 0 \\ e_j^{(i)} & f_j^{(i)} & 0 & p_j^{(i)} & q_j^{(i)} \end{bmatrix} \quad (79)$$

$$L_j^{(i)} = \begin{bmatrix} 0 & 1 & h_j/2 & 0 & 0 \\ 0 & 0 & 0 & 1 & h_j/2 \\ 1 & h_j/2 & 0 & 0 & 0 \\ \tilde{a}_j^{(i)} & \tilde{b}_j^{(i)} & \tilde{c}_j^{(i)} & 0 & 0 \\ \tilde{e}_j^{(i)} & \tilde{f}_j^{(i)} & 0 & \tilde{p}_j^{(i)} & \tilde{q}_j^{(i)} \end{bmatrix} \quad (80)$$

and

$$H_j^{(i)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ s_j^{(i)} \\ t_j^{(i)} \end{bmatrix} \quad (81)$$

Again the abbreviations for matrix and vector elements are expanded in the appendix. The boundary conditions (67) yield for our iteration scheme

$$\begin{aligned} \delta g_0^{(i)} &= -g_0^{(i)}, \quad \delta u_0^{(i)} = -u_0^{(i)}, \quad \delta \varphi_0^{(i)} = 1 - \varphi_0^{(i)}, \\ \delta \varphi_{J_1-0}^{(i)} &= -\varphi_{J_1-0}^{(i)}, \quad \delta \varphi_{J_1+0}^{(i)} = -\varphi_{J_1+0}^{(i)}, \\ \delta g_{J_1-0}^{(i)} - C_0 \delta g_{J_1+0}^{(i)} &= C_0 g_{J_1+0}^{(i)} - g_{J_1-0}^{(i)}, \\ \delta u_{J_1-0}^{(i)} - C_1 \delta u_{J_1+0}^{(i)} &= C_1 u_{J_1+0}^{(i)} - u_{J_1-0}^{(i)}, \\ \delta v_{J_1-0}^{(i)} - C_2 \delta v_{J_1+0}^{(i)} &= C_2 v_{J_1+0}^{(i)} - v_{J_1-0}^{(i)}, \\ \delta u_{J_2}^{(i)} - U_\epsilon(0) \delta \eta_\delta^{(i)}(0) &= U_\epsilon(0) \eta_\delta^{(i)}(0) - u_{J_2}^{(i)} \quad n = 0, \end{aligned} \quad (82)$$

and

$$\delta v_{j_2}^{(i)} = -v_{j_2}^{(i)} \quad n = 1, 2, \dots,$$

$$\delta \varphi_{j_2}^{(i)} = -\varphi_{j_2}^{(i)}. \quad (83)$$

Clearly the right hand sides in each of these equations will vanish if the initial iterated variables satisfy the correct boundary conditions. Assuming this to be the case the entire linear system (72), (73) and (82) can be written in the block arrow-like matrix form.

$$A^{(i)} \Delta^{(i)} = \mathbf{q}^{(i)} \quad i = 0, 1, 2, \dots \quad (84)$$

where

$$\Delta^{(i)} \equiv (\delta_0^{(i)\top}, \dots, \delta_{j_1-0}^{(i)\top}, \delta_{j_1+0}^{(i)\top}, \dots, \delta_{j_2}^{(i)\top}, \delta \eta_\delta^{(i)}(\xi_n), \delta S_1, \delta S_2, \delta S_3, \delta S_4)^\top \quad (85)$$

$$\mathbf{q}^{(i)} \equiv (0, 0, 0, \mathbf{r}_{1/2}^{(i)\top}, \dots, \mathbf{r}_{j_1-1/2}^{(i)\top}, 0, 0, 0, 0, 0, \mathbf{r}_{j_1+1/2}^{(i)\top}, \dots, \mathbf{r}_{j_2-1/2}^{(i)\top}, 0, 0, \gamma_\delta^{(i)}, 0, 0, 0, 0)^\top. \quad (86)$$

The matrix $A^{(i)}$ can be expanded by four extra rows and columns to form a block arrow-like matrix with 5×5 blocks if we include four extra unknowns S_1, S_2, S_3 and S_4 and four extra equations $S_1 = 0, S_2 = 0, S_3 = 0$ and $S_4 = 0$. The ordering of equations is (i) the three boundary conditions (82) at $\phi = 0$, (ii) equation (72) at the centred location $j = 1/2, \dots, j_1 - 1/2$, (iii) the five boundary conditions (82) at $\phi = 1$, (iv) equation (72) at the centred location $j = j_1 + 1/2, \dots, j_2 - 1/2$, (v) the two equations (82) at $\phi = \phi_\infty$, (vi) equation (73) and (vii) the four dummy variable equations. We now have $5j_2 + 15$ equations and unknowns and the matrix $A^{(i)}$ has the form

$$A^{(i)} = \begin{pmatrix} A_0 & C_0 & & & & & & D_0 \\ B_1 & A_1 & C_1 & & & & & D_1 \\ & B_2 & A_2 & C_2 & & & & D_2 \\ & & & \cdot & \cdot & \cdot & & \cdot \\ & & & & \cdot & \cdot & \cdot & \cdot \\ & & & & & \cdot & \cdot & \cdot \\ & & & & & & B_{N-1} & A_{N-1} & C_{N-1} & D_{N-1} \\ & & & & & & & B_N & A_N & D_N \\ E_0 & E_1 & E_2 & \cdot & \cdot & & E_{N-1} & E_N & A_{N+1} \end{pmatrix} \quad (87)$$

7. DIRECT FACTORIZATION METHOD OF BLOCK ARROW-LIKE MATRIX

The matrix $A^{(i)}$ is called a block arrow-like matrix here due to its shape. Now we seek a factorization of the form

$$A^{(i)} = LU = \begin{pmatrix} F_0 & & & & & & & & & \\ B_1 & F_1 & & & & & & & & \\ & B_2 & F_2 & & & & & & & \\ & & & \cdot & \cdot & & & & & \\ & & & & \cdot & \cdot & & & & \\ & & & & & \cdot & \cdot & & & \\ & & & & & & B_{N-1} & F_{N-1} & & \\ & & & & & & & B_N & F_N & \\ G_0 & G_1 & G_2 & \cdot & \cdot & \cdot & G_{N-1} & G_N & F_{N+1} \end{pmatrix}$$

$$\times \begin{bmatrix} I_0 & R_0 & & & & & P_0 \\ & I_1 & R_1 & & & & P_1 \\ & & I_2 & R_2 & & & P_2 \\ & & & \cdot & \cdot & & \cdot \\ & & & & \cdot & \cdot & \cdot \\ & & & & & \cdot & \cdot \\ & & & & & I_{N-1} & R_{N-1} & P_{N-1} \\ & & & & & & I_N & P_N \\ & & & & & & & I_{N+1} \end{bmatrix} \quad (88)$$

where the I_j are identity matrices of order 5 and $N = J_2 + 1$. Then we find that

$$\begin{aligned} F_0 &= A_0, \quad P_0 = F_0^{-1} D_0, \quad G_0 = E_0; \\ R_j &= F_j^{-1} C_j, \quad j = 0, 1, 2, \dots, N-1; \\ G_j &= E_j - G_{j-1} R_{j-1}, \quad j = 1, 2, \dots, N; \\ F_j &= A_j - B_j R_{j-1}, \quad j = 1, 2, \dots, N; \\ P_j &= F_j^{-1} (D_j - B_j P_{j-1}), \quad j = 1, 2, \dots, N; \\ F_{N+1} &= A_{N+1} - \sum_{k=0}^N G_k P_k. \end{aligned} \quad (89)$$

