Diffusion in a symmetric sphere (spherincl.m)

For a radiogenic isotope in a sphere

$$\frac{\partial C}{\partial t} = \frac{1}{r^2} * \frac{\partial\left(r^2 * D * \frac{\partial C}{\partial r}\right)}{\partial r} + P,$$

where P is the amount of radiogenic isotope generated via parent isotope decay.

Explicit finite difference scheme for this equation is

$$\frac{C_i^{t+1} - C_i^t}{\delta t} = \frac{1}{r_i^2} * D \frac{r^2_{i+\frac{1}{2}} * \frac{C_{i+1}^t - C_i^t}{\delta r} - r^2_{i-\frac{1}{2}} * \frac{C_i^t - C_{i-1}^t}{\delta r}}{\delta r} + P$$

For the case of a mineral boundary at $r_i = R$, where the rightmost part of the inclusion is located, this can be rewritten into:

$$\frac{C_i^{t+1} - C_i^t}{\delta t} = \frac{1}{r_i^2} * \frac{r^2_{i+\frac{1}{2}} * D_{i+1} * \frac{C_{i+1}^t - C_i^t * Kd}{\delta r} - r^2_{i-\frac{1}{2}} * D_i * \frac{C_i^t - C_{i-1}^t}{\delta r}}{\delta r} + P$$

for this grain boundary node, and

$$\frac{C_i^{t+1} - C_i^t}{\delta t} = \frac{1}{r_i^2} * \frac{r^2_{i+\frac{1}{2}} * D_{i+1} * \frac{C_{i+1}^t - C_i^t}{\delta r} - r^2_{i-\frac{1}{2}} * D_i * \frac{C_i^t - C_{i-1}^t * Kd}{\delta r}}{\delta r} + P$$

for the first node of the host mineral, where $Kd = \frac{C_{host}}{C_{inclusion}}$.

To apply the same equation for all the internal nodes of the model, it is convenient to rewrite the diffusion equation in this way

$$\frac{C_i^{t+1} - C_i^t}{\delta t} = \frac{1}{r_i^2} * \frac{\frac{r^2_{i+\frac{1}{2}} * D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} * \frac{C_{i+1}^t * Kd^*_{i+1} - C_i^t * Kd^*_i}{\delta r} - \frac{r^2_{i-\frac{1}{2}} * D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}} * \frac{C_i^t * Kd^*_i - C_{i-1}^t * Kd^*_{i-1}}{\delta r}}{\delta r} + P \ ,$$

where $Kd^* = Kd$ for the inclusion and $Kd^* = 1$ for the host mineral.

Replacing all the concentrations right of the equal sign with those at the next time layer gives an equation for implicit scheme. Crank-Nicolson scheme is the average of the explicit and implicit solutions

$$\frac{C_i^{t+1} - C_i^t}{\delta t} = \frac{1}{r_i^2} * \frac{\frac{r^2_{i+\frac{1}{2}} * D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} * \frac{C_{i+1}^{t+1} * Kd^*_{i+1} - C_i^{t+1} * Kd^*_i}{\delta r} - \frac{r^2_{i-\frac{1}{2}} * D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}} * \frac{C_i^{t+1} * Kd^*_i - C_{i-1}^{t+1} * Kd^*_{i-1}}{\delta r}}{\delta r} * \frac{1}{2} +$$

$$\frac{1}{r_i^2} * \frac{\frac{(r^2_{i+\frac{1}{2}} * D_{i+\frac{1}{2}})}{Kd^*_{i+\frac{1}{2}}} * \frac{C_{i+1}^t * Kd^*_{i+1} - C_i^t * Kd^*_i}{\delta r} - \frac{(r^2_{i-\frac{1}{2}} * D_{i-\frac{1}{2}})}{Kd^*_{i-\frac{1}{2}}} * \frac{C_i^t * Kd^*_i - C_{i-1}^t * Kd^*_{i-1}}{\delta r}}{\delta r} * \frac{1}{2} + P$$

