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FARF31 – A far field radionuclide migration code for use with the PROPER package

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A Far Field Radionuclide Migration Code for use with the PROPER Package

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ABSTRACT

The far field radionuclide migration computer code FARF31 has been developed as a submodel to the probabilistic package PROPER, and can be considered a refined and less CPU-time consuming version of the far field models used in the KBS -3 study.

FARF31 constitutes the numerical equivalent of a dual porosity model for radionuclide migration along a stream tube in fractured rock. It calculates the migration rate of the radionuclide chains at the exit of the tube given the input rates at the entrance. Advection, dispersion and one dimensional matrix diffusion is taken into account as well as chain decay.

The underlying equations are formulated in terms of groundwater travel time and Peclet number, thus allowing for the groundwater travel time to be computed outside FARF31 by a separate submodel fitted to handle Darcy velocities and kinematic porosities which vary in space.

Input migration rate boundary conditions are arbitrary.

Contents

1. INTRODUCTION

The purpose of the PROPER code package is to provide the analyst with a computerized methodology that enables him/her to study the propagation of parameter uncertainties in performance-assessment-related model calculations. The core of PROPER is the Monitor that is used to interconnect the desired submodels, selected from a library at runtime, and to propagate the input parameter uncertainties to find the associated uncertainties in the results, cf. Figure 1.1. This is accomplished without any intervention in the source code of the Monitor or the submodels. The submodels typically deal with groundwater flow and radionuclide migration.

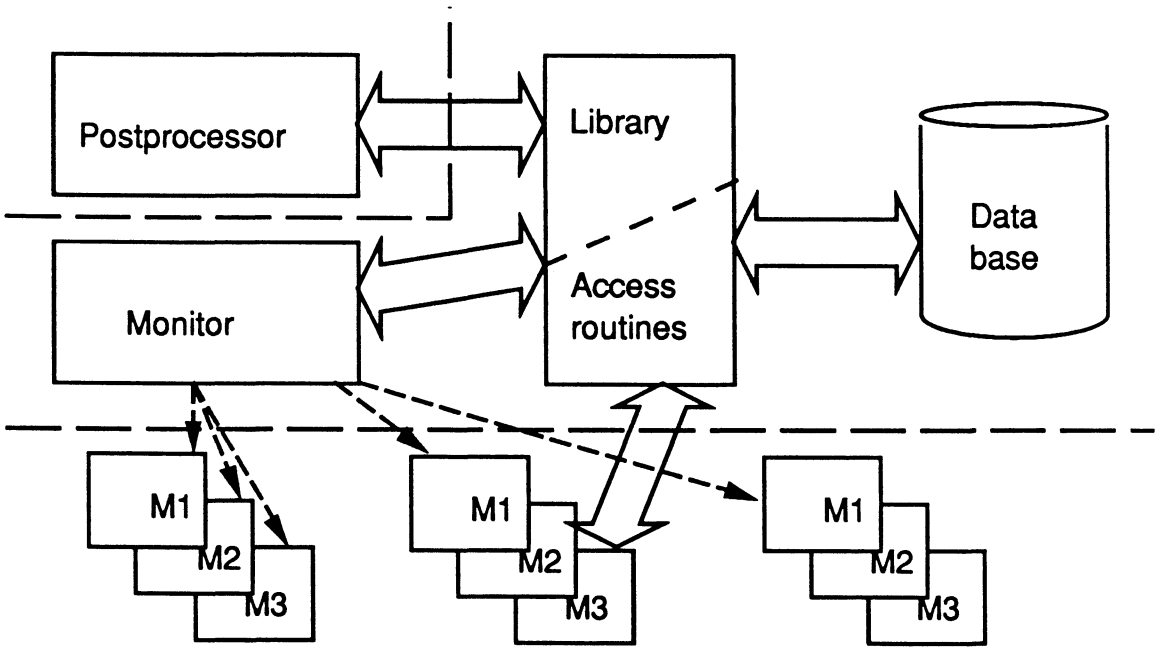

Figure 1.1 Schematic illustration of the function of PROPER.

The numerical integration method used in PROPER is a Monte Carlo procedure using repeated sampling of parameter values. The PROPER Monitor only collects crude statistics. Further evaluation must be carried out using a suitable post-processor. The Monte Carlo approach requires that submodels are simplified and/or use very fast numerical algorithms.

The present report presents a submodel designed to calculate the rate of radionuclide transport in fractured rock. It is based on the dual porosity farfield model that was used in the KBS-3 study /1-1/ and on work that was reported with that study. The submodel, named FARF31, represents a further development of the zero:th generation farfield model FARF30 which does not treat radionuclide chain decay , uses a simplified treatment of matrix diffusion and handles only a limited number of input boundary conditions. FARF31 is based on a more pronounced stream tube formulation than was adopted in the KBS-3 study and a more elaborate description of matrix diffusion than FARF30 , accepts any input boundary conditions and it takes chain decay into account.

FARF31 is coded in FORTRAN77 and was produced in accordance with the PROPER standard software engineering procedures.The following chapters contain descriptions of the basic model (Chapter 2), the simplifications made including an associated minimal set of assumptions (Chapter 3), the method of numerical solution (Chapter 4), the inputs to and outputs from FARF31 (Chapter 5) and a test example (Chapter 6).

2. BASIC MODEL

2.1 Flow Porosity Portion

FARF31 constitutes the numerical equivalent of a dual porosity model for radionuclide migration along a stream tube, cf. Figure 2.1. With a stream tube we mean the surface created by the stream lines going through a closed contour Γ_0 or , equivalently , the surface created by sweeping the contour Γ_0 through space along the stream lines . Streamlines are the curves defined by tangency to the velocity field. In the following we summarize the stream tube formulation detailed in Appendix A.

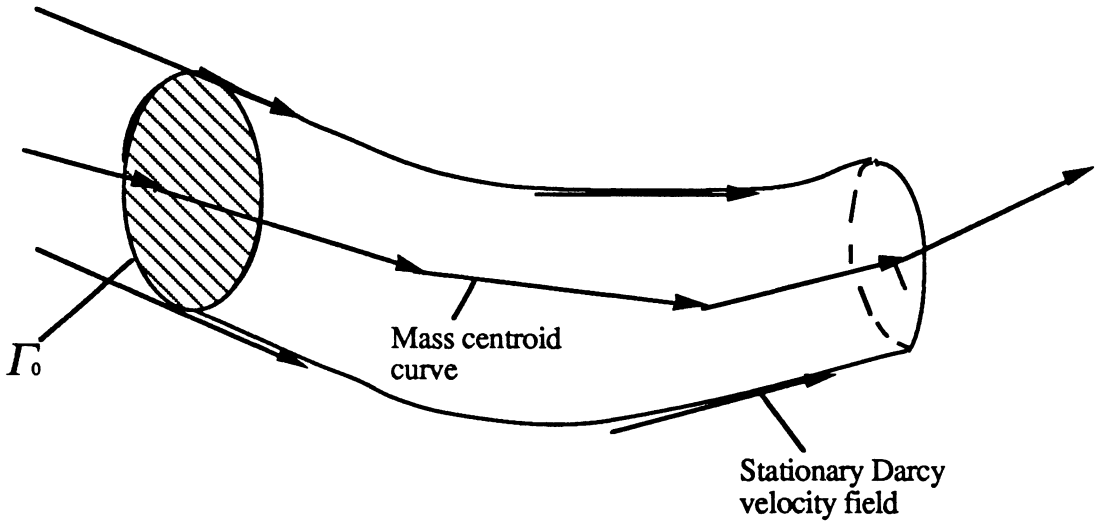

Figure 2.1 Stream tube geometry.

Under the assumptions that

(i) stationary flow conditions prevail,
(ii) we may neglect transversal dispersion,
(iii) the longitudinal dispersion coefficient and the exchange terms between flow- and diffusional porosity may be replaced by averages over the stream tube cross section,
(iv) the density is constant and the variation of porosity is small compared to the variation of concentration and
(v) the stream tube is sufficiently narrow to warrant the assumption that the pore velocity may be replaced by some average over the cross section

the basic transport equation is :

$$\frac{\partial C_f^{\,i}}{\partial t} = - U_f \frac{\partial C_f^{\,i}}{\partial z} + U_f \frac{\partial}{\partial z} \frac{D_L}{U_f} \frac{\partial C_f^{\,i}}{\partial z} - w^i - \lambda^i C_f^{\,i} + \lambda^{i-1} C_f^{\,i-1} \qquad (2.1)$$

where

t = time [T],

z = distance in flow direction along the mass centroid with respect to mobile liquid of the tube [L] ,

$C_f^{\,i}(z,t)$ = an effective stream tube average of the concentration of nuclide i in the mobile liquid [ML^{-3}]

$U_f(z)$ = an effective stream tube average of the pore velocity i.e. velocity of the mobile liquid [LT^{-1}],

$D_L(z)$ = longitudinal dispersion coefficient averaged over the cross - section of the tube [L^2T^{-1}] . The dispersive flux through an area A is given by $\phi_{dispersion} = -([D]\nabla C_f)\varepsilon_f A$ where $[D]$ signifies the dispersion tensor. See Appendix A , p. A4.

Finally

$w^i(z)$ = an effective stream tube average of the macroscopic exchange term from the flow porosity to the diffusional porosity per unit volume of mobile liquid [$MT^{-1}L^{-3}$]

and

λ^i = decay constant for nuclide i [T^{-1}].

The solutions to (2.1) are restricted by the following initial and boundary conditions:

$$C_f^{\,i}(z,t)\Big|_{t=0} = 0 \tag{2.2}$$

$$\lim_{z\to\infty} C_f^{\,i}(z,t) = 0 \tag{2.3}$$

$$Q_{tube}\left(C_f^{\,i}(z,t) - \frac{D_L(z)}{U_f(z)}\frac{\partial C_f^{\,i}(z,t)}{\partial z}\right)\Bigg|_{z=0} = F_{in}^{\,i}(t) \tag{2.4}$$

where we have introduced

Q_{tube} = the volume flow in the tube. [M^3T^{-1}]. This is constant since nothing may flow through the side boundaries and the density is assumed constant

and

$F_{in}^{\,i}(t)$ = input flux of nuclide i to stream tube [MT^{-1}].

The desired quantity is the output flux at some distance z_0 :

$$F_{out}^{\ i}(t) = Q_{tube}\left(C_f^{\ i}(z,t) - \frac{D_L(z)}{U_f(z)} \frac{\partial C_f^{\ i}(z,t)}{\partial z} \right)\Bigg|_{z=z_0} . \qquad (2.5)$$

2.2 Diffusive Porosity Portion and the Exchange Term

Assuming a simple model for the diffusive porosity i.e that it can be represented by one dimensional non intersecting finite tubes we can deduce a one dimensional diffusion equation for a macroscopic (surface) average , C_p^i , of the concentration in the micro fissures. This is done in Appendix B and results in the equation

$$D_e \frac{\partial^2}{\partial x^2} C_p^i(z,x,t) - \lambda^i R^i C_p^i(z,x,t) +$$

$$\lambda^{i-1} R^{i-1} C_p^{i-1}(z,x,t) = R^i \frac{\partial}{\partial t} C_p^i(z,x,t) \qquad (2.6)$$

and the boundary conditions

$$C_p^i(z,x,t)\Big|_{x=0} = C_f^i(z,t) \qquad (2.7)$$

$$\frac{\partial}{\partial x} C_p^i(z,x,t)\Big|_{x=\langle L\rangle(z)} = 0 \qquad (2.8)$$

where we added the notation

$\langle L\rangle(z)$ = the surface average of micro fissure length or of depth of diffusive penetration,[L]

x = relative penetration depth [L], $0 \le x \le \langle L\rangle(z)$, see Appendix B,

$C_p^i(x,z,t)$ = a surface and stream tube averaged concentration of nuclide i dissolved in the stagnant pore liquid in the impervious rock matrix [ML^{-3}], see equation (B.4) and (B.10),

$D_e(x,\zeta)$ = effective rock matrix diffusion coefficient for non sorbed species [L^2T^{-1}] ,see equation (B.7),

$R^i(x,\zeta)$ = effective matrix volume sorption retention factor for nuclide i [-] ,see equation (B.8).

The exchange term is now expressed in terms of the above averaged quantities as

$$w^i(z) = -\alpha(z) D_e(z) \frac{\partial}{\partial x} C_p^i(z,x,t)\Big|_{x=0} \qquad (2.9)$$

where now

$a(z)$ = total surface area of the boundary of the flow porosity per unit volume of mobile liquid [L^{-1}],

3. SIMPLIFIED MODEL

3.1.Treatment of Flow Porosity Portion

In the above differential equation (2.1), the ground water pore velocity (and, hence, kinematic porosity) and the dispersion coefficient are allowed to vary along the stream tube. This complication can be handled reasonably well using a simplification taken from Neretnieks and Rasmuson /3-1/.

It would be desirable to formulate the equations in terms of groundwater traveltime and Peclet number instead of pore velocity and dispersion coefficient. One major advantage would be that the groundwater travel time could be computed outside the migration model by a separate submodel which is more fitted to handle Darcy velocities and kinematic porosities which vary in space.

A transformation is made along the lines of /3-1/:

$$\zeta = \int_0^z \frac{dz'}{U_f(z')} \tag{3.1}$$

yielding

$$\frac{\partial C_f^{\,i}}{\partial t} = -\frac{\partial C_f^{\,i}}{\partial \zeta} + \frac{\partial}{\partial \zeta}\frac{D_L}{U_f^{\,2}}\frac{\partial C_f^{\,i}}{\partial \zeta} - w^i - \lambda^i C_f^{\,i} + \lambda^{i-1} C_f^{\,i-1} \tag{3.2}$$

with

$$F_{in}^{\,i}(t) = Q_{tube}\left(C_f^{\,i}(\zeta, t) - \frac{D_L(\zeta)}{U_f(\zeta)^2}\frac{\partial C_f^{\,i}(\zeta, t)}{\partial \zeta}\right)\Bigg|_{\zeta=0} \tag{3.3}$$

at the inlet, and

$$F_{out}^{\,i}(t) = Q_{tube}\left(C_f^{\,i}(\zeta, t) - \frac{D_L(\zeta)}{U_f(\zeta)^2}\frac{\partial C_f^{\,i}(\zeta, t)}{\partial \zeta}\right)\Bigg|_{\zeta=\zeta_0} \tag{3.4}$$

at the outlet, where

$$\zeta_0 = \int_0^{z_0} \frac{dz'}{U_f(z')} = t_w \tag{3.5}$$

is the groundwater travel time over the entire migration distance (a constant), now in place of the pore velocity and the migration distance as such.

An approximation is made with respect to the dispersive term in Equations (3.2) - (3.4), assuming that the pore velocity and dispersion coefficient in that term can be averaged along the stream tube so that

$$\frac{D_L(z)}{U_f(z)^2} \approx \frac{\overline{D_L(z)}}{U_f(z)^2} = \frac{1}{z_0}\int_0^{z_0} \frac{D_L(z)}{U_f(z)U_f(z)}dz \approx \frac{z_0}{z_0^2}\frac{\overline{D_L(z)}}{U_f(z)}\int_0^{z_0}\frac{dz}{U_f(z)} = \frac{t_w}{Pe} \qquad (3.6)$$

where Pe is an effective Peclet number. The sacrifice associated with the approximation is, actually, a somewhat shaky definition of the Peclet number which could be partly justified by the assumption of a constant dispersivity.