The system (84) is now equivalent to

$$L \mathbf{z}^{(i)} = \mathbf{q}^{(i)}, \quad U \Delta^{(i)} = \mathbf{z}^{(i)} \quad i = 0, 1, 2, \dots \quad (90)$$

and the intermediate vectors $\mathbf{z}^{(i)} \equiv (\mathbf{z}_0^{(i)\top}, \dots, \mathbf{z}_{J_2+2}^{(i)\top})^\top$, where $\mathbf{z}_j^{(i)}$ are 5-component column vectors, are computed from:

$$\begin{aligned} \mathbf{z}_0^{(i)} &= F_0^{-1} \mathbf{q}_0^{(i)}; \\ \mathbf{z}_j^{(i)} &= F_j^{-1} (\mathbf{q}_j^{(i)} - B_j \mathbf{z}_{j-1}^{(i)}) \quad j = 1, 2, \dots, J_2 + 1; \\ \mathbf{z}_{J_2+2}^{(i)} &= F_{J_2+2}^{-1} (\mathbf{q}_{J_2+2}^{(i)} - \sum_{k=0}^{J_2+1} G_k \mathbf{z}_k^{(i)}) \end{aligned} \quad (91)$$

where

$$\mathbf{q}_0^{(i)} = (0, 0, 0, \beta_{1/2}^{(i)}, \tau_{1/2}^{(i)})^\top \quad (92)$$

$$\mathbf{q}_j^{(i)} = (\alpha_{j-1/2}^{(i)}, \gamma_{j-1/2}^{(i)} + S_{j-1/2}^{n-1}, \sigma_{j-1/2}^{(i)} + T_{j-1/2}^{n-1}, \beta_{j+1/2}^{(i)}, \tau_{j+1/2}^{(i)})^\top \quad j = 1, 2, \dots, J_1 - 1 \quad (93)$$

$$\mathbf{q}_{J_1}^{(i)} = (\alpha_{J_1-1/2}^{(i)}, \gamma_{J_1-1/2}^{(i)} + S_{J_1-1/2}^{n-1}, \sigma_{J_1-1/2}^{(i)} + T_{J_1-1/2}^{n-1}, 0, 0)^\top \quad (94)$$

$$\mathbf{q}_{J_1+1}^{(i)} = (0, 0, 0, \beta_{J_1+1/2}^{(i)}, \tau_{J_1+1/2}^{(i)})^\top \quad (95)$$

$$\mathbf{q}_j^{(i)} = (\alpha_{j-3/2}^{(i)}, \gamma_{j-3/2}^{(i)} + S_{j-3/2}^{n-1}, \sigma_{j-3/2}^{(i)} + T_{j-3/2}^{n-1}, \beta_{j-1/2}^{(i)}, \tau_{j-1/2}^{(i)})^\top \quad j = J_1 + 2, J_1 + 3, \dots, J_2 \quad (96)$$

$$\mathbf{q}_{J_2+1}^{(i)} = (\alpha_{J_2-1/2}^{(i)}, \gamma_{J_2-1/2}^{(i)} + S_{J_2-1/2}^{n-1}, \sigma_{J_2-1/2}^{(i)} + T_{J_2-1/2}^{n-1}, 0, 0)^\top \quad (97)$$

$$\mathbf{q}_{J_2+2}^{(i)} = (\gamma_8^{(i)}, 0, 0, 0, 0)^\top. \quad (98)$$

Finally the solution components $\Delta_j^{(i)}$ are obtained as:

$$\begin{aligned} \Delta_{J_2+2}^{(i)} &= \mathbf{z}_{J_2+2}^{(i)} \\ \Delta_{J_2+1}^{(i)} &= \mathbf{z}_{J_2+1}^{(i)} - P_{J_2+1} \Delta_{J_2+2}^{(i)} \\ \Delta_j^{(i)} &= \mathbf{z}_j^{(i)} - R_j \Delta_{j+1}^{(i)} - P_j \Delta_{J_2+2}^{(i)} \quad j = J_2, J_2 - 1, \dots, 0 \end{aligned} \quad (99)$$

where

$$\begin{aligned}\Delta_j^{(i)} &= \delta_j^{(i)} \quad j = 0, 1, 2, \dots, J_1 \\ \Delta_j^{(i)} &= \delta_{j-1}^{(i)} \quad j = J_1 + 1, J_1 + 2, \dots, J_2 + 1 \\ \Delta_{J_2+2}^{(i)} &= (\delta \eta_\delta^{(i)}(\xi_n), \delta S_1, \delta S_2, \delta S_3, \delta S_4)^T.\end{aligned}\quad (100)$$

Note again that the matrix $A^{(i)}$ is not block diagonal as is usual with the Keller box method and consequently the solution of equation (84) needs to be modified to take account of the column of D s and the row of E s. A suitable algorithm for solving the matrix equation in (84) is

$$\begin{aligned}Q &\leftarrow A_0^{-1}, \quad \mathbf{q}_0^{(i)} \leftarrow Q \mathbf{q}_0^{(i)}, \quad D_0 \leftarrow Q D_0, \\ \left. \begin{aligned} A_{j-1} &\leftarrow Q C_{j-1}, \quad E_j \leftarrow E_j - E_{j-1} A_{j-1} \\ Q &\leftarrow (A_j - B_j A_{j-1})^{-1} \\ \mathbf{q}_j^{(i)} &\leftarrow Q(\mathbf{q}_j^{(i)} - B_j \mathbf{q}_{j-1}^{(i)}), \quad D_j \rightarrow Q(D_j - B_j D_{j-1}) \end{aligned} \right\} j = 1, 2, \dots, J_2 + 1 \\ Q &\leftarrow \left(A_{J_2+2} - \sum_{k=0}^{J_2+1} E_k D_k \right)^{-1} \\ \Delta_{J_2+2}^{(i)} &\leftarrow Q \left(\mathbf{q}_{J_2+2}^{(i)} - \sum_{k=0}^{J_2+1} E_k \mathbf{q}_k^{(i)} \right) \\ \Delta_{J_2+1}^{(i)} &\leftarrow \mathbf{q}_{J_2+1}^{(i)} - D_{J_2+1} \Delta_{J_2+2}^{(i)} \\ \Delta_j^{(i)} &\leftarrow \mathbf{q}_j^{(i)} - A_j \Delta_{j+1}^{(i)} - D_j \Delta_{J_2+2}^{(i)} \quad j = J_2, J_2 - 1, \dots, 0\end{aligned}\quad (101)$$

where $\leftarrow$ denotes replacement. Algorithmically this is simply a modification of the usual solution of a block tridiagonal system to include the D_j and E_j . The algorithm can be made efficient by taking account of the zeros appearing in matrices.

