2. GOVERNING EQUATIONS FOR TRANSPORT

2.1 Introduction

Four types of governing equations are incorporated in RMA-11. These represent the various levels of approximation that are used in the model. In the sections that follow, the advection diffusion equations are presented in generalised form with sources sinks and reactions represented by generic terms. The equations are shown in both conservative and conservative form. A more complete derivation of the vertical transformation and a description of the finite element approach is given in King (1993).

2.2 Governing Equations for Three Dimensional Transport

The governing transport equations may be transformed to a constant water surface elevation (r) and the following form is be derived for the case where the principal diffusion direction is at angle to the x axis:

Continuity

$$h\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)+(r-a)\frac{\partial w}{\partial z} - (r-a)\left(T_x\frac{\partial u}{\partial z}+T_y\frac{\partial v}{\partial z}\right) - hq_0 = 0$$

where q_0 = inflow per unit volume.

Constituent transport

$$\begin{aligned}
&h\frac{\partial C}{\partial t} + h\frac{\partial (uC)}{\partial x} + h\frac{\partial (vC)}{\partial y} + (r-a)\frac{\partial (wC)}{\partial z} - (r-a)T_x\frac{\partial (uC)}{\partial z} - (r-a)T_y\frac{\partial (vC)}{\partial z} - (z-a)\frac{\partial h}{\partial t}\frac{\partial C}{\partial z}\\
&- h\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right) + h\frac{\partial}{\partial x}\left(\frac{(r-a)}{h}\{D_xT_x + D_{xy}T_y\}\frac{\partial C}{\partial z}\right) + (r-a)T_x\frac{\partial}{\partial z}\left(D_x\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right)\\
&- (r-a)T_x\frac{\partial}{\partial z}\left(\frac{(r-a)}{h}\{D_xT_x + D_{xy}T_y\}\frac{\partial C}{\partial z}\right) - h\frac{\partial}{\partial y}\left(D_{xy}\frac{\partial C}{\partial x} + D_y\frac{\partial C}{\partial y}\right) + h\frac{\partial}{\partial y}\left(\frac{(r-a)}{h}\{D_{xy}T_x\right.\\
&\left.+ D_yT_y\}\frac{\partial C}{\partial z}\right) + (r-a)T_y\frac{\partial}{\partial z}\left(D_{xy}\frac{\partial C}{\partial x} + D_y\frac{\partial C}{\partial y}\right) - (r-a)T_y\frac{\partial}{\partial z}\left(\frac{(r-a)}{h}\{D_{xy}T_x + D_yT_y\}\frac{\partial C}{\partial z}\right)\\
&- (r-a)\frac{\partial}{\partial z}\left(D_z\frac{(r-a)}{h}\frac{\partial C}{\partial z}\right) - KhC - h\,\theta_s - (r-a)\frac{\partial (V_sC)}{\partial z} = 0
\end{aligned}$$

where T_x and T_y are defined by

$$T_x = \left[\frac{\partial a}{\partial x} + \frac{(z-a)}{(r-a)}\frac{\partial h}{\partial x} - \frac{h}{(r-a)}\frac{\partial a}{\partial x} + \frac{(z-a)}{(r-a)^2}h\frac{\partial a}{\partial x}\right]$$

$$T_y = \left[\frac{\partial a}{\partial y} + \frac{(z-a)}{(r-a)}\frac{\partial h}{\partial y} - \frac{h}{(r-a)}\frac{\partial a}{\partial y} + \frac{(z-a)}{(r-a)^2}h\frac{\partial a}{\partial y}\right]$$

After substitution of the continuity equation the transport equation may be written as