The resulting equation is

$$\frac{\partial C_f^{\,i}}{\partial t} \approx -\frac{\partial C_f^{\,i}}{\partial \zeta} + \frac{t_w}{Pe}\frac{\partial^2 C_f^{\,i}}{\partial \zeta^2} - w^i - \lambda^i C_f^{\,i} + \lambda^{i-1} C_f^{\,i-1} \qquad (3.7)$$

with

$$F_{in}^{\,i}(t) \approx Q_{tube}\left(C_f^{\,i}(\zeta,t) - \frac{t_w}{Pe}\frac{\partial C_f^{\,i}(\zeta,t)}{\partial \zeta}\right)\Bigg|_{\zeta=0} \qquad (3.8)$$

at the inlet, and

$$F_{out}^{\,i}(t) \approx Q_{tube}\left(C_f^{\,i}(\zeta,t) - \frac{t_w}{Pe}\frac{\partial C_f^{\,i}(\zeta,t)}{\partial \zeta}\right)\Bigg|_{\zeta=t_w} \qquad (3.9)$$

at the outlet. Rasmuson and Neretnieks /3-2/ claim this to be a good approximation in general.

3.2 Treatment of Diffusive Porosity Portion

The equations (2.6) - (2.9) are only simplified with respect to the variation of the parameters along the stream tube. Thus we assume that the average micro fissure length or alternatively the maximal diffusive penetration depth is constant i.e. $\langle L\rangle(z) = x_0$, the average total surface area of the flow porosity $a(z)$,the effective rock matrix diffusion coefficient $D_e(z)$ and the effective matrix volume sorption retention factor for nuclide i , $R^i(z)$ all are independent of any stream tube coordinate spatial (z) or temporal (ζ).

3.3 Summary of Equations

The equations to solve are, in summary:

$$\frac{\partial C_f^{\,i}}{\partial t} = -\frac{\partial C_f^{\,i}}{\partial \zeta} + \frac{t_w}{P_e}\frac{\partial^2 C_f^{\,i}}{\partial \zeta^2} + aD_e\frac{\partial C_p^i}{\partial x}\Bigg|_{x=0} - \lambda^i C_f^{\,i} + \lambda^{i-1} C_f^{\,i-1} \qquad (3.10)$$

where we have substituted (2.9) for the exchange term,

$$R^i\frac{\partial C_p^i}{\partial t} = D_e\frac{\partial^2 C_p^i}{\partial x^2} - R^i\lambda^i C_p^i + R^{i-1}\lambda^{i-1}C_p^{i-1} \qquad (3.11)$$

and

$$F_{out}{}^{i}(t) = Q_{tube}\left(C_f{}^{i}(\zeta, t) - \frac{t_w}{P_e}\frac{\partial C_f{}^{i}(\zeta, t)}{\partial \zeta} \right)\Bigg|_{\zeta = t_w} \tag{3.12}$$

under the following initial and boundary conditions:

$$C_p^i(x, \zeta, t)\Big|_{t=0} = 0 \tag{3.13}$$

$$C_f{}^{i}(\zeta, t)\Big|_{t=0} = 0 \tag{3.14}$$

$$\lim_{\zeta \to \infty} C_f{}^{i}(\zeta, t) = 0 \tag{3.15}$$

$$F_{in}{}^{i}(t) = Q_{tube}\left(C_f{}^{i}(\zeta, t) - \frac{t_w}{P_e}\frac{\partial C_f{}^{i}(\zeta, t)}{\partial \zeta} \right)\Bigg|_{\zeta = 0} \tag{3.16}$$

$$\frac{\partial C_p^i(x, \zeta, t)}{\partial x}\Bigg|_{x = x_0} = 0 \tag{3.17}$$

$$C_p^i(x, \zeta, t)\Big|_{x=0} = C_f^i(\zeta, t) \tag{3.18}$$

where

x = relative penetration depth [L], $0 \le x \le \langle L \rangle(z)$, see Appendix B,

$C_p^i(x, z, t)$ = a surface and stream tube averaged concentration of nuclide i dissolved in the stagnant pore liquid in the impervious rock matrix [ML^{-3}], see equation (B.4) and (B.10),

$D_e(x, \zeta)$ = effective rock matrix diffusion coefficient for non sorbed species [L^2T^{-1}] ,see equation (B.7),

$R^i(x, \zeta)$ = effective matrix volume sorption retention factor for nuclide i [-] ,see equation (B.8)

x_0 = $\langle L \rangle(z)$ the surface average of micro fissure length or of maximal diffusive penetration ,[L] ,

t = time [T],

ζ = distance in flow direction expressed in terms of groundwater travel time [T],

$C_f^{\,i}(\zeta, t)$ = concentration of nuclide i in the mobile liquid [ML^{-3}],

t_w = groundwater travel time over entire flow path [T],

$a(z)$ = total surface area of the boundary of the flow porosity per unit volume of mobile liquid [L^{-1}] ,

λ^i = decay constant of nuclide i [T^{-1}],

Q_{tube} = flow rate in the stream tube [L^3T^{-1}],

$F_{in}^{\,i}(t)$ = input flux of nuclide i to stream tube [MT^{-1}],

and finally

$F_{out}^{\,i}(t)$ = output flux of nuclide i from stream tube [MT^{-1}].

The equations summarized above are in principle those of /3-3/ and /3-4/ which treats more explicit fracture geometries. In these references exact solutions are developed for one nuclide with the use of Laplace transforms. In /3-3/ a single planar fracture is treated giving rise to the boundary condition $C_p^i(\infty, \zeta, t) = 0$ replacing (3.17) , /3-4/ treats an aggregate of planar equidistant cracks also producing the condition (3.17). The reference /4-2/ considers the same equations as those above expressed in a length coordinate i.e without the transformation (3.1). We will return to this reference in Paragraph 4. We also mention that the diffusion equation for the matrix could be based on other assumptions than ours thus producing other equations. See for example /3-5/.

4. NUMERICAL SOLUTION OF THE TRANSPORT EQUATIONS

4.1 General Procedure

The approach chosen for numerically solving the system of partial differential equations (3.10) - (3.11) with boundary and initial conditions given by (3.13) - (3.18) is a semi analytical one dependent on three major steps. This approach is also employed in /4-2/.

(i) Take the Laplace transform of (3.10) - (3.18) with respect to t and derive an analytical expression for the solution of the arisen system of ordinary differential equations.

(ii) Utilize a numerical inversion algorithm to transform the solution(s) to the time domain. The numerical Laplace inversion algorithm presently used in FARF31 is that invented by Talbot /4-1/ and employed in /4-2/. FARF31 is however modularized such that any inversion routine can be plugged in with minor effort.

(iii) Make use of the linearity of the equations to express the solution to any input function $F_{in}^{\ j}(t)$ as

$$C_f^{\ i}(\zeta, t) = \sum_{j=1}^{i} \int_0^t F_{in}^{\ j}(\tau) C_f^{\ i,j}(\zeta, t-\tau)\, d\tau \tag{4.1}$$

where $C_f^{\ i,j}(\zeta, t-\tau)$ is the concentration response of nuclide i at a time t given a unit pulse, Dirac function, input of nuclide j upstream in the chain at time τ .To perform the convolution operations a straight forward numerical algorithm based on the trapezoidal rule has been developed[1].

Next we detail these three steps. The step (i) is detailed even more in Appendix C.

4.2 Analytical Solution in Laplace Space

This chapter is a summary of the results given in Appendix C. As the appendix is self contained readers who want to get directly into business may therefore skip this paragraph.

Taking the Laplace transform of the governing equations (3.10) - (3.11) and the initial and boundary conditions (3.13) - (3.18) we obtain

$$\frac{d^2\bar{C}_f^{\ i}}{d\zeta^2} - \frac{P_e}{t_w}\frac{d\bar{C}_f^{\ i}}{d\zeta} - \frac{P_e}{t_w}(s + \lambda^i)\bar{C}_f^{\ i} + \frac{P_e}{t_w} a D_e \frac{d\bar{C}_p^{\ i}}{dx}\bigg|_{x=0} = -\frac{P_e}{t_w}\lambda^{i-1}\bar{C}_f^{\ i-1} \tag{4.2}$$

$$\frac{d^2\bar{C}_p^{\ i}}{dx^2} - \frac{R^i}{D_e}(s + \lambda^i)\bar{C}_p^{\ i} = -\frac{R^{i-1}}{D_e}\lambda^{i-1}\bar{C}_p^{\ i-1} \tag{4.3}$$

---

[1] A variation of this technique is to perform numerical Laplace transformation on $F_{in}^{i}(t)$ and perform inversion on the solution directly. This has not yet been done but would be interesting especially to compare the computational efficiency of the two variants

$$Q_{tube}\left[\tilde{C}_f^i(\zeta, s) - \frac{t_w}{P_e}\frac{d\tilde{C}_f^i}{d\zeta}(\zeta, s)\right]\Bigg|_{\zeta = t_w} = \tilde{F}_{out}^i(s) \qquad (4.4)$$

with boundary conditions

$$\lim_{\zeta \to \infty} \tilde{C}_f^i(\zeta, s) = 0 \qquad (4.5)$$

$$Q_{tube}\left[\tilde{C}_f^i(\zeta, s) - \frac{t_w}{P_e}\frac{d\tilde{C}_f^i}{d\zeta}(\zeta, s)\right]\Bigg|_{\zeta = 0} = \tilde{F}_{in}^i(s) \qquad (4.6)$$

$$\left.\frac{d\tilde{C}_p^i}{dx}\right|_{x = x_0} = 0 \qquad (4.7)$$

$$\tilde{C}_p^i(x, \zeta, s)\Big|_{x=0} = \tilde{C}_f^i(\zeta, s). \qquad (4.8)$$

Using N to denote the total number of equations and $\delta^{i,j}$ to denote the Kronecker delta we write the input as

$$\sum_{j=1}^{N} F_{in}^j(s)\delta^{i,j},$$

i.e viewing the input as a vector indexed by i. We may use the linearity of the system to deduce that the solution may be written

$$\sum_{j=1}^{N} F_{in}^j(s)\tilde{C}_f^{i,j}(\zeta, s)$$

and

$$\sum_{j=1}^{N} F_{in}^j(s)\tilde{C}_p^{i,j}(x, \zeta, s)$$

where $\tilde{C}_f^{i,j}$ and $\tilde{C}_p^{i,j}$ are the solutions of this system of ordinary differential equations for each of the cases where $\tilde{F}_{in}^i(s) = \delta^{i,j}$, $j = 1,2 \ldots N$. As already stated above the corresponding functions in the time domain, $C_f^{i,j}$ and $C_p^{i,j}$, should be thought of as the concentration response of nuclide i given a unit pulse - Dirac function - inlet of nuclide j upstream in the chain, at time zero. In particular

$$C_f^{i,j} = C_p^{i,j} = 0 \qquad \text{if} \qquad j > i.$$

The first thing to note is that s acts as a parameter in the equations (4.2) -(4.3) and that the solutions must be analytic in s to the right of some vertical line. One may show that:

(a) There is a large set of points s such that the system (4.2) -(4.3) has a solution . Note that there does not exist a solution for all s . See Appendix C, Proposition 2 .

(b) The solutions may be continued as analytical functions to the complex plane cut along the negative real axis from infinity to the largest of the numbers $-\lambda^i$,i = 1, 2, ... N . This is important for the Laplace inversion. See Appendix C, Proposition 4.

(c) The solutions may expressed as

$$\bar{C}_f^{i,j} = \sum_{k=j}^{i} P_{i,j,k}(s)\, h_f^k(\zeta, s)$$

$$\bar{C}_p^{i,j} = \sum_{k=j}^{i}\sum_{l=k}^{i} Q_{i,j,k,l}(s)\, h_f^k(\zeta, s)\, h_p^l(x, s)$$

where

$$h_p^i(x, s) = \frac{\cosh(h_i(s)(x_0 - x))}{\cosh(h_i(s)x_0)}$$

$$h_f^i(\zeta, s) = \frac{e^{f_i(s)\zeta}}{Q_{eq}\left[1 - \frac{t_w}{Pe} f_i(s)\right]}$$

and in turn $f_i(s)$ may be expressed as

$$f_i(s) = \frac{Pe}{2t_w}\left[1 - \left(1 + \frac{t_w}{Pe}\left[(s + \lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right]\right)^{1/2}\right]$$

in which the square root always will denote the principal branch i.e the one that is positive for positive arguments and $h_i(s)$ is defined in Ω_i by

$$h_i(s) = \left(\frac{R^i}{D_e}(s + \lambda^i)\right)^{1/2}.$$

The functions $P_{i,j,k}(s)$ and $Q_{i,j,k,l}(s)$ can be calculated from the recursive equations

$$P_{i,j,i}(s) = -\sum_{k=j}^{i-1} P_{i,j,k}(s)$$

$$Q_{i,j,k,l}(s) = Q_{i-1,j,k,l}(s)\frac{R^{i-1}}{D_e}\lambda^{i-1}\frac{1}{h_i^2(s) - h_l^2(s)} \qquad j \le k < i-1,\ k \le l < i-1$$

$$Q_{i,j,k,i}(s) = P_{i,j,k}(s) - \sum_{l=k}^{i-1} Q_{i,j,k,l}(s) \qquad j \le k < i-1$$

$$Q_{i,j,i,i}(s) = P_{i,j,i}(s)$$

see Appendix C, Proposition 3 and the subsequent discussion.

These solutions are equivalent to those of /4-2/. However the solutions have different appearance. The solution presented above is recursive which has turned out to be computational more efficient on the SKB -VAX. This may be the other way around on a vector machine. Also since the solution involves multiple valued functions and seems to possess poles it is not at all clear where one can place a contour to perform an inverse transformation without traversing a branch cut or being tricked by a forgotten pole on the wrong side of the contour. These questions are answered in Appendix C.

4.3 Numerical Laplace Inversion

The Laplace space expression from Section 4.2 cannot be inverted analytically; a numerical technique must be employed. FARF31 uses a special service routine that has been developed based on the Talbot algorithm /4-1/,which also has been used by Hodginson and Maul /4-2/ on a very similar problem. Two alternative inversion routines have also been developed based on other algorithms. They have not yet been subjected to formal testing. In any case, FARF31 is designed so as to facilitate the replacement of the inversion routine. The resulting response time series are put out with a controlled interpolation error using the PROPER Time Series Manager. First guess upper temporal bounds are obtained from the first two moments of the response time series, which can be obtained directly from the Laplace transforms by differentiation and subsequent use of the Chebyshev inequality.