Rearranging gives

$$C_i^{t+1} - C_i^t = \frac{\delta t*Kd_{i+1}^*}{2*r_i^2*\delta r^2} * \frac{r^2_{i+\frac{1}{2}}*D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} * C_{i+1}^{t+1} - \frac{\delta t*Kd_i^*}{2*r_i^2*\delta r^2} * \left(\frac{r^2_{i+\frac{1}{2}}*D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} + \frac{r^2_{i-\frac{1}{2}}*D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}}\right) * C_i^{t+1} + \frac{\delta t*Kd_{i-1}^*}{2*r_i^2*\delta r^2} * \frac{r^2_{i-\frac{1}{2}}*D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}} * C_{i-1}^{t+1} + \frac{\delta t*Kd_{i+1}^*}{2*r_i^2*\delta r^2} * \frac{r^2_{i+\frac{1}{2}}*D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} * C_{i+1}^{t} - \frac{\delta t*Kd_i^*}{2*r_i^2*\delta r^2} * \left(\frac{r^2_{i+\frac{1}{2}}*D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} + \frac{r^2_{i-\frac{1}{2}}*D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}}\right) * C_i^{t} + \frac{\delta t*Kd_{i-1}^*}{2*r_i^2*\delta r^2} * \frac{r^2_{i-\frac{1}{2}}*D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}} * C_{i-1}^{t} + P$$

Say $A_i = \frac{\delta t*Kd_{i+1}^*}{2*r_i^2*\delta r^2} * \frac{r^2_{i+\frac{1}{2}}*D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}}$, $B_i = \frac{\delta t*Kd_i^*}{2*r_i^2*\delta r^2} * \left(\frac{r^2_{i+\frac{1}{2}}*D_{i+\frac{1}{2}}}{Kd^*_{i+\frac{1}{2}}} + \frac{r^2_{i-\frac{1}{2}}*D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}}\right)$, $E_i = \frac{\delta t*Kd_{i-1}^*}{2*r_i^2*\delta r^2} * \frac{r^2_{i-\frac{1}{2}}*D_{i-\frac{1}{2}}}{Kd^*_{i-\frac{1}{2}}}$,

$P = C_{parent\ i} * (1 - e^{-\lambda*\delta t})$, then

$$C_i^{t+1} - C_i^t = A_i * C_{i+1}^{t+1} - B_i * C_i^{t+1} + E_i * C_{i-1}^{t+1} + A_i * C_{i+1}^t - B_i * C_i^t + E_i * C_{i-1}^t + C_{parent\ i} * (1 - e^{-\lambda*\delta t})$$

Rearranging gives

$$-A_i * C_{i+1}^{t+1} + (1 + B_i) * C_i^{t+1} - E_i * C_{i-1}^{t+1} = A_i * C_{i+1}^t + (1 - B_i) * C_i^t + E_i * C_{i-1}^t + C_{parent\ i} * (1 - e^{-\lambda*\delta t})$$

The rightmost boundary of the model is treated as open (there is no diffusion ingrowth there, but ther is radiogenic). Equations for the leftmost boundary (with $r = 0$) are derived from the condition of zero flux across this point, which is required by the symmetry. Since we stay within the same mineral, D can be considered as a constant and Kd^* can be omitted.

$$\begin{cases} \frac{\partial C}{\partial t} = \frac{D}{r^2} * \frac{\partial\left(r^2*\frac{\partial C}{\partial r}\right)}{\partial r} + P \\ \frac{\partial C}{\partial r} = 0 \end{cases}$$

$$\frac{\partial C}{\partial t} = \frac{D}{r^2} * \frac{\partial r^2}{\partial r}\frac{\partial C}{\partial r} + \frac{r^2 D}{r^2}\frac{\partial^2 C}{\partial r^2} + P = \frac{2*D*\partial C/\partial r}{r} + D\frac{\partial^2 C}{\partial r^2} + P$$

according to L'Hôpital's rule

$$\lim_{r\to 0}\frac{2*D*\partial C/\partial r}{r} = \lim_{r\to 0}\frac{\partial(2*D*\partial C/\partial r)/\partial r}{\partial r/\partial r} = 2D * \frac{\partial^2 C}{\partial r^2}$$

which gives

$$\frac{\partial C}{\partial t} = 3D * \frac{\partial^2 C}{\partial r^2} + P$$

Finite difference expression for this is derived by introducing virtual node left of the coordinate origin (here with an index *-1*, explicit scheme is used)