8. EXTRAPOLATING THE RESULTS

Since central differences are used the exact numerical solution of our difference equations (61)–(65), (67) and (70) is a second order accurate approximation. The local truncation errors of this difference scheme can be written as a Taylor series in powers of h^2 and k^2 where $k = \max_n k_n$ and $h = \max_j h_j$. It is therefore possible, as pointed out by Keller, by solving the problem on different sized grids and using Richardson's extrapolation, to produce results of high accuracy provided the truncation errors are larger than the iteration errors. For example each cell of the net (60) is divided into m subintervals both in the ξ direction and in the ϕ direction where m is an integer. The problem is solved numerically for $m = 1, 2, 3$ and 4. If z_m denotes the results of any actual variable function $z(\xi, \phi)$ at a common grid point then the z_m has accuracy $O(k^2 + h^2)$. Since the truncation error is proportional to the square of k and h then

$$z_{12} = \frac{1}{3}(4z_2 - z_1), \quad z_{23} = \frac{1}{5}(9z_3 - 4z_2), \quad z_{34} = \frac{1}{7}(16z_4 - 9z_3)$$

have errors $O(k^4 + h^4)$ and

$$z_{123} = \frac{1}{8}(9z_{23} - z_{12}), \quad z_{234} = \frac{1}{12}(16z_{34} - 4z_{23}) \quad (102)$$

will be in error by $O(k^6 + h^6)$ and finally

$$z_{1234} = \frac{1}{15}(16z_{234} - z_{123}).$$

The results quoted are z_{1234} and error is estimated by maximum of the difference $|z_{1234} - z_{234}|$, which being a global error estimate measures the actual error in z .

9. RESULTS FOR THE PROTOTYPE PROBLEM—MIXED CONDENSATION

The numerical scheme described in previous sections was introduced in the context of combined body force and forced convection laminar condensation. To demonstrate the scheme a detailed examination of this problem has been performed.

Table 1. Exact numerical characteristics for various Prandtl numbers for $\xi = 0$, $H_0 = 0.008191$ and $\omega = 10$

P_r	$\eta_\delta(0)$	$F_{\phi\phi}(0, 0)$	$\Theta_\phi(0, 0)$	$Nu_x R_c^{-1/2}$	$C_f R_c^{-1/2}$	$\delta R_c^{1/2}/x$
1.0	0.66484	0.02460	-1.00068	1.06430	0.07870	0.94022
2.0	0.66444	0.02456	-1.00136	1.06566	0.07868	0.93966
3.0	0.66404	0.02453	-1.00204	1.06702	0.07866	0.93910
4.0	0.66364	0.02449	-1.00271	1.06838	0.07864	0.93853
5.0	0.66325	0.02446	-1.00338	1.06973	0.07863	0.93797
6.0	0.66285	0.02442	-1.00404	1.07108	0.07861	0.93741
7.0	0.66246	0.02439	-1.00471	1.07243	0.07859	0.93686
8.0	0.66206	0.02435	-1.00537	1.07377	0.07858	0.93630
9.0	0.66167	0.02432	-1.00603	1.07511	0.07856	0.93575
10.0	0.66129	0.02429	-1.00668	1.07644	0.07854	0.93520

The appropriate ξ -dependent parameters of the general scheme must be chosen as

$$\alpha(\xi) = \frac{1 + 24\xi}{(1 + \xi)^{1/4}(1 + 16\xi)^{3/4}}, \quad \beta(\xi) = \frac{\xi(17 + 32\xi)}{2(1 + \xi)^{5/4}(1 + 16\xi)^{3/4}},$$

$$\gamma(\xi) = \frac{4(1 + \xi)^{1/2}(1 + 16\xi)^{1/2}}{17 + 32\xi}, \quad p(\xi) = \frac{(1 + 16\xi)^{1/4}}{(1 + \xi)^{1/4}}, \quad (103)$$

and the constants are prescribed as $C_0 = 1/\lambda\omega$, $C_1 = 1/\lambda^2$, $C_2 = 1/\lambda^3\omega$, where λ , ω are two physical constants whose values depend on the flow under examination. In fact a very good approximation to λ is just unity and accordingly $\lambda = 1$ has been adopted in all that follows. With $U_c(0) = 1$ equation (39) leads to

$$U_c(\xi) = \frac{1}{(1 + \xi)^{1/4}(1 + 16\xi)^{1/4}}. \quad (104)$$

The non-dimensional characteristics of any given flow are

(i) the skin friction coefficient

$$C_f R_c^{1/2} = \sqrt{2}(1 + 16\xi)^{1/4}(1 + \xi)^{1/2} f_{\eta\eta}(\xi, 0) = \frac{\sqrt{2}(1 + 16\xi)^{1/4}(1 + \xi)^{1/2} F_{\phi\phi}(\xi, 0)}{\eta_\delta^2(\xi)} \quad (105)$$

where $C_f = \mu(\partial u/\partial y)_{y=0}/\frac{1}{2}\rho U_\infty^2$

(ii) the heat transfer coefficient

$$Nu_x R_c^{-1/2} = -\frac{1}{\sqrt{2}}(1 + \xi)^{1/4} \theta_\eta(\xi, 0) = -\frac{1}{\sqrt{2}} \frac{(1 + \xi)^{1/4} \Theta_\phi(\xi, 0)}{\eta_\delta(\xi)} \quad (106)$$

(iii) the dimensionless film thickness

$$\delta R_c^{1/2}/x = \frac{\sqrt{2}}{(1 + \xi)^{1/4}} \eta_\delta(\xi). \quad (107)$$

A detailed solution should also identify velocity and temperature profiles as well as the interfacial free surface velocity of the condensate film. Once values have been specified for the physical constants H_0 , P_r and ω as they relate to a given physical configuration a complete solution can be obtained from the scheme which supplies any such information as desired.