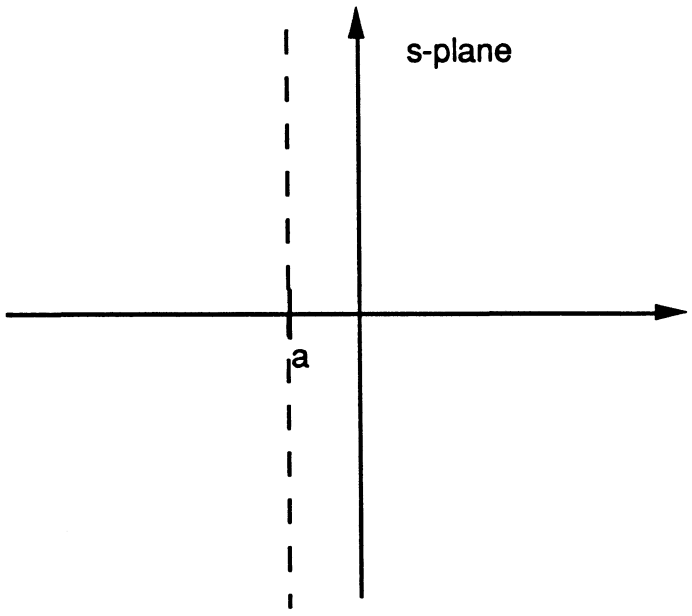

Figure 4.1

The standard inversion formula is based on integration on the so called Bromwich contour:

$$c(t) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{st} \tilde{c}(s) ds \qquad , \quad t > 0$$

where $\tilde{c}(s)$ must be analytic in $\{s : \mathrm{Re}(s) > a\}$ cf. Figure. 4.1

The basis of the Talbot algorithm is the choice of an alternative integration contour and a change of variables, introducing a scale and a shift parameter

$$c(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \int_{L} e^{\lambda s t} \tilde{c}(\lambda s + \sigma) ds \qquad , \quad t > 0$$

with the contour L starting and ending in the left half plane, so that $\mathrm{Re}(s) \to -\infty$ at each end. This contour still has to pass to the left of all singularities, which could be made hold by the appropriate choice of λ and σ .

The general idea is to obtain faster convergence when using trapezoidal integration (via a mapping function) through e^{st} as $\mathrm{Re}(s) \to -\infty$. The contour presently used by the inversion routine is the one recommended by Talbot

$$L_v : s = s_v(\theta) = \theta \cot \theta + vi\theta \qquad -\pi < \theta < \pi$$

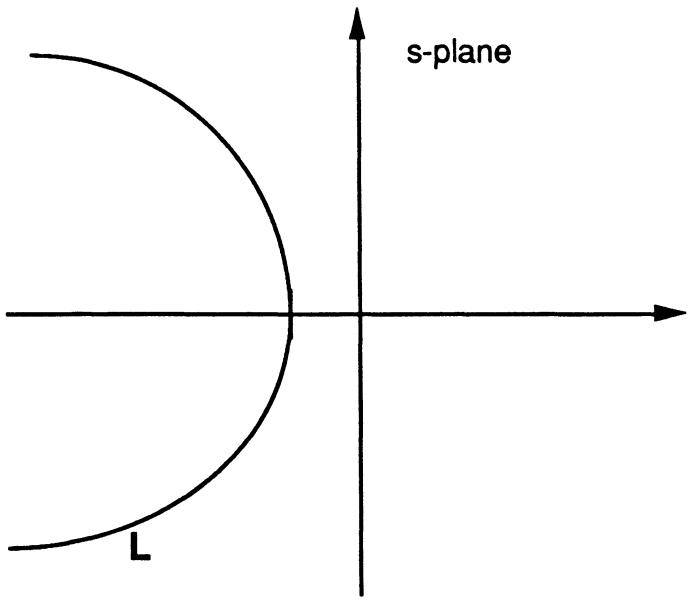

Figure 4.2

The functions appearing in Section 4.2 are rather complicated and it is not at all clear where these functions are analytic. Before an inversion routine is used, it must be made certain that the contour is correctly placed. This is dealt with in Appendix C.

If all non analytic points are on the real axis, better numerical accuracy is obtained if the contour passes very close to the rightmost such point. This point is given by

$\max_i \{-\lambda^i\}$. This is used by FARF31 to compute the correct choice for σ (cf Appendix C). Constant defaults are used for $\tau = \lambda t$, ν and the number of integration points.

4.4 Numerical Convolution

To convolve the input time series with the response time series, FARF31 uses a PROPER service routine designed for convolving two time series in the time domain (the PROPER Numerical Convolution Routine, originally developed for FARF31). The union of all points in both series are used in a trapezoidal quadrature scheme. The output series from convolution are put out with a controlled interpolation error using the PROPER Time Series Manager.

5. INPUTS AND OUTPUTS

Since FARF31 is a PROPER submodel, the input and output data must follow the format imposed by the PROPER Monitor.

In principle , FARF31 demands the following inputs:

* From other models:
  - groundwater travel time over far field migration path, t_w ,
  - migration rate from near field (for each nuclide), $F_{in}^{i}(t)$.
* Sampled parameters:
  - longitudinal dispersion Peclet number, Pe ,
  - total surface area of the boundary of the flow porosity per unit volume of mobile liquid , a ,
  - matrix porosity, ε_p ,
  - effective matrix diffusion coefficient, D_e ,
  - surface average of the maximum depth of diffusive penetration into rock matrix or of microfissure length, x_0,
  - mass based distribution coefficient (for each chemical element), $K_d^{\ i}$.
* Other data:
  - data describing the decay chains, i.e half lives etc.

and returns the following output series:

- Migration rate from far field (for each nuclide), $F_{out}^{\ i}(t)$.

Q_{tube} is cancelled out in the final expression for $F_{out}^{\ i}(t)$ and is not needed in the input, cf Chapter 4.

The bulk density of the rock is automatically set to 2700 kg/m^3.

6. TEST EXAMPLE

To demonstrate the type of results obtained by the FARF31 submodel, a single-realization test example was designed.

The output fluxes of Uranium-238, the Neptunium-237 chain (Np237 - U233 - Th229) and Cesium-135 were computed for constant band inputs of Uranium-238 and Neptunium-237, and for decaying band input of Cesium-135.

The following data were used:

-	groundwater travel time	100	yrs
-	Peclet number	2	-
-	specific surface	4000	m^2/m^3
-	matrix porosity	0.002	-
-	matrix diffusion coefficient	1.58E-6	m^2/yr
-	penetration depth	2.5	m
-	distribution coefficient		
	Uranium	5	m^3/kg
	Neptunium	5	m^3/kg
	Thorium	5	m^3/kg
	Cesium	0.05	m^3/kg

Half lives:		
	U-238	4.47 Gyrs
	Np - 237	2.14 Myrs
	U -233	0.159 Myrs
	Th -229	7.3 kyrs
	Cs -135	2.95 Myrs

The output time series are shown in Figures 6.1 - 6.3 which also show the input series. The inputs start at time zero.

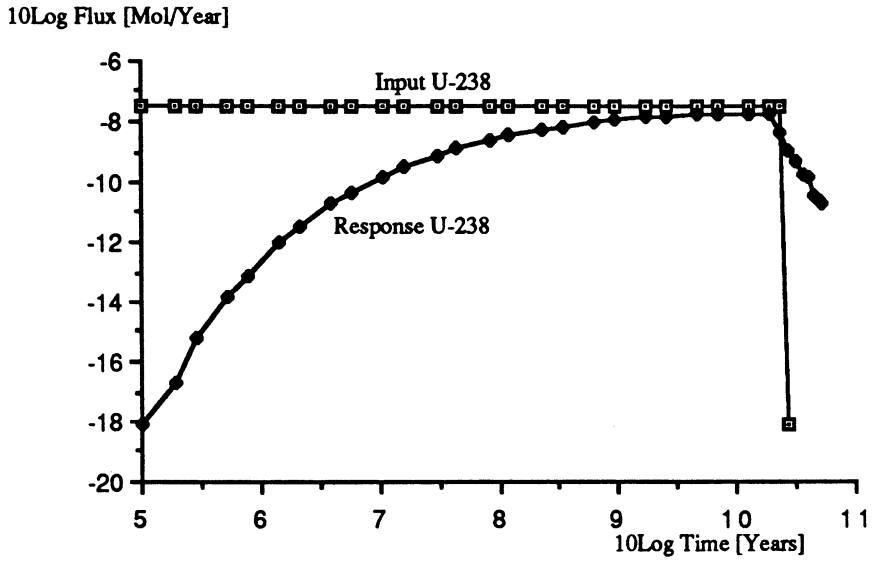

Figure 6.1

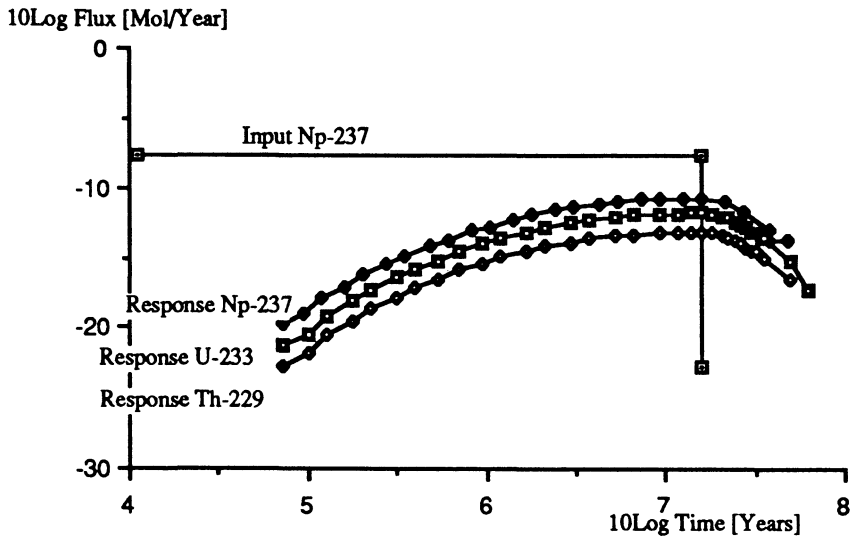

Figure 6.2

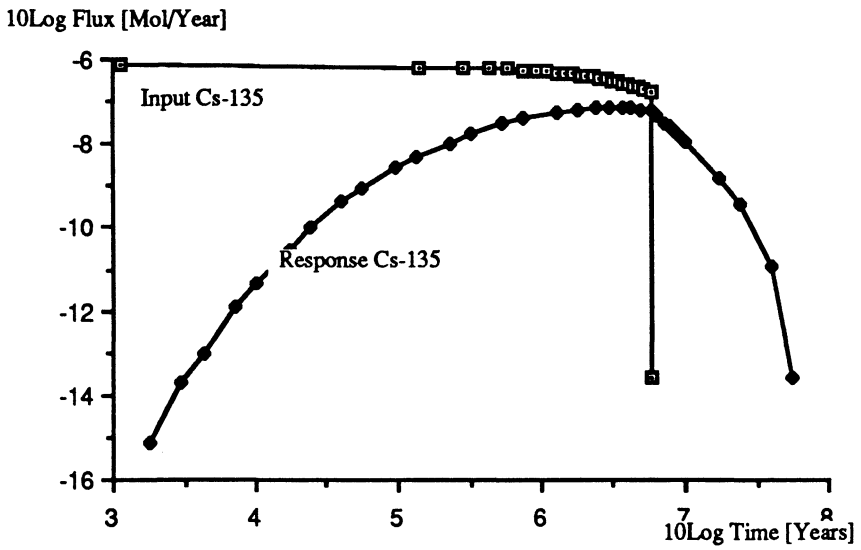

Figure 6.3

ACKNOWLEDGEMENTS

The authors wish to thank Mr. Per Söderberg, Starprog AB for actually coding most of the FARF31 submodel, and Prof. Sven-Åke Gustafsson , presently at the Rogaland University , for designing and implementing the first version of the Talbot inversion routine and for designing and implementing the PROPER Time Series Manager used in FARF31. The contributions from Mss. Mercedes Prieto and Anna Lidman to the Laplace inversion scheme are also gratefully acknowledged.

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Appendix A. Stream Tube Transport Equation

Given a stationary Darcy velocity field $U_0(x)$ and a flow porosity $\varepsilon_f(x)$ we define the pore velocity field as

$$U_f(x) = \frac{U_0(x)}{\varepsilon_f(x)}.$$

Then we produce , or define, a stream tube by taking an arbitrary closed contour Γ_0 , bounding a surface A_0 and sweep it through space along the solution curves of

$$\frac{dX_f(a,\zeta)}{d\zeta} = U_f(X_f(a,\zeta)) \quad , \quad X_f(a,0) = a \in A_0 \quad . \qquad (A.1)$$

If we like to we can interpret ζ as a travel time coordinate for a particle travelling with speed U_f .The notion of surface will in the sequel always mean an orientable surface equipped with a continuous normal vector field. The surface A_0 will then be continuously transformed into the surfaces $A(\zeta)$ and $A(0) = A_0$. It follows from the continuity equation , Gauss formula and our definition of a stream tube that the mass flow through any such surface is a constant i.e

$$\int_{A(\zeta)} \rho(\xi)U_0(\xi)dA(\xi) = \int_{A(\zeta)} \rho(\xi)U_f(\xi)\varepsilon_f(\xi)dA(\xi) = Q_{tube,M}\,.^{1}$$

Note that dA is a vectorial quantity. We define a representative pore velocity for this stream tube as

$$U_f^{tube}(\zeta) = \frac{1}{Q_{tube,M}}\int_{A(\zeta)} U_f(\xi)dq_M(\xi)$$

where

$$dq_M(\xi) = \rho(\xi)U_0(\xi)dA(\xi).$$

The stream tube may be represented with a single curve consisting of the averages

$$X_f^{tube}(A_0,\zeta) = \frac{1}{Q_{tube,M}}\int_{A(\zeta)} \xi\, dq_M(\xi).$$

We note the interesting fact that $X_f^{tube}(A_0,\zeta)$ is the point of gravity of the surface $A(\zeta)$ in fact using the definition of $X_f^{tube}(A_0,\zeta)$ and equation (A.1) we have

---

[1]The Darcy velocity is a phase average whereas the density here is a intrinsic phase average. In this case the continuity equation is $\nabla(\rho U_0)+\frac{\partial(\rho\varepsilon)}{\partial t}=0$ where ε is porosity.

$$X_f^{tube}(A_0, \zeta) = \lim_{\Delta\zeta \to 0} \frac{1}{Q_{tube,M}\Delta\zeta} \int_{\zeta}^{\zeta+\Delta\zeta} d\tau \int_{A(\tau)} \xi \left[\rho(\xi) U_f(\xi) \varepsilon_f(\xi) dA(\xi)\right] =$$

$$\lim_{\Delta\zeta \to 0} \frac{1}{Q_{tube,M}\Delta\zeta} \int_{\zeta}^{\zeta+\Delta\zeta} \iint_{\Omega} X_f(a, \tau)$$

$$\left[\frac{\partial X_f(a, \tau)}{\partial \tau} \rho(X(a, \tau)) \left(\frac{\partial X_f(a, \tau)}{\partial a_1} \times \frac{\partial X_f(a, \tau)}{\partial a_2}\right) \varepsilon_f(X_f(a, \tau)) da_1 da_2\right] d\tau =$$

$$\lim_{\Delta t \to 0} \frac{1}{Q_{tube,M}\Delta\zeta} \int_{V(\zeta, \Delta\zeta)} \xi dm(\xi)$$

where $V(\zeta, \Delta\zeta)$ is the volume of the tube between $A(\zeta)$ and $A(\zeta + \Delta\zeta)$ and (a_1, a_2) are some curvilinear coordinate system on A_0 with domain of definition Ω i.e. A_0 is parameterized by (a_1, a_2). Here we used the form of the Jacobian for the coordinate system on the stream tube defined by the map

$$(a_1, a_2) \in A_0, \zeta > 0 \to X_f(a_1, a_2, \zeta)$$

to deduce that the mass of a mobile fluid particle is

$$dm(a, \tau) =$$

$$\frac{\partial X_f(a, \tau)}{\partial \zeta} \rho(X_f(a, \tau)) \left(\frac{\partial X_f(a, \tau)}{\partial a_1} \times \frac{\partial X_f(a, \tau)}{\partial a_2}\right) \varepsilon_f(X_f(a, \tau)) da_1 da_2 d\tau .$$

Moreover this relation can be concisely expressed as

$$dm(a, \tau) = dq_M(a) d\tau \qquad (*)$$

where our notation implies that dq_M only depends on a. We can easily see this is true since

$$\int_{\omega} dq_M(X_f(a, \zeta))$$

is independent of ζ for any $\omega \subset \Omega$ by the same reasoning as for $Q_{tube,M}$ above. Physically this has the intuitively appealing meaning that the mass flow through (a_1, a_2) is independent of ζ. As a consequence of this and (*) we get the conclusion that the mass of a mobile fluid particle is only dependent on the incremental length ($d\tau$) and the stream line (a). We stress that dm is not a differential so that $\frac{dm(a, \tau)}{d\tau}$ is *not* a derivative.