$$
\begin{aligned}
&(h\frac{\partial C}{\partial t} + hu\frac{\partial C}{\partial x} + hv\frac{\partial C}{\partial y} + [(r\text{-}a)\,(w\text{-}uT_X\text{-}vT_y)\text{-}(z\text{-}a)\,\frac{\partial h}{\partial t}]\frac{\partial C}{\partial z} - h\,\frac{\partial}{\partial x}\,(D_X\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y})\\
&+ h\,\frac{\partial}{\partial x}(\,\frac{(r\text{-}a)}{h}\{D_XT_X + D_{xy}T_y\}\frac{\partial C}{\partial z}\,)\; + (r\text{-}a)T_X\frac{\partial}{\partial z}(D_X\,\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y})\\
&- (r\text{-}a)T_X\frac{\partial}{\partial z}(\,\frac{(r\text{-}a)}{h}\{D_XT_X + D_{xy}T_y\}\frac{\partial C}{\partial z}) - h\,\frac{\partial}{\partial y}(\,D_{xy}\frac{\partial C}{\partial x} + D_y\frac{\partial C}{\partial y})\\
&+ h\,\frac{\partial}{\partial y}(\,\frac{(r\text{-}a)}{h}\{D_{xy}T_X + D_yT_y\}\frac{\partial C}{\partial z}) + (r\text{-}a)T_y\frac{\partial}{\partial z}(D_{xy}\,\frac{\partial C}{\partial x} + D_y\,\frac{\partial C}{\partial y})\\
&- (r\text{-}a)T_y\frac{\partial}{\partial z}(\,\frac{(r\text{-}a)}{h}\{D_{xy}T_X + D_yT_y\}\frac{\partial C}{\partial z}) - (r\text{-}a)\,\frac{\partial}{\partial z}(D_Z\frac{(r\text{-}a)}{h}\frac{\partial C}{\partial z})\\
&+ (q_0 - K)\,hC - h\,\theta_S\; - (r\text{-}a)\,\frac{\partial (V_SC)}{\partial z} = 0
\end{aligned}
$$

For the finite element formulation partial integration is applied to the diffusive and settling terms. The element residual contribution may then be written

$$
\begin{aligned}
\mathbf{f_C} \quad = \int_V \; &\mathbf{N^T[}h\frac{\partial C}{\partial t} + hu\frac{\partial C}{\partial x} + hv\frac{\partial C}{\partial y} + \quad [(r\text{-}a)\,(w\text{-}uT_X\text{-}vT_y)\text{-}\,(z\text{-}a)\,\frac{\partial h}{\partial t}]\frac{\partial C}{\partial z}\\
&+ \frac{\partial h}{\partial x}\;\;(D_X\,\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}) - \;\frac{\partial h}{\partial x}\,\frac{(r\text{-}a)}{h}(D_XT_X + D_{xy}T_y)\frac{\partial C}{\partial z} + \frac{\partial h}{\partial y}\,(D_{xy}\frac{\partial C}{\partial x} + D_y\,\frac{\partial C}{\partial y}\,)\\
&- \frac{\partial h}{\partial y}\,\frac{(r\text{-}a)}{h}(D_{xy}T_X + D_yT_y)\frac{\partial C}{\partial z} + (q_0 - K)\,hC - h\theta_S\mathbf{]} + \mathbf{N_X^T}\,h\;\mathbf{[}(D_X\frac{\partial C}{\partial x} + D_{xy}\,\frac{\partial C}{\partial y}\,) - \frac{(r\text{-}a)}{h}(D_XT_X +\\
&D_{xy}T_y)\frac{\partial C}{\partial z}\mathbf{]} + \mathbf{N_y^T}\,h\;\;\mathbf{[}(\,D_{xy}\frac{\partial C}{\partial x} + D_y\frac{\partial C}{\partial y})\;\, - \frac{(r\text{-}a)}{h}(\,D_{xy}T_X + D_yT_y)\frac{\partial C}{\partial z}\mathbf{]}\\
&- \mathbf{N_Z^T}\;\mathbf{[}\text{-}(r\text{-}a)T_X\,\{(D_X\,\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}) - \frac{(r\text{-}a)}{h}(D_XT_X + D_{xy}T_y)\,\frac{\partial C}{\partial z}\}\;\, - \;(r\text{-}a)T_y\,\{(\,D_{xy}\frac{\partial C}{\partial x} + D_y\,\frac{\partial C}{\partial y}\,) -\\
&\frac{(r\text{-}a)}{h}(\,D_{xy}T_X + D_yT_y)\frac{\partial C}{\partial z}\} + D_Z\,\frac{(r\text{-}a)^2}{h}\frac{\partial C}{\partial z}\\
&+ (r\text{-}a)V_SC\mathbf{]}
\end{aligned}
$$

