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RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

TWIST - A NUMERICAL TECHNIQUE FOR CALCULATING THE STEADY-STATE MASS FRACTION VARIATION IN AN AXI-SYMMETRIC BINARY GAS MIXTURE SUBJECTED TO PRESSURE GRADIENTS

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April 1973

ISBN 0 642 99557 5

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ABSTRACT

The equation for diffusion in a binary gas mixture is integrated over each of a number of elements into which the R-Z system volume is divided. The resulting equations are soluble using the TWIST programme to give the mass fraction variation through the system. The Programme is suitable for analysis of any device which utilises pressure diffusion for the separation of a binary gas mixture, the components of which have approximately equal molecular weights and is describable in the R-Z coordinate system. Applications include the centrifuge, the vortex tube and the Vortex Matrix.

A knowledge of the mixture mass flow and pressure distribution throughout the system is assumed. A weakness of this method is the requirement of a fine subdivision of the system volume when such flows are large.

The TWIST programme has been applied to a counter-current centrifuge and the results compared with those from Cohen's theory.

National Library of Australia card number and ISBN 0 642 99557 5

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BOUNDARY CONDITIONS; CYLINDRICAL CONFIGURATION; DIFFUSION; BINARY MIXTURES; FINITE DIFFERENCE METHOD; FORTRAN; GASES; MASS; MASS TRANSFER; PRESSURE DEPENDENCE; SYMMETRY; T CODES; ULTRACENTRIFUGATION; VARIATIONS

CONTENTS

1. INTRODUCTION

Although the time dependant behaviour of an isotope separating device can be quite an important subject, much can be learnt from a study of its steady-state behaviour.

Pressure diffusion is employed in most separative devices, including the ultra-centrifuge, the vortex tube, and the Becker Nozzle. We concentrate here on those devices in which the binary gas mixture is caused to rotate about an axis.

Cylindrical coordinates are convenient for the description of these systems, but to avoid the calculational complexity and expense of a full 3D solution, it is necessary to eliminate at least one of the three spatial variables, R, Z or θ. For the ultra-centrifuge and, to a lesser extent, the vortex tube, RZ modelling should be satisfactory. For the vortex matrix, an RZ model could be considered adequate.

Rotation of the gas induces a centrifugal field which, whilst it has no intrinsic separating effect, induces a pressure gradient which performs the separation. Although its tangential component is predominant, the gas velocity will also have radial and axial components. These 'secondary' flows will affect the radial pressure gradient and will also induce an axial pressure gradient. As it is the resultant pressure gradient vector which performs the separation, we must allow for both radial and axial components. This is particularly necessary for the vortex tube device where rapid axial deterioration of the radial pressure gradient could occur.

It is assumed that the pressure field and secondary flow distributions are known throughout the volume of the device. A knowledge of the secondary flows is required for the calculation of mass transport resulting from bulk fluid flow.

It is further assumed that the difference between the molecular weights of the component gases is small so that the mixture molecular weight can be taken to be independent of position.

For the complex secondary flow patterns possible in a vortex device, it appears that the mass diffusion equations can only be solved by numerical methods. For more simple secondary flows in certain devices, analytical solutions are available (Cohen 1951), and their use is recommended. Cohen obtained an analytical solution for the counter-current centrifuge by neglecting the effect of axial diffusion on the radial concentration gradient. Here the numerical method would be useful only to cross-check results.

Before proceeding to the numerical method, the mass diffusion equation is

cast in dimensionless form. The input data for the resulting computer programme (see Appendix B) becomes dimensionless, thus avoiding the restrictions of a specific set of units. In addition, the result of any computer run is easily recognisable as being applicable to any system described by the particular set of dimensionless data.

The numerical method seeks to evaluate the mass fraction at the centre of each of a number of elements into which the volume is divided. A feature of this method is the use of an integral rather than a differential approach; this conserves matter irrespective of the coarseness of subdivision of the system volume.

The method produces a set of simultaneous equations for the unknown mass fractions. Following a description of the computer programme TWIST for the solution of these equations, an application of the programme to a counter-current centrifuge is discussed, with the results compared to those from Cohen's theory.

2. DIMENSIONLESS EQUATIONS

For a binary mixture, the steady-state equation of continuity of species A is, from equation 18.3-4 of Bird, Stewart and Lightfoot (1960),

$$\nabla \cdot (\rho_A v + j_A) = 0 \qquad \ldots(1)$$

where v and j_A are vector quantities, v being the mass averaged velocity and j_A being the mass flux of species A with respect to v; ρ_A is the density of species A.

Considering only ordinary (concentration) diffusion and pressure diffusion fluxes to be relevant, then

$$j_A = j_A^{(c)} + j_A^{(P)} \quad . \qquad \ldots(2)$$

From equation c of table 16.2-1 of Bird et al. (1960)

$$j_A^{(c)} = -\rho D \nabla \omega_A \qquad \ldots(3)$$

where ρ is the mixture density, D is the mass diffusivity and ω_A is the mass fraction of species A. From equation 18.4-9 of Bird et al. (1960)

$$j_A^{(P)} = \frac{-c^2}{\rho . R . T} \cdot M_A \cdot M_B \cdot D \left[x_A \cdot M_A \left(\frac{\bar{V}_A}{M_A} - \frac{1}{\rho} \right) \cdot \nabla_P \right] \qquad \ldots(4)$$

where c is the molar density and x_A is the mole fraction of A, the lighter of the species, D is the diffusion coefficient, M the molecular weight, R the gas constant and P and T are the pressure and temperature. As it is preferable to

work in terms of mass fraction, we write

$$c \cdot x_A \cdot M_A = \rho \cdot \omega_A \quad . \qquad \ldots(5)$$

This gives,

$$j_A^{(P)} = \frac{c}{R.T} \cdot M_B \cdot D \cdot \omega_A \left(\bar{V}_A - M_A/\rho\right) \cdot \nabla P \quad . \qquad \ldots(6)$$

For a perfect gas,

$$\bar{V}_A^{-1} = c = \frac{\rho}{M} = \rho\left(\frac{\omega_A}{M_A} + \frac{1-\omega_A}{M_B}\right) \qquad \ldots(7)$$

so,

$$j_A^{(P)} = -\rho D \cdot \frac{\Delta M}{M} \cdot \omega (1-\omega) \cdot \nabla \ell n\ P \quad . \qquad \ldots(8)$$

Substituting $\rho_A = \rho.\omega_A$ in equation 1, we can drop the subscript A and use equations 3 and 8 to obtain

$$\nabla \cdot (\rho v \omega) = \nabla \cdot \left(\rho D \nabla \omega + \rho D \cdot \frac{\Delta M}{M} \cdot \omega\ (1-\omega) \cdot \nabla \cdot \ell n\ P\right) \quad . \qquad \ldots(9)$$

Defining a characteristic length L* and a characteristic product of density and diffusion coefficient $(\rho.D)^*$, and then multiplying equation 9 through by $(L^*)^2/(\rho.D)^*$, the following dimensionless form is achieved:

$$\tilde{\nabla} \cdot \tilde{G}\omega = \tilde{\nabla} \cdot \left(\eta \cdot \tilde{\nabla}\omega + \eta \cdot \frac{D}{D} \cdot \frac{\Delta M}{M} \omega\ (1-\omega)\ \tilde{\nabla}\ \ell n\ P\right) \qquad \ldots(10)$$

where $\tilde{\nabla} = L^*\nabla$

and $\tilde{G}$ is the dimensionless mass flux

$$\tilde{G} = \frac{\rho v}{(\rho D)^*/L^*} \quad . \qquad \ldots(11)$$

Also,

$$\eta = \frac{\rho D}{(\rho D)^*} \qquad \ldots(12)$$

and, since it is generally accepted that ρD is independent of pressure, η reflects the temperature dependence of ρD.

Integrating equation 10 over a volume enclosed by a surface S, then by Green's theorem

$$-\int \tilde{G}\omega d\tilde{S} + \int \eta \tilde{\nabla}\omega \cdot d\tilde{S} + \int \eta \frac{D}{D} \frac{\Delta M}{M} \omega\ (1-\omega)\ \tilde{\nabla}\ \ell n\ P \cdot dS = 0 \qquad \ldots(13)$$

where

$$\tilde{S} = S/(L^*)^2 \quad . \qquad \ldots(14)$$

The *tilda* in equation 13 can be discarded provided it is noted that all length measurements must be expressed as multiples of L* and all mass fluxes as multiples of $(\rho D)^*/L^*$. It follows that any mass flow integrated over a given area must be expressed as a multiple of $(\rho D)^*/L^*$. With this understanding, we can write,

$$-\int G\omega \cdot dS + \int \eta \cdot \nabla\omega \, dS + \int \eta \cdot \frac{D}{D} \cdot \frac{\Delta M}{M} \cdot \omega(1-\omega) \nabla \ell n P \cdot dS = 0 \qquad \ldots(15)$$

3. FINITE DIFFERENCE APPROXIMATION

3.1 Introduction

The volume of the cylindrical system is divided into a number of intervals separated by surfaces with areas

$$A_i^{(Z)} = \pi (r_{i+1}^2 - r_i^2) = \pi (r_{i+1} + r_i) \delta r_i \qquad \ldots(16)$$

and $$A_{i,j}^{(R)} = 2\pi r_i (z_{j+1} - z_j) = 2\pi r_i \delta z_j \qquad \ldots(17)$$

where r_i and z_j are the coordinates of mesh lines defining the intervals. Figure 1 shows how the mass flow rates $w_{ij}^{(Z)}$ and $w_{ij}^{(R)}$ are defined at the surfaces of each interval whilst other quantities ω_{ij} are defined at the mid points of each interval.

3.2 Convective Flow

In applying equation 15 to one of the above intervals, we first consider the term representing convective flow of the desired species across the surface. We require values of ω at the surfaces, and these are obtained by linear interpolation. For example, the value of ω corresponding to $w_{i,j}^{(Z)}$ is

$$\omega_{i,j-\frac{1}{2}} = (1-q_j^{(Z)}) \omega_{i,j} + q_j^{(Z)} \omega_{i,j-1} \qquad \ldots(18)$$

where

$$q_j^{(Z)} = \delta z_j/(\delta z_j + \delta z_{j-1}) \qquad \ldots(19)$$

then with

$$q_i^{(R)} = \delta r_i/(\delta r_i + \delta r_{i-1}) \qquad \ldots(20)$$

we obtain

$$-\int_{ij} G\omega dS = w_{ij}^{(Z)} \left[\left(1-q_j^{(Z)}\right)\omega_{ij} + q_j^{(Z)}\,\omega_{ij-1}\right] -$$
$$-w_{ij+1}^{(Z)} \left[\left(1-q_{j+1}^{(Z)}\right)\omega_{ij+1} + q_{j+1}^{(Z)}\,\omega_{ij}\right] +$$
$$+w_{ij}^{(R)} \left[\left(1-q_i^{(R)}\right)\omega_{ij} + q_i^{(R)}\,\omega_{i-1,j}\right] -$$
$$-w_{i+1,j}^{(R)} \left[\left(1-q_{i+1}^{(R)}\right)\omega_{i+1,j} + q_{i+1}^{(R)}\,\omega_{ij}\right]. \qquad \ldots(21)$$

Using mass conservation,

$$W_{ij}^{(Z)} + W_{ij}^{(R)} - W_{ij+1}^{(Z)} - W_{i+1,j}^{(R)} = 0 \qquad \ldots(22)$$

and equation 21 can be cast in the more convenient form

$$-\int_{ij} G\omega dS = w_{ij}^{(Z)}\, q_j^{(Z)}\, (\omega_{i,j-1} - \omega_{ij})$$
$$-w_{ij+1}^{(Z)}\, (1-q_{j+1}^{(Z)})\, (\omega_{i,j+1} - \omega_{i,j})$$
$$+w_{i,j}^{(R)}\, q_i^{(R)}\, (\omega_{i-1,j} - \omega_{i,j})$$
$$-w_{i+1,j}^{(R)}\, (1-q_{i+1}^{(R)})\, (\omega_{i+1,j} - \omega_{i,j}) \quad . \qquad \ldots(23)$$

This equation gives the convective flow of the desired species into a volume element located away from boundary surfaces. Boundary intervals are considered in section 3.5.

3.3 Concentration Diffusion

The concentration diffusion current across surface $A_{i,j}^{(Z)}$ is approximated, from equation 15, by

$$C_{ij}^{(Z)} = A_{ij}^{(Z)} \left[\frac{\omega_{i,j-1} - \omega}{\delta z_{j-1}/(2\eta_{i,j-1})}\right] = A_{ij}^{(Z)} \left[\frac{\omega - \omega_{i,j}}{\delta z_j/(2\eta_{ij})}\right]$$
$$= 2A_{i,j}^{(Z)} \left[\frac{\omega_{i,j-1} - \omega_{i,j}}{(\delta z_{j-1}/\eta_{i,j-1}) + (\delta z_j/\eta_{i,j})}\right] \qquad \ldots(24)$$

where ω is an interpolated concentration of surface $A_{ij-1}^{(Z)}$. The total concentration diffusion current into volume interval i,j, is

$$\int \eta.\nabla\omega.dS = C_{i,j}^{(Z)} - C_{i,j+1}^{(Z)} + C_{i,j}^{(R)} - C_{i+1,j}^{(R)}$$

$$= C_{ij}^{(Z)} \ (\omega_{i,j-1} - \omega_{ij}) + C_{i,j-1}^{(Z)} \ (\omega_{i,j+1} - \omega_{i,j})$$

$$+ C_{ij}^{(R)} \ (\omega_{i-1,j} - \omega_{ij}) + C_{i+1,j}^{(R)} \ (\omega_{i+1,j} - \omega_{i,j}) \qquad \ldots(25)$$

where,

$$C_{ij}^{(Z)} = 2A_{ij}^{(Z)} / (\delta z_{j-1}/\eta_{i,j-1} + \delta z_j/\eta_{ij}) \qquad \ldots(26)$$

and

$$C_{ij}^{(R)} = 2A_{ij}^{(R)} / (\delta r_{i-1}/\eta_{i-1,j} + \delta r_i/\eta_{i,j}) \quad . \qquad \ldots(27)$$

Boundary terms in equation 25 will be considered after expressions have been generated for pressure diffusion.