Next by this relation (*)

$$Q_{tube,M}\,\Delta\zeta = \int_{\zeta}^{\zeta+\Delta\zeta} d\zeta \int_{A(\tau)} \rho(\xi) U_0(\xi)\, dA(\xi) = \int_{V(\zeta,\Delta\zeta)} dm(x)$$

so that we see that $X_f^{tube}(A_0, \zeta)$ is the limit of the points of gravities of layers around $A(\zeta)$ as the layer thickness tends to zero.

We will now show , as a final point of the hydraulic part , that the point of gravity so defined follows a trajectory defined by tangency to the representative pore velocity U_f^{tube}. With the results already established this is an easy matter. In fact since dq_M only depends on a we differentiate the expression for $X_f^{tube}(A_0, \zeta)$ under the integral sign and use (A.1) to obtain

$$\frac{dX_f^{tube}(A_0, \zeta)}{d\zeta} = \frac{1}{Q_{tube,M}} \int_{\Omega} \frac{dX_f(a, \zeta)}{d\zeta} dq_M(a_1, a_2) = U_f^{tube}(\zeta)$$

which is what we wanted to show.

Turning to the transport of solutes in this stream tube we want to express the mass balance for the volume $V(\zeta, \Delta\zeta)$ introduced above. First, the amount of dissolved substance in this volume is

$$\int_{V(\zeta,\Delta\zeta)} C^i_{f,M}(x)\varepsilon_f(x)\rho(x)dV(x) = \int_{V(\zeta,\Delta\zeta)} C^i_{f,M}(x)dm(x) =$$

$$\int_{\zeta}^{\zeta+\Delta\zeta} d\tau \int_{A(\tau)} C^i_{f,M}(\xi)\, dq_M(\xi) d\tau = Q_{tube,M} \int_{\zeta}^{\zeta+\Delta\zeta} C^{i,tube}_{f,M}(\tau) d\tau$$

where $C^i_{f,M}$ denotes an intrinsic phase average [1]of mass based concentration in the mobile fluid and we have implicitly defined

$$C^{i,tube}_{f,M}(\zeta) = \int_{A(\zeta)} C^i_{f,M}(\xi) \frac{dq_M(\xi)}{Q_{tube,M}} \qquad \text{(A.2)}$$

which is an effective stream tube concentration as an intrinsic phase average.

To continue, the convective flux through $A(\zeta)$ is

---

[1]When discussing continuum descriptions of porous media one uses different averaged quantities. Taking an elementary volume V we define a phase average of a quantity Q defined in a part of the porous media Ω_f as $\frac{1}{V}\int_{V\cap\Omega_f} Q dV$ whereas an intrinsic average is defined as $\frac{1}{V\cap\Omega_f}\int_{V\cap\Omega_f} Q dV$. See for instance /A-1, p. 45/ although he does not use this nomenclature.

$$\int_{A(\zeta)} C^i_{f,M}(\xi)\rho(\xi)U_0(\xi)dA(\xi) = \int_{A(\zeta)} C^i_{f,M}(\xi)dq_M(\zeta) = Q_{tube,M}\, C^{i,tube}_{f,M}(\zeta)$$

So far we have not done any approximations. However to treat the dispersive flux we must unfortunately make some serious approximations. The dispersive flux through $A(\zeta)$ is written as

$$-\int_{A(\zeta)} [D](\xi)\nabla\left(\varepsilon_f(\xi)\rho(\xi)C^i_{f,M}(\xi)\right)dA(\xi)$$

where $[D]$ denotes the dispersion tensor with respect to a phase average of volume based concentration. Now we neglect the transversal dispersion which in mathematical language may be stated as

$$-\int_{A(\zeta)} [D](\xi)\nabla\left(\varepsilon_f(\xi)\rho(\xi)C^i_{f,M}(\xi)\right)dA(\xi) \approx$$

$$-\int_{A(\zeta)} D_L(\xi)\frac{\nabla\left(\varepsilon_f(\xi)\,\rho(\xi)C^i_{f,M}(\xi)\right)U_0(\xi)}{\|U_0(\xi)\|^2}U_0(\xi)dA(\xi)$$

where D_L is the longitudinal dispersion coefficient. This approximation is the most serious one in this analysis, it implies also that the dispersive flux through the stream tube boundary is zero, which we use later on when we set up the mass balance equation for $V(\zeta,\ \zeta + \Delta\zeta)$. The subsequent approximations are, save for one which neglects the variation of density times porosity compared to the variation of concentration, of the type replacing integrands with their averages, which may always be justified taking the stream tube sufficiently narrow.

To continue we neglect $\nabla[\varepsilon_f(\xi)\rho(\xi)]$ [1] to obtain

$$-\int_{A(\zeta)} D_L(\xi)\frac{\nabla\left(C^i_{f,M}(\xi)\right)U_f(\xi)}{\|U_f(\xi)\|^2}dq_M(\xi),$$

approximate the dispersion coefficient with its average and pore velocity by effective Darcy velocity U_f^{tube} so the final result becomes

$$-\frac{\langle D_L\rangle(\zeta)}{\|U_f^{tube}(\zeta)\|^2}\int_{A(\zeta)}\frac{\partial\left[C^i_{f,M}(\xi)\right]}{\partial\zeta}dq_M(\xi) = -\langle D_L\rangle(\zeta)\frac{Q_{tube,M}}{\|U_f^{tube}(\zeta)\|^2}\frac{\partial}{\partial\zeta}C^{i,tube}_{f,M}(\zeta)$$

where the last step follows as above from the fact that $dq_M(\xi)$ is independent of ζ. In fact

---

[1] To really see what the approximation is we write it as $\frac{\nabla\varepsilon_f\rho}{\varepsilon_f\rho} << \frac{\nabla C^i_{f,M}}{C^i_{f,M}}$.

$$\frac{\partial}{\partial\zeta}\int_{A(\zeta)} C^i_{f,M}(\xi)\,dq_M(\xi) = \int_{\Omega}\frac{\partial}{\partial\zeta}C^i_{f,M}(X_f(a,\zeta))\,dq_M(a) = \int_{A(\zeta)}\frac{\partial}{\partial\zeta}C^i_{f,M}(\xi)\,dq_M(\xi).$$

The exchange term ${w_M}^i(x)$ defined as the macroscopic flux of substance i per unit weight of mobile water from the flow porosity to the diffusional porosity is simply averaged as

$$\int_{V(\zeta,\Delta\zeta)} {w_M}^i(\xi)\,\rho(\xi)\varepsilon_f(\xi)\,dV(\xi) = \int_{V(\zeta,\Delta\zeta)} {w_M}^i(\xi)\,dm(\xi) =$$

$$\int_{\zeta}^{\zeta+\Delta\zeta} d\tau \int_{A(\tau)} {w_M}^i(\xi)\,dq_M(\xi) \approx Q_{tube,M}\int_{\zeta}^{\zeta+\Delta\zeta} {w_M}^{i,tube}(\tau)\,d\tau$$

where we implicitly have defined

$${w_M}^{i,tube}(\zeta) = \int_{A(\zeta)} {w_M}^i(\xi)\frac{dq_M(\xi)}{Q_{tube,M}}.$$

The last term in the mass balance is the production term due radioactive decay which is treated exactly as the accumulation term to get

$$\int_V \left[-\lambda^i C^i_{f,M}(\xi) + \lambda^{i-1}C^{i-1}_{f,M}(\xi)^i\right]\varepsilon_f(\xi)\rho(\xi)\,dV(\xi) =$$

$$Q_{tube,M}\left[-\lambda^i\int_{\zeta}^{\zeta+\Delta\zeta} C^{i,tube}_{f,M}(\tau)\,d\tau + \lambda^{i-1}\int_{\zeta}^{\zeta+\Delta\zeta} C^{i-1,tube}_{f,M}(\tau)\,d\tau\right].$$

Putting it all together in a mass balance equation for $V(\zeta,\Delta\zeta)$ dividing with $\Delta\zeta$ and letting $\Delta\zeta$ tend to zero we obtain

$$\frac{\partial}{\partial\zeta}\left[\frac{\langle D_L\rangle(\zeta)}{\left\|U_f^{tube}(\zeta)\right\|^2}\frac{\partial}{\partial\zeta}C^{i,tube}_{f,M}(\zeta) - C^{i,tube}_{f,M}(\zeta)\right] - w_M^{i,tube}$$

$$-\lambda^i C^{i,tube}_{f,M}(\zeta) + \lambda^{i-1}C^{i-1,tube}_{f,M}(\zeta) = \frac{\partial C^{i,tube}_{f,M}}{\partial t}.$$

Note again that since we have neglected transversal dispersion we only have to take the dispersive flux through $A(\zeta)$ and $A(\zeta+\Delta\zeta)$ into account.

Now , it is more standard to use volume concentration. The reason for using mass based concentration is of course that the continuity equation holds for mass flux and not volume flux. However in the case of constant density we may just drop the index M

since we only have to multiply through the above equation with the constant density. Hence we write

$$\frac{\partial}{\partial\zeta}\left[\frac{\langle D_L\rangle(\zeta)}{\left\|U_f^{tube}(\zeta)\right\|^2}\frac{\partial}{\partial\zeta}C_f^{i,tube}(\zeta) - C_f^{i,tube}(\zeta)\right] - w^{i,tube}$$

$$- \lambda^i C_f^{i,tube}(\zeta) + \lambda^{i-1} C_f^{i-1,tube}(\zeta) = \frac{\partial C_f^{i,tube}}{\partial t}$$

and

$$C_f^{i,tube}(\zeta) = \int_{A(\zeta)} C_f^i(\xi)\frac{dq(\xi)}{Q_{tube}}.$$

We also define another coordinate system for the stream tube by arc length , z , on the representing stream line that is

$$dz = \left\|U_f^{tube}(\zeta)\right\| d\zeta ,$$

this relation are the same as (3.1). Hence we can write down a third form of the mass balance equation as

$$\left\|U_f^{tube}(\zeta)\right\|\frac{\partial}{\partial z}\left[\frac{\langle D_L\rangle(\zeta)}{\left\|U_f^{tube}(\zeta)\right\|}\frac{\partial}{\partial z}C_f^{i,tube}(\zeta) - C_f^{i,tube}(\zeta)\right] - w^{i,tube}$$

$$- \lambda^i C_f^{i,tube}(\zeta) + \lambda^{i-1} C_f^{i-1,tube}(\zeta) = \frac{\partial C_f^{i,tube}}{\partial t}$$

which is the same as (2.1) after dropping the superscript *tube* and the angle brackets around D_L .

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Appendix B. The Exchange Term

The exchange term arises from the division of the void space into two parts. This division is in principle arbitrary but the point is to chose one of the parts such that the convective transport in it can safely be assumed to be negligible. Thus we chose it to be the microfissures i.e fractures which are orders of magnitude smaller then the main water bearing channels. Denoting this set of micro fissures with Ω_p ,the remaining porosity , the flow porosity ,Ω_f and the mutual boundary between the sets , B we may write the total exchange rate into Ω_p , Φ^i , as

$$\Phi^i = - D_0 \int_B \frac{\partial c^i}{\partial n} dA$$

where the normal of B points out from Ω_f and D_0 is the diffusion coefficient in water. We now propose a simple model for the micro fissures. We assume that at each point β of B there is a finite one dimensional tube of width $dA(\beta)$ and finite length $L(\beta)$. Tubes for different β may have different lengths but are assumed not to intersect.

Let us denote the concentration in the tube at β with $c_p{}^i(\beta, \xi, t)$ where ξ is the linear coordinate in the tube and $0 \le \xi \le L(\beta)$. Then we may write for each tube i.e for each β

$$D(\beta)\frac{\partial^2 c_p^i(\beta, \xi, t)}{\partial \xi^2} - \lambda^i R^i(\beta) c_p^i(\beta, \xi, t) + \lambda^{i-1} R^{i-1}(\beta) c_p^{i-1}(\beta, \xi, t) =$$

$$R^i(\beta)\frac{\partial c_p^i(\beta, \xi, t)}{\partial t}$$

where $D(\beta)$ is some effective diffusion coefficient and $R^i(\beta)$ is some effective retention factor for the one dimensional micro fissure. These effective constants should be understood in the same sense as for instance hydraulic conductivity and could in principle be measured by response methods.

Natural boundary conditions are

$$c_p^i(\beta, \xi, t)\Big|_{\xi=0} = c_f^i(\beta, t)$$

$$\frac{\partial c_p^i(\beta, \xi, t)}{\partial \xi}\Bigg|_{\xi=L(\beta)} = 0$$

where and the part of the exchange rate into Ω_p corresponding to this tube is written

$$d\Phi^i(\beta) = - D_0 \frac{\partial c_p^i(\beta, \xi, t)}{\partial \xi}\Bigg|_{\xi=0} dA(\beta).$$

Here $c_f^i(\beta, t)$ signifies the concentration in the water bearing fracture at the mouth of the micro fissure and D_0 denotes ordinary diffusion coefficient in water.