Table 2. Exact numerical characteristics for various H_0 for $\xi = 0$, $P_r = 10$ and $\omega = 10$

H_0	$\eta_\delta(0)$	$F_{\phi\phi}(0, 0)$	$\Theta_\phi(0, 0)$	$Nu_x R_c^{-1/2}$	$C_f R_c^{1/2}$	$\delta R_c^{1/2}/x$
0.00002	0.1	0.00047	-1.00002	7.07121	0.06658	0.14142
0.00019	0.2	0.00191	-1.00016	3.53610	0.06736	0.28284
0.00066	0.3	0.00437	-1.00055	2.35831	0.06859	0.42426
0.00160	0.4	0.00796	-1.00133	1.77011	0.07040	0.56569
0.00325	0.5	0.01288	-1.00268	1.41801	0.07285	0.70711
0.00589	0.6	0.01937	-1.00484	1.18421	0.07609	0.84853
0.00998	0.7	0.02783	-1.00811	1.01834	0.08031	0.98995
0.01614	0.8	0.03883	-1.01292	0.89530	0.08581	1.13137
0.02545	0.9	0.05329	-1.01992	0.80133	0.09305	1.27279
0.03975	1.0	0.07625	-1.03013	0.72841	0.10275	1.41421

Table 3. Exact numerical characteristics for various ω for $\xi = 0$, $P_r = 10$ and $H_0 = 0.008191$

ω	$\eta_\delta(0)$	$F_{\phi\phi}(0, 0)$	$\Theta_\phi(0, 0)$	$Nu_x R_c^{-1/2}$	$C_f R_c^{1/2}$	$\delta R_c^{1/2}/x$
10	0.66128	0.02429	-1.00668	1.07644	0.07854	0.93519
100	1.16768	0.01375	-1.00668	0.60962	0.01427	1.65134
150	1.24507	0.01290	-1.00668	0.57172	0.01177	1.76080
500	1.38315	0.01161	-1.00668	0.51465	0.00858	1.95607
600	1.39237	0.01153	-1.00668	0.51124	0.00841	1.96911

Table 4. Comparison of $Nu_x R_c^{-1/2}$ from exact results and the correlation of Fujii and Uehara [18], $Nu_x R_c^{-1/2} = 0.450 (1.20 + 1/\omega H_0)^{1/3}$

ωH_0	Shu and Wilks	Fujii and Uehara
10^{-2}	2.05545	2.09704
$10^{-3/2}$	1.42379	1.44080
10^{-1}	1.00591	1.00682
$10^{-1/2}$	0.73967	0.73528
10^0	0.58704	0.58527
$10^{1/2}$	0.52113	0.51697
10^1	0.50622	0.49113

Note that the solution at $\xi = 0$ recovers the solutions of pure forced convection condensation and results at this station may be expected simply to be more accurate solutions of the associated similarity equations. Table 1 presents exact numerical data at $\xi = 0$ for a range of Prandtl numbers with H_0 and ω held at constant representative values. There is clearly relatively little formal dependence on P_r . By way of contrast Table 2 presents data at $\xi = 0$ for a prescribed Prandtl number and the same ω as before. Here however initial film thicknesses over the range $\eta_\delta(0) = 0.1(0.1)1.0$ have been prescribed and the associated values of the parameter H_0 have been established. Table 3 again relates to $\xi = 0$ and indicates the effect of variations in the interfacial shear stress parameter ω on the various flow characteristics. A valuable correlation of initial data

Table 5. Exact numerical characteristics for various Prandtl numbers as $\xi \rightarrow +\infty$, $H_0 = 0.008191$ and $\omega = 10$

P_r	$\bar{\eta}_\delta(+\infty)$	$F_{\phi\phi}(\infty, 0)$	$\Theta_\phi(\infty, 0)$	$\frac{Nu_x R_c^{-1/2}}{\xi^{1/4}}$	$\frac{C_f R_c^{1/2}}{2\xi^{3/4}}$	$\frac{\delta R_c^{1/2} \xi^{1/4}}{x}$
1.0	0.30164	0.02721	-1.00082	2.34615	0.42289	0.42658
2.0	0.30147	0.02716	-1.00163	2.34938	0.42266	0.42634
3.0	0.30130	0.02712	-1.00245	2.35261	0.42243	0.42610
4.0	0.30113	0.02707	-1.00325	2.35582	0.42219	0.42586
5.0	0.30096	0.02703	-1.00406	2.35903	0.42197	0.42562
6.0	0.30079	0.02698	-1.00486	2.36222	0.42173	0.42539
7.0	0.30063	0.02694	-1.00565	2.36541	0.42151	0.42515
8.0	0.30046	0.02689	-1.00645	2.36858	0.42128	0.42492
9.0	0.30029	0.02685	-1.00724	2.37175	0.42106	0.42468
10.0	0.30013	0.02680	-1.00802	2.37489	0.42083	0.42445

Table 6. Exact numerical characteristics for various H_0 as $\xi \rightarrow +\infty$, $P_r = 10$ and $\omega = 10$

H_0	$\bar{\eta}_\delta(+\infty)$	$F_{\phi\phi}(\infty, 0)$	$\Theta_\phi(\infty, 0)$	$\frac{Nu_x R_c^{-1/2}}{\pm \xi^{3/4}}$	$\frac{C_f R_c^{1/2}}{2\xi^{3/4}}$	$\frac{\delta R_c^{1/2} \xi^{1/4}}{x}$
0.00818	0.3	0.02677	-1.00801	2.37590	0.42065	0.42426
0.02660	0.4	0.06270	-1.02489	1.81177	0.55418	0.56569
0.06920	0.5	0.11983	-1.05893	1.49756	0.67786	0.70711
0.16089	0.6	0.20022	-1.11632	1.31559	0.78653	0.84853
0.35828	0.7	0.30388	-1.20092	1.21311	0.87705	0.98995
0.80248	0.8	0.42969	-1.31327	1.16078	0.94948	1.13137
1.87632	0.9	0.57642	-1.45054	1.13965	1.00640	1.27279
4.71390	1.0	0.74337	-1.60749	1.13666	1.05128	1.41421

Table 7. Exact numerical characteristics for various ω as $\xi \rightarrow +\infty$, $P_r = 10$ and $H_0 = 0.008191$

ω	$\bar{\eta}_\delta(+\infty)$	$F_{\phi\phi}(\infty, 0)$	$\Theta_\phi(\infty, 0)$	$\frac{Nu_x R_c^{-1/2}}{\xi^{1/4}}$	$\frac{C_f R_c^{1/2}}{2\xi^{3/4}}$	$\frac{\delta R_c^{1/2} \xi^{1/4}}{x}$
10	0.30013	0.02680	-1.00802	2.37489	0.42083	0.42445
100	0.29977	0.02679	-1.00802	2.37772	0.42167	0.42394
150	0.29977	0.02679	-1.00802	2.37774	0.42167	0.42394
500	0.29977	0.02679	-1.00802	2.37777	0.42168	0.42393
600	0.29977	0.02679	-1.00802	2.37777	0.42168	0.42393

Fig. 2. Dimensionless film thickness profiles $\eta_\delta(\xi)$.

obtained by earlier workers is provided by Fujii and Uehara [18] who suggest that over the various parameter ranges on ω and H_0

$$Nu_x R_e^{-1/2} = 0.450 \left(1.20 + \frac{1}{\omega H_0} \right)^{1/3} \quad \text{at } \xi = 0. \quad (108)$$

Notice that this is independent of the Prandtl number except for its role in the definition of H_0 . Our results have in essence substantiated the independence. As an indicator of the precision of (108) Table 4 draws a comparison between its predictions and the exact numerical results. For the most part agreement is very good. As expected the greatest variations occur in the transition range from small to large ωH_0 i.e. between $0.1 < \omega H_0 < 4$.