$$\begin{cases} \frac{C_1^{t+1} - C_1^t}{\delta t} = 3D * \frac{C_2^t - 2*C_1^t + C_{-1}^t}{\delta r^2} + P \\ \frac{C_2^t - C_{-1}^t}{\delta r^2} = 0 \end{cases} \rightarrow \begin{cases} \frac{C_1^{t+1} - C_1^t}{\delta t} = 6D * \frac{C_2^t - C_1^t}{\delta r^2} + P \\ C_2^t = C_{-1}^t \end{cases}$$

The equation to be used in the Crank-Nicolson scheme looks like this

$$C_1^{t+1} - C_1^t = \frac{3D\delta t}{\delta r^2} * C_2^{t+1} - \frac{3D\delta t}{\delta r^2} C_1^{t+1} + \frac{3D\delta t}{\delta r^2} * C_2^t - \frac{3D\delta t}{\delta r^2} C_1^t + C_{parent\ i} * (1 - e^{-\lambda * \delta t})$$

$$-\frac{3D\delta t}{\delta r^2} * C_2^{t+1} + \left(1 + \frac{3D\delta t}{\delta r^2}\right) C_1^{t+1} = \frac{3D\delta t}{\delta r^2} * C_2^t + \left(1 - \frac{3D\delta t}{\delta r^2}\right) C_1^t + C_{parent\ i} * (1 - e^{-\lambda * \delta t})$$

(so $A_1 = B_1 = \frac{3D\delta t}{\delta r^2}$)

Diffusion in an axisymmetric finite cylinder (cylincl.m)

For a radiogenic isotope in a finite cylinder symmetric around the main axis.

$$\frac{\partial C}{\partial t} = \frac{1}{r} * \frac{\partial\left(r * D * \frac{\partial C}{\partial r}\right)}{\partial r} + \frac{\partial\left(D * \frac{\partial C}{\partial z}\right)}{\partial z} + P,$$

where P the amount of radiogenic isotope generated via parent isotope decay.

Explicit finite difference scheme for this equation is

$$\frac{C_{i,j}^{t+1} - C_{i,j}^t}{\delta t} = \frac{1}{r_{i,j}} * D \frac{r_{i,j+\frac{1}{2}} * \frac{C_{i,j+1}^t - C_{i,j}^t}{\delta r} - r_{i,j-\frac{1}{2}} * \frac{C_{i,j}^t - C_{i,j-1}^t}{\delta r}}{\delta r} + D \frac{\frac{C_{i+1,j}^t - C_{i,j}^t}{\delta z} - \frac{C_{i,j}^t - C_{i-1,j}^t}{\delta z}}{\delta z} + P$$

There are many cases of possible orientation of the grain boundary, so for simplicity we only provide a generalised equation. To apply the same equation for all the internal nodes of the model, it is convenient to rewrite diffusion equation in this way

$$\frac{C_{i,j}^{t+1} - C_{i,j}^t}{\delta t} = \frac{1}{r_{i,j}} * \frac{\frac{r_{i,j+\frac{1}{2}} * D_{i,j+\frac{1}{2}}}{Kd^*_{i,j+\frac{1}{2}}} * \frac{C_{i,j+1}^t * Kd^*_{i,j+1} - C_{i,j}^t * Kd^*_{i,j}}{\delta r} - \frac{r_{i,j-\frac{1}{2}} * D_{i,j-\frac{1}{2}}}{Kd^*_{i,j-\frac{1}{2}}} * \frac{C_{i,j}^t * Kd^*_{i,j} - C_{i,j-1}^t * Kd^*_{i,j-1}}{\delta r}}{\delta r} +$$
$$\frac{\frac{D_{i+\frac{1}{2},j}}{Kd^*_{i+\frac{1}{2},j}} * \frac{C_{i+1,j}^t * Kd^*_{i+1,j} - C_{i,j}^t * Kd^*_{i,j}}{\delta z} - \frac{D_{i-\frac{1}{2},j}}{Kd^*_{i-\frac{1}{2},j}} * \frac{C_{i,j}^t * Kd^*_{i,j} - C_{i-1,j}^t * Kd^*_{i-1,j}}{\delta z}}{\delta z} + P$$

where $Kd = \frac{C_{host}}{C_{inclusion}}$, $Kd^* = Kd$ for the inclusion and $Kd^* = 1$ for the host mineral.