For technical reasons, that will be obvious to the reader in a short while, we switch to the coordinate $\xi = \frac{L(\beta)}{\langle L\rangle(z)}x$ where $\langle L\rangle(z)$ denotes the volume average of the micro fissure depths i.e

$$\langle L\rangle(z) = \frac{1}{|V(z)\cap B|}\int_{V(z)\cap B} L(\beta)dA(\beta) \tag{B.1}$$

and obtain after some rearrangements

$$\frac{D_0\langle L\rangle(z)}{L(\beta)}\frac{\partial^2 c_p^i(\beta, x, t)}{\partial x^2} - \lambda^i\frac{D_0 L(\beta)}{D(\beta)\langle L\rangle(z)}R^i(\beta)c_p^i(\beta, x, t) +$$

$$\lambda^{i-1}\frac{D_0 L(\beta)}{D(\beta)\langle L\rangle(z)}R^{i-1}(\beta)c_p^{i-1}(\beta, x, t) = R^i(\beta)\frac{D_0 L(\beta)}{D(\beta)\langle L\rangle(z)}\frac{\partial c_p^i(\beta, x, t)}{\partial t}$$

(B.2)

$$c_p^i(\beta, x, t)\Big|_{x=0} = c_f^i(\beta, t)$$

$$\frac{\partial c_p^i(\beta, x, t)}{\partial x}\Big|_{x=\langle L\rangle(z)} = 0.$$

Now in order to find an expression for the macroscopic exchange term we must average these equations over a volume , say $V(z)$. This results in the equation

$$\frac{\partial^2}{\partial x^2}\int_{V(z)\cap B}\frac{D_0\langle L\rangle(z)}{L(\beta)}c_p^i(\beta, x, t)dA(\beta) -$$

$$\lambda^i\int_{V(z)\cap B}\frac{D_0 L(\beta)}{D(\beta)\langle L\rangle(z)}R^i(\beta)c_p^i(\beta, \xi, t)dA(\beta) +$$

$$\lambda^{i-1}\int_{V(z)\cap B}\frac{D_0 L(\beta)}{D(\beta)\langle L\rangle(z)}R^{i-1}(\beta)c_p^{i-1}(\beta, x, t)dA(\beta) =$$

$$\frac{\partial}{\partial t}\int_{V(z)\cap B}\frac{D_0 L(\beta)}{D(\beta)\langle L\rangle(z)}R^i(\beta)c_p^i(\beta, \xi, t)dA(\beta) \tag{B.3}$$

and the boundary conditions

$$\int_{V(z)\cap B} c_p^i(\beta, x, t)\,dA(\beta)\Big|_{x=0} = \int_{V(z)\cap B} c_f^i(\beta, t)\,dA(\beta)$$

$$\frac{\partial}{\partial x}\int_{V(z)\cap B} c_p^i(\beta, x, t)\,dA(\beta)\Big|_{x=\lfloor L\rfloor(z)} = 0.$$

We want to express the boundary condition at $x = 0$ in terms of a volume average. In order to achieve this we assume that

$$\frac{1}{|V(z)\cap B|}\int_{V(z)\cap B} c_f^i(\beta, t)\,dA(\beta) \approx \frac{1}{|V(z)\cap \Omega_f|}\int_{V(z)\cap \Omega_f} c_f^i(y, t)\,dV(y) = C_f^i(z, t)$$

i.e. that there is little difference between the volume averaged - and the surface averaged concentrations. This assumption seems reasonable even if the we note that the surface average is taken over the micro fissure mouths only. Introducing the macroscopic micro fissure concentration $C_p^i(z, x, t)$ as

$$C_p^i(z, x, t) = \frac{1}{|V(z)\cap B|}\int_{V(z)\cap B} c_p^i(\beta, x, t)\,dA(\beta) \tag{B.4}$$

we can write the boundary conditions as

$$C_p^i(z, x, t)\Big|_{x=0} = C_f^i(z, t) \tag{B.5}$$

$$\frac{\partial}{\partial x} C_p^i(z, x, t)\Big|_{x=\lfloor L\rfloor(z)} = 0. \tag{B.6}$$

The crux then is , as often when trying to deduce averaged equations , the product terms

$$\int_{V(z)\cap B} \frac{D_0\lfloor L\rfloor(z)}{L(\beta)} c_p^i(\beta, x, t)\,dA(\beta),$$

$$\int_{V(z)\cap B} \frac{D_0 L(\beta)}{D(\beta)\lfloor L\rfloor(z)} R^i(\beta) c_p^i(\beta, \xi, t)\,dA(\beta) \qquad i = 1,2,...N\ .$$

If we assume that $\frac{D_0\lfloor L\rfloor(z)}{L(\beta)}$ and $\frac{D_0 L(\beta)}{D(\beta)\lfloor L\rfloor(z)} R^i(\beta)$ $i = 1,2,...N$ are approximately constant or include some assumption of uncorrelation we obtain the equation

$$D_e \frac{\partial^2}{\partial x^2} C_p^i(z,x,t) - \lambda^i R_e^{\ i} C_p^i(z,x,t) +$$

$$\lambda^{i-1} R_e^{\ i-1} C_p^{i-1}(z,x,t) = R_e^{\ i} \frac{\partial}{\partial t} C_p^i(z,x,t) \qquad \text{(B.7)}$$

where we have defined the effective quantities,

$$D_e(z) = \frac{\varepsilon_p(z)}{|V(z) \cap B|} \int_{V(z) \cap B} \frac{D_0 \langle L \rangle(z)}{L(\beta)} dA(\beta) \qquad \text{(B.8)}$$

and

$$R_e^{\ i}(z) = \frac{\varepsilon_p(z)}{|V(z) \cap B|} \int_{V(z) \cap B} \frac{D_0 L(\beta)}{D(\beta) \langle L \rangle(z)} R^i(\beta) dA(\beta) \quad i = 1,2,...N \qquad \text{(B.9)}$$

with the boundary conditions (B.5) and (B.6). These effective quantities may also be defined without the factor $\varepsilon_p(z)$ but in this way they allude to the total area of the boundary of the flow porosity, $\partial\Omega_f$.

Of course the assumption of uncorrelation is the favored one but it is difficult to assess. Regard for example the first term of (B.3) and the following heuristic reasoning. It is clear that for a given point x and time t a large value of $L(\beta)$ will tend to produce a low value of the concentration if the matrix porosity is recharging and the other way around if the matrix porosity is decharging. The effect of this coupling thus seems to be nullified if the volume $V(z)$ is sufficiently large to contain several locations with different recharge/discharge at each time. To even more complicate the picture there is also a coupling from $L(\beta)$ via c_f^i to c_p^i which is even more difficult to understand properly. So even if lack of knowledge is not a good reason for an assumption at least this reasoning shows that the assumption of uncorrelation is not easy to refute in particular if the averaging volume $V(z)$ is large.

Finally the macroscopic exchange term can then be written

$$-w^i(z) = \frac{1}{|V(z) \cap \Omega_f|} \int_{V(z) \cap B} \frac{D_0 \langle L \rangle(z)}{L(\beta)} \frac{\partial}{\partial x} c_p^i(\beta,x,t)\Big|_{x=0} dA(\beta) \approx$$

$$\frac{|V(z) \cap B|}{\varepsilon_p(z) |V(z) \cap \Omega_f|} D_e \frac{\partial}{\partial x} C_p^i(z,x,t)\Big|_{x=0} \approx a(z) D_e(z) \frac{\partial}{\partial x} C_p^i(z,x,t)\Big|_{x=0}$$

where we have introduced some more notation in defining the total surface area of the boundary of the flow porosity per unit volume of mobile fluid, $a(z)$, by

$$a(z) = \frac{|V(z) \cap B|}{\varepsilon_p(z) |V(z) \cap \Omega_f|}. \qquad \text{(B.10)}$$

Now we want to perform an stream tube averaging of this. That is of course just to use the definition from Appendix A i.e

$$w^{i,tube}(\zeta) = \int_{A(\zeta)} w^i(\xi) \frac{dq(\xi)}{Q_{tube}}$$

and to make the necessary assumption that $\alpha(z)$ and $D_e(z)$ do not vary to much over the stream tube cross section so as to obtain

$$w^{i,tube}(\zeta) = -\alpha(\zeta) D_e(\zeta) \frac{\partial}{\partial x} C_p^{i,tube}(\zeta, x, t)\Big|_{x=0} \qquad \text{(B.11)}$$

where ζ is as in Appendix A the travel time coordinate along the stream tube and

$$C_p^{i,tube}(\zeta, x, t) = \int_{A(\zeta)} C_p^i(\xi, x, t) \frac{dq(\xi)}{Q_{tube}}. \qquad \text{(B.12)}$$

Appendix C. Analytical Solution

C.1 Development of the Solution

The equation for $\tilde{C}_p^i$ becomes after transforming (3.11) and using the initial conditions

$$\frac{d^2\tilde{C}_p^i}{dx^2} - \frac{R^i}{D_e}(s + \lambda^i)\tilde{C}_p^i = -\frac{R^{i-1}}{D_e}\lambda^{i-1}\tilde{C}_p^{i-1} \quad . \tag{C.1}$$

Similarly the boundary conditions (3.17) - (3.18) transform to

$$\left.\frac{d\tilde{C}_p^i}{dx}\right|_{x=x_0} = 0$$

$$\left.\tilde{C}_p^i(x, \zeta, s)\right|_{x=0} = \tilde{C}_f^i(\zeta, s). \tag{C.2}$$

The general solution of the corresponding homogeneous equation is

$$A\cosh(h_i(s)x) + B\sinh(h_i(s)x)$$

where $h_i(s)$ is the principal branch of $(\frac{R^i}{D_e}(s + \lambda^i))^{1/2}$ unless of course $s = -\lambda^i$ but this is a case of no importance. For later use we name the domain of holomorphy of $h_i(s)$ to Ω_i. Thus Ω_i denotes the complex plane cut from infinity to $-\lambda^i$ along the negative real axis see Figure C.1. Now invoking the boundary conditions we easily obtain the solution to the homogeneous equation as

$$H_p^i(x, \zeta, s) = \tilde{C}_f^i(\zeta, s)\frac{\cosh(h_i(s)(x_0 - x))}{\cosh(h_i(s)x_0)}.$$

This is of course obtained under the assumption that

$$h_i(s)x_0 \neq \pi i + n2\pi i \qquad n \in Z$$

which is the same thing as to say that the boundary value problem (C.1) - (C.2) is well set i.e. that the homogeneous problem (zero right hand side and zero boundary conditions) does

not have non -trivial solutions. This assumption however does always hold if $s \in \Omega_i$ which we shall always assume.

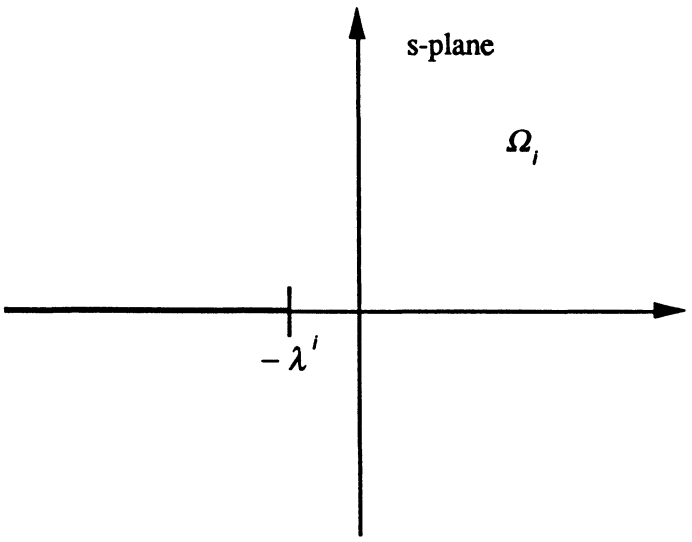

Figure C.1. The domain of holomorphy of $h_i(s)$, Ω_i.

Now we put

$$H_p^i(x, \zeta, s) + u_i(x, \zeta, s) = \tilde{C}_p^i(x, \zeta, s)$$

then $u_i(x, \zeta, s)$ satisfies

$$\frac{d^2 u_i}{dx^2} - h_i(s)^2 u_i = -\frac{R^{i-1}}{D_e}\lambda^{i-1}\tilde{C}_p^{i-1}$$

with homogeneous boundary conditions. Referring to for instance /C-5/, p 53, we infer that if the problem is well set then there the exist a Greens function $G_p^i(x, \xi)$ for this differential equation indeed

$$G_p^i(x, \xi, s) = \begin{cases} \dfrac{-\cosh(h_i(s)(\xi - x_0))\sinh(h_i(s)x)}{h_i(s)\cosh(h_i(s)x_0)} & 0 \le x \le \xi \\ \dfrac{-\cosh(h_i(s)(x - x_0))\sinh(h_i(s)\xi)}{h_i(s)\cosh(h_i(s)x_0)} & \xi \le x \le x_0 \end{cases} \qquad \text{(C.3)}$$

and

$$\tilde{C}_p^i(x, \xi) = -\frac{R^{i-1}}{D_e}\lambda^{i-1}\int_0^{x_0} G_p^i(x, \xi, s) C_p^{i-1}(\xi, \zeta, s)\, d\xi + H_p^i(x, \zeta, s).$$

We may write this in a more compact way if we define the integral operator K_p^i by

$$K_p^i \alpha = -\frac{R^{i-1}}{D_e}\lambda^{i-1}\int_0^{x_0} G_p{}^i(x,\ \xi,\ s)\alpha(\xi)d\xi$$

as

$$\tilde{C}_p^i = K_p^i C_p^{i-1} + H_p^i. \tag{C.4}$$

Iterating this we can express $\tilde{C}_p^n$ in terms of $\tilde{C}_f^j$ $j=1,...n$ as

$$\tilde{C}_p^n = \sum_{j=1}^{n} \tilde{C}_f^j \prod_{l=j+1}^{n} K_p^l h_p^j \tag{C.5}$$

where

$$h_p^i(x,\ s) = \frac{\cosh(h_i(s)(x_0 - x))}{\cosh(h_i(s)x_0)}$$

and an empty product is defined to be equal one.