As a further test of the effectiveness of the numerical scheme special consideration can also be given to large ξ . With computations extending to $\xi = 10^{24}$ equations (105) can also be interpreted as asymptotes to the pure body force convection condensation data. Associated values are presented in Tables 5–7. In Table 5 the Prandtl number has been varied and the values for heat transfer and skin friction coefficients and film thickness identified. As in Table 1 the dependence

Table 8. Dimensionless film thickness profile for the parameter $H_0 = 0.008191$, $P_r = 10$ and $\omega = 10$

ξ	$\eta_\delta(\xi)$	ξ	$\eta_\delta(\xi)$	ξ	$\eta_\delta(\xi)$
0.0	0.661	0.3	0.414	15	0.305
10^{-6}	0.661	0.4	0.396	20	0.303
10^{-5}	0.661	0.6	0.374	30	0.302
10^{-4}	0.661	0.8	0.360	60	0.301
5×10^{-4}	0.659	1.0	0.351	100	0.301
10^{-3}	0.657	1.3	0.341	250	0.301
4×10^{-3}	0.645	1.6	0.335	10^3	0.301
0.01	0.624	2.0	0.329	10^4	0.301
0.025	0.585	2.5	0.324	10^5	0.301
0.05	0.542	3.2	0.319	10^6	0.301
0.075	0.513	4.0	0.316	10^8	0.301
0.1	0.492	5.0	0.312	10^{10}	0.301
0.15	0.462	7.0	0.309	10^{16}	0.301
0.2	0.441	10	0.306	10^{24}	0.301

Fig. 3. Development of interfacial velocity.

Fig. 4. Development of skin friction coefficient.

Fig. 5. Development of heat transfer coefficient.

on P_r for fixed H_0 is seen to be remarkably slight. By far the most significant influence of the Prandtl number is again its role in the definition of H_0 . This feature may be expected to persist throughout the full mixed condensation range. In Table 6 further information in the limit $\xi \rightarrow +\infty$ has been extracted from numerical solutions. The values of H_0 associated with $\eta_s = 0.3(0.1)1.0$ have been obtained together with values for the physical characteristics. Table 7, in contrast to Table 2, indicates the minimal role of ω in pure body force condensation.

It is clear that the numerical scheme captures entirely satisfactorily the correct details of the flow characteristics at the extremes $\xi = 0$ and $\xi \rightarrow +\infty$. Of greater significance however is the opportunity to obtain exact information over the full range of ξ . For three representative values of $H_0 = 0.001, 0.01, 0.1$ the precise values of the film thickness $\eta_s(\xi)$ have been obtained. The Prandtl number has been nominally taken as the single value 10. From earlier remarks no significant dependence on Prandtl number is expected. In view of the dependence on ω at small ξ two representative values of $\omega = 10, 100$ have also been used. The results are illustrated in Fig. 2 using the convenient ordinate variable $(\xi/(1+\xi))^{1/4}$ to cover the range $0 < \xi < +\infty$. For each set of fixed parameters the accelerating flow of the condensate under gravity together with the accompanying relative film thinning is apparent. Numerical data for a typical parameter set as

Table 9. Heat transfer coefficient comparison between exact results and approximate correlation (109)

$\frac{\xi}{H_0}$	$Nu_x R_c^{-1/2}$			
	$\omega = 10, H_0 = 0.008191$		$\omega = 100, H_0 = 0.02468$	
	Shu and Wilks Exact	Fujii and Uehara Equation (109)	Shu and Wilks Exact	Fujii and Uehara Equation (109)
10^{-2}	1.077	1.070	0.531	0.531
10^{-1}	1.083	1.074	0.577	0.565
10^0	1.133	1.117	0.778	0.756
10^1	1.432	1.397	1.281	1.267
10^2	2.305	2.265	2.244	2.238
10^3	4.022	3.982	3.928	3.977
10^4	7.137	7.072	6.999	7.071
10^5	12.682	12.575	11.156	12.574

Fig. 6. Dimensionless temperature profiles at $\omega = 10$.

Fig. 7. Dimensionless velocity profile at $\xi = 0.2$, $Pr = 1$, $\omega = 100$ and $H_0 = 0.02468$.

Fig. 8. Dimensionless velocity profile at $\xi = 250$, $P_r = 1$, $\omega = 100$ and $H_0 = 0.02468$.

quoted in [15] is included for additional information in Table 8. The asymptote as $\xi \rightarrow +\infty$ is in exact agreement with the similarity solution of [15]. The specific development of the free surface velocity for various cases is presented in Fig. 3. Here log-log plots more readily capture the

Fig. 9. Developing velocity profiles over ξ at $P_r = 1$, $\omega = 100$ and $H_0 = 0.02468$.

transition between similarity states. The acceleration of the free surface under gravity naturally implies that its velocity will go through a transition from $< U_\infty$ to $> U_\infty$. This feature is notable in all plots in Fig. 3. Similarly skin friction and heat transfer coefficients are plotted for the given range of parameter values in Figs 4 and 5. Fujii and Uehara [18] have proposed an estimate of the heat transfer coefficient based on an approximate solution. In the present notation this correlation reads

$$Nu_x R_c^{-1/2} = K(\omega H_0) \left(1 + \frac{1}{4K^4(\omega H_0)} \frac{\xi}{H_0} \right)^{1/4} \quad (109)$$

Table 9 presents comparisons between estimates from (109) and exact numerical solutions for representative small and moderate values of ωH_0 . For a typical thin film setting e.g. $\omega = 10$ and $H_0 = 0.008191$, the correlation is seen to be a valuable close approximation to the exact results. Its success is related to the validity of a linear temperature profile approximation across the film. This feature for small ωH_0 is confirmed in Fig. 6 where temperature profiles in the mixed condensation range for $\omega = 10$ are presented. The thin film approximation deteriorates however as ωH_0 increases. There is a corresponding deterioration in heat transfer estimates from (109). This is noticeable in Table 9 where exact results for $\omega = 100$, $H_0 = 0.02468$ are compared with (109).