3.4 Pressure Diffusion

The pressure diffusion current across surface $A_{ij}^{(Z)}$ is approximated, from equation 15, by

$$P_{ij}^{(Z)} = A_{ij}^{(Z)} \cdot \frac{\ell n \ P_{ij-1} - \ell n \ P}{\Omega_{i,j-1}^{(Z)}} = A_{ij}^{(Z)} \frac{\ell n \ P - \ell n \ P_{ij}}{\Omega_{ij}^{(Z)}}$$

$$= A_{ij}^{(Z)} \frac{\ell n (P_{ij-1}/P_{ij})}{\Omega_{ij-1}^{(Z)} + \Omega_{ij}^{(Z)}} \qquad \ldots(28)$$

where P is an interpolated pressure at $A_{ij}^{(Z)}$ and

$$\Omega_{ij}^{(Z)} = \delta z_j / [\, 2\eta \, \frac{D}{D} \cdot \frac{\Delta M}{M} \, \omega(1-\omega)]_{ij} \quad . \qquad \ldots(29)$$

Similarly, the pressure diffusion current across surface $A_{ij}^{(R)}$ is:

$$P_{ij}^{(R)} = A_{ij}^{(R)} \cdot \frac{\ell n (P_{i-1,j}/P_{i,j})}{\Omega_{i-1,j}^{(R)} + \Omega_{ij}^{(R)}} \qquad \ldots(30)$$

where

$$\Omega_{ij}^{(R)} = \delta r_i / [\, 2\eta \, \frac{D}{D} \frac{\Delta M}{M} \, \omega(1-\omega)]_{ij} \quad . \qquad \ldots(31)$$

The total pressure diffusion current into volume interval i,j is:

$$\int_{ij} \eta \cdot \frac{D}{D} \cdot \frac{\Delta M}{M} \cdot \omega(1-\omega) \nabla \ \ell n \ P \ dS = S_{i,j}$$

$$S_{ij} = P_{i,j}^{(Z)} - P_{i,j+1}^{(Z)} + P_{i,j}^{(R)} - P_{i+1,j}^{(R)} \quad . \qquad \ldots(32)$$

For elements adjacent to boundaries, it is assumed that the nett diffusion from both pressure and concentration effect, is zero across the boundary surface. For example, if element i,j-1 is outside the boundary whilst i,j is inside, then

$$C^{(Z)}_{i,j} \ (\omega_{i,j-1} - \omega_{i,j}) + P^{(Z)}_{i,j} = 0 \quad . \qquad \ldots(33)$$

3.5 Boundary Conditions

In sections 3.2, 3.3 and 3.4 above, volume intervals located away from boundary surfaces have been considered. For an interval adjacent to a solid boundary surface, the convective flow across that boundary must be zero, as must diffusion from both pressure and concentration effects. Hence the relevant terms in equations 23, 25, 32 are set to zero. For positive outflow, it is assumed that ω outside the boundary is equal to that just inside. In addition, pressure diffusion across the boundary can be ignored and the relevant terms in equations 23, 25 and 32 can be discarded. For positive inflow, the convective flow of desired species, $W_{in} \cdot \omega_{in}$ is usually known at a large distance from the boundary where mass diffusion can be neglected. At the boundary, the total flow of desired species must also equal $W_{in} \cdot \omega_{in}$ but because of the possibility of mass diffusion across the boundary, the concentration at the boundary will not necessarily equal ω_{in}. This does not affect the application of the boundary condition (that the total flow of desired species equals $W_{in} \cdot \omega_{in}$) which is accounted for by setting the concentration and pressure diffusion terms to zero and the convective flow equal to $W_{in} \cdot \omega_{in}$. The appropriate term of equation 23 then becomes $W_{in}(\omega_{in} - \omega_{i,j})$.

3.6 Mass Balance for Volume Interval

Collecting the various terms for flow of the desired species into volume element i,j we have from equations 15, 23, 25 and 32

$$W^{(Z)}_{i,j} \cdot q^{(Z)}_{j} \ (\omega_{i,j-1} - \omega_{i,j}) - W^{(Z)}_{i,j+1} \ (1-q^{(Z)}_{j+1}) \ (\omega_{i,j+1} - \omega_{i,j}) +$$

$$+ W^{(R)}_{i,j} \cdot q^{(R)}_{i} \ (\omega_{i-1,j} - \omega_{ij}) - W^{(R)}_{i+1,j} \ (1-q^{(R)}_{i+1}) (\omega_{i+1,j} - \omega_{i,j}) +$$

$$+ C^{(Z)}_{i,j} \ (\omega_{i,j-1} - \omega_{i,j}) + C^{(Z)}_{i,j+1} \ (\omega_{i,j+1} - \omega_{i,j}) +$$

$$+ C^{(R)}_{i,j} \ (\omega_{i-1,j} - \omega_{i,j}) + C^{(R)}_{i+1,j} \ (\omega_{i+1,j} - \omega_{i,j}) +$$

$$+ S_{i,j} = 0 \quad . \qquad \ldots(34)$$

Define

$$h^{(Z-)}_{i,j} = C^{(Z)}_{i,j} + W^{(Z)}_{i,j}\ q^{(Z)}_{j} \qquad \ldots(35)$$

$$h^{(Z+)}_{i,j} = C^{(Z)}_{i,j+1} - W^{(Z)}_{i,j+1}\ (1-q^{(Z)}_{j+1}) \qquad \ldots(36)$$

$$h^{(R-)}_{i,j} = C^{(R)}_{i,j} + W^{(R)}_{i,j}\ q^{(R)}_{i} \qquad \ldots(37)$$

$$h^{(R+)}_{i,j} = C^{(R)}_{i+1,j} - W^{(R)}_{i+1,j}\ (1-q^{(R)}_{i+1}) \quad . \qquad \ldots(38)$$

Then

$$\omega_{i,j}(\textstyle\sum_4 h) = S_{i,j} + h^{(Z-)}_{i,j} \cdot \omega_{i,j-1} + h^{(Z+)}_{i,j}\ \omega_{i,j+1} + h^{(R-)}_{i,j}\ \omega_{i-1,j} + \\ + h^{(R+)}_{i,j}\ \omega_{i+1,j} \quad . \qquad \ldots(39)$$

3.7 Iterative Solution of Finite Difference Equations

The non-linear dependence of $S_{i,j}$ and $\omega_{i,j}$ and its neighbouring ω's suggests an iterative scheme to obtain a solution. An initial guess of the concentration (ω) field allows the S field to be calculated from equation 32 (using equations 28 to 31) then a new ω field can be calculated using the linear equation 39 for each volume interval.

In general, the number of volume intervals will be too large to contemplate a direct solution of equation 39 so an inner iterative loop is required with an outer iteration loop working on $S_{i,j}$. For the non-symmetric matrix involved in the inner loop, the extrapolated successive iteration method (Lee and Stone 1959) has been applied. This method is convergent provided that the h's of equations 35 to 38 are positive. From equations 26 and 27, it is noted that the C's are positive hence it is required that:

$$C^{(Z)}_{i,j} > |w^{(Z)}_{i,j}| \ .\ (q^{(Z)}_{j} \text{ or } 1-q^{(Z)}_{j}) \qquad \ldots(40)$$

and $$C^{(R)}_{i,j} > |w^{(R)}_{i,j}| \ .\ (q^{(R)}_{i} \text{ or } 1-q^{(R)}_{i}) \qquad \ldots(41)$$

depending on the flow direction.

Substituting for the q's from equations 19 and 20 and for the C's from equations 26 and 27 and ignoring any small differences between η_{ij} and its neighbours, we obtain the convergence criteria:

$$(\delta z_{j} \text{ or } \delta z_{j-1}) < \frac{2\eta_{ij}}{|W^{(Z)}_{ij}/A^{(Z)}_{ij}|} = 2\eta_{i,j}|G^{(Z)}_{i,j}| \qquad \ldots(42)$$

and

$$(\delta r_i \text{ or } \delta r_{i-1}) < \frac{2\eta_{ij}}{|W_{ij}^{(R)}/A_{ij}^{(R)}|} = 2\eta_{ij} |G_{ij}^{(R)}| \quad \ldots(43)$$

where the G's are mass fluxes.

The extrapolated successive iteration method requires an acceleration parameter, the ω in equation 3.16 of Lee and Stone (1959), ω=1 gives unaccelerated successive iteration. It was found that a value of ω of between 1.5 and 1.7 has halved the number of iterations required for problems so far attempted.

4. THE COMPUTER PROGRAMME TWIST

The computer programme TWIST has been developed to solve the equations derived in the previous sections. A FORTRAN IV listing is given in Appendix C.

4.1 Input Data

The necessary input data for the TWIST4 version are detailed in Appendix B. It should be noted that these must be expressed in dimensionless form in terms of the characteristic variables as defined in Section 2.

4.2 Convergence Problems

Initial difficulties associated with the stability of the programme have been overcome to some extent by adopting a more flexible programming philosophy. It was found necessary at an early stage to build in procedures to check the convergence or otherwise of both the inner and outer iteration loops, to terminate the programme if there was no convergence. This did not prove to be as simple as expected as an initial fluctuation must be permitted due to the arbitrary nature of the initial guess at the concentration field. Also, convergence to a requested accuracy may not be possible due to the quasi-stationary nature of the solution when the 'final' value has been reached, where slight fluctuations may occur due to round off errors. The programme will terminate after 10 successive divergences in either the inner or outer iteration loops.

4.3 Switching Between Iteration Loops

The optimum point at which to switch between the inner and outer iteration loops will depend on how strongly the coefficients determined in the outer loop depend on the parameter determined in the inner loop. Two alternatives have been made available in TWIST4. The user may specify the number of inner and outer loops to be traversed after which the programme will terminate. The default option will proceed with the inner loop iteration either until the convergence has reached the required accuracy or until the convergence (change in concentration between successive iterations) is less than 10% of the

maximum change between the first and second iterations of the loop, whichever occurs first. The programme will then return to the outer loop to recalculate coefficients. These criteria reduce significantly the computer time involved in reaching the final solution. In addition the programme will return to the outer loop immediately if there is a concentration change of 50% or more between successive iterations.

4.4 Problem Size

To alleviate problems caused by the small mesh intervals required when large flows are involved, the overall mesh size has been made flexible within the limits of IMAX*JMAX = 2000 rather than having a fixed size in either direction.

IMAX = number of points in the radial direction

JMAX = number of points in the axial direction.

5. COMPARISON WITH COHEN'S THEORY FOR THE COUNTER-CURRENT CENTRIFUGE

A flow distribution which could be readily treated by both TWIST and by Cohen's centrifuge theory was

$$G_Z = \left.\begin{matrix} +g, 0 < r < r_i \\ -g, r_i < r < r_o \end{matrix}\right\} \text{ g constant}$$

where G_Z is the axial mass flux and r_o the outer radius of the device. The relative proportions of product and re-circulating flow can be varied by changing r_i.

Appendix A gives the equations resulting when Cohen's theory is applied to such a flow distribution. To compare TWIST to this theory, the enricher end of the centrifuge is isolated and our parameters chosen as,

$$r_o = 3.87 \quad , \quad Z = 30$$

and

$$ar_o^2 = \frac{\Delta M V^2}{RT} = 0.2 \quad ,$$

V being the peripheral velocity.

The case of complete recirculation (zero product flow) was chosen with down flow L set at the optimum value of equation A15. For our selected value of r_o, this is L = 55.335.

For numerical stability, TWIST requires a mesh increment

$$\delta z < 2/g = \frac{2\pi r_o^2}{L} = 2r_o \sqrt{\left[\frac{2 \ln 2 - 1}{8}\right]}$$

or $\delta z < 1.7$ for our selected value of r_o.

Choosing 20 axial mesh intervals, with $\delta z = 1.5$, we have more than enough for accuracy, but a basic difficulty of the TWIST method is revealed, for larger flows would require a proportionately larger number of mesh points, and realistic centrifuges could have flows which are an order of magnitude greater than L_{opt}, making data preparation tedious and lengthening computer time.

In the radial direction, six annuli of equal flow area $A_{ij}^{(Z)}$ were chosen. Figure 2 shows the internal flow distribution, with the length of the smallest arrow being equal to L/6, that is 9.22. TWIST requires an inflow with concentration defined at at least one point, so a small through flow of magnitude 0.01 had to be imposed and added to the flows in the centre core. An extra axial mesh interval was needed for definition of the feed concentration which was taken as 0.007.

For the particular problem under consideration, Cohen's theory (equation A16) gives a separation factor of 1.554. The computed concentration profile from TWIST is plotted in Figure 3. Although the concentration profile itself has converged, the level has not. This was evident from the outflow concentration which should have converged to that of the feed stream. The lack of convergence produced mass balance errors of the same order of magnitude as the feed flow of the desired isotope. However, no convergence difficulties were experienced with more realistic feed flows.

The maximum separation factor calculated by TWIST was 1.576. This included radial separation which was neglected in Cohen's axial separation factor. The TWIST axial separation factor varied from 1.478 at the inner core to 1.501 at the outer annulus.

This good agreement shows that results from the code are valid for this type of device. Further comparisons of the code with experimental measurements would be an advantage.

6. CONCLUSIONS

The computer programme TWIST is available for the solution of pressure-diffusion problems describable in an R-Z coordinate system. The programme would be particularly suited to the analysis of separation in vortex tube devices with their complex secondary flow patterns, but also has application to the counter-current centrifuge, if only to validate the results of simpler theories. Such an application has indeed confirmed the result of Cohen's theory for the case of complete re-circulation.

The particular numerical technique used in TWIST was chosen so that mass is conserved irrespective of the coarseness of subdivision of the system volume.

However, for numerical stability, the method is found to require a very fine subdivision of the system volume when the internal mass flux is large. Its applicability to realistic counter-current centrifuges is doubtful.

For problems with realistic throughput (feed, product and waste mass flows) no severe convergence problems arise. Typically, each outer loop requires several hundred inner iterations and some five to ten outer loops are needed. The concentration level itself is slow to converge for problems with small mass throughput, but this is understandable in terms of round off errors and is of little consequence.

7. REFERENCES

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8. NOTATION

(Notation is as follows except where otherwise defined in the text).

A	Lighter component of binary gas mixture.
$A_{ij}^{(R)}$	Area in radial direction of interval ij defined by equation 17.
$A_{ij}^{(Z)}$	Area in axial direction of interval ij defined by equation 16.
A*	Characteristic area (multiple of $(L^*)^2$).
B	Heavier component of binary gas mixture.
$C_{ij}^{(R)}$	Coefficient defined by equation 27.
$C_{ij}^{(Z)}$	Coefficient defined by equation 26.
$\mathcal{C}_{ij}^{(R)}$	Concentration diffusion current across surface $A_{ij}^{(R)}$.
$\mathcal{C}_{ij}^{(Z)}$	Concentration diffusion current across surface $A_{ij}^{(Z)}$.
c	Molar density.
D	Diffusion coefficient.
$\mathcal{D}$	Mass diffusivity.
G	Mass flux.
$\tilde{G}$	Dimensionless mass flux (defined by equation 11).
$G_{ij}^{(R)}$	Radial mass flux at interval ij.

$G_{ij}^{(Z)}$ Axial mass flux at interval ij.

G_Z Axial mass flux.

$h_{ij}^{(R-)}$, $h_{ij}^{(R+)}$, $h_{ij}^{(Z-)}$, $h_{ij}^{(Z+)}$ Iteration coefficients for mass fractions as defined by equations 35 to 38.

j_A Mass flux of species A with respect to V

$j_A^{(c)}$ Concentration diffusion mass flux.

$j_A^{(p)}$ Pressure diffusion mass flux.

L^* Characteristic length.

M Mixture molecular weight.

M_A Molecular weight of species A.

M_B Molecular weight of species B.

P Pressure.

P_{ij} Pressure at interval ij.

$p_{ij}^{(R)}$ Pressure diffusion current across surface $A_{ij}^{(R)}$.

$p_{ij}^{(Z)}$ Pressure diffusion current across surface $A_{ij}^{(Z)}$.

$q_i^{(R)}$, $q_j^{(Z)}$ Variables related to mesh intervals, as defined by equations 19 and 20.

R Gas constant.

r Radius

r_i Radial coordinate of mesh line i.

r_o Outer radius of device.

S Surface

$\tilde{S}$ Dimensionless surface defined by equation 14.

S_{ij} Total pressure diffusion current into volume interval ij.