Next, transforming (3.10) , (3.15) - (3.16) and the taking the initial condition (3.14) into account the equation for $\tilde{C}_f^i$ becomes

$$\frac{d^2\tilde{C}_f^i}{d\zeta^2} - \frac{Pe}{t_w}\frac{d\tilde{C}_f^i}{d\zeta} - \frac{Pe}{t_w}(s + \lambda^i)\tilde{C}_f^i + \frac{Pe}{t_w}aD_e\frac{d\tilde{C}_p^i}{dx}\bigg|_{x=0} = -\frac{Pe}{t_w}\lambda^{i-1}\tilde{C}_f^{i-1} \tag{C.6}$$

with boundary conditions

$$\lim_{\zeta\to\infty} \tilde{C}_f^i(\zeta,\ s) = 0 \tag{C.7}$$

and

$$Q_{sub}\left[\tilde{C}_f^i(\zeta,\ s) - \frac{t_w}{Pe}\frac{d\tilde{C}_f^i}{d\zeta}(\zeta,\ s)\right]_{\zeta=0} = \tilde{F}_{in}^i(s). \tag{C.8}$$

Using the solution (C.4) for $\tilde{C}_p^i$ previously obtained we have

$$\left.\frac{\tilde{C}_p^{\,i}(x,\xi)}{dx}\right|_{x=0} = -\frac{R^{i-1}}{D_e}\lambda^{i-1}\int_0^{x_0}\left.\frac{\partial G_p^i}{\partial x}(x,\xi)\right|_{x=0}\tilde{C}_p^{\,i-1}(\xi,\zeta,s)d\xi -$$

$$\tilde{C}_f^{\,i}(\zeta,s)\tanh(h_i(s)x_0)h_i(s)$$

and hence we obtain an equation solely in $\tilde{C}_f^{\,i}$

$$\frac{d^2\tilde{C}_f^{\,i}}{d\zeta^2} - \frac{Pe}{t_w}\frac{d\tilde{C}_f^{\,i}}{d\zeta} - \frac{Pe}{t_w}\left[(s+\lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right]\tilde{C}_f^{\,i} =$$

$$-\frac{Pe}{t_w}\lambda^{i-1}\left[\tilde{C}_f^{\,i-1} - aR^{i-1}\int_0^{x_0}\left.\frac{\partial G_p^i}{\partial x}(x,\xi)\right|_{x=0}\tilde{C}_p^{\,i-1}(\xi,\zeta,s)d\xi\right].$$

In analogy with the $\tilde{C}_p^{\,i}$-equation we first study the homogeneous equation. It is an easy consequence of the argument principle that the characteristic polynomial i.e

$$P(z) = z^2 - \frac{Pe}{t_w}z - \frac{Pe}{t_w}\left[(s+\lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right]$$

has precisely one root with strictly negative real part and one root with strictly positive real part if and only if

$$\frac{Pe}{t_w}\mathrm{Re}\left[(s+\lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right] +$$

$$\left(\mathrm{Im}\left[(s+\lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right]\right)^2 > 0.$$

This can be expressed in a more compact way if we define the set

$$D = \left\{ z : \frac{Pe}{t_w}x + y^2 > 0 \right\}$$

and the function holomorphic in Ω_i

$$z = F_i(s) = (s+\lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)$$

as

$$s \in F_i^{-1}(D).$$

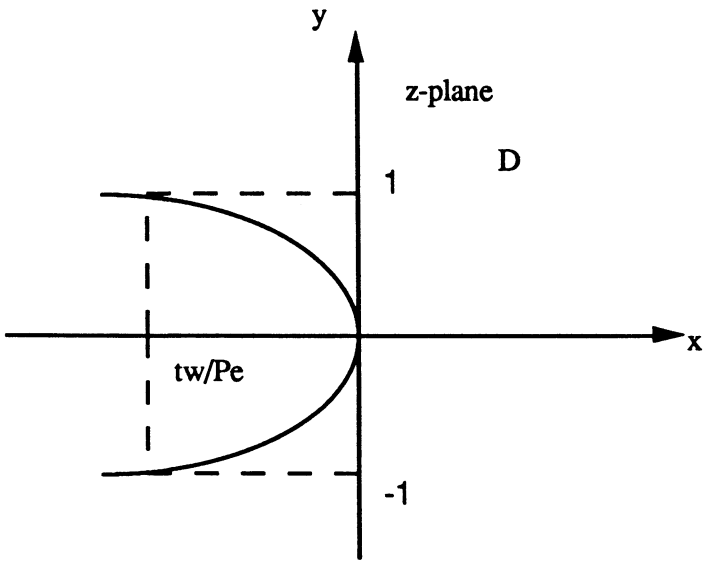

Figure C.2. The definition of D.

Proposition 1. The homogeneous $\tilde{C}_f^i$ -equation has a unique solution satisfying the boundary conditions if and only if $s \in F_i^{-1}(D) \cap \Omega_i$.

Proof. First let us assume that $s \in F_i^{-1}(D) \cap \Omega_i$. It is easy to write down the solution to the homogeneous equation. Letting $f_i(s)$ denote the unique root of $P(z)$ with negative real part we have

$$H_f^i(\zeta, s) = A_i e^{f_i(s)\zeta}$$

where A_i is determined from

$$Q_{tube}\left[1 - \frac{t_w}{Pe} f_i(s)\right] A_i = \tilde{F}_{in}^i(s)$$

i.e

$$A_i = \frac{\tilde{F}_{in}^i(s)}{Q_{tube}\left[1 - \frac{t_w}{Pe} f_i(s)\right]} .$$

Note that this is well defined since $f_i(s)$ has negative real part.

Secondly if $s \notin F_i^{-1}(D)$ there are two cases either both roots of the characteristic polynomial has positive real parts and then there is no solution satisfying the boundary condition at infinity or both roots has negative real parts thus producing infinitely many solutions to the problem.

Let us continue with

Lemma 1. $f_i(s)$ is holomorphic, that is analytic and single valued in $F_i^{-1}(D) \cap \Omega_i$.

Proof. The function

$$P(z, s) = z^2 - \frac{Pe}{t_w} z - \frac{Pe}{t_w}\left[(s + \lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right]$$

is analytic in $C \times \Omega_i$ (since $h_i(s)$ maps Ω_i onto the open right half-plane and tanh has all its poles on the imaginary axis). From Proposition 1 we know that for each point $s_0 \in F_i^{-1}(D) \cap \Omega_i$ there exist a z_0 such that

$$\mathrm{Re}\, z_0 < 0 \qquad \& \qquad P(z_0, s_0) = 0.$$

Now, since

$$\mathrm{Re}\left.\frac{\partial P}{\partial z}\right|_{z=z_0} = \mathrm{Re}(2z_0 - \frac{Pe}{t_w}) < 0$$

it follows from the implicit function theorem /C-3/, p. 24 that there exist a function $z(s)$ and a neighborhood U_0 of s_0 such that

(i) $z(s)$ is analytic in U_0
(ii) $\mathrm{Re}\, z(s) < 0$ in U_0
(iii) $P(z(s), s) = 0$ in U_0

Since $z(s)$ is unique we see that an analytic continuation must give back a single valued function namely $f_i(s)$.

Here it would be appropriate to try and gain some more grip on the domain of holomorphy $F_i^{-1}(D) \cap \Omega_i$ of $f_i(s)$. In particular in order for the obtained solution of the homogeneous $\tilde{C}_f^i$-equation to be a Laplace transform it has to be holomorphic to the left of some real number σ_0. This is possible to prove at this stage, however we defer this to a later paragraph. Instead we continue the development by finding the full solution of the $\tilde{C}_f^i$-equation.

As in the previously solved $\tilde{C}_p^i$-equation we put

$$\tilde{C}_f^i(\zeta, s) = v^i(\zeta, s) + H_f^i(\zeta, s)$$

then $v^i(\zeta, s)$ satisfies

$$\frac{d^2v^i}{d\zeta^2} - \frac{Pe}{t_w}\frac{dv^i}{d\zeta} - \frac{Pe}{t_w}\left[(s + \lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right]v^i =$$

$$-\frac{Pe}{t_w}\lambda^{i-1}\left[\bar{C}_f^{\,i-1} - aR^{i-1}\int_0^{x_0}\frac{\partial G_p^i}{\partial x}(x,\xi)\Big|_{x=0}\bar{C}_p^{\,i-1}(\xi,\zeta,s)d\xi\right]$$

with homogeneous boundary conditions

$$\left[v^i(\zeta,s) - \frac{t_w}{Pe}\frac{dv^i}{d\zeta}(\zeta,s)\right]\Big|_{\zeta=0} = 0$$

$$\lim_{\zeta\to\infty} v^i(\zeta,s) = 0.$$

Here we cannot refer to simple theorems on existence of Greens functions since this is a singular boundary value problem in view of the semi infinite interval. Moreover the kind of boundary condition at infinity given above does not always result in well posed problems /C-2/, p495. Instead we will in fact construct a solution by hand utilizing the standard construction of a Greens function and then show that the resulting function has all the desired properties.

To that end we simplify the notation and study

$$v'' + pv' + qv = f$$
$$v + cv'\big|_{\zeta=0} = 0$$
$$\lim_{\zeta\to\infty} v(\zeta) = 0$$

where p is a real constant less than zero and q is an arbitrary complex number. We construct a Greens function with the aid of two solutions of the homogeneous differential equation. One of these should satisfy the first boundary condition i.e

$$v_1 = -(1+\sigma_2)e^{r_1\zeta} + (1+\sigma_1)e^{r_2\zeta}$$

and the other should satisfy the second boundary condition

$$v_2 = e^{r_1\zeta}.$$

Here r_1 and r_2 are the roots of the characteristic polynomial and we assume that $\mathrm{Re}(r_1) < 0$ and $\mathrm{Re}(r_2) > 0$. We know that a good guess for a Greens function is

$$G(\zeta,\eta) = \begin{cases} \dfrac{v_1(\zeta)v_2(\eta)}{W(\zeta)} & \text{if } 0 \le \zeta \le \eta \\ \dfrac{v_1(\eta)v_2(\zeta)}{W(\zeta)} & \text{if } \eta < \zeta \end{cases}$$

where W is the Wronskian defined by

$$W(\zeta) = v_1(\zeta)v_2'(\zeta) - v_2(\zeta)v_1'(\zeta).$$

Lemma 2. If f is continuous on the positive real axis and moreover $f(\eta) \in O(e^{\varepsilon\eta})$ for some $\varepsilon < 0$ then

$$v(\zeta) = \int_0^{\infty} G(\zeta, \eta) f(\eta) d\eta$$

solves the inhomogeneous differential equation and $v(\eta) \in O(e^{\varepsilon'\eta})$ where $\varepsilon' = \max(\varepsilon, \mathrm{Re}(r_1))$.

Proof. First the Wronskian is easily calculated explicitly in fact

$$W(\zeta) = (1 + \sigma_1)e^{(r_1 + r_2)\zeta}(r_1 - r_2)$$

and thus

$$G(\zeta, \eta) = \begin{cases} \left[e^{r_2(\zeta - \eta)} - \dfrac{1 + \sigma_2}{1 + \sigma_1} e^{r_1\zeta - r_2\eta}\right] \dfrac{1}{r_1 - r_2} & 0 \le \zeta \le \eta \\ \left[e^{r_1(\zeta - \eta)} - \dfrac{1 + \sigma_2}{1 + \sigma_1} e^{r_1\zeta - r_2\eta}\right] \dfrac{1}{r_1 - r_2} & \eta < \zeta \end{cases} . \qquad \text{(C.9)}$$

Explicitly then v is given by

$$v(\zeta) = \frac{e^{r_1\zeta}}{r_1 - r_2}\int_0^{\zeta} e^{-r_1\eta} f(\eta) d\eta + \frac{e^{r_2\zeta}}{r_1 - r_2}\int_{\zeta}^{\infty} e^{-r_2\eta} f(\eta) d\eta -$$

$$\frac{e^{r_1\zeta}}{r_1 - r_2}\frac{1 + \sigma_2}{1 + \sigma_1}\int_0^{\infty} e^{-r_2\eta} f(\eta) d\eta . \qquad \text{(C.10)}$$

Note that the generalized integrals exist since we have assumed that $\mathrm{Re}(r_2) > 0$ and $f(\eta) \in O(e^{\varepsilon\eta})$. Upon differentiating, where we use the hypothesis that f is continuous we obtain

$$\frac{dv(\zeta)}{d\zeta} = \frac{r_1 e^{r_1\zeta}}{r_1 - r_2}\int_0^{\zeta} e^{-r_1\eta} f(\eta) d\eta + \frac{r_2 e^{r_2\zeta}}{r_1 - r_2}\int_{\zeta}^{\infty} e^{-r_2\eta} f(\eta) d\eta -$$

$$\frac{r_1 e^{r_1\zeta}}{r_1 - r_2}\frac{1 + \sigma_2}{1 + \sigma_1}\int_0^{\infty} e^{-r_2\eta} f(\eta) d\eta$$

for the first derivative and

$$\frac{d^2v(\zeta)}{d\zeta^2} = \frac{r_1^2 e^{r_1\zeta}}{r_1 - r_2}\int_0^{\zeta} e^{-r_1\eta} f(\eta)d\eta + \frac{r_2^2 e^{r_2\zeta}}{r_1 - r_2}\int_{\zeta}^{\infty} e^{-r_2\eta} f(\eta)d\eta -$$
$$\frac{r_1^2 e^{r_1\zeta}}{r_1 - r_2}\frac{1+cr_2}{1+cr_1}\int_0^{\infty} e^{-r_2\eta} f(\eta)d\eta + f(\zeta)$$

for the second so that clearly

$$\frac{d^2v(\zeta)}{d\zeta^2} + p\frac{dv(\zeta)}{d\zeta} + qv(\zeta) = f(\zeta).$$

Next we verify that the proposed solution also satisfies the boundary conditions. By hypothesis $|f(\eta)| \le Ce^{\varepsilon\eta}$ for some positive constants C and ε and for η large enough. Hence , as is easy to see

$$\left|\frac{e^{r_1\zeta}}{r_1 - r_2}\int_0^{\zeta} e^{-r_1\eta} f(\eta)d\eta\right| \le e^{\mathrm{Re}(r_1)\zeta}\left(C_1 + C_2 e^{-\mathrm{Re}(r_1)\zeta + \varepsilon\zeta}\right) \in O(e^{\varepsilon\zeta}).$$

Similarly for ζ large enough

$$\left|\frac{e^{r_2\zeta}}{r_1 - r_2}\int_{\zeta}^{\infty} e^{-r_2\eta} f(\eta)d\eta\right| \le C_3 e^{\mathrm{Re}(r_2)\zeta}\left(e^{-\mathrm{Re}(r_2)\zeta + \varepsilon\zeta}\right) \in O(e^{\varepsilon\zeta})$$

and the last term of (C.10) clearly belongs to $O(e^{\varepsilon\zeta})$ so that the assertion of the Lemma is proved save for the boundary condition at zero. Now this is an easy matter since

$$v(\zeta) + c\frac{dv(\zeta)}{d\zeta}\bigg|_{\zeta=0} = \frac{1}{r_1 - r_2}\int_0^{\infty} e^{-r_2\eta} f(\eta)d\eta - \frac{1}{r_1 - r_2}\frac{1+cr_2}{1+cr_1}\int_0^{\infty} e^{-r_2\eta} f(\eta)d\eta +$$
$$\frac{cr_2}{r_1 - r_2}\int_0^{\infty} e^{-r_2\eta} f(\eta)d\eta - \frac{cr_1}{r_1 - r_2}\frac{1+cr_2}{1+cr_1}\int_0^{\infty} e^{-r_2\eta} f(\eta)d\eta = 0$$

and we are done.