The Newton Raphson derivative then becomes:

$$
\begin{aligned}
\frac{\partial \mathbf{f_C}}{\partial C} \quad = \int_V &\mathbf{N^T[}h\frac{\alpha}{\Delta t} + (q_0 - K)\,h\mathbf{]N} + \mathbf{N^T[}hu + D_X\,\frac{\partial h}{\partial x}\;\; + \;\;D_{xy}\frac{\partial h}{\partial y}\,\mathbf{]N_x} + \mathbf{N^T[}hv + D_{xy}\frac{\partial h}{\partial x} + D_y\frac{\partial h}{\partial y}\,\mathbf{]N_y}\\
&+ \mathbf{N^T[}(r\text{-}a)\,(w\text{-}uT_x\text{-}vT_y) - (z\text{-}a)\frac{\partial h}{\partial t} - \frac{(r\text{-}a)}{h}\,\frac{\partial h}{\partial x}\,(D_xT_x + D_{xy}T_y)\\
&- \frac{(r\text{-}a)}{h}\,\frac{\partial h}{\partial y}\,(D_{xy}T_x + D_yT_y\mathbf{]N_z} + \mathbf{N_x^T}hD_x\mathbf{N_x} + \mathbf{N_x^T}hD_{xy}\mathbf{N_y}\\
&- \mathbf{N_x^T}(r\text{-}a)(D_xT_x + D_{xy}T_y)\mathbf{N_z} + \mathbf{N_y^T}hD_{xy}\mathbf{N_x} + \mathbf{N_y^T}hD_y\mathbf{N_y} - \mathbf{N_y^T}(r\text{-}a)(\,D_{xy}T_x + D_yT_y)\mathbf{N_z}\\
&+ \mathbf{N_Z^T}(r\text{-}a)V_S\mathbf{N} - \mathbf{N_Z^T}\,(r\text{-}a)(T_x\,D_x + D_{xy}T_y)\,\mathbf{N_x} - \mathbf{N_Z^T}(r\text{-}a)(D_{xy}T_x + T_yD_y)\,\mathbf{N_y}\\
&+ \mathbf{N_Z^T[}\frac{(r\text{-}a)^2}{h}\{T_x\,(D_xT_x + D_{xy}T_y) + T_y(\,D_{xy}T_x + D_yT_y) + D_Z\}\mathbf{]}\;\mathbf{N_Z}\,dV
\end{aligned}
$$

2.3 Governing Equations for Two Dimensional Laterally Averaged Transport

Lateral averaging eliminates the momentum equation associated with the horizontal direction normal to flow and enforces the assumption that derivatives with respect to this direction are zero. In order to develop a consistent form of the governing equations, the three dimensional equations must be integrated in the lateral direction over the channel width b. In RMA-11 it is assumed that b may vary as a function of x and z.

The transformed equations take the form:

Continuity

$$h\frac{\partial(ub)}{\partial x} + (r-a)\frac{\partial(wb)}{\partial z}) - (r-a)T_X\frac{\partial(ub)}{\partial z} - hq_2 = 0$$

where q_2 = inflow per unit vertical area.

Constituent transport

$$h\frac{\partial(bC)}{\partial t} + h\frac{\partial(buC)}{\partial x} - (r-a)T_X\frac{\partial(buC)}{\partial z} + (r-a)\frac{\partial(bwC)}{\partial z} - (z-a)\frac{\partial h}{\partial t}\frac{\partial(bC)}{\partial z} - h\frac{\partial}{\partial x}(D_X b\frac{\partial C}{\partial x})$$
$$+ h\frac{\partial}{\partial x}(D_X\frac{(r-a)}{h}T_X b\frac{\partial C}{\partial z}) + (r-a)T_X\frac{\partial}{\partial z}(D_X b\frac{\partial C}{\partial x}) - (r-a)T_X\frac{\partial}{\partial z}(D_X\frac{(r-a)}{h}T_X b\frac{\partial C}{\partial z})$$
$$- (r-a)\frac{\partial}{\partial z}(D_Z\frac{(r-a)}{h}b\frac{\partial C}{\partial z}) - KbhC - bh\,\theta_S - (r-a)\frac{\partial(bV_SC)}{\partial z} = 0$$

Note that in this equation settling is incorporated in the 1st order rate coefficient K