T Temperature.

V Peripheral velocity.

v mass averaged velocity.

$W_{ij}^{(R)}$ Mass flow rate in radial direction at interval ij.

$W_{ij}^{(Z)}$ Mass flow rate in axial direction at interval ij.

X_A Mole fraction of species A.

Z Length of device.

Z_j Axial coordinate of mesh line j.

ΔM Difference in molecular weights of species.

δr Radial mesh interval.

δz Axial mesh interval.

ρ Mixture density.

ρ_A Density of species A.

η Defined by equation 12 to reflect temperature dependence of (ρD)

η_{ij} Value of η applicable at interval ij.

ω_A Mass fraction of species A.

ω Interpolated mass fraction at surface $A_{ij-1}^{(Z)}$.

ω_{ij} Mass fraction of species A at interval ij.

$\Omega_{ij}^{(R)}$ Variable defined by equation 31.

$\Omega_{ij}^{(Z)}$ Variable defined by equation 29.

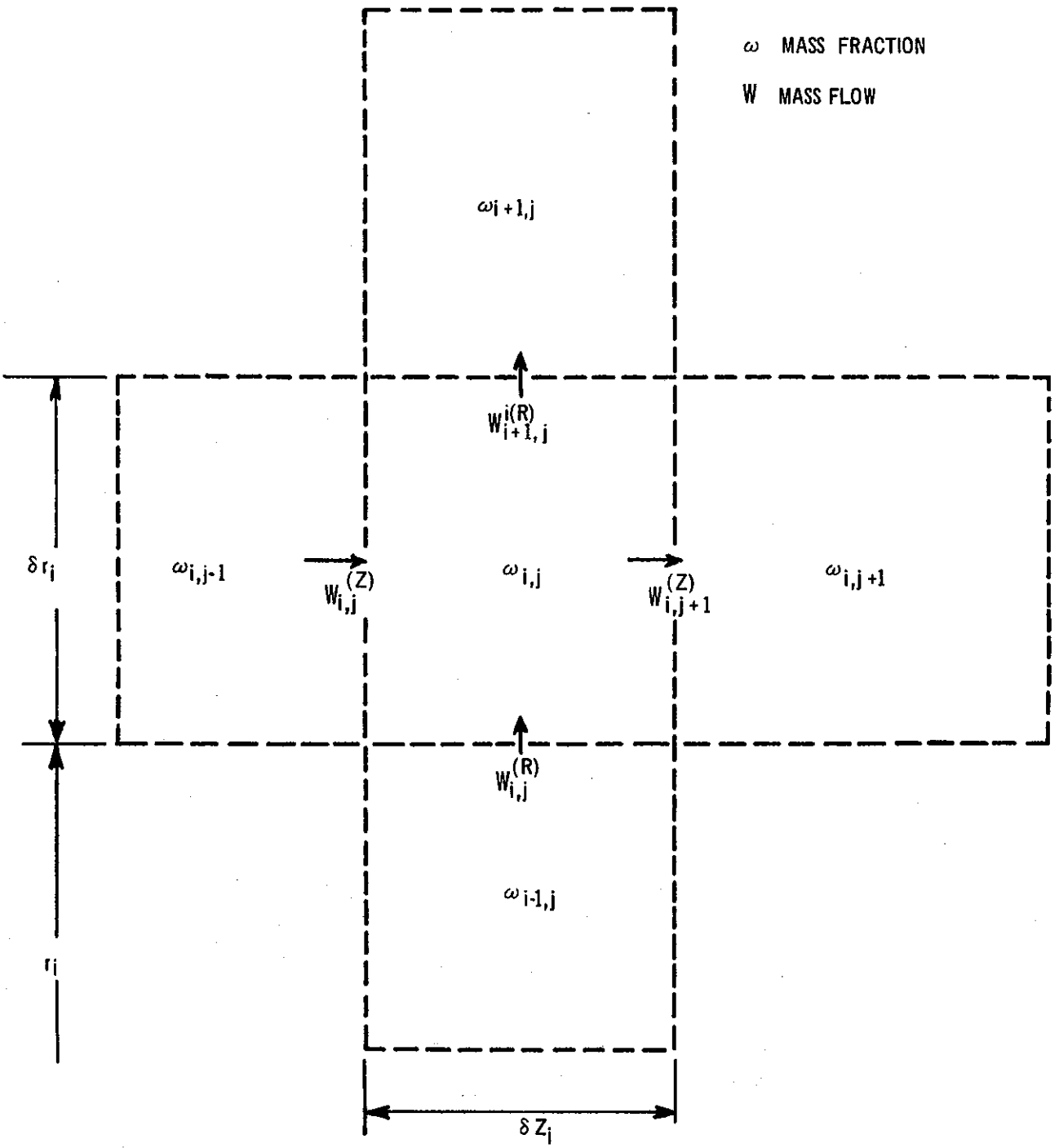

FIGURE 1. A FINITE VOLUME ELEMENT WITH NEIGHBOURS

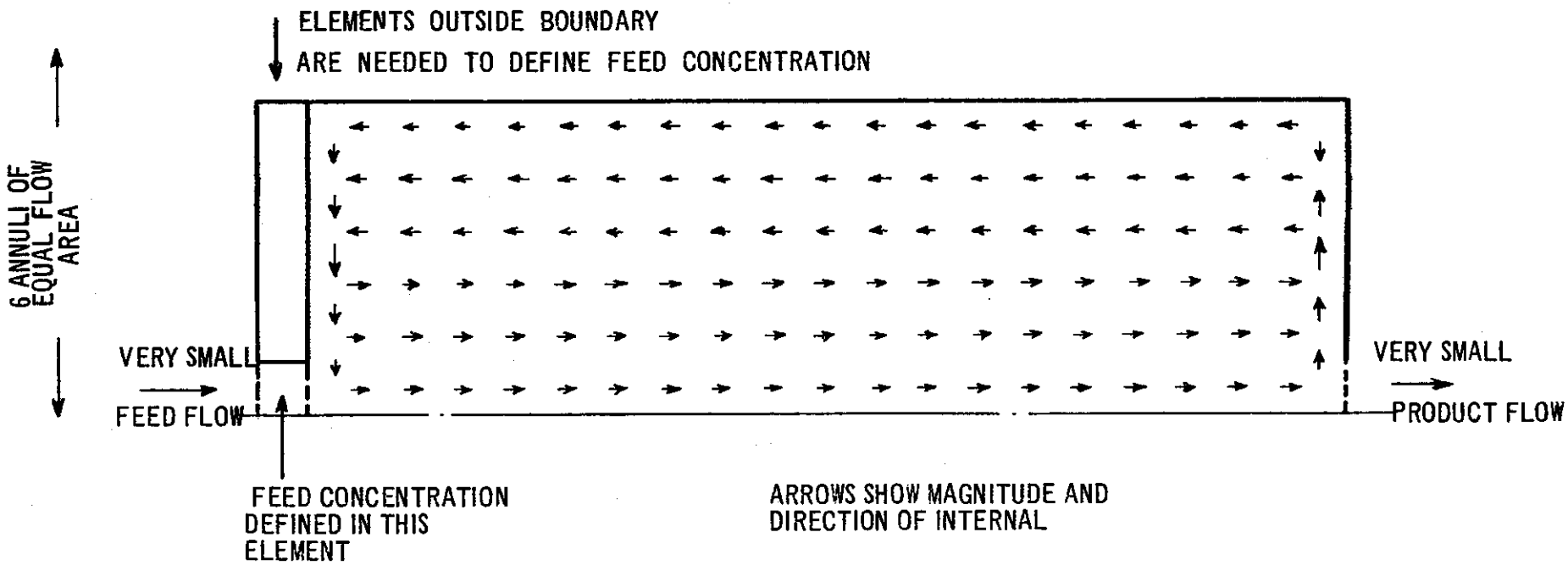

FIGURE 2. COUNTER-CURRENT FLOW DISTRIBUTION FOR TWIST

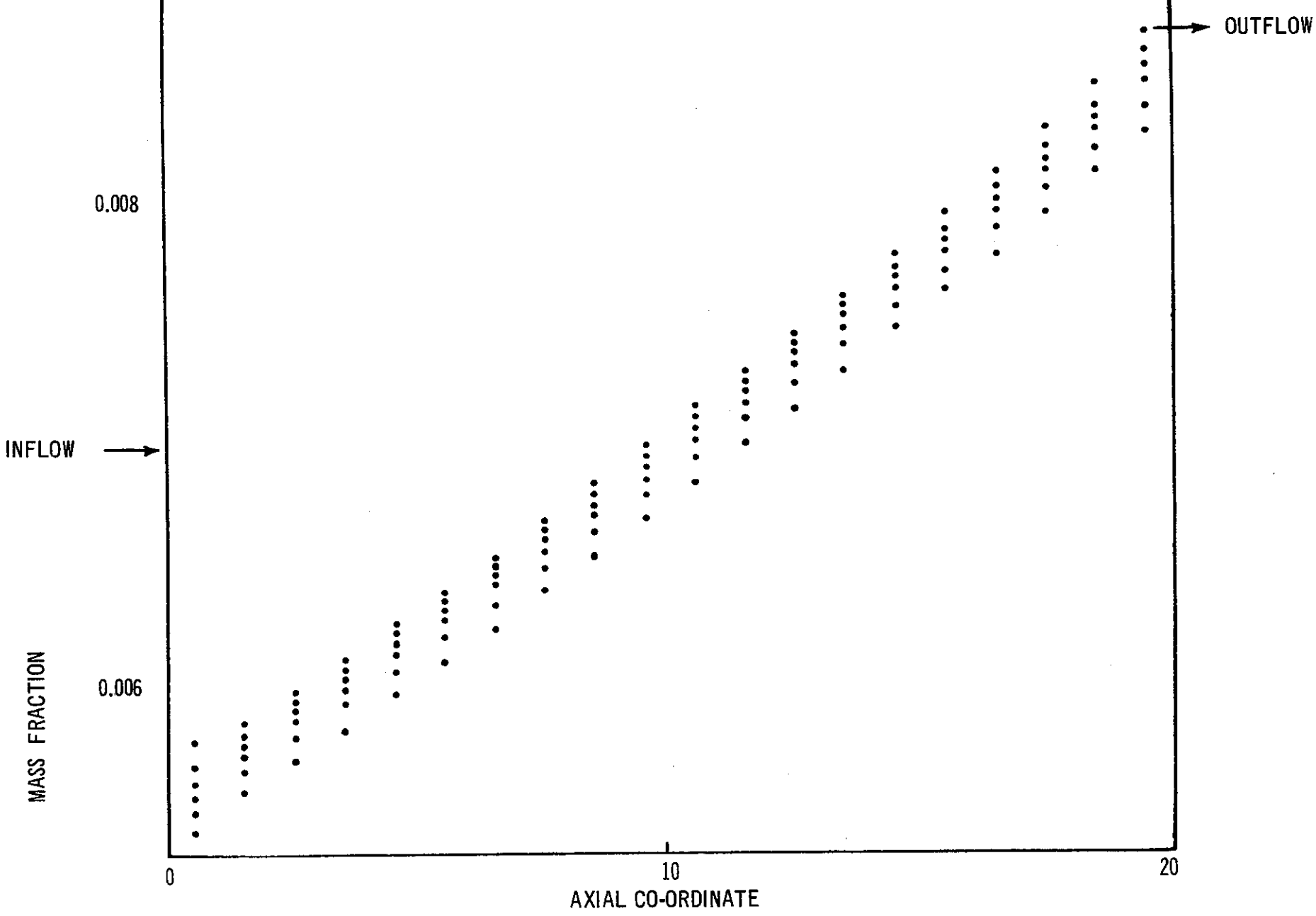

FIGURE 3. CONCENTRATION PROFILE FROM TWIST FOR COUNTER-CURRENT CENTRIFUGE

APPENDIX A

COHEN'S APPROACH FOR THE COUNTER-CURRENT CENTRIFUGE

By recognising that all length measurements are expressed in multiples of L* and all mass fluxes are expressed as multiples of $(\rho.D)^*/L^*$, equation 10 can be written without the *tilda* as:

$$\nabla.G\omega = \nabla.(\eta\nabla\omega + \eta\,\frac{D}{D}\,.\,\frac{\Delta M}{M}\,.\,\omega\,(1-\omega)\,\nabla.\ell n\,P) \quad . \qquad \ldots A1$$

For zero radial flow, zero axial pressure gradient, uniform temperature ($\eta = 1$), $D = D$ and $\omega \ll 1$, this equation reduces to:

$$G_Z\,\frac{\partial\omega}{\partial z} = \frac{\partial^2\omega}{\partial z^2} + \frac{1}{r}\,\frac{\partial}{\partial r}\,.\,r\left[\frac{\partial\omega}{\partial r} + \frac{\Delta M}{M}\,.\,\omega\,.\,\frac{\partial\ell n\,P}{dr}\right] \quad . \qquad \ldots A2$$

Taking the radial pressure distribution as that for a solid body,

$$G_Z\,.\,\frac{\partial\omega}{\partial z} = \frac{\partial^2\omega}{\partial z^2} + \frac{1}{r}\,\frac{\partial}{\partial r}\,.\,r\left[\frac{\partial\omega}{\partial r} + a.r.\omega\right] \quad , \qquad \ldots A3$$

where

$$a = \frac{\Delta M\,.\,(\Omega L^*)^2}{RT} \qquad \ldots A4$$

with due regard to the dimensionless form of equation A3 it is the same as Cohen's equation 6.45. Using his method of eliminating the r dependence of ω we obtain the simplification:

$$(c_2 + c_3)\,\frac{d\omega}{dz} - (P + c_1)\,\omega = -P\omega_p \qquad \ldots A5$$

where

$$c_1 = a\int_o^r r\int_o^r G_Z\,.\,2\pi r'dr'dr \qquad \ldots A6$$

$$c_2 = \pi r_o^2 \qquad \ldots A7$$

and $$c_3 = \int_o^r r^{-1}\left[\int_o^r G_Z\,.\,2\pi r'dr'\right]^2 dr/2\pi \qquad \ldots A8$$

where ω_p is the concentration at the product end and P is the product flow (in multiples of $(\rho D)^*L^*$). Consider the flow distribution

$$G_Z = \begin{Bmatrix} +g, 0 < r < r_i \\ -g, r_i < r < r_o \end{Bmatrix} \quad g \text{ constant} \quad . \qquad \ldots A9$$

The total up and down flow is

$$L = \pi r_o^2 g \qquad \ldots A10$$

and the product flow

$$P = \pi g \left[2r_i^2 - r_o^2 \right] \qquad \ldots A11$$

is varied by changing r_i.

In terms of L and P, equations A6 and A8 yield

$$c_1 = a \cdot \frac{r_o^2}{8} \cdot \frac{L^2 + 2PL - P^2}{L} \qquad \ldots A12$$

and

$$c_3 = \frac{1}{2\pi} \left\{ \frac{2P^2 - L^2}{4} + \frac{(P+L)^2}{2} \cdot \ell n \left(\frac{2L}{P+L} \right) \right\} \qquad \ldots A13$$

The solution to equation A5 is, for the enricher end of the centrifuge,

$$\alpha = \frac{\omega P}{\omega_F} = (P+c_1) / \left[P + c_1 . \exp \left(- \frac{P+c_1}{c_2+c_3} . Z \right) \right] \qquad \ldots A14$$

where ω_F is the feed concentration and Z is the enricher length. By allowing negative L, equation A14 is also valid for the stripper, in which case P would denote the waste rather than product flow.