Now we can apply this Lemma to our $\tilde{C}_f^{\,i}$ –equation. First it is clear that $v^1(\zeta) = 0$ so that $\tilde{C}_f^{\,1} \in O(e^{\mathrm{Re}(f_1(s))\zeta})$. Assume that $\tilde{C}_f^{\,i} \in O(e^{m_i\zeta})$ where $m_i = \max_{0\le j\le i} \mathrm{Re}(f_j(s))$ then the right hand side of the differential equation for v^{i+1} i.e

$$-\frac{Pe}{t_w}\lambda^i\left[\tilde{C}_f^{\,i} - aR^i\int_0^{x_0}\frac{\partial G_p^{i+1}}{\partial x}(x,\xi)\bigg|_{x=0}\tilde{C}_p^{\,i}(\xi,\zeta,s)d\xi\right]$$

is in $O(e^{m_i\zeta})$. To see this we need only to review (C.5). It now follows from the Lemma that ν^{i+1} belongs in $O(e^{m_{i+1}\zeta})$ which a fortiori holds for $\tilde{C}_f^{i+1}$ as well.

By induction we have proved :

Proposition 2. If $s \in \bigcap_{j=1}^{N}\left(F_j^{-1}(D) \cap \Omega_j\right)$, where N is the number of equations , then there is a solution $\tilde{C}_f^i \quad i = 1,2,\ldots N$ of (C.6) - (C.8). Moreover $\tilde{C}_f^i \in O(e^{m_i\zeta})$ where $m_i = \max_{0\le j\le i} \mathrm{Re}(f_j(s))$.

Explicitly , translating the simplified notations used into those of the $\tilde{C}_f^i$ -equations and introducing the notation $f_i^*(s)$ for the root of the characteristic polynomial with positive real part we have for the Greens function (C.9)

$$G_f^i(\zeta,\eta,s) = \begin{cases} \dfrac{1}{f_i(s)-f_i^*(s)} e^{f_i^*(s)(\zeta-\eta)} - \dfrac{f_i(s)}{f_i^*(s)} e^{f_i(s)\zeta - f_i^*(s)\eta} & \text{for } 0 \le \zeta \le \eta \\ \dfrac{1}{f_i(s)-f_i^*(s)} e^{f_i(s)(\zeta-\eta)} - \dfrac{f_i(s)}{f_i^*(s)} e^{f_i(s)\zeta - f_i^*(s)\eta} & \text{for } \eta \le \zeta \end{cases}$$

and for the solution (C.10)

$$\tilde{C}_f^i(\zeta,s) = -\lambda^{i-1}\frac{Pe}{t_w}\int_0^{\infty} G_f^i(\zeta,\eta,s)\tilde{C}_f^{i-1}(\eta,s)d\eta$$

$$+\lambda^{i-1}\frac{Pe}{t_w}aR^{i-1}\int_0^{\infty} G_f^i(\zeta,\eta,s)\int_0^{x_0}\frac{\partial G_p^i}{\partial x}(x,\xi,s)\Big|_{x=0}\tilde{C}_p^{i-1}(\xi,\eta,s)d\xi d\eta + H_f^i(\zeta,s).$$

Let us introduce the integral operators

$$K_f^i(\alpha(\eta)) = -\lambda^{i-1}\frac{Pe}{t_w}\int_0^{\infty} G_f^i(\zeta,\eta,s)\alpha(\eta)d\eta$$

$$K_\partial^i(\beta(\xi)) = -aR^{i-1}\int_0^{x_0}\frac{\partial G_p^i}{\partial x}(x,\xi,s)\Big|_{x=0}\beta(\xi)d\xi$$

we may then write

$$\tilde{C}_f^i(\zeta,s) = K_f^i\tilde{C}_f^{i-1} + K_f^iK_\partial^i\tilde{C}_p^{i-1} + H_f^i.$$

Now we recall the solution of the $\tilde{C}_p^i$-equation (C.4) and rewrite it using the appearance of the homogeneous solution as

$$\tilde{C}_p^i = K_p^i C_p^{i-1} + \tilde{C}_f^i h_p^i$$

where as before

$$h_p^i(x, \zeta, s) = \frac{\cosh(h_i(s)(x_0 - x))}{\cosh(h_i(s)x_0)}.$$

It is advantageous to write the equations in recursive form i.e express the quantities of label i in the quantities with label i-1. To that end we write in matrix notation

$$\begin{bmatrix} 1 & 0 \\ -h_p^i & 1 \end{bmatrix} \begin{bmatrix} \tilde{C}_f^i \\ \tilde{C}_p^i \end{bmatrix} = \begin{bmatrix} K_f^i & K_f^i K_\partial^i \\ 0 & K_p^i \end{bmatrix} \begin{bmatrix} \tilde{C}_f^{i-1} \\ \tilde{C}_p^{i-1} \end{bmatrix} + \begin{bmatrix} H_f^i \\ 0 \end{bmatrix}$$

and whence upon inverting we get the solution in recursive form as

$$\begin{bmatrix} \tilde{C}_f^i \\ \tilde{C}_p^i \end{bmatrix} = \begin{bmatrix} K_f^i & K_f^i K_\partial^i \\ h_p^i K_f^i & K_p^i + h_p^i K_f^i K_\partial^i \end{bmatrix} \begin{bmatrix} \tilde{C}_f^{i-1} \\ \tilde{C}_p^{i-1} \end{bmatrix} + \begin{bmatrix} H_f^i \\ h_p^i H_f^i \end{bmatrix}.$$

By linearity we see that it is sufficient to study the case

$$\tilde{F}_{in}^m(s) = \begin{cases} 1 & \text{if } m = j \\ 0 & \text{if } m \neq j \end{cases}$$

since any other inflow can be represented as a linear combination of these solutions. Recalling standard transform theory we see that this corresponds to the response of a unit pulse of substance j at time zero. The solutions are denoted $\tilde{C}_f^{i,j}$ and $\tilde{C}_p^{i,j}$ and are thought of as the response in substance i to a unit pulse in substance j. This simplifies the equations above in that we may write

$$\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix} = \begin{bmatrix} K_f^i & K_f^i K_\partial^i \\ h_p^i K_f^i & K_p^i + h_p^i K_f^i K_\partial^i \end{bmatrix} \begin{bmatrix} \tilde{C}_f^{i-1\,j} \\ \tilde{C}_p^{i-1\,j} \end{bmatrix} \qquad i - 1 \geq j$$

$$\begin{bmatrix} \tilde{C}_f^{j,j} \\ \tilde{C}_p^{j,j} \end{bmatrix} = \begin{bmatrix} h_f^j \\ h_p^j h_f^j \end{bmatrix} \tag{C.11}$$

where h_f^j is the same quantity as H_f^j except that the boundary condition at zero is

$$Q_{eq}\left(1-\frac{t_w}{Pe}\frac{\partial}{\partial\zeta}\right)h_f^j\Big|_{\zeta=0}=1.$$

This formula suggests that we can calculate the solution through iteration in fact we have

$$\begin{bmatrix}\tilde{C}_f^{i,j}\\ \tilde{C}_p^{i,j}\end{bmatrix}=\begin{bmatrix}K_f^i & K_f^iK_\partial^i\\ h_p^iK_f^i & K_p^i+h_p^iK_f^iK_\partial^i\end{bmatrix}^{i-j}\begin{bmatrix}h_f^j\\ h_p^jh_f^j\end{bmatrix}\qquad i\geq j. \tag{C.12}$$

The direct calculation using this formula would nescessitate calculation of many integral operators. Fortunately this can be avoided by use of the following three Lemmas.

Lemma 3. $$K_f^n h_f^m=\frac{\lambda^{n-1}}{F_n(s)-F_m(s)}\left[h_f^m(\zeta,s)-h_f^n(\zeta,s)\right]$$

Proof. Define

$$D_f^n=\frac{\partial^2}{\partial\zeta^2}-\frac{Pe}{t_w}\frac{\partial}{\partial\zeta}-\frac{Pe}{t_w}F_n(s)$$

then

$$D_f^nh_f^m=D_f^mh_f^m+\frac{Pe}{t_w}(F_n(s)-F_m(s))h_f^m=\frac{Pe}{t_w}(F_n(s)-F_m(s))h_f^m.$$

We note in passing that this is to say that h_f^m is an eigenvector of D_f^n. Applying K_f^n to this equation we see that

$$K_f^nD_f^nh_f^m=\frac{Pe}{t_w}(F_n(s)-F_m(s))K_f^nh_f^m.$$

Now the right hand side is by definition $-\lambda^{n-1}\frac{Pe}{t_w}$ times the unique solution α of

$$\begin{cases}D_f^n\alpha=D_f^nh_f^m\\ \left(1-\frac{t_w}{Pe}\frac{\partial}{\partial\zeta}\right)\alpha\Big|_{\zeta=0}=0\\ \lim_{\zeta\to-\infty}\alpha(\zeta)=0\end{cases}$$

so that we must have

$$K_f^n D_f^n h_f^m = -\lambda^{n-1}\frac{P_e}{t_w}\left(h_f^m - h_f^n\right)$$

which proves the assertion.

Lemma 4. $K_p^n h_p^m = \frac{R^{n-1}}{D_e}\lambda^{n-1}\frac{1}{h_n^2(s) - h_m^2(s)}\left(h_p^m - h_p^n\right)$.

Proof. This goes in the same style as the previous one. Define $D_p^n = \frac{\partial^2}{\partial x^2} - h_n^2(s)$ then

$$D_p^n h_p^m = \left[D_p^m + h_m^2(s) - h_n^2(s)\right]h_p^m = \left(h_m^2(s) - h_n^2(s)\right)h_p^m .$$

Apply K_p^n on this equality to obtain

$$K_p^n h_p^m = \frac{K_p^n D_p^n h_p^m}{h_m^2(s) - h_n^2(s)} = -\frac{R^{n-1}}{D_e}\lambda^{n-1}\frac{h_p^m - h_p^n}{h_m^2(s) - h_n^2(s)}$$

which was to be proved.

Lemma 5.

$$K_\partial^n h_p^m = \frac{aR^{n-1}}{h_m^2(s) - h_n^2(s)}\left[h_m(s)\tanh(h_m(s)x_0) - h_m(s)\tanh(h_m(s)x_0)\right]$$

Proof. Recall that K_∂^n is defined by

$$K_\partial^i(\beta(\xi)) = -aR^{i-1}\int_0^{x_0}\frac{\partial G_p^i}{\partial x}(x, \xi, s)\Big|_{x=0}\beta(\xi)d\xi$$

thus $-\frac{1}{aR^{n-1}}K_\partial^n h_p^m$ is obtained as $\frac{\partial}{\partial x}\bullet\Big|_{x=0}$ onto the solution α of $D_p^n\alpha = h_p^m$ that is to

$$-\frac{D_e}{R^{n-1}\lambda^{n-1}}K_p^n h_p^m = \frac{h_p^m - h_p^n}{h_m^2(s) - h_n^2(s)}$$

where the last equality follows from the previous Lemma. Now

$$\frac{\partial}{\partial x}h_p^j\Big|_{x=0} = h_j(s)\tanh(h_j(s)x_0)$$

and thus the Lemma follows.

We see that these Lemmas together with the recursion relation (C.11) or (C.12) enables us to develop the influence functions $\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix}$ in terms of the homogeneous solutions $\begin{bmatrix} h_f^k \\ h_p^l h_f^k \end{bmatrix}$ $i \geq k \geq l \geq j$ in fact we have

Proposition 3. We have

$$\tilde{C}_f^{i,j} = \sum_{k=j}^{i} P_{i,j,k}(s) h_f^k(\zeta, s)$$

$$\tilde{C}_p^{i,j} = \sum_{k=j}^{i} \sum_{l=k}^{i} Q_{i,j,k,l}(s) h_f^k(\zeta, s)\, h_p^l(x, s)$$

where $P_{i,j,k}(s)$ and $Q_{i,j,k,l}(s)$ satisfy the recursive relations

$$P_{j,j,j}(s) = Q_{j,j,j,j}(s) = 1$$

$$P_{i,j,k}(s) = \frac{\lambda^{i-1}}{F_i(s) - F_k(s)} \left[P_{i-1,j,k}(s) + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}(s) \left(K_\partial^i h_p^l \right)(s) \right] \qquad k \in [j, i-1]$$

$$P_{i,j,i}(s) = -\sum_{k=j}^{i-1} \frac{\lambda^{i-1}}{F_i(s) - F_k(s)} \left[P_{i-1,j,k}(s) + \sum_{l=j}^{i-1} Q_{i-1,j,k,l}(s) \left(K_\partial^i h_p^l \right)(s) \right]$$

$$Q_{i,j,k,l}(s) = \frac{R^{i-1}}{D_e} \lambda^{i-1} Q_{i-1,j,k,l}(s) \frac{1}{h_i^2(s) - h_l^2(s)} \qquad k, l \in [j, i-1]$$

$$Q_{i,j,k,i}(s) = \frac{\lambda^{i-1}}{F_i(s) - F_k(s)} \left[P_{i-1,j,k}(s) + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}(s) \left(K_\partial^i h_p^l \right)(s) \right]$$

$$- \sum_{l=k}^{i-1} Q_{i-1,j,k,l}(s) \frac{R^{i-1}}{D_e} \lambda^{i-1} \frac{1}{h_i^2(s) - h_l^2(s)} \qquad k \in [j, i-1]$$

$$Q_{i,j,i,i}(s) = -\sum_{k=j}^{i-1} \left[P_{i-1,j,k}(s) + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}(s) \left(K_\partial^i h_p^l \right)(s) \right] \frac{\lambda^{i-1}}{F_i(s) - F_k(s)}$$

Corollary 1. If i is not equal j then

$$\sum_{k=j}^{i} P_{i,j,k}(s) = 0$$

$$\sum_{k=j}^{i}\sum_{l=k}^{i} Q_{i,j,k,l}(s) = 0.$$

Proof of the Proposition. The assertion is trivially true for $i = j$. Assume that the assertion holds for $i - j = N$. Let $i - j = N + 1$ and use (C.11) and the induction assumption to obtain

$$\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix} = \begin{bmatrix} K_f^i & K_f^i K_\partial^i \\ h_p^i K_f^i & K_p^i + h_p^i K_f^i K_\partial^i \end{bmatrix} \begin{bmatrix} \sum_{k=j}^{i-1} P_{i-1,j,k}(s) h_f^k(\zeta, s) \\ \sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i-1,j,k,l}(s) h_f^k(\zeta, s) h_p^l(x, s) \end{bmatrix} =$$

$$\begin{bmatrix} \sum_{k=j}^{i-1} P_{i-1,j,k} K_f^i h_f^k + \sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i-1,j,k,l} K_f^i h_f^k K_\partial^i h_p^l \\ \sum_{k=j}^{i-1} P_{i-1,j,k} h_p^i K_f^i h_f^k + \sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i-1,j,k,l} h_f^k K_p^i h_p^l + \sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i-1,j,k,l} h_p^i K_f^i h_f^k K_\partial^i h_p^l \end{bmatrix}.$$