Expanding and substituting the continuity equation

$$bh\frac{\partial C}{\partial t} + hu\,(b\frac{\partial C}{\partial x} + C\frac{\partial b}{\partial x}) + [(r-a)\,(w-uT_X)\,(b\frac{\partial C}{\partial z} + C\frac{\partial b}{\partial z}) - (z-a)\frac{\partial h}{\partial t}\frac{\partial(bC)}{\partial z}] - h\frac{\partial}{\partial x}(D_X b\frac{\partial C}{\partial x}) + h\frac{\partial}{\partial x}($$
$$D_X\frac{(r-a)}{h}T_X b\frac{\partial C}{\partial z}) + (r-a)T_X\frac{\partial}{\partial z}(D_X b\frac{\partial C}{\partial x}) - (r-a)T_X\frac{\partial}{\partial z}(D_X\frac{(r-a)}{h}T_X b\frac{\partial C}{\partial z})$$
$$- (r-a)\frac{\partial}{\partial z}(D_Z\frac{(r-a)}{h}b\frac{\partial C}{\partial z}) + (q_2 - Kb)hC - bh\,\theta_S - (r-a)\frac{\partial(bV_SC)}{\partial z} = 0$$

For the finite element formulation partial integration is applied to the diffusive and settling terms. The element residual contribution may then be written

$$\mathbf{f_C} = \int_{A_V}\mathbf{N^T[}hb\frac{\partial C}{\partial t} + hu\,(b\frac{\partial C}{\partial x} + C\frac{\partial b}{\partial x}) + [(r-a)\,(w-uT_X) - (z-a)\frac{\partial h}{\partial t}]\,(b\frac{\partial C}{\partial z} + C\frac{\partial b}{\partial z})$$
$$+ D_X\frac{\partial h}{\partial x}b\frac{\partial C}{\partial x} - D_X\frac{\partial h}{\partial x}\frac{(r-a)}{h}T_X b\frac{\partial C}{\partial z} + (q_2 - Kb)hC - bh\theta_S\mathbf{]}$$

$$+ \mathbf{N_x}^{\mathbf{T}} \mathbf{[}\ hD_X\, b\frac{\partial C}{\partial x} - hD_X \frac{(r-a)}{h} T_X b\frac{\partial C}{\partial z}\ \mathbf{]}$$

$$+ \mathbf{N_z}^{\mathbf{T}}\ \mathbf{[}\ -(r-a)T_X D_X b\frac{\partial C}{\partial x} + \frac{(r-a)^2}{h}(T_X^2\, D_X + D_Z)b\frac{\partial C}{\partial z} + (r-a)\, bV_S C]dA$$

The Boundary integral has the following form

$$- \int_{L_B} \mathbf{N^T} D_X \mathbf{[}\ h - (r-a)T_X]\mathbf{[}\ b\frac{\partial C}{\partial x} - \frac{(r-a)}{h} T_X b\frac{\partial C}{\partial z}\ ] + \mathbf{N^T}(r-a)\, bV_S C\, dL$$

The Newton Raphson derivative then becomes:

$$\frac{\partial \mathbf{f_C}}{\partial C} = \int_{A_V} \mathbf{N^T[}bh\frac{\alpha}{\Delta t} + hu\frac{\partial b}{\partial x} + [(r-a)\,(w-uT_X) - (z-a)\frac{\partial h}{\partial t}]\frac{\partial b}{\partial z} + (\ h\frac{\partial (ub)}{\partial x} + (r-a)\frac{\partial (wb)}{\partial z})$$

$$- (r-a)T_X\frac{\partial (ub)}{\partial z}) + (q_2 - Kb)h\ \mathbf{]N} + \mathbf{N^T[}buh + D_X\frac{\partial h}{\partial x} b\ \mathbf{]N_x}$$

$$+ \mathbf{N^T[}[b(r-a)\,(w-uT_X) - (z-a)\frac{\partial h}{\partial t}] - D_X\frac{\partial h}{\partial x}\frac{(r-a)}{h}T_X b\ \mathbf{]N_z}$$

$$+ \mathbf{N_x}^{\mathbf{T}} bhD_X \mathbf{N_x} - \mathbf{N_x}^{\mathbf{T}} hD_X\frac{(r-a)}{h}T_X b\mathbf{N_z} + \mathbf{N_z}^{\mathbf{T}}\mathbf{[}\ + (r-a)\, bV_S\mathbf{]N - N_z}^{\mathbf{T}}(r-a)T_X D_X b\mathbf{N_x}$$

$$+ \mathbf{N_z}^{\mathbf{T}}\frac{(r-a)^2}{h}(T_X^2\, D_X + D_Z)b\ \mathbf{N_z}\ dA$$

2.4 Governing Equations for Two Dimensional Depth Averaged Transport

The governing transport equations may be integrated over the vertical dimension with the assumption that C is independent of elevation (z). Under these conditions all derivatives with respect to z are eliminated.