At zero production, α is stationary when

$$L = L_{opt} = \pm \pi r_o \sqrt{\left[\frac{8}{2 . \ell n\ 2 - 1} \right]} \qquad \ldots A15$$

The positive result gives the optimum enricher flow and the negative result gives the optimum stripper flow. The maximum separation factor is

$$\alpha_{max} = \exp \left(\frac{a . r_o . Z}{16} \right) \sqrt{\left[\frac{8}{2 . \ell n\ 2 - 1} \right]} \qquad \ldots A16$$

APPENDIX B

PREPARATION OF INPUT DATA FOR TWIST4

1. INPUT DATA FOR TWIST4

Card 1: (Format 20A4)
Card 2: (Format 20A4) — Title cards to describe the run.

Card 3: (Format I3)

NC — Number of cases to be processed (programme terminates when NC becomes zero).

2. FIRST CASE SPECIFICATION

Card 4: (Format 3I3,6E10.0)

IMAX,JMAX — Number of Radial and Axial mesh spaces. (Maximum problem size IMAX*JMAX=2000).

NBF — Number of points at which concentration is to be defined. (Must be at least 1).

AM,BM — Molecular weights of species A and B with respect to characteristic mixture mean, (species A being the lighter). (Must be non-zero, and unequal.)

AREA — Characteristic area A* as a multiple of (characteristic length, L*)^2.

RD — Ratio D/D (must be non-zero), normally = 1.0.

ACC — Accuracy for the final iteration of the inner and outer loops. (Maximum variation in concentration between successive iterations.) This figure will be used to terminate the iteration if NINNER and NØUTER are not specified on the next card.

GUESS — Guess at concentration for all undefined internal points (must not be zero or 1.0). This figure is not required for cases when a variable initial guess is to be made (see card 16) or when restarting a case from punched cards (NPUNCH=2).

Card 5: (Format 4I3,2E10.0)

NPUNCH — To determine punched card outputs.
NPUNCH=0, No punched card output.
NPUNCH=1, Punched card output of final concentration field.
NPUNCH=2, For case being restarted with punched cards from previous run.

NINNER≠0 — Number of iterations for inner loop.

NØUTER≠0 Number of iterations for outer loop.

W Acceleration coefficient.
Usually 1.0≤W≤2.0, the default option being W=1.5.

Card 6: (Format 36I2)

N(I,J) Boundary specification for all elements.
N=0 for elements outside the boundary.
N=1 for elements inside the boundary.

Card 7: (Format 2I3, E10.0)

I,J,F(I,J) There will be NBF cards in this set (i.e. at least one) as specified on Card 2.
The concentration, F, is specified for point (I,J) for which N(I,J) must equal 0 (F(I,J)≠0 or 1).

Card 8: (Format I3)

IN To determine the method of reading in the radial mesh.
IN=1, Read in mesh in Format (E6.0,I3) as cards 9a.
IN≠1, Read in mesh spaces individually as cards 9b.

Cards 9a: (Format E6.0,I3)

DR(I),N Indicates N radial mesh spaces of width DR(I). A new card is required for each change in mesh width until $\Sigma(N)=IMAX$. DR(I) must be a multiple of the chosen characteristic length, L*.

Cards 9b: (Format 12E6.0)

DR(I) Radial mesh spacing for each interval as a multiple of characteristic length, L*.

Card 10: (Format I3)

IN To determine the method of reading in the axial mesh, cards 11a or 11b. (Similar to card 8 for radial mesh).

Cards 11a: (Format E6.0,I3)

DZ(I),N Indicates N axial mesh spaces of width DZ(I) similar to cards 9a for the radial mesh.

Cards 11b: (Format 12E6.0)

DZ(J) Axial mesh spacing for each interval as a multiple of characteristic length, L*.

Cards 12: (Format 12E6.0)

P(I,J) Relative Pressure field. (New card required for each change in axial position.)

Card 13: (Format I3)

ITEMP To determine the temperature field.

ITEMP=1 read in an eta field on cards 14

ITEMP≠1 assume a uniform eta field, next cards type 15.

Cards 14: (Format 12E6.0)

T(I,J) Eta field referred to characteristic eta.

(New card required for each change in axial position.)

Cards 15: (Format (3X,11E6.0)/12E6.0...)

WZ(1,1) . . .

WR(1,1) WR(2,1) . . . Flow field

WZ(1,2) . . .

. . . . . .

The flow field is input with axial and radial elements on alternate lines. Due regard must be taken of mass conservation requirements.

Flows are calculated with respect to A*(δD)*/L*.

Card 16A: (Format I3)

(If NPUNCH.EQ.2 only cards 16C are required)

KZ Determines guess for initial concentration iteration.

KZ=0 will set all non defined concentrations=GUESS.

KZ=1 will read in a variable guess (see cards 16B).

KZ=Ø or 1 programme terminates.

Cards 16B: (Format 12E6.0)

F(I,J) Initial guess at concentration for all points (I,J), including specified points (only if KZ=1 on card 14, otherwise omit these cards).

Cards 16C: (Format 6E12.5)

(only used if NPUNCH.EQ.2)

F(I,J) Initial guess at concentration field for all points. Read in punched cards as output from the previous run.

3. CHANGE OF DATA FOR NEXT CASE

(Provided NC was specified as greater than 1)

Card 18: (Format I3)

NCHTP Type of data change for next case.

NCHTP less than zero, programme terminates.

NCHTP=0 all data to be changed, requires a new set of cards 4 to 17.

NCHTP=1 a few data items to be changed in the same problem geometry (see card 19 et sequens).

Card 19: (Format 2I3)

NN Specifies which items are to be changed as follows:

NN=-3 change entire flow field but no other items.

NN=-2 change some values of flow field and some P, T, or molecular weights.

NN=-1 change some P, T, or molecular weights.

NN=0 change some items in flow field but no other items.

NN=+1 change accuracy or acceleration scheme, but no other items.

NN=+2 change pressure field but no other items.

NN=+3 change eta field but no other items.

NM Total number of changes to flow, eta and pressure fields (options NN=-2, -1 and 0 only).
(N.B. In option NN=-2,NM is number of items to be changed in flow field and number of items in eta + pressure.)

If more complex data changes are required it is recommended that the facility NCHTP=0 be used on CARD 18.

Cards 20

NN=-3 New set of cards 15.

NN=-2 (i) Namelist, changes in molwts AM or BM using namelist e.g. Ø$$MØLWT AM=1.001 $END.

(ii) Changes in Pressure or temp using Format
(A1,2(LX;I3), 2X,E13.6)
e.g. P(I,J) = +1.005071E+00
T(I,J) = +0.999999E+00

(iii) For changes in flow field Format
(A2,2(1X,I3), 2X,E13.6)
e.g. WZ(I,J)=+1.000000E+00

(iv) Changes in iteration scheme use namelist $NEWACC for any of items ACC,W,ALAMAX,ALAMIN,NSPEED.

NN=-1 As for items (i) and (ii) of NN=-2

NN=0 As for item (iii) of NN=-2

NN=+1 As for item (iv) of NN=-2

NN=+2 New set of cards 12

NN=+3 New set of cards 14.

APPENDIX C

PROGRAMME LISTING

```
C                                                                       10
C     MAINLINE                                                          20
C                                                                       30
C     TWIST  FOUR                                                       40
C                                                                       50
      DIMENSION CR(2000),CZ(2000),GR(2000),QZ(2000),AR(2000),AZ(2000),  60
     1P(2000),T(2000),F(2000),FM1(2000),FP1(2000),FF(2000),HL(2000),    70
     2HR(2000),HU(2000),HD(2000),SUM(2000),S(2000)                      80
      DIMENSION DR(2001),DZ(2001)                                       90
      DIMENSION A(2002)                                                100
      DIMENSION WR(2004),WZ(2004),NS(2004)                             110
      READ(1,2000) IMAX,JMAX                                           120
      IMP1=IMAX+1                                                      130
      IMP2=IMAX+2                                                      140
      JMP1=JMAX+1                                                      150
      JMP2=JMAX+2                                                      160
      CALL MAIN2 (CR,CZ,GR,GZ,AR,AZ,P,T,F,FM1,FP1,FF,HL,HR,HU,HD,SUM,S,  170
     1DR,DZ,A,WR,WZ,NS,IMAX,JMAX,IMP1,IMP2,JMP1,JMP2)                   180
 2000 FORMAT(2I3)                                                      190
      END                                                              200



      SUBROUTINE  MAIN2 (CR,CZ,GR,QZ,AR,AZ,P,T,F,FM1,FP1,FF,HL,HR,HU,HD,  210
     1SUM,S,DR,DZ,A,WR,WZ,NS,IMAX,JMAX,IIMP1,IIMP2,JJMP1,JJMP2)         220
C     MAINLINE INPUT DATA:   NC, NCHTP                                  230
C     NC=NO. OF CASES TO PROCESS                                        240
C     NCHTP=TYPE OF DATA CHANGE FOR NEXT CASE.                          250
C     NCHTP=0,  CHANGE ALL DATA.                                        260
C     NCHTP=1,  CHANGE A FEW ITEMS  (SEE SUBROUTINE DATACH).            270
C                                                                       280
      COMMON /AREA/ AREA                                               290
      COMMON /GUESS/ GUESS                                             300
      COMMON /WGHTS/ AM,BM                                             310
      COMMON /NBF/ NBF                                                 320
      COMMON /PUNCH/ NPUNCH                                            330
      COMMON /LAMBDA/ ALAMAX,ALAMIN                                    340
      COMMON /LIMITS/ IMP1,IMP2,JMP1,JMP2                              350
      COMMON /ACC/ ACC,EMAX1,ALPHA,BETA,NJ,W,NSPEED,NINNER,NOUTER      360
      COMMON /CONVRG/ CONV1,KK                                         370
C                                                                      380
      IMP1=IIMP1                                                       390
      IMP2=IIMP2                                                       400
      JMP1=JJMP1                                                       410
      JMP2=JJMP2                                                       420
      DIMENSION CR(IMP1),DZ(JMP1)                                      430
      DIMENSION WR(IMP2,JMP2),WZ(IMP2,JMP2)                            440
      DIMENSION  P(IMAX,JMAX),T(IMAX,JMAX)                             450
      DIMENSION F(IMAX,JMAX),FM1(IMAX,JMAX),FP1(IMAX,JMAX)             460
```

```
      DIMENSION N(IMP1,JMP1)                                            470
      DIMENSION AR(IMAX,JMAX),AZ(JMAX)                                  480
      DIMENSION GR(IMAX),GZ(JMAX)                                       490
      DIMENSION CR(IMAX,JMAX),CZ(IMAX,JMAX)                             500
      DIMENSION FF(IMAX,JMAX)                                           510
      DIMENSION NS(IMP2,JMP2)                                           520
      DIMENSION  S(IMAX,JMAX)                                           530
      DIMENSION HL(IMAX,JMAX),HR(IMAX,JMAX),HU(IMAX,JMAX),              540
     1HD(IMAX,JMAX),SUM(IMAX,JMAX)                                      550
      DIMENSION CHAR(40)                                                560
      READ(1,2001)(CHAR(I),I=1,40)                                      570
      WRITE(3,2001)(CHAR(I),I=1,40)                                     580
      NN=0                                                              590
      NK=0                                                              600
      NJ=0                                                              610
      KK=0                                                              620
      READ(1,2000) NC                                                   630
      WRITE(3,3000) NC                                                  640
      IF(NC.LE.0) GO TO 1000                                            650
 1001 CALL CASEIN(F,FM1,FP1,WR,WZ,DR,DZ,P,T,RO,ALAMAX                  660
     1 , ALAMIN,NS,IMAX,JMAX,IMP1,IMP2,JMP1,JMP2)                       670
      CALL IDNTFY(N,NS,IMAX,JMAX,IMP1,IMP2,JMP1,JMP2)                   680
      CALL INLSET(F,FM1,FF,NS,IMAX,JMAX)                                690
      CALL FFCOEF(AR,AZ,DR,DZ,GR,GZ,R,IMAX,JMAX)                        700
      CALL CDIFF(CR,CZ,AR,AZ,DR,DZ,T,NS,IMAX,JMAX,C3,C4)                710
 1002 CALL PDIFF(F,AR,AZ,S,P,T,RO,DR,DZ,NS,IMAX,JMAX,U3,U4,UR,UZ)       720
 1003 CALL ILPREP(WR,WZ,GR,GZ,CR,CZ,HL,HR,HU,HD,SUM,IMAX,JMAX)          730
 1004 CALL INLOOP(F,FM1,FP1,S,HL,HR,HU,HD,SUM,NS,IMAX,JMAX)             740
      NK=NK+1                                                           750
      IF(NK.GE.NOUTER.AND.NOUTER.GE.1.AND.NINNER.GE.1) GO TO 1011       760
C                                                                       770
C     IF NJ=1, INNER LOOP HAS GONE AS FAR AS POSSIBLE AND CAN ACHIEVE NO  780
C     BETTER ACCURACY DUE TO ROUND OFF ERRORS, GO TO NEXT CASE.         790
C                                                                       800
      IF(NJ.EQ.1) GO TO 1009                                            810
      CALL MXCNCH(F,FF,IMAX,JMAX,CONV2)                                 820
C                                                                       830
C     CHECK IF OUTER LOOP DIVERGING.                                    840
C                                                                       850
      IF(CONV2.GT.CONV1)  KK=KK+1                                       860
      IF(KK.GT.10) GO TO 1005                                           870
      CONV1=CONV2                                                       880
C                                                                       890
C     TEST IF BOTH INNER AND OUTER LOOPS SUFFICIENTLY CONVERGED.        900
C                                                                       910
      IF(CONV2.LT.ACC.AND.EMAX1.LT.ACC) GO TO 1006                      920
C                                                                       930
C     OUTER LOOP NOT CONVERGED. PRINT PRESENT RESULT AND RETURN TO      940
C     RECALCULATE COEFFICIENTS.                                         950
C                                                                       960
      WRITE(3,3001)                                                     970
      CALL FPRINT(F,IMAX,JMAX)                                          980
      GO TO  1002                                                       990
C                                                                      1000
C     CASE CONVERGED, PRINT ANSWER.                                    1010
C                                                                      1020
 1006 WRITE(3,3002)                                                    1030
```

```
      WRITE(3,3001)                                                     1040
      CALL FPRINT(F,IMAX,JMAX)                                          1050
      GO TO 1007                                                        1060
 1009 IF(W.EQ.1.0.AND.NSPEED.EQ.0) GO TO 1010                           1070
      NJ=0                                                              1080
      NSPEED=0                                                          1090
      WRITE(3,3005)                                                     1100
      CALL FPRINT(F,IMAX,JMAX)                                          1110
      W=1.0                                                             1120
      GO TO 1002                                                        1130
 1010 WRITE(3,3004)                                                     1140
      CALL FPRINT(F,IMAX,JMAX)                                          1150
      GO TO 1007                                                        1160
 1011 WRITE(3,3006)                                                     1170
      CALL FPRINT(F,IMAX,JMAX)                                          1180
      GO TO 1007                                                        1190
 1005 WRITE(3,3003)                                                     1200
      CALL FPRINT(F,IMAX,JMAX)                                          1210
C                                                                       1220
C     PREPARE FOR NEXT CASE.                                            1230
C                                                                       1240
 1007 NC=NC-1                                                           1250
      IF(NPUNCH.EQ.1) CALL FPUNCH(F,IMAX,JMAX)                          1260
      WRITE(3,3000) NC                                                  1270
      IF(NC.LE.0) GO TO 1000                                            1280
      READ(1,2000) NCHTP                                                1290
C                                                                       1300
C     DETERMINE METHOD FOR CHANGING DATA FOR NEXT CASE.                 1310
C                                                                       1320
      KK=0                                                              1330
      IF(NCHTP)1000,1001,1008                                           1340
 1008 CALL DATACH (NNN,P,T,RO,WR,WZ,NS,IMAX,JMAX)                       1350
C                                                                       1360
C     FROM TYPE OF DATA CHANGE MADE, DETERMINE WHERE TO RESTART PROBLEM.1370
C                                                                       1380
      IF(NNN.EQ.5) GO TO 1007                                           1390
      IF(NNN) 1002,1003,1004                                            1400
 1000 CONTINUE                                                          1410
 2000 FORMAT(I3)                                                        1420
 2001 FORMAT(20A4)                                                      1430
 3000 FORMAT('1','NO. OF CASES TO SOLVE=',I3)                           1440
 3001 FORMAT('0 CALCULATED CONCENTRATION FIELD',//)                     1450
 3002 FORMAT('0 OUTER LOOP CONVERGED')                                  1460
 3003 FORMAT('0 OUTER ITERATION NOT CONVERGING. PROGRAMME TERMINATING.') 1470
 3004 FORMAT('0 THIS CASE WILL NOT CONVERGE BEYOND PRESENT VALUES DUE TO 1480
     1 ROUND OFF ERRORS. PROCEEDING TO NEXT CASE.')                     1490
 3005 FORMAT('0FURTHER CONVERGENCE IS INHIBITED BY ACCELERATION TECHNIQUE1500
     1.',/,' PROGRAMME WILL REVERT TO NON-ACCELERATED SCHEME TO ACHIEVE  1510
     2FINAL RESULT.')                                                   1520
 3006 FORMAT('0 REQUESTED NUMBER OF OUTER LOOPS COMPLETED.')            1530
      STOP                                                              1540
      END                                                               1550
```

```
      SUBROUTINE CASIN (F,FM1,FF1,WF,WZ,DR,DZ,P,T,RD,ALAMAX,ALAMIN      1560
     1  , NS,IMAX,JMAX,IMP1,IMP2,JMP1,JMP2)                             1570
C                                                                       1580
C     INPUT DATA FOR THIS CASE:                                         1590
C                                                                       1600
C     CARD 1:(FORMAT 3I3,5E10.0)                                        1610
C                                                                       1620
C         IMAX=NUMBER OF RADIAL MESH SPACES (                           1630
C         JMAX=NUMBER OF AXIAL MESH SPACES  (IMAX*JMAX.LE.2000)         1640
C         NBF=NUMBER OF POINTS AT WHICH CONCENTRATIONS DEFINED (GE.1)   1650
C         AM=MOLECULAR WEIGHT OF SPECIES A ( WRT MIXTURE MEAN)          1660
C         BM=MOLECULAR WEIGHT OF SPECIES B ( WRT MIXTURE MEAN)          1670
C         AREA=CHARACTERISTIC AREA                                      1680
C         RD=(PRESSURE DIFFUSION COEF)/(CONCENTRATION DIFFUSION COEF)   1690
C         ACC=ACCURACY                                                  1700
C         GUESS=GUESS AT CONCENTRATION FOR ALL UNKNOWN POINTS(NE.0.OR.1)1710
C                                                                       1720
C     CARD 2: FORMAT(3I3,2E10.0)                                        1730
C                                                                       1740
C     NPUNCH=0 NO PUNCHED CARD INPUT OR OUTPUT                          1750
C     NPUNCH=1 FOR PUNCHED OUTPUT OF FINAL CONCCENTRATION FIELD         1760
C     NPUNCH=2 FOR CASE BEING RESTARTED WITH CARDS FROM PREVIOUS RUN    1770
C                                                                       1780
C                                                                       1790
C     NINNER = NUMBER OF ITERATIONS FOR INNER LOOP. (OPTIONAL)          1900
C                                                                       1810
C     NOUTER = NUMBER OF ITERATIONS FOR OUTER LOOP. (OPTIONAL)          1820
C                                                                       1830
C     W=ACCELERATION PARAMETER                                          1840
      ZC=1.                                                             1850
C                                                                       1860
C     CARD SET 3:(FORMAT 24I3)                                          1870
C         N(I,J) I=1,IMAX;J=1,JMAX                                      1880
C         N=0 FOR VOLUME ELEMENTS OUTSIDE BOUNDARY                      1890
C         N=1 FOR VOLUME ELEMENTS INSIDE  BOUNDARY                      1900
C                                                                       1910
C     CARD SET 4:(FORMAT(2I3,E10.0))                                    1920
C         I,J,F(I,J)                                                    1930
C         POINTS (I,J) AT WHICH CONCENTRATION IS DEFINED                1940
C         AND F(I,J) CONCENTRATION AT THIS POINT (NOT 0 OR 1)           1950
C                                                                       1960
C     CARD 5:(FORMAT I3)                                                1970
C         IN, METHOD FOR READING IN RADIAL MESH                         1980
C         IN=0, INPUT MESH AS CARDS 6A                                  1990
C         IN=1, INPUT MESH AS CARDS 6B                                  2000
C                                                                       2010
C     CARD SET 6A:(FORMAT 12E6.0)                                       2020
C         DR(I) I=1,IMAX                                                2030
C         INDIVIDUAL RADIAL MESH SPACINGS (DIMENSIONLESS)               2040
C                                                                       2050
C     CARD SET 6B:(FORMAT E6.0,I3)                                      2060
C         A,N  DENOTES N MESH SPACES OF WIDTH A                         2070
C              A NEW CARD IS REQUIRED FOR EACH CHANGE IN MESH WIDTH     2080
C             UNTIL SIGMA(N)=IMAX                                       2090
C                                                                       2100
C     CARD 7:(FORMAT I3)                                                2110
C         IN, METHOD FOR READING IN AXIAL MESH (SEE CARD 5)             2120
C                                                                       2130
      ZB=0.5                                                            2140
C     CARD SET 7A:(FORMAT 12E.0)                                        2150
```