Finally velocity profiles have been considered. Again representative ξ stations have been chosen for comparison with approximate results. At $\xi = 0.2$ Fig. 7 displays a wide discrepancy between the actual velocity in the vapour boundary layer and that predicted by Jacobs approximate method. At large ξ , Fig. 8, Jacobs' results are remarkably good with discrepancies again mostly associated with details in the vapour boundary layer. A display of progressively developing profiles as ξ increases is presented in Fig. 9. The transition of interfacial velocity from less than to greater than U_∞ is clearly accommodated by the numerical scheme.

10. CONCLUSION

In this paper we have presented an extension of the Keller box numerical scheme for a single boundary layer to a multilayer setting. The extended scheme has been successfully developed in a multiphase, non-similar boundary layer context. As has been displayed in a prototype configuration the scheme retains the accuracy and robustness of the original Keller box scheme. The scheme may be applied to a wide variety of non-similar physical configurations governed by differentio-integral systems reflecting inherent multiphase, multilayer features.

REFERENCES

1. H. B. Keller, Numerical methods in boundary-layer theory. *Ann. Rev. Fluid Mech.* **10**, 417 (1978).
2. H. B. Keller and T. Cebeci, Accurate numerical methods for boundary layer flows—I. Two dimensional laminar flows. In *Proc. of the 2nd Int. Conf. on Numerical Methods in Fluid Dynamics*, Berkeley, California, pp. 92–100 (1971).
3. H. B. Keller and T. Cebeci, Accurate numerical methods for boundary-layer flows—II. Two-dimensional turbulent flows. *AIAA J.* **10**(9), 1193 (September 1972).
4. G. Wilks and R. Hunt, Vertical mixed convection flow about a horizontal line source of heating or cooling. *Int. J. Heat Mass Transfer* **30**(6), 1119 (1987).
5. G. Wilks and R. Hunt, The assimilation of a strong, two-dimensional laminar jet into an aligned uniform stream. *The R. Soc. Edinburgh Proc. Sec. A Maths* **90A**, 13 (1981).
6. G. Wilks, R. Hunt and D. S. Riley, The two-dimensional laminar vertical jet with positive or adverse buoyancy. *Numerical Heat Transfer* **8**(4), 449 (1985).
7. G. Wilks and R. Hunt, The axisymmetric, turbulent, buoyant jet—numerical-solution for a semiempirical theory. *Numerical Heat Transfer* **9**(4), (1986).
8. R. Hunt and G. Wilks, On the behaviour of the laminar boundary-layer equations of mixed convection near a point of zero skin friction. *J. Fluid Mech.* **101**, 377 (1980).
9. J. H. Merkin, The effect of buoyancy forces on the boundary-layer flow over a semi-infinite vertical flat plate in a uniform free stream. *J. Fluid Mech.* **35**, 439 (1969).
10. G. Wilks, The flow of a uniform stream over a semi-infinite vertical flat plate with uniform surface heat flux. *Int. J. Heat Mass Transfer* **17**, 743 (1974).
11. R. Hunt and G. Wilks, Continuous transformation computation of boundary layer equations between similarity regimes. *J. Comput. Phys.* **40**(2), 478 (1981).
12. M. S. Raju, X. Q. Liu and C. K. Law, A formulation of combined forced and free convection past horizontal and vertical surfaces. *Int. J. Heat Mass Transfer* **27**(12), 2215 (1984).
13. H.-T. Lin and C. C. Chen, Mixed convection on vertical plate for fluids of any Prandtl number. *Warme Stoffübertragung-Thermo Fluid Dynamics* **22**(3–4), 159 (1988).

14. H.-T. Lin and W.-T. Cheng, Comprehensive correlations for laminar mixed convection line plume and wall plume. *Int. J. Heat Mass Transfer* **35**(10), 2751 (1992).
15. J. C. Y. Koh, E. M. Sparrow and J. P. Hartnett, The two phase boundary layer in laminar film condensation. *Int. J. Heat Mass Transfer* **2**, 69 (1961).
16. P. Beckett and G. Poots, Laminar film condensation in forced flows. *Q. J. Mech. Appl. Maths* **XXV**, 125 (1972).
17. R. D. Cess, Laminar-film condensation on a flat plate in the absence of a body force. *Z Angew. Math. Phys.* **11**, 426 (1960).
18. T. Fujii and H. Uehara, Laminar filmwise condensation on a vertical surface. *Int. J. Heat Mass Transfer* **15**, 217 (1972).
19. H. R. Jacobs, An integral treatment of combined body force and forced convection in laminar film condensation. *Int. J. Heat Mass Transfer* **9**, 637 (1966).
20. J. C. Y. Koh, Film condensation in a forced-convection boundary-layer flow. *Int. J. Heat Mass Transfer* **5**, 941 (1962).

APPENDIX

Details of Abbreviations Used in the Difference Equations of Section 6

(a) Inhomogeneous terms

$$\begin{aligned} S_{j-1/2}^{n-1} = & -v_{j-1/2}^{n-1} + v_{j-1/2}^{n-1} - \alpha_{n-1/2} h_j \eta_\delta(\xi_{n-1})(g v)_{j-1/2}^{n-1} \\ & - \beta_{n-1/2} h_j \eta_\delta(\xi_{n-1}) [\gamma_{n-1/2} \eta_\delta^2(\xi_{n-1}) H(J_1 - j + 1/2) - (u^2)_{j-1/2}^{n-1}] \\ & - \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} h_j \eta_\delta(\xi_{n-1}) [(u_{j-1/2}^{n-1})^2 - (u^2)_{j-1/2}^{n-1} - g_{j-1/2}^{n-1} v_{j-1/2}^{n-1}] \end{aligned} \quad (A1)$$

$$T_{j-1/2}^{n-1} = -w_{j-1/2}^{n-1} + w_{j-1/2}^{n-1} - P_r \alpha_{n-1/2} h_j \eta_\delta(\xi_{n-1})(g w)_{j-1/2}^{n-1} - \frac{2\xi_{n-1/2}}{k_n} P_r p_{n-1/2} h_j \eta_\delta(\xi_{n-1}) [u_{j-1/2}^{n-1} \varphi_{j-1/2}^{n-1} - g_{j-1/2}^{n-1} w_{j-1/2}^{n-1}] \quad (A2)$$

$$\begin{aligned} R_\delta^{n-1} = & -H_0 \left\{ w_\delta^{n-1} + P_r \alpha_{n-1/2} \eta_\delta(\xi_{n-1}) \sum_{j=1}^{J_1} (u \varphi)_{j-1/2}^{n-1} h_j \right. \\ & \left. - \frac{4\xi_{n-1/2}}{k_n} P_r p_{n-1/2} \eta_\delta(\xi_{n-1}) \sum_{j=1}^{J_1} u_{j-1/2}^{n-1} \varphi_{j-1/2}^{n-1} h_j \right\} \\ & - \left(\alpha_{n-1/2} - \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} \right) \eta_\delta(\xi_{n-1}) g_{J_1}^{n-1} \end{aligned} \quad (A3)$$

