ALGORITHM FOR RUNGE-KUTTA NUMERICAL KINETICS UP TO 4TH ORDER

(See Rao, Singiresu. *Applied Numerical Methods for Engineers and Scientists.* Prentice-Hall, Upper Saddle River, NJ, pp. 654-665.)

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Let  m, n     index orders of approximation (or interpolation)
     p        index chemical species
     u, w     index reaction steps, forward or reverse direction,
     i, i-1   index time steps.
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Let $C_p(t_i)$ be concentration of p at time t_i,
$C_p^{(n)}$ be nth order interpolation correction to concentration of p,
$V_u^{(n)}$ be velocity of reaction step u to nth order, and
$R_p^{(n)}$ be the nth order correction to rate of production of p,
k_u be rate constant of step u, and
ν_{pw} be the signed (- for reactants, + for products) stoichiometric coefficient of p in step w.

Algorithm:

do for each t_i
    $\{C_p^{(0)}\} = \{C_p(t_{i-1})\}$ OR $\{C_p(t_{init})\}$
    $\{C_p(t_i)\} = \{C_p(t_{i-1})\}$ OR $\{C_p(t_{init})\}$
    for n = 1 to maxord
        for each step, u
            $V_u^{(n)} = k_u$
            for each species, p, in u

$$V_u^{(n)} = k_u \prod_p^{\text{in } u} C_p^{(n-1)}$$

            next p
        next u
        for each species, p
            $R_p^{(n)} = 0$
            for each step, w, involving p

$$R_p^{(n)} = \sum_{\mathrm{w}}^{\text{involving } p} \nu_{p\mathrm{w}} V_{\mathrm{w}}^{(n)}$$

            next w
            $C_p^{(n)} = C_p^{(0)}$
            for each order, m

$$C_p^{(n)} = C_p^{(0)} + \Delta t \sum_{m=1}^{n} a_{(n+1),m} R_p^{(m)}$$

            next m

            $C_p(t_i) = C_p(t_{i-1}) + \ldots$

$$C_p(t_i) = C_p(t_{i-1}) + \Delta t \sum_{n=1}^{\max n} b_n R_p^{(n)}$$

        next p
    next n
next t_i (old $t_i \rightarrow t_{i-1}$)

The $\{a_{nm}\}$ and $\{b_n\}$ are constants determined by the methodology (see reference).