Two alternative formulations have been created. The basic form is suitable for applications that consist only of one-dimensional and depth-averaged two-dimensional elements. The transformed form is suitable for combinations of all element types. For this latter form the transport equation must be multiplied by (r-a) to be consistent after integration with the more general transport equations presented above, the equations may be stated as follows:

Continuity

$$(h\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}) + u\frac{\partial h}{\partial x} + v\frac{\partial h}{\partial y} + \frac{\partial h}{\partial t} - q_1 = 0$$

where q_1 = inflow per unit area.

Constituent transport

$$\frac{\partial (hC)}{\partial t} + u\frac{\partial (hC)}{\partial x} + v\frac{\partial (hC)}{\partial y} - \frac{\partial}{\partial x}(D_X\, h\frac{\partial C}{\partial x} + D_{xy}\, h\frac{\partial C}{\partial y}) - \frac{\partial}{\partial y}(\ D_{xy}\, h\frac{\partial C}{\partial x} + D_y\, h\frac{\partial C}{\partial y})$$

$$- KhC - h\theta_S = 0$$

After substitution of the continuity equation the transport equation may be written as

$$h\left(\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial x}\left(D_x h \frac{\partial C}{\partial x} + D_{xy} h \frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial y}\left(D_{xy} h \frac{\partial C}{\partial x} + D_y h \frac{\partial C}{\partial y}\right)$$
$$+ (q_1 - Kh)C - h\theta_s = 0$$

For the finite element formulation partial integration is applied to the diffusive terms. The element residual contribution may then be written:

$$\mathbf{f_c} = \int_{A_h} \mathbf{N^T} \mathbf{[} h \left(\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y}\right) + (q_1 - Kh)\, C - h\theta_s \mathbf{]} + \mathbf{N_x}^\mathbf{T}\mathbf{[} h \left(D_x \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y}\right)\mathbf{]}$$
$$+ \mathbf{N_y}^\mathbf{T}\mathbf{[} h \left(D_{xy} \frac{\partial C}{\partial x} + D_y \frac{\partial C}{\partial y}\right)\mathbf{]}\, dA$$

After the (r-a) multiplier is incorporated, the element residual contribution may be written

$$\mathbf{f_{ct}} = \int_{A_h} \mathbf{N^T} \mathbf{[} h(r-a) \left(\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y}\right) - h\frac{\partial a}{\partial x}\left(D_x \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y}\right) - h\frac{\partial a}{\partial y}\left(D_{xy} \frac{\partial C}{\partial x} + D_y \frac{\partial C}{\partial y}\right)$$
$$+ (r-a) \{(q_1 - Kh)C - h\theta_s\}\mathbf{]} + \mathbf{N_x}^\mathbf{T}\mathbf{[}(r-a)\, h\left(D_x\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}\right)\mathbf{]}$$
$$+ \mathbf{N_y}^\mathbf{T}\mathbf{[}(r-a)\, h\left(D_{xy}\frac{\partial C}{\partial x} + D_y\frac{\partial C}{\partial y}\right. \mathbf{]}dA$$

The Newton Raphson derivative then becomes:

$$\frac{\partial \mathbf{f_c}}{\partial C} = \int_{A_h} \mathbf{N^T} \mathbf{[}\{h \frac{\alpha}{\Delta t} + (q_1 - Kh)\}\mathbf{]N} + \mathbf{N^T}\, hu\, \mathbf{N_x} + \mathbf{N^T}\, hv\, \mathbf{N_y} + \mathbf{N_x}^\mathbf{T} D_x h \mathbf{N_x} + \mathbf{N_x}^\mathbf{T} D_{xy} h \mathbf{N_y}$$
$$+ \mathbf{N_y}^\mathbf{T} D_{xy} h \mathbf{N_x} + \mathbf{N_y}^\mathbf{T} D_y h \mathbf{N_y}\, dA$$