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C          DZ(J) J=1,JMAX                                                    2160
C          INDIVIDUAL AXIAL MESH SPACINGS                                    2170
C                                                                            2180
C      CARD SET 7B:(FORMAT E6.0,I3)                                          2190
C          A,N  MESH WIDTH AND NO. OFF AS CARD SET 6B                        2200
C                                                                            2210
C      CARD SET 8:(FORMAT 12E6.0)                                            2220
C          P(I,J) I=1,IMAX;J=1,JMAX                                          2230
C      PRESSURE FIELD (NEW CARD FOR EACH CHANGE IN AXIAL POSITION)           2240
C                                                                            2250
C      CARD 9:(FORMAT I3)                                                    2260
C          ITEMP, METHOD OF READING IN ETA FIELD                             2270
C          ITEMP=1, READ IN ETA FIELD ON CARD SET 9A                         2280
C                                                                            2290
C      CARD SET 9A:(FORMAT 12E6.0)                                           2300
C          T(I,J) I=1,IMAX;J=1,JMAX                                          2310
C            ETA FIELD, REFLECTS TEMPERATURE DEPENDANCE OF RO*D              2320
C                                                                            2330
       Z9=1.                                                                2340
C      CARD SET 10:(FORMAT (2X, 11E6.0 / 12E6.3))                            2350
C                                                                            2360
C          RADIAL AND AXIAL FLOW FIELD IN UNITS OF RO*, A*, V*               2370
C                                                                            2380
C            WZ(1,1)          WZ(2,1)              ...    WZ(IMAX,1)       2390
C      WR(1,1)          WR(2,1)          ...WR(IMAX,1)  WR(IMAX+1,1)        2400
C            WZ(1,2)          WZ(2,2)              ...    WZ(IMAX,2)       2410
C      WR(1,2)          WR(2,2)          ...WR(IMAX,2)  WR(IMAX+1,2)        2420
C            WZ(1,JMAX)       WZ(2,JMAX)           ...    WZ(IMAX,JMAX)    2430
C      WR(1,JMAX)     WR(2,JMAX)  ...WR(IMAX,JMAX)   WR(IMAX+1,JMAX)        2440
C            WZ(1,JMAX+1)     WZ(2,JMAX+1)         ...WZ(IMAX,JMAX+1)      2450
C                                                                            2460
C      ALL ARRAYS BASED ON MAXIMUM MESH OF 30 * 30                           2470
C                                                                            2480
       DIMENSION F(IMAX,JMAX),FM1(IMAX,JMAX),FP1(IMAX,JMAX),                2490
      1P(IMAX,JMAX),T(IMAX,JMAX),CR(IMP1  ),DZ(JMP1),                        2500
      2 NS(IMP2,JMP2),WR(IMP2,JMP2),WZ(IMP2,JMP2)                            2510
       COMMON /AREA/ AREA                                                    2520
       COMMON /ACC/ ACC,EMAX1,ALPHA,BETA,NJ,W,NSPEED,NINNER,NOUTER           2530
       COMMON /GUESS/ GUESS                                                  2540
       COMMON /MOMENTS/ AM,BM                                                2550
       COMMON /PUNCH/ NPUNCH                                                 2560
       COMMON /NBF/ NBF                                                      2570
       COMMON /TIGHT/ ACC1                                                   2580
C                                                                            2590
       WRITE(3,3000)                                                         2600
C                                                                            2610
C      READ FIRST CARD FOR SIZE OF PROBLEM                                   2620
C                                                                            2630
       READ(1,2000,END=1004)IMAX,JMAX,NBF,AM,BM,AREA,RD,ACC,GUESS            2640
       WRITE(3,3001)IMAX,JMAX,NBF,AM,BM,AREA,RD,ACC,GUESS                    2650
       NPUNCH=0                                                              2660
       READ(1,2000,END=1004) NPUNCH,NINNER,NOUTER,W                          2670
       IF(NINNER.GE.1.AND.NOUTER.GE.1) WRITE(3,3015) NOUTER,NINNER           2680
C                                                                            2690
C      CHECK VALIDITY OF INPUT DATA.                                         2700
C                                                                            2710
       IF(W.NE.0.0) GO TO 1002                                               2720
       W=1.5                                                                 2730
       WRITE(3,3009)                                                         2740
 1002  CONTINUE                                                              2750
       WRITE(3,2010) W                                                       2760
```

```
      CALL TRVIAL (RC,IMAX,JMAX)                                        2770
C                                                                       2780
C     SET ALL CONCENTRATIONS F(I,J) TO ZERO                             2790
C     SET ALL POINTS AS OUTSIDE PROBLEM BOUNDARY UNTIL SPECIFIED.       2800
C                                                                       2810
      DO 1000 I=1,IMAX                                                  2820
      DO 1000 J=1,JMAX                                                  2830
      F(I,J)=0.0                                                        2840
      NS(I+1,J+1)=0                                                     2850
 1000 CONTINUE                                                          2860
      CALL CONDEF (F,FMI,FPI,N,IMAX,JMAX)                               2870
      CALL ACCTST (ACC)                                                 2880
C                                                                       2890
C     PRINT CONCENTRATION FOR EACH DEFINED POINT.                       2900
C                                                                       2910
      WRITE(3,3013)                                                     2920
      WRITE(3,3002)                                                     2930
      DO 1001 I=1,IMAX                                                  2940
      DO 1001 J=1,JMAX                                                  2950
      IF(F(I,J).NE.0) WRITE(3,3003) I,J,F(I,J)                          2960
 1001 CONTINUE                                                          2970
C                                                                       2980
C     READ IN MESH SPACINGS DR,DZ                                       2990
C                                                                       3000
      WRITE(3,3013)                                                     3010
      WRITE(3,3004)                                                     3020
      CALL MESHIN (DR,IMAX)                                             3030
      WRITE(3,3005)                                                     3040
      CALL MESHIN (DZ,JMAX)                                             3050
C                                                                       3060
C     READ IN PRESSURE & TEMPERATURE FIELDS.                            3070
C                                                                       3080
      WRITE(3,3006)                                                     3090
      CALL FREAD (P,IMAX,JMAX,NS)                                       3100
      CALL FPRINT (P,IMAX,JMAX)                                         3110
      READ(1,2001) ITEMP                                                3120
      IF(ITEMP.EQ.1) GO TO 1005                                         3130
      WRITE(3,3014)                                                     3140
      DO 1007 I=1,IMAX                                                  3150
      DO 1007 J=1,JMAX                                                  3160
 1007 T(I,J)=1.0                                                        3170
      GO TO 1006                                                        3180
 1005 WRITE(3,3007)                                                     3190
      CALL FREAD (T,IMAX,JMAX,NS)                                       3200
      CALL FPRINT (T,IMAX,JMAX)                                         3210
C                                                                       3220
C     READ IN FLOW FIELD AND PERFORM A MASS BALANCE CHECK.              3230
C                                                                       3240
 1006 CALL FLOWIN (WR,WZ,IMAX,JMAX)                                     3250
      CALL FLWCHK (WR,WZ,IMAX,JMAX)                                     3260
      RETURN                                                            3270
 1004 WRITE(3,3012)                                                     3280
      STOP                                                              3290
C                                                                       3300
 2000 FORMAT(3I3,6E10.0)                                                3310
 2001 FORMAT(4I3,2E10.0)                                                3320
 3000 FORMAT('1','INPUT DATA',//)                                       3330
 3001 FORMAT('0','MESH SIZE:',I3,' RADIAL *',I3,' AXIAL',//,' NBF=',I3,/3340
     1,' AM=',1PE10.3,/' BM=',1PE10.3,/' AREA=',1PE10.3,                3350
     2 /,' RO=',1PE10.3,/,' ACC=',1PE10.3,/,' GUESS=',1PE10.3//)        3360
 3002 FORMAT('0 SPECIFIED CONCENTRATIONS')                              3370
```

```
 3001 FORMAT('0 POINT, I=',I3,2X,' J=',I3,3X,'CONC=',1PE10.3)
 3002 FORMAT('0 RADIAL MESH',/)
 3003 FORMAT('0 AXIAL MESH',/)
 3004 FORMAT('0 PRESSURE FIELD')
 3007 FORMAT('0 ETA FIELD (TEMPERATURE DEPENDANCE OF RO*D)')
 3008 FORMAT('0',///' ACCELERATION CRITERIA, W, WAS SPECIFIED AS ZERO.
     1AS THIS WOULD NOT ENABLE THE PROBLEM TO BE SOLVED,',/,' THE VALUE
     2HAS BEEN RESET TO 1.5')
 3009 FORMAT('0 FIRST ORDER ACCELERATION WILL BE USED FOR INNER LOOP ITE
     1RATION.',/,' W = ',1PE10.3)
 3012 FORMAT('1','PROGRAMME TERMINATING DUE TO UNEXPECTED END OF INPUT D
     1ATA (SUBROUTINE CASEIN)')
 3013 FORMAT('0')
 3014 FORMAT('1 UNIFORM TEMPERATURE ASSUMED.')
 3015 FORMAT('0 REQUESTED TO RUN PROGRAMME FOR ',I4,' OUTER LOOPS,  EACH
     2 OF ',I4,'  INNER LOOPS.')
C
      END