Replacing all the concentrations right of the equal sign with those at next time layer gives an equation for implicit scheme. Crank-Nicolson scheme is the average of explicit and implicit solutions

$$\frac{C_{i,j}^{t+1} - C_{i,j}^t}{\delta t} = \frac{1}{2} * \frac{1}{r_i} * \frac{\frac{r_{i,j+\frac{1}{2}} * D_{i,j+\frac{1}{2}}}{Kd^*_{i,j+\frac{1}{2}}} * \frac{C_{i,j+1}^t * Kd^*_{i,j+1} - C_{i,j}^t * Kd^*_{i,j}}{\delta r} - \frac{r_{i,j-\frac{1}{2}} * D_{i,j-\frac{1}{2}}}{Kd^*_{i,j-\frac{1}{2}}} * \frac{C_{i,j}^t * Kd^*_{i,j} - C_{i,j-1}^t * Kd^*_{i,j-1}}{\delta r}}{\delta r} +$$
$$\frac{1}{2} * \frac{\frac{D_{i+\frac{1}{2},j}}{Kd^*_{i+\frac{1}{2},j}} * \frac{C_{i+1,j}^t * Kd^*_{i+1,j} - C_{i,j}^t * Kd^*_{i,j}}{\delta z} - \frac{D_{i-\frac{1}{2},j}}{Kd^*_{i-\frac{1}{2},j}} * \frac{C_{i,j}^t * Kd^*_{i,j} - C_{i-1,j}^t * Kd^*_{i-1,j}}{\delta z}}{\delta z} +$$

$$\frac{1}{2}*\frac{1}{r_i}*\frac{\frac{r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}}{Kd^*_{i,j+\frac{1}{2}}}*\frac{C^{t+1}_{i,j+1}*Kd^*_{i,j+1}-C^{t+1}_{i,j}*Kd^*_{i,j}}{\delta r}-\frac{r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}}{Kd^*_{i,j-\frac{1}{2}}}*\frac{C^{t+1}_{i,j}*Kd^*_{i,j}-C^{t+1}_{i,j-1}*Kd^*_{i,j-1}}{\delta r}}{\delta r}+$$

$$\frac{1}{2}*\frac{\frac{D_{i+\frac{1}{2},j}}{Kd^*_{i+\frac{1}{2},j}}*\frac{C^{t+1}_{i+1,j}*Kd^*_{i+1,j}-C^{t+1}_{i,j}*Kd^*_{i,j}}{\delta z}-\frac{D_{i-\frac{1}{2},j}}{Kd^*_{i-\frac{1}{2},j}}*\frac{C^{t+1}_{i,j}*Kd^*_{i,j}-C^{t+1}_{i-1,j}*Kd^*_{i-1,j}}{\delta z}}{\delta z}+P$$

Rearranging gives

$$C^{t+1}_{i,j}-C^{t}_{i,j}=\frac{\delta t*r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}*Kd^*_{i,j+1}}{2*r_i*Kd^*_{i,j+\frac{1}{2}}*\delta r^2}*C^{t}_{i,j+1}+\frac{\delta t*r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}*Kd^*_{i,j-1}}{2*r_i*Kd^*_{i,j-\frac{1}{2}}*\delta r^2}*C^{t}_{i,j-1}+\frac{\delta t*D_{i+\frac{1}{2},j}*Kd^*_{i+1,j}}{2*Kd^*_{i+\frac{1}{2},j}*\delta z^2}*C^{t}_{i+1,j}+$$