The transformed Newton Raphson derivatives become:

$$\frac{\partial \mathbf{f_{ct}}}{\partial C} = \int_{A_h} \mathbf{N^T} \mathbf{[}(r-a)\{h \frac{\alpha}{\Delta t} + (q_1 - Kh)\} \mathbf{]N} + \mathbf{N^T} \mathbf{[}h(r-a)u - h\frac{\partial a}{\partial x}D_x - h\frac{\partial a}{\partial y}D_{xy}\mathbf{]N_x}$$

$$+ \mathbf{N^T} \mathbf{[}h(r-a)v - h\frac{\partial a}{\partial x}D_{xy} - h\frac{\partial a}{\partial y}D_y\mathbf{]N_y} + \mathbf{N_x}^\mathbf{T} D_x h(r-a) \mathbf{N_x} + \mathbf{N_x}^\mathbf{T} D_{xy}h(r-a) \mathbf{N_y}$$

$$+ \mathbf{N_y}^\mathbf{T} D_{xy}h(r-a) \mathbf{N_x} + \mathbf{N_y}^\mathbf{T} D_y h(r-a) \mathbf{N_y}\, dA$$

2.5 Governing Equations for One Dimensional Transport

For this approximation, integration is applied in both the vertical and the horizontal direction normal to the desired flow direction. The basic equations for this approximation are once again independent of depth, however to introduce some generality when one dimensional approximations are used the equations are constructed to permit trapezoidal cross-sections and off channel storage.

Two alternative formulations have been created. The basic form is suitable for applications that consist only of one-dimensional and depth-averaged two-dimensional elements. The transformed form is suitable for combinations of all element types. For this latter form the transport equation must be multiplied by (r-a) to be consistent after integration with the more general transport equations presented above, the equations may be stated as follows:

Continuity

$$\frac{\partial A_s}{\partial t} + A\frac{\partial u}{\partial x} + u\frac{\partial A}{\partial x} - q_3 = 0$$

where A = flowing cross-sectional area of the one-dimensional element
A_s = storage cross-sectional area of the one-dimensional element
q_3 = inflow per unit length

Constituent transport

$$\frac{\partial (A_s C)}{\partial t} + \frac{\partial (AuC)}{\partial x} - \frac{\partial}{\partial x}(D_x A \frac{\partial C}{\partial x}) - KA_s C - A_s \theta_s = 0$$

Note that in this equation settling is incorporated in the 1st order rate coefficient K

After substitution of the continuity equation the transport equation may be written as

$$A_s\frac{\partial C}{\partial t} + Au\frac{\partial C}{\partial x} - \frac{\partial}{\partial x}(D_x A \frac{\partial C}{\partial x}) + (q_3 - KA_s)\, C - A_s \theta_s = 0$$

For the finite element formulation partial integration is applied to the diffusive term. The element residual contribution may then be written

$$\mathbf{f_c} = \int_L \mathbf{N^T[}\, A\frac{\partial C}{\partial t} + Au\frac{\partial C}{\partial x} + (C\,(q_3 - KA_s) - A_s\theta_{s-})\mathbf{]} + \mathbf{N_x}^\mathbf{T} D_x A \frac{\partial C}{\partial x}\, dL$$

After the (r-a) multiplier is incorporated, the element residual contribution may be written

$$\mathbf{f_{ct}} = \int_L \mathbf{N^T[}(r\text{-}a)\left(A_S\frac{\partial C}{\partial t} + Au\frac{\partial C}{\partial x}\right) - D_X\frac{\partial a}{\partial x}A\frac{\partial C}{\partial x} + (r\text{-}a)(C\,(q_3 - KA_S) - A_S\theta_{S\text{-}})\mathbf{]}$$

$$+ \mathbf{N_X}^{\mathbf{T}}(r\text{-}a)D_X A\frac{\partial C}{\partial x}\,dL$$

The Newton Raphson derivatives then become:

$$\frac{\partial \mathbf{f_c}}{\partial C} = \int_{\mathbf{L}} \mathbf{N^T[}A_{\mathbf{S}}\left(\frac{\alpha}{\Delta t} - K\right) + q_3\ \mathbf{]\ N + N^T}\ Au\ \mathbf{N_X + N_X}^{\mathbf{T}}\ D_X A\mathbf{N_X}\ \ dL$$

The transformed Newton Raphson derivatives become:

$$\frac{\partial \mathbf{f_{ct}}}{\partial C} = \int_{\mathbf{L}} \mathbf{N^T[}(r\text{-}a)\ \{A_{\mathbf{S}}\left(\frac{\alpha}{\Delta t} - K\right) + q_3\}\ \mathbf{]\ N + N^T\ [}(r\text{-}a)\ Au - D_X\ A\frac{\partial a}{\partial x}\mathbf{]N_X}$$

$$+ \mathbf{N_X}^{\mathbf{T}}\ (r\text{-}a)D_X A\mathbf{N_X}dL$$