      SUBROUTINE TRVIAL (RO,IMAX,JMAX)
C
C     CHECK INPUT FOR TRIVIAL CASES.
C
      COMMON /AREA/AREA
      COMMON /MCLWTS/ AM,BM
      COMMON /NBF/ NBF
C
      IF(IMAX*JMAX.GT.2000) GO TO 1000
      IF(IMAX.LE.0.OR.JMAX.LE.0) GO TO 1001
      DM=BM-AM
      IF(DM.EQ.0) GO TO 1002
      IF(AM.LE.0.OR.BM.LE.0) GO TO 1003
      IF(AREA.LE.0) GO TO 1004
      IF(RO.EQ.0) GO TO 1005
 1007 IF(NBF.LE.0) GO TO 1006
      WRITE(3,3007)
      RETURN
C
 1000 WRITE(3,3000)
      STOP
 1001 WRITE(3,3001)
      STOP
 1002 WRITE(3,3002)
      STOP
 1003 WRITE(3,3003)
      STOP
 1004 WRITE(3,3004)
      STOP
 1005 WRITE(3,3005)
      RO=1.0
      GO TO 1007
 1006 WRITE(3,3006)
      STOP
C
 3000 FORMAT('1','MESH SIZE HAS BEEN SPECIFIED AS GREATER THAN2000  0 PR
     1OBLEM IS TOO LARGE FOR THE PROGRAMME.',/,' REDEFINE THE PROBLEM WI
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     2TH LESS MESH SPACES.')                                                    3930
 3001 FORMAT('1','MESH HAS BEEN SPECIFIED WITH IMAX OR JMAX AS ZERO OR          3940
     1NEGATIVE.  PROGRAMME TERMINATING.')                                       3950
 3002 FORMAT('1','ISOTOPES A + B HAVE SAME MOLECULAR WEIGHT SO THERE IS         3960
     1NO PROBLEM TO SOLVE. PROGRAMME TERMINATING.')                             3970
 3003 FORMAT('1','ONE ISOTOPE HAS ZERO MOLECULAR WEIGHT SO THERE IS NO          3980
     1PROBLEM TO SOLVE. PROGRAMME TERMINATING.')                                3990
 3004 FORMAT('1','CHARACTERISTIC AREA SPECIFIED AS ZERO OR NEGATIVE. PRO        4000
     1BLEM HAS NO PHYSICAL SIZE. PROGRAMME TERMINATING.')                       4010
 3005 FORMAT('1','RO SPECIFIED AS ZERO. VALUE OF RO=1.0 WILL BE SUBSTITU        4020
     1TED.')                                                                    4030
 3006 FORMAT('1','CONCENTRATION MUST BE DEFINED FOR AT LEAST ONE POINT.'        4040
     1,/,' PROGRAMME TERMINATING.')                                             4050
 3007 FORMAT('0 ',///,' DATA CHECK "TRVIAL" COMPLETED.')                        4060
      END                                                                       4070


      SUBROUTINE MESHIN(AMESH,MAXDIM)                                           4080
C                                                                               4090
C     SUBROUTINE TO READ IN MESH SPACINGS.                                      4100
C                                                                               4110
      DIMENSION AMESH(MAXDIM)                                                   4120
      READ(1,2000) IN                                                           4130
      IF(IN.EQ.0)GO TO 1000                                                     4140
      READ(1,2002)(AMESH(I),I=1,MAXDIM)                                         4150
      GO TO 1001                                                                4160
 1000 I=1                                                                       4170
      NN=0                                                                      4180
 1002 READ(1,2001) A,N                                                          4190
      NN=NN+N                                                                   4200
      DO 1002 J=I,NN                                                            4210
 1002 AMESH(J)=A                                                                4220
      I=NN+1                                                                    4230
      IF(NN.LT.MAXDIM) GO TO 1002                                               4240
 1001 DO 1004 I=1,MAXDIM                                                        4250
      IF(AMESH(I).LE.0.0) GO TO 1005                                            4260
 1004 WRITE(3,3000)AMESH(I)                                                     4270
      RETURN                                                                    4280
 1005 WRITE(3,3001) I,AMESH(I)                                                  4290
      STOP                                                                      4300
 2000 FORMAT(I2)                                                                4310
 2001 FORMAT(E4.0,I3)                                                           4320
 2002 FORMAT(12E6.0)                                                            4330
 3000 FORMAT(12(1X,1PE10.3))                                                    4340
 3001 FORMAT(' MESH INTERVAL SPECIFIED AS ZERO OR NEGATIVE. POINT IS=',         4350
     1I3,'INTERVAL VALUE=',1PE10.3,/,' PROGRAMME TERMINATING.')                 4360
      END                                                                       4370


      SUBROUTINE FLOWIN (WR,WZ,IMAX,JMAX)                                       4380
C                                                                               4390
C     READ IN FLOW FIELD                                                        4400
C                                                                               4410
      COMMON /LIMITS/ IMP1,IMP2,JMP1,JMP2                                       4420
      DIMENSION WR(IMP2,JMP2),WZ(IMP2,JMP2)                                     4430
C                                                                               4440
C     SET LOOP LIMITS                                                           4450
```

```
C                                                                       4460
      IM=IMAX                                                           4470
      IK=0                                                              4480
      II=1                                                              4490
 1000 IF(IM.LE.10) GO TO 1001                                           4500
      IK=IK+10                                                          4510
      GO TO 1002                                                        4520
 1001 IK=IM                                                             4530
 1002 DO 1003 J=1,JMAX                                                  4540
      IKP1=IK+1                                                         4550
      READ(1,2001)(WZ(I,J),I=II,IK)                                     4560
 1003 READ(1,2000)(WR(I,J),I=II,IKP1)                                   4570
      READ(1,2001)(WZ(I,JMP1),I=II,IK)                                  4580
      IF(IM.LE.10)GO TO 1004                                            4590
      IM=IM-10                                                          4600
      II=IK+1                                                           4610
      GO TO 1000                                                        4620
 1004 CONTINUE                                                          4630
      WRITE(3,3001)                                                     4640
      II=1                                                              4650
      IK=0                                                              4660
      IM=IMAX                                                           4670
 1005 IF(IM.LE.6) GO TO 1006                                            4680
      IK=IK+6                                                           4690
      GO TO 1007                                                        4700
 1006 IK=IM+IK                                                          4710
 1007 IKP1=IK+1                                                         4720
      WRITE(3,3000)                                                     4730
      DO 1008 J=1,JMAX                                                  4740
      WRITE(3,3002)(WZ(I,J),I=II,IK)                                    4750
 1008 WRITE(3,3003)((WR(I,J),I,J),I=II,IK),WR(IKP1,J)                   4760
      WRITE(3,3002)(WZ(I,JMP1),I=II,IK)                                 4770
      IF(IM.LE.6) GO TO 1009                                            4780
      IM=IM-6                                                           4790
      II=IK                                                             4800
      GO TO 1005                                                        4810
 1009 CONTINUE                                                          4820
      RETURN                                                            4830
 2000 FORMAT(12E6.0)                                                    4840
 2001 FORMAT(59.0,10E6.0)                                               4850
 3000 FORMAT('0',////)                                                  4860
 3001 FORMAT('1','FLOW FIELD')                                          4870
 3002 FORMAT('0',6(10X,1PE10.3))                                        4880
 3003 FORMAT('0',6(1PE10.3,   '(',I3,',',I3,')',1X),1PE10.3)            4890
      END                                                               4900