$$\frac{\delta t*D_{i-\frac{1}{2},j}*Kd^*_{i-1,j}}{2*Kd^*_{i-\frac{1}{2},j}*\delta z^2}*C^{t}_{i-1,j}-\frac{\delta t*Kd^*_{i,j}}{2}*\left(\frac{r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}}{r_i*Kd^*_{i,j+\frac{1}{2}}*\delta r^2}+\frac{r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}}{r_i*Kd^*_{i,j-\frac{1}{2}}*\delta r^2}+\frac{D_{i+\frac{1}{2},j}}{Kd^*_{i+\frac{1}{2},j}*\delta z^2}+\frac{D_{i-\frac{1}{2},j}}{Kd^*_{i-\frac{1}{2},j}*\delta z^2}\right)*C^{t}_{i,j}+$$

$$\frac{\delta t*r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}*Kd^*_{i,j+1}}{2*r_i*Kd^*_{i,j+\frac{1}{2}}*\delta r^2}*C^{t+1}_{i,j+1}+\frac{\delta t*r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}*Kd^*_{i,j-1}}{2*r_i*Kd^*_{i,j-\frac{1}{2}}*\delta r^2}*C^{t+1}_{i,j-1}+\frac{\delta t*D_{i+\frac{1}{2},j}*Kd^*_{i+1,j}}{2*Kd^*_{i+\frac{1}{2},j}*\delta z^2}*C^{t+1}_{i+1,j}+$$

$$\frac{\delta t*D_{i-\frac{1}{2},j}*Kd^*_{i-1,j}}{2*Kd^*_{i-\frac{1}{2},j}*\delta z^2}*C^{t+1}_{i-1,j}-\frac{\delta t*Kd^*_{i,j}}{2}*\left(\frac{r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}}{r_i*Kd^*_{i,j+\frac{1}{2}}*\delta r^2}+\frac{r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}}{r_i*Kd^*_{i,j-\frac{1}{2}}*\delta r^2}+\frac{D_{i+\frac{1}{2},j}}{Kd^*_{i+\frac{1}{2},j}*\delta z^2}+\frac{D_{i-\frac{1}{2},j}}{Kd^*_{i-\frac{1}{2},j}*\delta z^2}\right)*C^{t+1}_{i,j}+P$$

Say $A_{i,j}=\frac{\delta t*r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}*Kd^*_{i,j+1}}{2*r_i*Kd^*_{i,j+\frac{1}{2}}*\delta r^2}$, $B_{i,j}=\frac{\delta t*r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}*Kd^*_{i,j-1}}{2*r_i*Kd^*_{i,j-\frac{1}{2}}*\delta r^2}$, $E_{i,j}=\frac{\delta t*D_{i+\frac{1}{2},j}*Kd^*_{i+1,j}}{2*Kd^*_{i+\frac{1}{2},j}*\delta z^2}$,

$F_{i,j}=\frac{\delta t*D_{i-\frac{1}{2},j}*Kd^*_{i-1,j}}{2*Kd^*_{i-\frac{1}{2},j}*\delta z^2}$, $G_{i,j}=\frac{\delta t*Kd^*_{i,j}}{2}*\left(\frac{r_{i,j+\frac{1}{2}}*D_{i,j+\frac{1}{2}}}{r_i*Kd^*_{i,j+\frac{1}{2}}*\delta r^2}+\frac{r_{i,j-\frac{1}{2}}*D_{i,j-\frac{1}{2}}}{r_i*Kd^*_{i,j-\frac{1}{2}}*\delta r^2}+\frac{D_{i+\frac{1}{2},j}}{Kd^*_{i+\frac{1}{2},j}*\delta z^2}+\frac{D_{i-\frac{1}{2},j}}{Kd^*_{i-\frac{1}{2},j}*\delta z^2}\right)$ and

$P=C_{parent\ i,j}*(1-e^{-\lambda*\delta t})$ then

$$C^{t+1}_{i,j}-C^{t}_{i,j}=A_{i,j}*C^{t}_{i,j+1}+B_{i,j}*C^{t}_{i,j-1}+E_{i,j}*C^{t}_{i+1,j}+F_{i,j}*C^{t}_{i-1,j}-G_{i,j}*C^{t}_{i,j}+A_{i,j}*C^{t+1}_{i,j+1}+$$

$$B_{i,j}*C^{t+1}_{i,j-1}+E_{i,j}*C^{t+1}_{i+1,j}+F_{i,j}*C^{t+1}_{i-1,j}-G_{i,j}*C^{t+1}_{i,j}+C_{parent\ i,j}*(1-e^{-\lambda*\delta t})$$

