Conversion of Pdes using **method of lines** to a system of Odes

For simplicity, let

(i) $C_{CO_2} = A$

(ii) $C_{H_2O} = B$

(iii) $\theta\, CO_2 = C$

(iv) $\theta\, H_2O = P$

Using method of lines to convert P.d.e.s to O.d.e.s

(i) $$\frac{\partial A}{\partial t} = -\frac{\partial A}{\partial x} + D\frac{\partial^2 A}{\partial x^2} - (k_1 \times C_{O_2})(1-C-P)$$

$$\cancel{\frac{\partial A}{\partial x} = A_{i+1} - A}$$

$$\frac{\partial A}{\partial x} = \frac{A_{i+1} - A_{i-1}}{2\Delta x}, \quad \frac{\partial^2 A}{\partial x^2} = \frac{A_{i+1} - 2A_i + A_{i-1}}{\Delta x^2}$$

(i)' $$\frac{\partial A_{(i)}}{\partial t} = -\left(\frac{A_{i+1} - A_{i-1}}{2\Delta x}\right) + D\left(\frac{A_{i+1} - 2A_i + A_{i-1}}{\Delta x^2}\right) - (k_1 \times C_{O_2})(1-C-P)$$

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$$(i)'\ \frac{\partial A_{(i)}}{\partial t} = -\left(\frac{A_{i+1} - A_{i-1}}{2\Delta x}\right) + D\left(\frac{A_{i+1} - 2A_i + A_{i-1}}{\Delta x^2}\right) - (k_1 \times C_{O_2})(1 - C - P)$$

$$(ii)\ \frac{\partial B_{(i)}}{\partial t} = -\left(\frac{B_{i+1} - B_{i-1}}{2\Delta x}\right) + D\left(\frac{B_{i+1} - 2B_i + B_{i-1}}{\Delta x^2}\right) + k_2 \cdot A \cdot P -$$

$$k_3(1 - C - P) - \frac{k_4 \cdot B \cdot C}{1 - kC_{O_2}A}$$

$$(iii)\ \frac{\partial C}{\partial t} = -\frac{(k_1 \times C_{O_2})(1 - C - P)}{\Omega C_{O_2}}$$

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(i) $$\frac{\partial A_{(i)}}{\partial t} = -\left(\frac{A_{i+1} - A_{i-1}}{2\Delta x}\right) + D\left(\frac{A_{i+1} - 2A_i + A_{i-1}}{\Delta x^2}\right) - (k_1 \times C_{O_2})(1-C-P)$$

(ii) $$\frac{\partial B}{\partial t}(i) = -\left(\frac{B_{i+1} - B_{i-1}}{2\Delta x}\right) + D\left(\frac{B_{i+1} - 2B_i + B_{i-1}}{\Delta x^2}\right) + k_2 \cdot A \cdot P - k_3(1-C-P) - \frac{k_4 \cdot B \cdot C}{1 - KC_{O_2}A}$$

(iii) $$\frac{\partial C}{\partial t} = -\frac{(k_1 \times C_{O_2})(1-C-P)}{\Omega C_{O_2}}$$

(iv) $$\frac{\partial P}{\partial t} = (k_2 \cdot A \cdot P) - k_3(1-C-P) - \frac{k_4(B \cdot C)}{1 + KC_{O_2} \cdot A} + k_5 \cdot A \cdot C \cdot P$$