

Details not shown on Web pages.

Derivations of Equations used in subroutine SLEEP and the S.O.R. equation.

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Started with 1971, CSC 333, class notes posted as equations (7) and (8) on the Web at:
http://www.sv.nv.edu/class/es/MSE2034_Notebook/MSE2034_kriz_NoteBook/diffusion/...
 .../numeric/numeric1.htm

$$\alpha = D\theta\Delta t/h^2, \beta = D(1-\theta)\Delta t/h^2, \text{ where for stability } \frac{2D\Delta t}{h^2} \leq \frac{1}{1-2\theta}$$

The finite difference equation (5) reduces to

$$-\alpha C_s^{n+1} - \alpha C_w^{n+1} + (1+4\alpha) C_o^{n+1} - \alpha C_E^{n+1} - \alpha C_N^{n+1} = (1-4\beta) C_o^n + \beta [C_s^n + C_w^n + C_E^n + C_N^n]$$

rearrange

$$(1+4\alpha) C_o^{n+1} = (1-4\beta) C_o^n + \beta [C_{NEWS}^n] + \alpha [C_{NEWS}^{n+1}] \text{ where } C_{NEWS}^n \equiv \uparrow$$

Let $A \equiv 1+4\alpha$ and $B \equiv 1-4\beta$ and multiply by ω

$$\omega C_o^{n+1} = \frac{\omega B}{A} C_o^n + \frac{\omega \beta}{A} [C_{NEWS}^n] + \frac{\omega \alpha}{A} [C_{NEWS}^{n+1}]$$

$$\omega C_o^{n+1} = \underbrace{+\omega C_o^{n+1} - \omega C_o^{n+1}} + \frac{\omega B}{A} C_o^n + \frac{\omega \beta}{A} [C_{NEWS}^n] + \frac{\omega \alpha}{A} [C_{NEWS}^{n+1}]$$

$$\omega C_o^{n+1} - \omega C_o^{n+1} \stackrel{\text{add zero}}{=} \frac{\omega B}{A} C_o^n + \frac{\omega \beta}{A} [C_{NEWS}^n] + \frac{\omega \alpha}{A} [C_{NEWS}^{n+1} - \frac{A}{\alpha} C_o^{n+1}]$$

$$0 = \frac{\omega}{A} \left\{ B C_o^n + \beta [C_{NEWS}^n] \right\} + \frac{\omega \alpha}{A} \left[C_{NEWS}^{n+1} - \frac{A}{\alpha} C_o^{n+1} \right]$$

SLEEP compare:

where diffusion Coef., $\sigma = D$: $0 = \frac{\omega}{A} \left\{ F + \alpha [C_{NEWS}^{n+1} - \frac{A}{\alpha} C_o^{n+1}] \right\}$ Compare with eqn. in subroutine SLEEP "same"

Compare

$$\beta = \sigma(1-\theta)\Delta t/\Delta h^2 \text{ same as array } H(k)$$

$$B = (1-4\beta) = 1-4\sigma(1-\theta)\Delta t/\Delta h^2 \text{ same as array } G(k)$$

$$A = 1+4\sigma\theta\Delta t/\Delta h^2 \text{ same as array } C(k)$$

$$\alpha = \sigma\theta\Delta t/\Delta h^2 \text{ same as arrays } A(k)=B(k)=D(k)=E(k)$$

$$F(k) = G(k)*U(k) + H(k)*(U(k-IC) + U(k-1) + U(k+1) + U(k+IC))$$

$$T = U(k) + (W/C(k))*$$

$$F(k) - (A(k)*U(k-IC) + B(k)*U(k-1) + C(k)*U(k) + D(k)*U(k+1) + E(k)*U(k+IC))$$

comparison checks except for $T = U(k)$ + "same"

If the correct values for C^n and C^{n+1} were substituted into the same term, this term would be zero. But, because C^{n+1} is not known, C^n is used as a guess for the concentration at the next time step, consequently the same term is not zero. This non zero term is used to adjust the current value of $U(k)$ which is then set equal to T . The Crank-Nicholson algorithm states that this adjustment goes to zero if we use the method of Successive Over Relaxation (SOR). The new "adjusted" values for $U(k)$ are substituted as a better guess which results in a smaller adjustment than before. This method is repeated until the same term becomes less than ERRSOR. Next we show that the same term has the same form as the SOR equation (7.88), Ref. [1], pg. 508.

SOR method, Ref. [1], pg 508.

Web
page
Eqn.
(9)

$$C'_{i,j} = C_{i,j} + \frac{\omega}{4} (C_{i-1,j} + C_{i+1,j} + C_{i,j-1} + C_{i,j+1} - 4C_{i,j})$$

Recall: $0 = \frac{\omega}{A} \left\{ F + \alpha \left[C_{NEWS}^{n+1} - \frac{A}{\alpha} C_o^{n+1} \right] \right\}$

expand:

$$0 = \frac{\omega B}{A} C_o^n + \frac{\omega \beta}{A} [C_N^n + C_E^n + C_W^n + C_S^n] + \frac{\omega \alpha}{A} [C_N^{n+1} + C_E^{n+1} + C_W^{n+1} + C_S^{n+1} - \frac{A}{\alpha} C_o^{n+1}]$$

add terms: $+4 \frac{\omega \beta}{A} C_o^n - 4 \frac{\omega \beta}{A} C_o^n = 0$

$$0 = \frac{4\omega \beta}{A} C_o^n + \frac{\omega B}{A} C_o^n + \frac{\omega \beta}{A} [C_N^n + C_E^n + C_W^n + C_S^n - 4C_o^n] + \frac{\omega \alpha}{A} [C_N^{n+1} + C_E^{n+1} + C_W^{n+1} + C_S^{n+1} - \frac{A}{\alpha} C_o^{n+1}]$$

recall $B = 1 - 4\beta$

$$-\frac{\omega \alpha}{A} [C_N^{n+1} + C_E^{n+1} + C_W^{n+1} + C_S^{n+1} - \frac{A}{\alpha} C_o^{n+1}] = \frac{\omega}{A} (4\beta + 1 - 4\beta) C_o^n + \frac{\omega \alpha}{A} [C_N^n + C_E^n + C_W^n + C_S^n - 4C_o^n]$$

Cancel's

$$-\frac{\omega \alpha}{A} [C_{NEWS}^{n+1} - \frac{A}{\alpha} C_o^{n+1}] = \frac{\omega}{A} C_o^n + \frac{\omega \alpha}{A} [C_{NEWS}^n - 4C_o^n], \text{ } \omega \text{ divides out!}$$

but o.k.

$n+1$ (next timestep) concentrations \leftarrow \rightarrow n (current time) concentrations

$$\alpha [C_N^{n+1} + C_E^{n+1} + C_W^{n+1} + C_S^{n+1}] - A C_o^{n+1} = C_o^n + \alpha [C_N^n + C_E^n + C_W^n + C_S^n - 4C_o^n]$$

insert Eqn. into Fig. 2

Equation above is of the form equation (7.88), Ref. [1], pg 508, except Form coeffs.

$$C'_{i,j} = C_{i,j} + \frac{\omega}{4} (C_{i-1,j} + C_{i+1,j} + C_{i,j-1} + C_{i,j+1} - 4C_{i,j})$$

22-141 50 SHEETS
22-142 100 SHEETS
22-144 200 SHEETS