Rearranging gives

$$-A_{i,j}*C^{t+1}_{i,j+1}-B_{i,j}*C^{t+1}_{i,j-1}-E_{i,j}*C^{t+1}_{i+1,j}-F_{i,j}*C^{t+1}_{i-1,j}+(1+G_{i,j})*C^{t+1}_{i,j}=A_{i,j}*C^{t}_{i,j+1}+$$

$$B_{i,j}*C^{t}_{i,j-1}+E_{i,j}*C^{t}_{i+1,j}+F_{i,j}*C^{t}_{i-1,j}+(1-G_{i,j})*C^{t}_{i,j}+C_{parent\ i,j}*(1-e^{-\lambda*\delta t})$$

The right, upper and bottom boundaries of the model are treated as open (there is no diffusion ingrowth there, but there is radiogenic). Equations for the left boundary (with $r=0$) are derived from the condition of zero flux across it which is required by the symmetry.

$$\begin{cases}\frac{\partial C}{\partial t}=\frac{1}{r}*\frac{\partial\left(r*D*\frac{\partial C}{\partial r}\right)}{\partial r}+\frac{\partial\left(D*\frac{\partial C}{\partial z}\right)}{\partial z}+P\\ \frac{\partial C}{\partial r}=0\end{cases}$$

$$\frac{\partial C}{\partial t}=\frac{D}{r}*\frac{\partial r}{\partial r}\frac{\partial C}{\partial r}+\frac{rD}{r}\frac{\partial^2 C}{\partial r^2}+\frac{\partial\left(D*\frac{\partial C}{\partial z}\right)}{\partial z}+P=\frac{D*\partial C/\partial r}{r}+D\frac{\partial^2 C}{\partial r^2}+D\frac{\partial^2 C}{\partial z^2}+P$$

according to L'Hôpital's rule

$$\lim_{r\to 0}\frac{D*\partial C/\partial r}{r}=\lim_{r\to 0}\frac{\partial(D*\partial C/\partial r)/\partial r}{\partial r/\partial r}=D*\frac{\partial^2 C}{\partial r^2}$$

which gives

$$\frac{\partial C}{\partial t} = 2D * \frac{\partial^2 C}{\partial r^2} + D\frac{\partial^2 C}{\partial z^2} + P$$

Finite difference expression of this derived by introducing virtual node left of coordinates origin (here with index *-1*, explicit scheme used)

$$\begin{cases} \frac{C_{i,1}^{t+1}-C_{i,1}^{t}}{\delta t} = 2*\frac{D_{i,1\frac{1}{2}}}{Kd^*_{i,1\frac{1}{2}}} * \frac{C_{i,2}^t*Kd^*_{i,2}-2*C_{i,1}^t*Kd^*_{i,1}+C_{i,-1}^t*Kd^*_{i,-1}}{\delta r^2} + \frac{D_{i+\frac{1}{2},1}}{Kd^*_{i+\frac{1}{2},1}}*\frac{C^t_{i+1,1}*Kd^*_{i+1,1}-C^t_{i,1}*Kd^*_{i,1}}{\delta z^2} \\ \qquad -\frac{D_{i-\frac{1}{2},1}}{Kd^*_{i-\frac{1}{2},1}}*\frac{C^t_{i,1}*Kd^*_{i,1}-C^t_{i-1,1}*Kd^*_{i-1,1}}{\delta z^2}+P \\ \frac{C_2^t-C_{-1}^t}{\delta r^2}=0 \\ Kd^*_{i,2}=Kd^*_{i,-1}\end{cases} \rightarrow$$

$$\begin{cases} \frac{C_{i,1}^{t+1}-C_{i,1}^{t}}{\delta t} = 4*\frac{D_{i,1\frac{1}{2}}}{Kd^*_{i,1\frac{1}{2}}} * \frac{C_{i,2}^t*Kd^*_{i,2}-C_{i,1}^t*Kd^*_{i,1}}{\delta r^2} + \frac{D_{i+\frac{1}{2},1}}{Kd^*_{i+\frac{1}{2},1}}*\frac{C^t_{i+1,1}*Kd^*_{i+1,1}-C^t_{i,1}*Kd^*_{i,1}}{\delta z^2} \\ \qquad -\frac{D_{i-\frac{1}{2},1}}{Kd^*_{i-\frac{1}{2},1}}*\frac{C^t_{i,1}*Kd^*_{i,1}-C^t_{i-1,1}*Kd^*_{i-1,1}}{\delta z^2}+P \\ C_2^t=C_{-1}^t \\ Kd^*_{i,2}=Kd^*_{i,-1}\end{cases}$$