      SUBROUTINE FLWCHK (WR,WZ,IMAX,JMAX)                               4910
C                                                                       4920
C     CHECK WR(1,J)=0, IE: NO FLOW RADIALLY ACROSS CENTRE LINE.         4930
C     PRINT OUT ANY OFFENDERS.                                          4940
C                                                                       4950
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                 4960
      DIMENSION WR(IMP2,JMP2),WZ(IMP2,JMP2)                             4970
      DO 1000 J=1,JMAX                                                  4980
 1000 IF(WR(1,J).NE.0.) WRITE(3,3000)J,WR(1,J)                          4990
```

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C                                                                       5000
C     CHECK MASS BALANCE, PRINT OUT ANY OFFENDERS.                      5010
C                                                                       5020
      WRITE(3,3003)                                                     5030
      NJ=0                                                              5040
      DO 1001 J=1,JMAX                                                  5050
      DO 1001 I=1,IMAX                                                  5060
      WW=WZ(I,J)+WR(I,J)-WZ(I,J+1)-WR(I+1,J)                            5070
      IF(WW.EQ.0.0) GO TO 1001                                          5080
      WRITE(3,3002)I,J,WW                                               5090
      NJ=NJ+1                                                           5100
 1001 CONTINUE                                                          5110
      IF(NJ.EQ.0) WRITE(3,3003)                                         5120
C                                                                       5130
C     SAY IF THERE ARE NO ERRORS IN MASS BALANCE.                       5140
C                                                                       5150
      RETURN                                                            5160
 3000 FORMAT('1','ERROR-ALL WR(1,J) SHOULD BE ZERO FOR SYMETTRY ABOUT R=  5170
     1 0.0',/2X,'WR(1,',I3,')=',1PE10.3)                                5180
 3001 FORMAT('1','ERRORS IN MASS BALANCE, ALL WW SHOULD BE ZERO.',/)     5190
 3002 FORMAT(' ','WW(',I3,',',I3,')=',1PE10.3)                          5200
 3003 FORMAT(' NO ERRORS IN MASS BALANCE.')                             5210
      END                                                               5220


      SUBROUTINE CATACH(NNN,P,T,RO,WR,WZ,NS,IMAX,JMAX)                  5230
C     SUBROUTINE TO VARY CERTAIN DATA ITEMS FOR A NEW CASE IN THE SAME  5240
C     GEOMETRY AS PREVIOUS CASE.                                        5250
C     DATA INPUT USING NAMELIST FORMAT..                                5260
C     SUBROUTINE PERFORMS CHECKS ON CHANGED ITEMS TO AVOID SPURIOUS     5270
C     ERRORS.                                                           5280
C     SPECIFY DATA ITEMS TO BE CHANGED USING 'NN'                       5290
C     NN=-3, CHANGE ENTIRE FLOW FIELD BUT NO OTHER ITEMS.               5300
C     NN=-2, CHANGE ITEMS IN NAMELISTS PLUS PRESS,TEMP, OR FLOW FIELDS  5310
C     NN=-1, CHANGE ITEMS IN NCLWT OR PRESS OR TEMP FIELDS              5320
C     NN= 0, CHANGE ITEMS IN FLOW FIELD ONLY                            5330
C     NN=+1, CHANGE ITEMS IN ACC ONLY.                                  5340
C     NN=+2, CHANGE ENTIRE PRESSURE FIELD ONLY                          5350
C     NN=+3, CHANGE ENTIRE ETA FIELD ONLY.                              5360
C     NM= TOTAL NUMBER OF CHANGES TO FLOW,TEMP+PRESS FIELDS.            5370
C     OPTIONS NN=-2,-1 AND 0 ONLY                                       5380
C                                                                       5390
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                 5400
      DIMENSION P(IMAX,JMAX),T(IMAX,JMAX),WR(IMP2,JMP2),                5410
     1 WZ(IMP2,JMP2),NS(IMP2,JMP2)                                      5420
      COMMON /ACC/ ACC,EMAX1,ALPHA,BETA,NJ,W,NSPEED,NINNER,NOUTER       5430
      COMMON /NCLWTS/ AN,BN                                             5440
      COMMON /AREA/ AREA                                                5450
      COMMON /NBF/ NBF                                                  5460
      COMMON /LAMBDA/ ALAMAX,ALAMIN                                     5470
       NAMELIST/NCLWT/ AN,BN                                            5480
      NAMELIST /NEWACC/ ACC,W,ALAMAX,ALAMIN,NSPEED                      5490
      DATA  PP/'P'/,TT/'T'/,WRR/'WR'/,WZZ/'WZ'/,ROO/'RO'/               5500
      WRITE(3,2000)                                                     5510
 2000 FORMAT('1','SUBROUTINE CATACH')                                   5520
      READ(1,1000)NN,NM                                                 5530
      WRITE(3,2001)NN,NM                                                5540
```

```
 1003 FORMAT('0','NN=',I2,'  MM=',I2)                                   5550
 1004 FORMAT(2I2)                                                       5560
      IF(NN-2) 1102,1104,1102                                           5570
 1104 CALL FREAD(P,IMAX,JMAX,NS)                                        5580
      WRITE(3,1200)                                                     5590
 1200 FORMAT('1','NEW PRESSURE FIELD')                                  5600
      CALL FPRINT (P,IMAX,JMAX)                                         5610
      NNN=-1                                                            5620
      RETURN                                                            5630
 1102 CALL FREAD(T,IMAX,JMAX,NS)                                        5640
      WRITE(3,1201)                                                     5650
 1201 FORMAT('1 NEW ETA FIELD')                                         5660
C                                                                       5670
C                                                                       5680
      CALL FPRINT (T,IMAX,JMAX)                                         5690
      NNN=-1                                                            5700
      RETURN                                                            5710
 1102 IF(NN.NE.-2) GO TO 1201                                           5720
      CALL FLOWIN (WR,WZ,IMAX,JMAX)                                     5730
      CALL FLWCHK (WR,WZ,IMAX,JMAX)                                     5740
      NNN=0                                                             5750
      RETURN                                                            5760
 1201 CONTINUE                                                          5770
      IF(NN)  1001,1002,1003                                            5780
 1001 READ(1,MCLWT)                                                     5790
      WRITE(3,MCLWT)                                                    5800
      CALL TRVIAL (RC,IMAX,JMAX)                                        5810
      DO 1400  II=1,NM                                                  5820
      READ(1,1401)CH,I,J,VAL                                            5830
      WRITE(3,1304)CH,I,J,VAL                                           5840
      IF(CH.EQ.PP) GO TO 1402                                           5850
      IF(CH.EQ.TT) GO TO 1403                                           5860
      WRITE(3,1305)                                                     5870
      GO TO 1400                                                        5880
 1402 P(I,J)=VAL                                                        5890
      GO TO 1400                                                        5900
 1403 T(I,J)=VAL                                                        5910
 1400 CONTINUE                                                          5920
 1401 FORMAT(A1,2(1X,I3),2X,E13.6)                                      5930
      IF(NN.EQ.-2) GO TO 1002                                           5940
      GO TO 1004                                                        5950
 1002 DO 1300 II=1,NM                                                   5960
      READ(1,1301) CH,I,J,VAL                                           5970
      WRITE(3,1304) CH,I,J,VAL                                          5980
      IF(CH.EQ.WRR) GO TO 1302                                          5990
      IF(CH.EQ.WZZ) GO TO 1303                                          6000
      IF(CH.EQ.RDD) GO TO 1306                                          6010
      WRITE(3,1305)                                                     6020
      GO TO 1300                                                        6030
 1302 WR(I,J)=VAL                                                       6040
      GO TO 1300                                                        6050
 1306 RD=VAL                                                            6060
      GO TO 1300                                                        6070
 1303 WZ(I,J)=VAL                                                       6080
 1300 CONTINUE                                                          6090
 1301 FORMAT(A2,2(1X,I3),2X,E13.6)                                      6100
 1304 FORMAT('0',A2,'(',I3,',',I3,')= ',1PE13.6)                        6110
 1305 FORMAT('+',30X,'ERROR IN FORMAT.')                                6120
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```
      CALL FLWCHK (WR,WZ,IMAX,JMAX)                                     613
      IF(NN.EQ.-2) GO TO 1003                                           614
      GO TO 1004                                                        615
 1003 ACC1=ACC                                                          616
      NO=NSPEED                                                         617
      A1=ALAMAX                                                         618
      A2=ALAMIN                                                         619
      READ(1,NEWACC)                                                    620
      WRITE(3,NEWACC)                                                   621
      IF(NO.NE.NSPEED.OR.A1.NE.ALAMAX.OR.A1.NE.ALAMIN) CALL EIGENV (ALPH 622
     1A,BETA)                                                           623
C                                                                       624
C     IF NEW ACC GT OLD ACC, CASE WILL BE BYPASSED.                     625
C                                                                       626
      IF(ACC.LE.ACC1) GO TO 1004                                        627
      WRITE(3,1202) ACC                                                 628
 1202 FORMAT('0 NEW ACCURACY IS NOT LESS THAN FOR PREVIOUS CASE,NO USEFU 629
     1L RESULT WOULD BE PRODUCED.',/,' PROGRAMME WILL BYPASS THIS CASE.' 630
     2)                                                                 631
      NNN=5                                                             632
      RETURN                                                            633
 1004 NNN=NN                                                            634
      IF(NN.EQ.-2) NNN=-1                                               635
      RETURN                                                            636
      END                                                               637

      SUBROUTINE IDNTFY (N,NS,IMAX,JMAX,IMP1,IMP2,JMP1,JMP2)            638
C                                                                       639
C     SET NS=0 FOR ELEMENTS OUTSIDE SIMPLE PROBLEM BOUNDARIES AND NS=N  640
C     FOR ALL DEFINED POINTS. HENCE, NS=0 FOR EXTERNAL POINTS,          641
C     NS=1 FOR INTERNAL POINTS, NS=2 FOR EXTERNAL POINTS WITH DEFINED   642
C     CONCENTRATION, F(I,J)                                             643
C                                                                       644
      DIMENSION N(IMP1,JMP1),NS(IMP2,JMP2)                              645
      DO 2020 I=1,IMP2                                                  646
      NS(I,1)=0.0                                                       647
 2020 NS(I,JMP2)=0.0                                                    648
      DO 2021 J=1,JMP2                                                  649
      NS(1,J)=0.0                                                       650
 2021 NS(IMP2,J)=0.0                                                    651
      DO 2023 J=1,JMAX                                                  652
      DO 2022 I=1,IMAX                                                  653
      IF(NS(I+1,J+1).EQ.2) GO TO 2022                                   654
      NS(I+1,J+1)=N(I,J)                                                655
 2022 CONTINUE                                                          656
 2023 CONTINUE                                                          657
C                                                                       658
C     PRINT OUT VALUES OF NS(I,J)                                       659
C                                                                       660
      WRITE(3,1117)                                                     661
      DO 2024 J=1,JMP2                                                  662
 2024 WRITE(3,1118)(NS(I,J),I=1,IMP2)                                   663
      RETURN                                                            664
 1117 FORMAT('1','VALUES OF NS',//,5X,'NS=0 -EXTERNAL',/,5X,'NS=1 -INTER 665
     1NAL,UNDEFINED CONC',/,5X,'NS=2 -EXTERNAL,CONC. DEFINED',/)        666
 1118 FORMAT('0',2X,32(2X,I2))                                          667
      END                                                               668
```

```
      SUBROUTINE FECOEF (AR,AZ,DR,DZ,GR,GZ,R,IMAX,JMAX)                 7290
                                                                        7300
C                                                                       7310
C     FINITE ELEMENT COEFFICIENTS                                       7320
C                                                                       7330
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                 7340
      COMMON /AREA/ AREA                                                7350
      DIMENSION AR(IMAX,JMAX),AZ(JMAX),DR(IMP1  ),DZ(JMP1  ),           7360
     1GR(IMAX),GZ(JMAX),R(IMP1)                                         7370
      PI=3.14159265                                                     7380
      R(1)=0.0                                                          7390
      R(2)=DR(1)                                                        7400
      AZ(1)=PI*R(2)*GR(1)/AREA                                          7410
      GR(1)=1.0                                                         7420
      GZ(1)=1.0                                                         7430
      DO 2102 J=1,JMAX                                                  7440
 2102 AR(1,J)=0.0                                                       7450
      DO 2100 I=2,IMAX                                                  7460
      GR(I)=DR(I)/(DR(I)+DR(I-1))                                       7470
      R(I+1)=R(I)+DR(I)                                                 7480
      AZ(I)=PI*(R(I+1)+R(I))*DR(I)/AREA                                 7490
      AR(I,1)=2.*PI*R(I)*DZ(1)/AREA                                     7500
      DO 2101 J=2,JMAX                                                  7510
      AR(I,J)=2.*PI*R(I)*DZ(J)/AREA                                     7520
 2101 GZ(J)=DZ(J)/(DZ(J)+DZ(J-1))                                       7530
 2100 CONTINUE                                                          7540
      RETURN                                                            7550
      END                                                               7560

      SUBROUTINE COEFF (CR,CZ,AR,AZ,DR,DZ,T,NS,IMAX,JMAX,C3,C4)         7570
C                                                                       7580
C     CONCENTRATION DIFFUSION TERM                                      7590
C                                                                       7600
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                 7610
      DIMENSION AR(IMAX,JMAX),AZ(JMAX),DR(IMP1),DZ(JMP1),               7620
     1T(IMAX,JMAX),NS(IMP2  ,JMP2  ),C3(JMAX),C4(JMAX),CR(IMAX,JMAX),   7630
     2CZ(IMAX,JMAX)                                                     7640
      DO 1000 I=1,IMAX                                                  7650
      IS=I+1                                                            7660
      DO 1000 J=1,JMAX                                                  7670
      JS=J+1                                                            7680
      IF(NS(IS,JS).EQ.0) GO TO 1000                                     7690
      IF(JS.NE.2) GO TO 1001                                            7700
      C1=DZ(1)/T(I,1)                                                   7710
 1001 IF(IS.NE.2) GO TO 1002                                            7720
      C3(J)=DR(1)/T(1,J)                                                7730
 1002 C2=DZ(J)/T(I,J)                                                   7740
      C4(J)=DR(I)/T(I,J)                                                7750
      IF(NS(IS,J).EQ.0) GO TO 1003                                      7760
      CZ(I,J)=2.*AZ(I)/(C1+C2)                                          7770
      C1=C2                                                             7780
 1003 IF(NS(I,JS).EQ.0) GO TO 1000                                      7790
      CR(I,J)=2.*AR(I,J)/(C3(J)+C4(J))                                  7800
      C3(J)=C4(J)                                                       7810
 1000 CONTINUE                                                          7820
      RETURN                                                            7830
      END                                                               7840
```

```
      SUBROUTINE PDIFF (F,AR,AZ,S,P,T,RD,DR,DZ,NS,IMAX,JMAX,                    7850
     1 U3,U4,U2,UZ)                                                             7860
C                                                                               7870
C     PRESSURE DIFFUSION TERM                                                   7880
C                                                                               7890
      COMMON /MCLWTS/ AM,BM                                                     7900
      COMMON /LIMITS/ IMP1,IMP2,JMP1,JMP2                                       7910
      DIMENSION F(IMAX,JMAX),AR(IMAX,JMAX),AZ(JMAX),S(IMAX,JMAX),              7920
     1P(IMAX,JMAX),T(IMAX,JMAX),DR(IMP1),DZ(JMP1),NS(IMP2,JMP2),               7930
     2U3(IMP2),U4(IMP2),UR(IMP2,JMP2),UZ(IMP2,JMP2)                            7940
      DM=BM-AM                                                                  7950
      DUMY=1./(2.*DM*RD)                                                        7960
C                                                                               7970
C     START OF OUTER ITERATION LOOP                                             7980
C                                                                               7990
      DO 1006 I=1,IMP1                                                          8000
      IS=I+1                                                                    8010
      DO 1006 J=1,JMP1                                                          8020
      JS=J+1                                                                    8030
      IF(NS(IS,JS).EQ.0) GO TO 1008                                             8040
      PDUM=DUMY/(T(I,J)*F(I,J)*(1.-F(I,J))*(F(I,J)/AM+(1.-F(I,J))/BM))          8050
      IF(JS.NE.2) GO TO 1000                                                    8060
      U1=DZ(1)*PDUM                                                             8070
 1000 IF(IS.NE.2) GO TO 1001                                                    8080
      U3(J)=DR(1)*PDUM                                                          8090
 1001 CONTINUE                                                                  8100
      U2=DZ(J)*PDUM                                                             8110
      U4(J)=DR(I)*PDUM                                                          8120
      IF(NS(IS,J).EQ.0) GO TO 1002                                              8130
      PZ=P(I,J-1)/P(I,J)                                                        8140
      IF(PZ.EQ.1) GO TO 1002                                                    8150
      UZ(I,J)=AZ(I)*ALOG(PZ)/(U1+U2)                                            8160
      GO TO 1003                                                                8170
 1002 UZ(I,J)=0.0                                                               8180
 1003 U1=U2                                                                     8190
      IF(NS(I,JS).EQ.0) GO TO 1004                                              8200
      PR=P(I-1,J)/P(I,J)                                                        8210
      IF(PR.EQ.1) GO TO 1004                                                    8220
      UR(I,J)=AR(I,J)*ALOG(PR)/(U3(J)+U4(J))                                    8230
        GO TO 1005                                                              8240
 1004 UR(I,J)=0.0                                                               8250
 1005 U3(J)=U4(J)                                                               8260
 1006 CONTINUE                                                                  8270
      DO 1007 I=1,IMAX                                                          8280
      IS=I+1                                                                    8290
      DO 1007 J=1,JMAX                                                          8300
      JS=J+1                                                                    8310
      IF(NS(IS,JS).EQ.0) GO TO 1007                                             8320
      S(I,J)=UR(I,J)+UZ(I,J)-UR(IS,J)-UZ(I,JS)                                  8330
 1007 CONTINUE                                                                  8340
      RETURN                                                                    8350
 1008 UZ(I,J)=0.0                                                               8360
      UR(I,J)=0.0                                                               8370
      GO TO 1006                                                                8380
      END                                                                       8390
```

```
      SUBROUTINE ILPREP (WR,WZ,CP,QZ,CR,CZ,HL,HR,HU,HD,SUM,NS,IMAX,JMAX)     8400
C                                                                            8410
C     PREPARATION OF SUM,AND HD,HU,HL,HR FOR INNER ITERATION                 8420
C                                                                            8430
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                      8440
      DIMENSION WR(IMP2,JMP2),WZ(IMP2,JMP2),                                 8450
     1QR(IMAX),QZ(JMAX),CR(IMAX,JMAX),CZ(IMAX,JMAX),HL(IMAX,JMAX),HR(IMA    8460
     2X,JMAX),HU(IMAX,JMAX),HD(IMAX,JMAX),SUM(IMAX,JMAX),NS(IMP2,JMP2)      8470
      K=1                                                                    8480
      DO 1012 I=1,IMAX                                                       8490
      IS=I+1                                                                 8500