(b) Column vector elements

$$\begin{aligned} \alpha_{j-1/2}^{(i)} = & -g_j^{(i)} + g_{j-1}^{(i)} + h_j u_{j-1/2}^{(i)} \\ \beta_{j-1/2}^{(i)} = & -u_j^{(i)} + u_{j-1}^{(i)} + h_j v_{j-1/2}^{(i)} \\ \tau_{j-1/2}^{(i)} = & -\varphi_j^{(i)} + \varphi_{j-1}^{(i)} + h_j w_{j-1/2}^{(i)} \end{aligned} \quad (A4)$$

$$\begin{aligned} \gamma_{j-1/2}^{(i)} = & -v_j^{(i)} + v_{j-1}^{(i)} - \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n)(g^{(i)} v^{(i)})_{j-1/2} \\ & - \beta_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) [\gamma_{n-1/2} \eta_\delta^2(\xi_n) H(J_1 - j + 1/2) - (u^{(i)2})_{j-1/2}] \\ & + \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n)(u_{j-1/2}^{(i)})^2 \\ & - (\eta_\delta^{(i)}(\xi_n) - \eta_\delta(\xi_{n-1}))(u_{j-1/2}^{(i)} u_{j-1/2}^{(i)} + (u^{(i)2})_{j-1/2}) \\ & - \eta_\delta^{(i)}(\xi_n)(u^2)_{j-1/2}^{n-1} - \eta_\delta^{(i)}(\xi_n)(g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) v_{j-1/2}^{(i)} \\ & - \eta_\delta(\xi_{n-1}) v_{j-1/2}^{n-1} v_{j-1/2}^{(i)} g_{j-1/2}^{(i)}] \end{aligned} \quad (A5)$$

$$\begin{aligned} \sigma_{j-1/2}^{(i)} = & -w_j^{(i)} + w_{j-1}^{(i)} - P_r \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n)(g^{(i)} w^{(i)})_{j-1/2} \\ & + \frac{2\xi_{n-1/2}}{k_n} P_r p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n)(\varphi_{j-1/2}^{(i)} - \varphi_{j-1/2}^{n-1}) u_{j-1/2}^{(i)} \\ & + \eta_\delta(\xi_{n-1}) u_{j-1/2}^{n-1} \varphi_{j-1/2}^{(i)} - \eta_\delta^{(i)}(\xi_n)(g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) w_{j-1/2}^{(i)} - \eta_\delta(\xi_{n-1}) w_{j-1/2}^{n-1} g_{j-1/2}^{(i)}] \end{aligned} \quad (A6)$$

(c) Matrix elements of (79), (80) and (81)

$$\alpha_j^{(i)} = 1/2 \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) v_j^{(i)} + \frac{\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n) v_{j-1/2}^{(i)} + \eta_\delta(\xi_{n-1}) v_{j-1/2}^{n-1}] \quad (A7)$$

$$\beta_j^{(i)} = -\beta_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) u_j^{(i)} - \frac{\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [2\eta_\delta^{(i)}(\xi_n) u_{j-1/2}^{(i)} - (\eta_\delta^{(i)}(\xi_n) - \eta_\delta(\xi_{n-1}))(2u_j^{(i)} + u_{j-1/2}^{n-1})] \quad (A8)$$

$$c_j^{(i)} = 1 + 1/2 \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) g_j^{(i)} + \frac{\xi_{n-1/2}}{k_n} p_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) (g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) \quad (A9)$$

$$e_j^{(i)} = 1/2 P_r \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) w_j^{(i)} + \frac{\xi_{n-1/2}}{k_n} P_r p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n) w_{j-1/2}^{(i)} + \eta_\delta(\xi_{n-1}) w_{j-1/2}^{n-1}] \quad (A10)$$

$$f_j^{(i)} = -\frac{\xi_{n-1/2}}{k_n} P_r p_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) (\varphi_{j-1/2}^{(i)} - \varphi_{j-1/2}^{n-1}) \quad (A11)$$

$$p_j^{(i)} = -\frac{\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n) u_{j-1/2}^{(i)} + \eta_\delta(\xi_{n-1}) u_{j-1/2}^{n-1}] \quad (\text{A12})$$

$$q_j^{(i)} = 1 + 1/2 P, \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) g_{j-1}^{(i)} + \frac{\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) (g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) \quad (\text{A13})$$

$$\tilde{a}_j^{(i)} = -1/2 \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) v_{j-1}^{(i)} - \frac{\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n) v_{j-1/2}^{(i)} + \eta_\delta(\xi_{n-1}) v_{j-1/2}^{n-1}] \quad (\text{A14})$$

$$\tilde{b}_j^{(i)} = \beta_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) u_{j-1}^{(i)} + \frac{\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [2\eta_\delta^{(i)}(\xi_n) u_{j-1/2}^{(i)} - (\eta_\delta^{(i)}(\xi_n) - \eta_\delta(\xi_{n-1}))(2u_{j-1}^{(i)} + u_{j-1/2}^{n-1})] \quad (\text{A15})$$

$$\tilde{c}_j^{(i)} = 1 - 1/2 \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) g_{j-1}^{(i)} - \frac{\xi_{n-1/2}}{k_n} p_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) (g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) \quad (\text{A16})$$

$$\tilde{e}_j^{(i)} = -1/2 P, \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) w_{j-1}^{(i)} - \frac{\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n) w_{j-1/2}^{(i)} + \eta_\delta(\xi_{n-1}) w_{j-1/2}^{n-1}] \quad (\text{A17})$$

$$\tilde{f}_j^{(i)} = \frac{\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) (\varphi_{j-1/2}^{(i)} - \varphi_{j-1/2}^{n-1}) \quad (\text{A18})$$

$$\tilde{p}_j^{(i)} = \frac{\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j [\eta_\delta^{(i)}(\xi_n) u_{j-1/2}^{(i)} + \eta_\delta(\xi_{n-1}) u_{j-1/2}^{n-1}] \quad (\text{A19})$$

$$\tilde{q}_j^{(i)} = 1 - 1/2 P, \alpha_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) g_{j-1}^{(i)} - \frac{\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j \eta_\delta^{(i)}(\xi_n) (g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) \quad (\text{A20})$$

$$s_j^{(i)} = \alpha_{n-1/2} h_j (g^{(i)} v^{(i)})_{j-1/2} + \beta_{n-1/2} h_j [3\gamma_{n-1/2} \eta_\delta^{(i)2}(\xi_n) H(J_1 - j + 1/2) - (u^{(i)2})_{j-1/2}] \\ - \frac{2\xi_{n-1/2}}{k_n} p_{n-1/2} h_j [(u_{j-1/2}^{(i)} - u_{j-1/2}^{n-1}) u_{j-1/2}^{(i)} - (u^{(i)2})_{j-1/2} - (u^2)_{j-1/2}^{n-1} - (g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) v_{j-1/2}^{(i)}] \quad (\text{A21})$$

$$t_j^{(i)} = P, \alpha_{n-1/2} h_j (g^{(i)} w^{(i)})_{j-1/2} - \frac{2\xi_{n-1/2}}{k_n} P, p_{n-1/2} h_j [(\varphi_{j-1/2}^{(i)} - \varphi_{j-1/2}^{n-1}) u_{j-1/2}^{(i)} - (g_{j-1/2}^{(i)} - g_{j-1/2}^{n-1}) w_{j-1/2}^{(i)}]. \quad (\text{A22})$$