The equation to be used in Crank-Nicolson scheme is derived in this way

$$C_{i,1}^{t+1}-C_{i,1}^{t} = 2*\frac{\delta t*D_{i,1+\frac{1}{2}}*Kd^*_{i,2}}{Kd^*_{i,1+\frac{1}{2}}*\delta r^2}*C^t_{i,2}+\frac{\delta t*D_{i+\frac{1}{2},1}*Kd^*_{i+1,1}}{2*Kd^*_{i+\frac{1}{2},1}*\delta z^2}*C^t_{i+1,1}+\frac{\delta t*D_{i-\frac{1}{2},1}*Kd^*_{i-1,1}}{2*Kd^*_{i-\frac{1}{2},1}*\delta z^2}*C^t_{i-1,1}-\delta t* Kd^*_{i,1}*\left(2*\frac{D_{i,1+\frac{1}{2}}}{Kd^*_{i,1+\frac{1}{2}}*\delta r^2}+\frac{D_{i+\frac{1}{2},1}}{2*Kd^*_{i+\frac{1}{2},1}*\delta z^2}+\frac{D_{i-\frac{1}{2},1}}{2*Kd^*_{i-\frac{1}{2},1}*\delta z^2}\right)*C^t_{i,1}+2*\frac{\delta t*D_{i,1+\frac{1}{2}}*Kd^*_{i,2}}{Kd^*_{i,1+\frac{1}{2}}*\delta r^2}*C^{t+1}_{i,2}+\frac{\delta t*D_{i+\frac{1}{2},1}*Kd^*_{i+1,1}}{2*Kd^*_{i+\frac{1}{2},1}*\delta z^2}*C^{t+1}_{i+1,1}+\frac{\delta t*D_{i-\frac{1}{2},1}*Kd^*_{i-1,1}}{2*Kd^*_{i-\frac{1}{2},1}*\delta z^2}*C^{t+1}_{i-1,1}-\delta t*Kd^*_{i,1}*\left(2*\frac{D_{i,1+\frac{1}{2}}}{Kd^*_{i,1+\frac{1}{2}}*\delta r^2}+\frac{D_{i+\frac{1}{2},1}}{2*Kd^*_{i+\frac{1}{2},1}*\delta z^2}+\frac{D_{i-\frac{1}{2},1}}{2*Kd^*_{i-\frac{1}{2},1}*\delta z^2}\right)*C^{t+1}_{i,1}+C_{parent\,i,j}*(1-e^{-\lambda*\delta t})$$

Say $A_{i,1}=2*\frac{\delta t*D_{i,1+\frac{1}{2}}*Kd^*_{i,2}}{Kd^*_{i,1+\frac{1}{2}}*\delta r^2}$, $B_{i,1}=0$, $E_{i,1}=\frac{\delta t*D_{i+\frac{1}{2},1}*Kd^*_{i+1,1}}{2*Kd^*_{i+\frac{1}{2},1}*\delta z^2}$, $F_{i,1}=\frac{\delta t*D_{i-\frac{1}{2},1}*Kd^*_{i-1,1}}{2*Kd^*_{i-\frac{1}{2},1}*\delta z^2}$, $G_{i,1}=\delta t*Kd^*_{i,1}*\left(2*\frac{D_{i,1+\frac{1}{2}}}{Kd^*_{i,1+\frac{1}{2}}*\delta r^2}+\frac{D_{i+\frac{1}{2},1}}{2*Kd^*_{i+\frac{1}{2},1}*\delta z^2}+\frac{D_{i-\frac{1}{2},1}}{2*Kd^*_{i-\frac{1}{2},1}*\delta z^2}\right)$, then