      DO 1012 J=1,JMAX                                                       8510
      JS=J+1                                                                 8520
      IF(NS(IS,JS).NE.1) GO TO 1002                                          8530
      IF(NS(I,JS).EQ.0) GO TO 1000                                           8540
      HD(I,J)=CR(I,J)+   WR(I,J)*QR(I)                                       8550
      GO TO 1001                                                             8560
 1000 HD(I,J)=0.0                                                            8570
      IF(WR(I,J).GT.0.0) HD(I,J)=WR(I,J)                                     8580
 1001 IF(NS(IS,J).EQ.0) GO TO 1002                                           8590
      HL(I,J)=CZ(I,J)+   WZ(I,J)*QZ(J)                                       8600
      GO TO 1003                                                             8610
 1002 HL(I,J)=0.0                                                            8620
      IF(WZ(I,J).GT.0.0) HL(I,J)=WZ(I,J)                                     8630
 1003 IF(NS(IS+1,JS).EQ.0) GO TO 1004                                        8640
      HU(I,J)=CR(IS,J)   *WR(IS,J)*(1.-QR(IS))                               8650
      GO TO 1005                                                             8660
 1004 HU(I,J)=0.0                                                            8670
      IF(WR(IS,J).LT.0.0) HU(I,J)=-WR(IS,J)                                  8680
 1005 IF(NS(IS,JS+1).EQ.0) GO TO 1006                                        8690
      HR(I,J)=CZ(I,JS)   *WZ(I,JS)*(1.-QZ(JS))                               8700
      GO TO 1007                                                             8710
 1006 HR(I,J)=0.0                                                            8720
      IF(WZ(I,JS).LT.0.0) HR(I,J)=-WZ(I,JS)                                  8730
 1007 SUM(I,J)=HR(I,J)+HU(I,J)+HL(I,J)+HD(I,J)                               8740
      IF(HL(I,J).LT.0.0) GO TO 1013                                          8750
 1008 IF(HR(I,J).LT.0.0) GO TO 1014                                          8760
 1009 IF(HU(I,J).LT.0.0) GO TO 1015                                          8770
 1010 IF(HD(I,J).LT.0.0) GO TO 1016                                          8780
 1011 IF(SUM(I,J).EQ.0.) WRITE(3,3000) I,J                                   8790
 1012 CONTINUE                                                               8800
      IF(K.EQ.1) WRITE(3,3001)                                               8810
      RETURN                                                                 8820
 1013 IF(K.EQ.1) WRITE(3,3002)                                               8830
      CALL UNSTBL (1,J,CZ(I,J),   WZ(I,J),QZ(J))                             8840
      K=K+1                                                                  8850
      GO TO 1009                                                             8860
 1014 IF(K.EQ.1) WRITE(3,3002)                                               8870
      CALL UNSTBL (2,JS,CZ(I,JS)   ,WZ(I,JS),QZ(JS)-1.)                      8880
      K=K+1                                                                  8890
      GO TO 1009                                                             8900
 1015 IF(K.EQ.1) WRITE(3,3002)                                               8910
      CALL UNSTBL (3,IS,CR(IS,J)   ,WR(IS,J),QR(IS)-1.)                      8920
      K=K+1                                                                  8930
      GO TO 1010                                                             8940
 1016 IF(K.EQ.1) WRITE(3,3002)                                               8950
      CALL UNSTBL (4,I,CP(I,J),   WR(I,J),QR(I))                             8960
      K=K+1                                                                  8970
      GO TO 1011                                                             8980
 3000 FORMAT('0','SUM(',I3,',',I3,')=0.0')                                   8990
```

```
 3001 FORMAT('0 ALL FF COEFFICIENTS ACCEPTED AS GE ZERO FOR STABILITY')      9000
 3002 FORMAT('1 WARNING--THIS PROBLEM MAY BE UNSTABLE AND NOT CONVERGE.'     9010
     1,/,'0 STABILITY AND CONVERGENCE MAY BE ACHIEVED BY USING A FINER M     9020
     2ESH.',/,'0 SUGGESTED ACTIONS : ',//)                                  9030
      END                                                                   9040


      SUBROUTINE INLOOP (F,FM1,FP1,S,HL,HR,HU,HD,SUM,NS,IMAX,JMAX)          9050
C                                                                           9060
C     INNER ITERATION FOR CONCENTRATIONS                                    9070
C                                                                           9080
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                     9090
      COMMON /ACC/ ACC,EMAX1,ALPHA,BETA,NJ,W,NSPEED,NINNER,NOUTER           9100
      DIMENSION F(IMAX,JMAX),FM1(IMAX,JMAX),FP1(IMAX,JMAX),                9110
     1S(IMAX,JMAX),HL(IMAX,JMAX),HR(IMAX,JMAX),HU(IMAX,JMAX),HD(IMAX,JMA   9120
     2X),SUM(IMAX,JMAX),NS(IMP2,JMP2)                                       9130
      K=0                                                                   9140
      EMAX2=0.0                                                             9150
      AA=100.0                                                              9160
      SMLACC=0.0                                                            9170
      WRITE(3,3002)                                                         9180
      CALL FPRINT(F,IMAX,JMAX)                                              9190
      JCT=0                                                                 9200
 1000 EMAX1=0.0                                                             9210
      JCT=JCT+1                                                             9220
      DO 1002 I=1, IMAX                                                     9230
      IS=I+1                                                                9240
      DO  1002J=1,JMAX                                                      9250
      JS=J+1                                                                9260
      IF(NS(IS,JS).NE.1) GO TO 1002                                         9270
      FN=(S(I,J)+HD(I,J)*F(I-1,J)+HL(I,J)*F(I,J-1)+HU(I,J)*F(I+1,J)+HR(I    9280
     1,J)*F(I,J+1))/SUM(I,J)                                                9290
      ERR=ABS(FN-F(I,J))                                                    9300
C     CHECK THAT STEPS IN F ARE NOT TOO GREAT AS TO INVALIDATE PRESENT      9310
C     COEFICIENTS, IF THEY ARE, SET K TO RETURN TO OUTER LOOP AFTER 2ITN    9320
      IF(ERR.GT.F(I,J)/2.0) K=K+6                                           9330
      IF(ERR.GT.EMAX1) EMAX1=ERR                                            9340
      IF(NSPEED.EQ.1) GO TO 1001                                            9350
      F(I,J)=W*FN+(1.-W)*F(I,J)                                             9360
      GO TO 1002                                                            9370
 1001 FP1(I,J)=F(I,J)*(1.+ALPHA-BETA)-FM1(I,J)*ALPHA+FN*BETA                9380
 1002 CONTINUE                                                              9390
      IF(NSPEED.EQ.1) CALL RESET (F,FM1,FP1,NS,IMAX,JMAX)                   9400
      IF(JCT/AA.LE.1.0) GO TO 1003                                          9410
      AA=AA+100.0                                                           9420
      WRITE(3,3002)                                                         9430
      CALL FPRINT(F,IMAX,JMAX)                                              9440
 1003 CONTINUE                                                              9450
C                                                                           9460
C     CHECK CONVERGENCE OF INNER ITERATION                                  9470
C                                                                           9480
      IF(EMAX2.LT.SMLACC) SMLACC=EMAX2                                      9490
      IF(EMAX1.GE.SMLACC)K=K+1                                              9500
      IF(NINNER.GT.JCT.OR.NINNER.LT.1.OR.NOUTER.LT.1) GO TO 1008            9510
      WRITE(3,3005)                                                         9520
      RETURN                                                                9530
 1008 IF(K-500) 1006,1004,1005                                              9540
 1004 WRITE(3,3004) ACC,JCT                                                 9550
```

```
      IF(JCT.GE.501) RETURN                                              956
      IF(NSPEED.EQ.0.AND.JCT.LT.500) GO TO 1000                          957
      NJ=1                                                               958
      RETURN                                                             959
 1005 IF(NSPEED.EQ.0.AND.JCT.LT.500) GO TO 1000                          960
      WRITE(3,3000)                                                      961
      RETURN                                                             962
 1004 EMAX2=EMAX1                                                        963
C                                                                        964
C     CHOOSE CONVERGENCE TOLERANCE FOR INNER LOOP TO BE 1/10 OF MAX      965
C     CHANGE ON FIRST ITERATION OR ACC WHICHEVER IS LEAST.               966
C                                                                        967
      IF(JCT.NE.1) GO TO 1007                                            968
      TOL=EMAX2/10.                                                      969
      IF(TOL.LT.ACC) TOL=ACC                                             970
      SMLACC=EMAX2                                                       971
 1007 IF(EMAX1.GT.TOL) GO TO 1000                                        972
      IF(NSPEED.EQ.0.AND.JCT.LT.500) GO TO 1000                          973
      WRITE(3,3001) TOL                                                  974
      WRITE(3,3002) JCT                                                  975
      RETURN                                                             976
 3000 FORMAT(' INNER ITERATION HAS CHANGED CONC BY 50%, RETURNING TO OUT 977
     1ER LOOP TO RECALCULATE COEFFICIENTS.')                             978
 3001 FORMAT('0CONVERGENCE TOLERANCE FOR THIS ITERATION = ',1PE10.3)     979
 3002 FORMAT('1')                                                        980
 3003 FORMAT('0INNER LOOP CONVERGED IN ',I4,' ITERATIONS.')              981
 3004 FORMAT(' INNER ITERATION NOT CONVERGING TO REQUIRED  ACCURACY,(=',  982
     1)1PE10.3,' ).AFTER ',I3,' ITERATIONS, RETURNING TO OUTER LOOP.')   983
 3005 FORMAT('0 REQUESTED NUMBER OF INNER LOOPS COMPLETED.')             984
      END                                                                985

      SUBROUTINE FREAD (X,NS,IMAX,JMAX)                                  986
C                                                                        987
C     SUBROUTINE TO READ IN VARIOUS FIELDS.                              988
C                                                                        989
      DIMENSION X(12,120)                                                990
      DO 1000 J=1,JMAX                                                   991
      READ(1,1001)(X(I,J),I=1,IMAX)                                      992
      DO 1002 I=1,IMAX                                                   993
      IF(X(I,J).LE.0) GO TO 2000                                         994
 1002 CONTINUE                                                           995
 1000 CONTINUE                                                           996
      RETURN                                                             997
 2000 IF(NS(I+1,J+1).EQ.0) GO TO 1002                                    998
      WRITE(3,1003) I,J,X(I,J)                                           999
      STOP                                                              1000
 1001 FORMAT(12E6.0)                                                    1001
 1003 FORMAT('1','ELEMENT OF PRESSURE OR TEMPERATURE FIELD SPECIFIED AS 1002
     1ZERO OR NEGATIVE. THIS HAS NO PHYSICAL MEANING.',/,' POINT IS, (', 1003
     2I3,',',I3,'). ELEMENT VALUE WAS =',1PE10.3,/,' PROGRAMME TERMINATI1004
     3NG')                                                              1005
      END                                                               1006
```

```
      SUBROUTINE FPRINT(X,IMAX,JMAX)                                    10070
C                                                                       10080
C     SUBROUTINE TO PRINT OUT VARIOUS FIELDS                            10090
C                                                                       10100
      DIMENSION X(IMAX,JMAX)                                            10110
      II=1                                                              10120
      IK=0                                                              10130
      IM=IMAX                                                           10140
 2220 IF(IM.LE.8) GO TO 2221                                            10150
      IK=IK+8                                                           10160
      GO TO 2222                                                        10170
 2221 IK=IM+IK                                                          10180
 2222 DO 2223 J=1,JMAX                                                  10190
 2223 WRITE(3,1122)(X(I,J),I=II,IK)                                     10200
      IF(IM.LE.8) GO TO 2224                                            10210
      IM=IM-8                                                           10220
      II=IK+1                                                           10230
      WRITE(3,1121)                                                     10240
      GO TO 2220                                                        10250
 2224 CONTINUE                                                          10260
 1121 FORMAT('0',//)                                                    10270
 1122 FORMAT('0',8(4X,1PE12.5))                                         10280
      RETURN                                                            10290
      END                                                               10300

      SUBROUTINE MXCNCH (F,FF,IMAX,JMAX,CONV2)                          10310
C                                                                       10320
C     DETERMINE MAX CONC CHANGE IN LAST INNER LOOP AS CONV2             10330
C     UPDATE FF ARRAY TO PRESENT CONCS.                                 10340
C                                                                       10350
      DIMENSION F(IMAX,JMAX),FF(IMAX,JMAX)                              10360
      COMMON /CONVRG/ CONV1,KK                                          10370
C                                                                       10380
      CONV2=0.0                                                         10390
      DO 1000 I=1,IMAX                                                  10400
      DO 1000 J=1,JMAX                                                  10410
      C=ABS(F(I,J)-FF(I,J))                                             10420
      IF(C.LT.CONV2) GO TO 1000                                         10430
      CONV2=C                                                           10440
      FF(I,J)=F(I,J)                                                    10450
 1000 CONTINUE                                                          10460
      RETURN                                                            10470
      END                                                               10480

      SUBROUTINE CONDEF (F,FM1,FP1,N,IMAX,JMAX)                         10490
C                                                                       10500
      DIMENSION F(IMAX,JMAX),FM1(IMAX,JMAX),FP1(IMAX,JMAX),N(IMAX,JMAX) 10510
      COMMON /NBF/ NBF                                                  10520
      COMMON /TIGHT/ ACC1                                               10530
C                                                                       10540
C     READ IN PROBLEM BOUNDARIES N(I,J)                                 10550
C                                                                       10560
      WRITE(3,3004)                                                     10570
      WRITE(3,3001)                                                     10580
      READ(2,2000)((N(I,J),I=1,IMAX),J=1,JMAX)                          10590
      WRITE(3,3002)((N(I,J),I=1,IMAX),J=1,JMAX)                         10600
C                                                                       10610
```

```
C     READ IN GIVEN CONCENTRATIONS F(I,J), CHECK THAT POSITION IS OUTSDE   10620
C      PROBLEM BOUNDARY                                                    10630
C     FORM ACC1 AS A TIGHT ACCURACY CRITERIA BASED ON THE DEFINED          10640
C     CONCENTRATION AT LAST SPECIFIED POINT, NBF.                          10650
C                                                                          10660
      DO 1000 II=1,NBF                                                     10670
      READ(1,2001) I,J,F(I,J)                                              10680
      ACC1=F(I,J)/1.0E+08                                                  10690
      IF(N(I,J).EQ.1) WRITE(3,3000) I,J                                    10700
      IF(F(I,J).EQ.0.0.OR.F(I,J).EQ.1.0) GO TO 3003                        10710
 1000 CONTINUE                                                             10720
      RETURN                                                               10730
 3003 WRITE(3,3004)                                                        10740
      STOP                                                                 10750
 2000 FORMAT(3512)                                                         10760
 2001 FORMAT(2I3,E10.0)                                                    10770
 3000 FORMAT('1','ERROR IN INPUT',/,' CONCENTRATION HAS BEEN DEFINED FOR   10780
     1 A POINT INSIDE  THE SYSTEM BOUNDARY',/,'POINT IS, I=',I3,2X,'J=',   10790
     2I3)                                                                  10800
 3001 FORMAT('0 BOUNDARY SPECIFICATION')                                   10810
 3002 FORMAT('0',33(2X,I2))                                                10820
 3003 FORMAT('1','CONCENTRATION FOR ABOVE POINT HAS BEEN SPECIFIED AS 1.   10830
     10 OR 0.0  THESE VALUES ARE IMPOSSIBLE FOR A FINITE PROBLEM.',/,      10840
     2' PROGRAMME TERMINATING.')                                           10850
 3004 FORMAT('0')                                                          10860
C                                                                          10870
      END                                                                  10880

      SUBROUTINE ACCTST (ACC)                                              10890
      COMMON /TIGHT/ ACC1                                                  10900
C                                                                          10910
C     CHECK THAT INPUT ACC FIGURE IS SUFFICIENTLY SMALL TO GIVE A          10920
C     MEANINGFUL ANSWER. IF IT IS NOT, PRINT RECOMMENDED VALUE.            10930
C                                                                          10940
      IF(ACC.LE.0.0) ACC=ACC1                                              10950
      IF(ACC.LT.ACC1) RETURN                                               10960
      WRITE(3,3001)                                                        10970
      WRITE(3,3000) ACC1                                                   10980
      RETURN                                                               10990
 3000 FORMAT('0 REQUESTED ACCURACY MAY NOT BE SUFFICIENTLY SMALL TO GIVE   11000
     1 A MEANINGFUL ANSWER.',/,' RECOMMENDED VALUE FOR THIS CASE IS ACC=   11010
     2 ',1PE10.3)                                                          11020
 3001 FORMAT('0')                                                          11030
      END                                                                  11040

      SUBROUTINE UNSTBL (I,J,C,   W,Q)                                     11050
      GO TO (1000,1001,1002,1003),I                                        11060
 1001 CONTINUE                                                             11070
 1000 WRITE(3,3000) J                                                      11080
      GO TO 1004                                                           11090
 1003 CONTINUE                                                             11100
 1002 WRITE(3,3001) J                                                      11110
 1004 F=(W*Q   /C)                                                         11120
      WRITE(3,3003) F                                                      11130
      RETURN                                                               11140
 3000 FORMAT('0 MAKE AXIAL MESH FINER AROUND  J =, ',I3,' BY FACTOR OF')   11150
 3001 FORMAT('0 MAKE RADIAL MESH FINER AROUND I =, ',I3,' BY FACTOR OF')   11160
 3003 FORMAT('+',58X,1PE12.5)                                              11170
      END                                                                  11180
```

```
      SUBROUTINE  RESET (F,FM1,FP1,NS,IMAX,JMAX)                        11190
C                                                                       11200
C     SUBROUTINE TO UPDATE CONC. VALUES AFTER EACH ITERATION LOOP       11210
C                                                                       11220
      COMMON/LIMITS/IMP1,IMP2,JMP1,JMP2                                 11230
      DIMENSION F(IMAX,JMAX),FM1(IMAX,JMAX),FP1(IMAX,JMAX),             11240
     1  NS(IMP2,JMP2)                                                   11250
      DO 1000 I=1,IMAX                                                  11260
      DO 1000 J=1,JMAX                                                  11270
      IF(NS(I+1,J+1).EQ.2) GO TO 1000                                   11280
      FM1(I,J)=F(I,J)                                                   11290
      F(I,J)=FP1(I,J)                                                   11300
 1000 CONTINUE                                                          11310
      RETURN                                                            11320
      END                                                               11330


      SUBROUTINE FPUNCH(X,IMAX,JMAX)                                    11340
      DIMENSION X(IMAX,JMAX)                                            11350
      DO 1000 J=1,JMAX                                                  11360
 1000 WRITE(2,4000)(X(I,J),I=1,IMAX)                                    11370
      RETURN                                                            11380
 4000 FORMAT(6(1PE12.5))                                                11390
      END                                                               11400

      SUBROUTINE RESTRT(X,IMAX,JMAX)                                    11410
      DIMENSION X(IMAX,JMAX)                                            11420
      DO 1000 J=1,JMAX                                                  11430
 1000 READ(1,2000)(X(I,J),I=1,IMAX)                                     11440
      RETURN                                                            11450
 2000 FORMAT(6(E12.5))                                                  11460
      END                                                               11470
```