Now using Lemma 3 and rearranging the first component is easily seen to be equal

$$\sum_{k=j}^{i-1}\left[P_{i-1,j,k} + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}\left(K_\partial^i h_p^l\right)(s)\right]\frac{\lambda^{i-1}}{F_i(s) - F_k(s)} h_f^k(\zeta, s) -$$

$$\left[\sum_{k=j}^{i-1}\frac{\lambda^{i-1}}{F_i(s) - F_k(s)}\left[P_{i-1,j,k} + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}\left(K_\partial^i h_p^l\right)(s)\right]\right] h_f^i(\zeta, s)$$

so that

$$P_{i,j,k} = \begin{cases} \left[P_{i-1,j,k} + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}\left(K_\partial^i h_p^l\right)(s)\right]\frac{\lambda^{i-1}}{F_i(s) - F_k(s)} & j \le k < i \\ -\sum_{k=j}^{i-1}\frac{\lambda^{i-1}}{F_i(s) - F_k(s)}\left[P_{i-1,j,k} + \sum_{l=k}^{i-1} Q_{i-1,j,k,l}\left(K_\partial^i h_p^l\right)(s)\right] & k = i \end{cases}$$

which is the first part of the Proposition. Now utilizing again Lemma 3 and Lemma 4 in the second component above and regrouping we obtain

$$\sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i-1,j,k,l}\frac{R^{i-1}}{D_e}\lambda^{i-1}\frac{1}{h_i^{\,2}(s)-h_l^{\,2}(s)}h_f^k h_p^l +$$

$$\sum_{k=j}^{i-1}\left[P_{i-1,j,k}\frac{\lambda^{i-1}}{F_i(s)-F_k(s)} -\right.$$

$$\left.\sum_{l=k}^{i-1} Q_{i-1,j,k,l}\left[\frac{R^{i-1}}{D_e}\lambda^{i-1}\frac{1}{h_i^{\,2}(s)-h_l^{\,2}(s)} - \frac{\lambda^{i-1}}{F_i(s)-F_k(s)}K_\partial^i h_p^l\right]\right]h_p^i h_f^k -$$

$$\sum_{k=j}^{i-1}\frac{\lambda^{i-1}}{F_i(s)-F_k(s)}\left[P_{i-1,j,k}+\sum_{l=k}^{i-1} Q_{i-1,j,k,l}K_\partial^i h_p^l\right]h_p^i h_f^i$$

which enables us to draw the conclusion

$$Q_{i,j,k,l}=\begin{cases} Q_{i-1,j,k,l}\dfrac{R^{i-1}}{D_e}\lambda^{i-1}\dfrac{1}{h_i^{\,2}(s)-h_l^{\,2}(s)} & j\le k<i-1,\ k\le l<i-1 \\[2ex] P_{i-1,j,k}\dfrac{\lambda^{i-1}}{F_i(s)-F_k(s)} - \displaystyle\sum_{l=k}^{i-1} Q_{i-1,j,k,l}\left[\frac{R^{i-1}}{D_e}\lambda^{i-1}\frac{1}{h_i^{\,2}(s)-h_l^{\,2}(s)} - \right. & \\ \qquad \left.\dfrac{\lambda^{i-1}}{F_i(s)-F_k(s)}K_\partial^i h_p^l\right] & l=i,\ j\le k<i-1 \\[2ex] -\displaystyle\sum_{k=j}^{i-1}\frac{\lambda^{i-1}}{F_i(s)-F_k(s)}\left[P_{i-1,j,k}+\sum_{l=k}^{i-1} Q_{i-1,j,k,l}K_\partial^i h_p^l\right] & l=i,\ k=i \end{cases}$$

which proves the Proposition by induction.

Proof of the Corollary. That $\sum_{k=j}^{i} P_{i,j,k}(s)=0$ follows directly from the form of the recursion relations in the previous Proposition. The second relation follows almost as easily in fact

$$\sum_{k=j}^{i}\sum_{l=k}^{i} Q_{i,j,k,l}=\left(Q_{i,j,i,i}+\sum_{k=j}^{i-1} Q_{i,j,k,i}\right)+\sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i,j,k,l}=$$
$$-\sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i-1,j,k,l}\frac{R^{i-1}}{D_e}\lambda^{i-1}\frac{1}{h_i^{\,2}(s)-h_l^{\,2}(s)}-\sum_{k=j}^{i-1}\sum_{l=k}^{i-1} Q_{i,j,k,l}=0$$

where we also have utilized the relations of the Proposition above.

In order to facilitate the numerical calculation of these relations we note that they can be written in a more efficient form as

$$P_{i,j,i}(s) = -\sum_{k=j}^{i-1} P_{i,j,k}(s)$$

$$Q_{i,j,k,l}(s) = Q_{i-1,j,k,l}(s)\frac{R^{i-1}}{D_e}\lambda^{i-1}\frac{1}{h_i^{\,2}(s) - h_l^{\,2}(s)} \qquad j \le k < i-1,\ k \le l < i-1$$

$$Q_{i,j,k,i}(s) = P_{i,j,k}(s) - \sum_{l=k}^{i-1} Q_{i,j,k,l}(s) \qquad j \le k < i-1$$

$$Q_{i,j,i,i}(s) = P_{i,j,i}(s)$$

Up to this point we have developed the solutions and designed an efficient way to compute them. We have also found the domain in the s -plane where these solutions are well defined and analytic. However one question remains unsettled namely what is the domain of holomorphy of the solutions i.e which is the maximal domain to which we may extend the solutions analytically. In particular this should contain a set $\{s : \mathrm{Re}(s) > \sigma\}$ since the solutions should be Laplace transforms. To answer these questions we open up a new paragraph

C.2 Analytic Continuation of the Solution

We start off by attacking the question of analytic continuation of $f_i(s)$. Referring to the proof of Lemma 1 we know that the branching points of $f_i(s)$ are given precisely by the zeros of

$$\frac{Pe}{4t_w} + \left(s + \lambda^i\right) + aD_e h_i(s)\tanh\left(h_i(s)x_0\right) \qquad s \in \Omega_i .$$

For reasons which will be evident as we proceed we will examine the possibility of solving the slightly more general equation

$$\Gamma(s) = \frac{Pe}{4t_w} + \left(s + \lambda^i\right) + aD_e h_i(s)\tanh\left(h_i(s)x_0\right) = x \qquad s \in \Omega_i \qquad \text{(C.13)}$$

where x a priori is a complex number. Putting $\zeta = h_i(s)x_0$ which transform Ω_i into the right half-plane we obtain instead

$$\Gamma(\zeta) = \frac{Pe}{4t_w} + \frac{D_e}{R^i x_0^{\,2}}\zeta^2 + \frac{aD_e}{x_0}\zeta\tanh(\zeta) = x \qquad \mathrm{Re}(\zeta) > 0 \qquad \text{(C.14)}$$

upon expanding the tanh -function and regrouping we see that this is equivalent to

$$\Gamma_x^*(\zeta) = P(\zeta)e^{\zeta} + P(-\zeta)e^{-\zeta} = 0 \qquad \mathrm{Re}(\zeta) > 0$$

where

$$P(\zeta) = \frac{D_e}{R^i x_0^2}\zeta^2 + \frac{dD_e}{x_0}\zeta + \frac{Pe}{4t_w} - x$$

Now it is an easy consequence of the argumentum principle and some trivial calculations that $P(\zeta)$ has no roots in the open right half plane precisely when x lies in the closed parabola

$$\mathrm{Im}(x)^2 + d^2 D_e R^i \mathrm{Re}(x) \le \frac{Pe}{4t_w} d^2 D_e R^i$$

From this it follows that when x satisfies this condition then $\frac{P(-\zeta)}{P(\zeta)}$ is holomorphic in the right half-plane. Moreover if we also assume that x is real we have on the imaginary axis

$$\left|\frac{P(-\zeta)}{P(\zeta)}\right| = \left|\frac{P(-iy)}{P(iy)}\right| = \left|\frac{\overline{P(iy)}}{P(iy)}\right| = 1$$

since this rational function also tends to 1 as $|z|$ tends to infinity it is easy to conclude from the maximum modulus principle that $\left|\frac{P(-\zeta)}{P(\zeta)}\right| \le 1$ in the right half plane. This implies that there are no roots of Γ^* in the open right half plane. Since Γ^* also is an even function there are also no roots of Γ^* in the left half plane either. This implies that a solution to (C.14) when x is real and less or equal than $\frac{Pe}{4t_w}$ is only possible for a purely imaginary ζ. This can be written as

$$\Gamma^{-1}\left(\left\{w : \mathrm{Im}(w) = 0, \mathrm{Re}(w) \le \frac{P_e}{4t_w}\right\}\right) \subset \{\zeta : \mathrm{Re}(\zeta) = 0\}$$

Now it is an easy matter to analyze $\Gamma(\zeta)$ for purely imaginary values and see that

$$\Gamma\{\zeta : \mathrm{Re}(\zeta) = 0\} = \left\{w : \mathrm{Im}(w) = 0, \mathrm{Re}(w) \le \frac{Pe}{4t_w}\right\}$$

We have found the following rather technical result

Lemma 6.

$$\Gamma^{-1}\left\{w : \mathrm{Im}(w) = 0, \mathrm{Re}(w) \le \frac{Pe}{4t_w}\right\} \subset \{\zeta : \mathrm{Re}(\zeta) = 0\}$$

$$\Gamma\{\zeta : \mathrm{Re}(\zeta) = 0\} = \left\{w : \mathrm{Im}(w) = 0, \mathrm{Re}(w) \le \frac{Pe}{4t_w}\right\}.$$

However from this result we deduce the following important

Corollary 2. $f_i(s)$ has an analytic continuation to Ω_i.

Proof. In fact the above reasoning for $x = 0$ shows that all branch points of $f_i(s)$ is on the imaginary axis in the ζ −plane i.e on the cut from $-\lambda_i$ to infinity in the s -plane. It then follows from the monodromy theorem /C-3/ , p295 or /C-4/ , p. 351 that $f_i(s)$ is holomorphic in Ω_i .

We may also deduce

Corollary 3. $h_f^i(s)$ has an analytic continuation to Ω_i .

Proof. We only need to show that $f_i(s) \neq \frac{Pe}{t_w}$. Now this is easy since by definition $f_i(s)$ satisfies

$$f_i(s)^2 - f_i(s)\frac{Pe}{t_w} - \frac{Pe}{t_w}\left[(s + \lambda^i) + aD_e h_i(s)\tanh(h_i(s)x_0)\right].$$

Hence $f_i(s) = \frac{Pe}{t_w}$ implies $\Gamma(s) = \frac{Pe}{4t_w}$ which cannot happen for $s \in \Omega_i$ in view of Lemma 6

These two corollaries are what we want. However we may draw some more information out of Lemma 6.

Corollary 4. The range of $f_i(s)$ denoted $\Re_f$ and the range of $f_i^*(s)$ denoted $\Re_f^*$ satisfies

$$\left\{w : \mathrm{Im}(w) = 0 \wedge 0 \leq \mathrm{Re}(w) \leq \frac{Pe}{t_w}\right\} \cup \left\{w : \mathrm{Re}(w) = \frac{Pe}{2t_w}\right\} \subset \Re_f \cup \Re_f^*$$

$$\Re_f - \frac{Pe}{2t_w} = -\left(\Re_f^* - \frac{Pe}{2t_w}\right).$$

Note. Both $f_i(s)$ and $f_i^*(s)$ are defined on Ω_i.

Proof. The second equality is just a consequence of the equality $f_i^*(s) + f_i(s) = \frac{Pe}{t_w}$. The first statement is also easily achieved . It follows as in the proof of Corollary 3 that

$$\left(f_i(s) - \frac{Pe}{2t_w}\right)^2 = \frac{Pe}{t_w}\Gamma(s)$$

so knowing that the right hand side does not attain values in the set

$$\left\{w : \mathrm{Im}(w) = 0, \mathrm{Re}(w) \leq \frac{Pe^2}{4t_w^2}\right\}$$

the first statement follows.

Now we have shown that the basis functions $h_f^k(\zeta, s)$, $1 \le k \le N$ where N is the number of equations , can be extended to holomorphic functions in s in $\bigcap_{j=1}^{N} \Omega_i$. This is also trivially true for $h_p^l(x, s)$, $1 \le l \le N$. The main goal of the present section is to extend this to the solutions $\tilde{C}_f^{i,j}(\zeta, s)$, $\tilde{C}_p^{i,j}(\zeta, x, s)$ i.e.

Proposition 4. The influence functions $\tilde{C}_f^{i,j}(\zeta, s)$, $\tilde{C}_p^{i,j}(\zeta, x, s)$ posess analytic continuations to $\bigcap_{j=1}^{N} \Omega_i$.

Proof. The proof is by induction. We know that

$$\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix} = \begin{bmatrix} K_f^i & K_f^i K_\partial^i \\ h_p^i K_f^i & K_p^i + h_p^i K_f^i K_\partial^i \end{bmatrix} \begin{bmatrix} \tilde{C}_f^{i-1,j} \\ \tilde{C}_p^{i-1,j} \end{bmatrix} \qquad i - 1 \ge j \qquad \text{(C.15)}$$

and

$$\begin{bmatrix} \tilde{C}_f^{j,j} \\ \tilde{C}_p^{j,j} \end{bmatrix} = \begin{bmatrix} h_f^j \\ h_p^j h_f^j \end{bmatrix}$$

hence $\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix}$ is analytic in $\bigcap_{j=1}^{N} \Omega_i$ for $i - j = 0$. Now assume inductively that $\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix}$ is analytic in $\bigcap_{j=1}^{N} \Omega_i$ for $i - j = n$ we want to show that this still is true when $i - j = n + 1$.

To achieve this aim we utilize (C.15). First we claim that $G_f^i(\zeta, \eta, s)$ is analytic in $\bigcap_{j=1}^{N} \Omega_i$. Reviewing the formula for $G_f^i(\zeta, \eta, s)$ we see that in order to validate the claim it is sufficient to show that $f_i(s) - f_i^*(s) \neq 0$ and $f_i^*(s) \neq 0$ in $\bigcap_{j=1}^{N} \Omega_i$. But we need only glance at Corollary 4 and remember the relation $f_i^*(s) + f_i(s) = \frac{Pe}{t_w}$ to see that this is so. From this fact it follows from differentiation under the integral sign and the induction assumption that $K_f^i \tilde{C}_f^{i-1,j}$ is analytic in $\bigcap_{j=1}^{N} \Omega_i$.

To continue we see that $G_p^i(x, \xi, s)$ and $\frac{\partial G_p^i}{\partial x}(x, \xi, s)\Big|_{x=0}$ is analytic in $\bigcap_{j=1}^{N}\Omega_i$ just by glancing on the definition (C.3) so again by the induction assumption , differentiation under the integral sign and (C.15) we obtain the result that $\begin{bmatrix} \tilde{C}_f^{i,j} \\ \tilde{C}_p^{i,j} \end{bmatrix}$ is analytic in $\bigcap_{j=1}^{N}\Omega_i$ which was what we wanted to prove.

Note. The coefficients $P_{i,j,k}(s)$ and $Q_{i,j,k,l}(s)$ in the recursive solution need not be analytic. In fact they are meromorphic functions i.e analytic with the exception of poles.

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