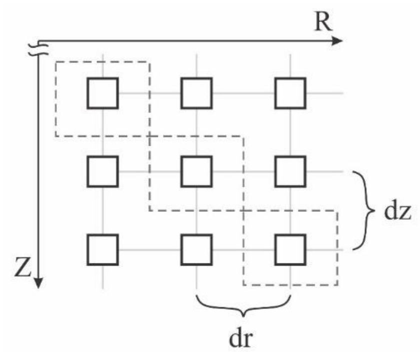
$$C_{i,j}^{t+1}-C_{i,j}^{t}=A_{i,j}*C^t_{i,j+1}+E_{i,j}*C^t_{i+1,j}+F_{i,j}*C^t_{i-1,j}-G_{i,j}*C^t_{i,j}+A_{i,j}*C^{t+1}_{i,j+1}+E_{i,j}*C^{t+1}_{i+1,j}+F_{i,j}*C^{t+1}_{i-1,j}-G_{i,j}*C^{t+1}_{i,j}+C_{parent\,i,j}*(1-e^{-\lambda*\delta t})$$

Rearranging gives

$$-A_{i,j} * C_{i,j+1}^{t+1} - E_{i,j} * C_{i+1,j}^{t+1} - F_{i,j} * C_{i-1,j}^{t+1} + \left(1 + G_{i,j}\right) * C_{i,j}^{t+1} = A_{i,j} * C_{i,j+1}^{t} + E_{i,j} * C_{i+1,j}^{t} + F_{i,j} * C_{i-1,j}^{t} + (1 - G_{i,j}) * C_{i,j}^{t} + C_{parent\ i,j} * (1 - e^{-\lambda * \delta t})$$

Integration of isotope quantities for the bulk date calculation

Quantities of isotopes within the modelled apatite crystal are calculated by integrating quantities of isotopes in the volumes around the model nodes. The latter are calculated by multiplying the isotope concentration in a given node by the volume of the $\pm\ \delta r/2$ and, if applicable, $\pm\ \delta z/2$ neighbourhood of this node. The nodes where the grain boundary is located must be ignores, since they are always in equilibrium with the host phase.



Squares with solid black outline depict the model nodes. Rectangles with dashed grey outline depict the $\pm\ \delta r/2$ and $\pm\ \delta z/2$ neighbourhoods for the diagonal nodes.

Formulas used in the symmetric sphere model (spherincl.m) are derived from the equation for a sphere volume

$$V_{sphere} = \frac{4}{3} * \pi * r^3$$

Volume around the node at the origin of the R axis is calculated using this formula:

$$V_{r=0} = \frac{4}{3} * \pi * \left(\frac{dr}{2}\right)^3$$

Volumes of all the others nodes are calculated using this formula:

$$V_{r>0} = \frac{4}{3}\pi * \left(\left(r + \frac{dr}{2}\right)^3 - \left(r - \frac{dr}{2}\right)^3\right) = \frac{4}{3}\pi * \left(r^3 + r^2 * dr + r\frac{dr^2}{4} + r^2 * \frac{dr}{2} + r * dr * \frac{dr}{2} + \frac{dr^3}{8} - r^3 + r^2 * dr - r\frac{dr^2}{4} + r^2 * \frac{dr}{2} - r * dr\frac{dr}{2} + \frac{dr^3}{8}\right) = 4\pi r^2 * dr + \frac{\pi dr^3}{3}$$

Formulas used in the axisymmetric finite cylinder model (cylincl.m) are derived from the equation for a cylinder volume

$$V_{cylinder} = \pi * r^2 * h$$

Volumes around the nodes at the origin of the R axis are calculated using this formula

$$V_{r=0} = \frac{\pi * dr^2 * dz}{4}$$

Volumes around all the others nodes are calculated using this formula:

$$V_{r>0} = \pi * \left(\left(r + \frac{dr}{2}\right)^2 - \left(r - \frac{dr}{2}\right)^2\right) * dz = \pi * \left(r^2 + r * dr + \frac{dr^2}{4} - r^2 + r * dr - \frac{dr^2}{4}\right) * dz = 2 * \pi * r * dr * dz$$