(d) Block matrices of $A^{(i)}$

$$A_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & -h_1/2 & 0 & 0 \\ 0 & 0 & 0 & -1 & -h_1/2 \end{pmatrix} \quad (\text{A23})$$

$$A_j = \begin{pmatrix} 1 & -h_j/2 & 0 & 0 & 0 \\ a_j^{(i)} & b_j^{(i)} & c_j^{(i)} & 0 & 0 \\ e_j^{(i)} & f_j^{(i)} & 0 & p_j^{(i)} & q_j^{(i)} \\ 0 & -1 & -h_{j+1}/2 & 0 & 0 \\ 0 & 0 & 0 & -1 & -h_{j+1}/2 \end{pmatrix} \quad (\text{A24})$$

for $j = 1, 2, \dots, J_1 - 1$

$$A_{J_1} = \begin{pmatrix} 1 & -h_{J_1}/2 & 0 & 0 & 0 \\ a_{J_1}^{(i)} & b_{J_1}^{(i)} & c_{J_1}^{(i)} & 0 & 0 \\ e_{J_1}^{(i)} & f_{J_1}^{(i)} & 0 & p_{J_1}^{(i)} & q_{J_1}^{(i)} \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A25})$$

$$A_{J_1+1} = \begin{pmatrix} -C_0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -C_2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & -h_{J_1+1}/2 & 0 & 0 \\ 0 & 0 & 0 & -1 & -h_{J_1+1}/2 \end{pmatrix} \quad (\text{A26})$$

$$A_j = \begin{pmatrix} 1 & -h_{j-1}/2 & 0 & 0 & 0 \\ a_{j-1}^{(0)} & b_{j-1}^{(0)} & c_{j-1}^{(0)} & 0 & 0 \\ e_{j-1}^{(0)} & f_{j-1}^{(0)} & 0 & p_{j-1}^{(0)} & q_{j-1}^{(0)} \\ 0 & -1 & -h_j/2 & 0 & 0 \\ 0 & 0 & 0 & -1 & -h_j/2 \end{pmatrix} \quad (A27)$$

for $j = J_1 + 2, J_1 + 3, \dots, J_2$

$$A_{J_2+1} = \begin{pmatrix} 1 & -h_{J_2}/2 & 0 & 0 & 0 \\ a_{J_2}^{(0)} & b_{J_2}^{(0)} & c_{J_2}^{(0)} & 0 & 0 \\ e_{J_2}^{(0)} & f_{J_2}^{(0)} & 0 & p_{J_2}^{(0)} & q_{J_2}^{(0)} \\ 0 & H(1-2n) & H(2n-1) & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (A28)$$

for $n = 0, 1, 2, \dots$

$$A_{J_2+2} = \begin{pmatrix} \tilde{h}_j^{(0)} & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad B_j = \begin{pmatrix} -1 & -h_j/2 & 0 & 0 & 0 \\ -\tilde{a}_j^{(0)} & -\tilde{b}_j^{(0)} & -\tilde{c}_j^{(0)} & 0 & 0 \\ -\tilde{e}_j^{(0)} & -\tilde{f}_j^{(0)} & 0 & -\tilde{p}_j^{(0)} & -\tilde{q}_j^{(0)} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (A29)$$

for $j = 1, 2, \dots, J_1$

$$B_{J_1+1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (A30)$$

$$B_j = \begin{pmatrix} -1 & -h_{j-1}/2 & 0 & 0 & 0 \\ -\tilde{a}_{j-1}^{(0)} & -\tilde{b}_{j-1}^{(0)} & -\tilde{c}_{j-1}^{(0)} & 0 & 0 \\ -\tilde{e}_{j-1}^{(0)} & -\tilde{f}_{j-1}^{(0)} & 0 & -\tilde{p}_{j-1}^{(0)} & -\tilde{q}_{j-1}^{(0)} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (A31)$$

for $j = J_1 + 2, J_1 + 3, \dots, J_2 + 1$

$$C_j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -h_{j+1}/2 & 0 & 0 \\ 0 & 0 & 0 & 1 & -h_{j+1}/2 \end{pmatrix} \quad C_{J_1} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -C_1 & 0 & 0 & 0 \end{pmatrix} \quad (A32)$$

for $j = 0, 1, \dots, J_1 - 1$

$$C_j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -h_j/2 & 0 & 0 \\ 0 & 0 & 0 & 1 & -h_j/2 \end{pmatrix} \quad D_0 = 0 \quad (A33)$$

for $j = J_1 + 1, J_1 + 2, \dots, J_2$

$$D_j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ s_j^{(0)} & 0 & 0 & 0 & 0 \\ t_j^{(0)} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad D_{J_1+1} = 0 \quad (A34)$$

for $j = 1, 2, \dots, J_1$

$$D_j = \begin{Bmatrix} 0 & 0 & 0 & 0 & 0 \\ s_{j-1}^{(j)} & 0 & 0 & 0 & 0 \\ t_{j-1}^{(j)} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{Bmatrix} \quad D_{J_1+1} = \begin{Bmatrix} 0 & 0 & 0 & 0 & 0 \\ s_{J_2}^{(j)} & 0 & 0 & 0 & 0 \\ t_{J_2}^{(j)} & 0 & 0 & 0 & 0 \\ -U_e(0)H(1-2n) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{Bmatrix} \quad (\text{A35})$$

for $j = J_1 + 2, J_1 + 3, \dots, J_2$ for $n = 0, 1, 2, \dots$

$$E_0 = \begin{Bmatrix} 0 & \tilde{\beta}_0^{(j)} & 0 & \tilde{s}_0^{(j)} & H_0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{Bmatrix} \quad E_j = \begin{Bmatrix} 0 & \tilde{\beta}_j^{(j)} & 0 & \tilde{s}_j^{(j)} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{Bmatrix} \quad (\text{A36})$$

for $j = 1, 2, \dots, J_1 - 1$

$$E_{J_1} = \begin{Bmatrix} \tilde{\alpha}_s^{(j)} & \tilde{\beta}_{J_1}^{(j)} & 0 & \tilde{s}_{J_1}^{(j)} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{Bmatrix} \quad E_j = 0 \quad \text{for } j = J_1 + 1, J_1 + 2, \dots, J_2 + 1. \quad (\text{A37})$$