Computer treatment of the chemical part in an air pollution model

1. *Computational problems* *in the chemical part*
2. *Treatment of the* *other parts* *of the model*
3. *QSSA* *method*
4. *Classical* **numerical methods**
5. *Rosenbrock methods*
6. *Special* **numerical methods**
7. *Numerical results*

1. Computational difficulties

Process	Computing time	Relative part
Chemistry	16147	83.09
Advection	3013	15.51
Initialization	2	0.00
Input operations	50	0.26
Output operations	220	1.13
Total	19432	100.00

2. Major parts of a model

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y}$$ hor. transport

$$+\frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right)$$ hor. diffusion

$$-\quad (k_{1s} + k_{2s})c_s$$ deposition

$$+ E_s + Q_s(c_1, c_2, \ldots, c_q)$$ chemistry

$$-\frac{\partial (wc_s)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s}{\partial z}\right)$$ vert. exchange

$$s = 1,2,\ldots,q$$

$$\frac{dg}{dt} = A_1(t)g + A_2 g + A_3(t)g + A_4(t,g) + A_5(t)g$$

3. Diffusion part

Horizontal diffusion:

1. If finite elements are used, it is treated together with the advection part
2. If the PS method is used, then the horizontal diffusion is treated separately

Vertical exchange: finite elements were always used

$$\frac{\partial c}{\partial t} = -\frac{\partial (wc)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z} \right)$$

$$P \frac{dg}{dt} = Hg$$

Implicit integration methods

$$P - \gamma \Delta tH$$

Shifted Jacobian matrix

4. Deposition part

$$\frac{\partial c_s}{\partial t} = -(k_{1s} + k_{2s})c_s \qquad s = 1,2,\ldots, q$$

$$\frac{dg}{dt} = -(k_{1s} + k_{2s})g \qquad g \in \Re^N$$

The last systems consists of independent linear equations and, thus, can be solved analytically

5. The QSSA method

$$\frac{dy_s}{dt} = P_s(t, y_1, y_2, \ldots, y_q) - L_s(t, y_1, y_2, \ldots, y_q) y_s$$

$$s = 1, 2, \ldots, q, \qquad y_s \in \Re, \quad y_s^{n+1} \approx y_s(t)$$

$$y_s^{n+1} = \frac{P_s}{L_s} \qquad \text{for} \qquad \Delta t L_s > 10$$

$$y_s^{n+1} = \frac{P_s}{L_s} + \left(y_s^n - \frac{P_s}{L_s} \right) e^{-\Delta t L_s} \qquad 0.01 < \Delta t L_s \le 10$$

$$y_s^{n+1} = y_s^n + \Delta t \left(P_s - L_s y_s^n \right) \qquad \Delta t L_s \le 0.01$$

1. Use the formulae as an explicit method
2. Combine them with an iterative process

5b. Improved QSSA method

$$y_s^{n+1} = \frac{P_s}{L_s} + \left(y_s^n - \frac{P_s}{L_s} \right) e^{-\Delta t L_s}$$

$$e^{-\Delta t L_s} \approx \frac{1}{1 + \Delta t L_s + 0.5 \left(\Delta t L_s \right)^2}$$

$$y_s^{n+1} = \frac{y_s^n + (1 + 0.5 \Delta t L_s) \Delta t P_s}{1 + \Delta t L_s + 0.5 \left(\Delta t L_s \right)^2}$$

6. Backward Euler

$$\frac{dy}{dt} = f(t, y)$$

$$y_{n+1} = y_n + \Delta t \; f_{n+1}, \qquad y_n \approx y(t_n), \quad f_n = f(t_n, y_n)$$

$$F(y_{n+1}) = 0, \qquad F(y_{n+1}) = y_{n+1} - y_n - \Delta t \; f_{n+1}$$

$$J_{n+1} = \frac{\partial f(t, y)}{\partial y}, \qquad for \qquad t = t_{n+1}, \quad y = y_{n+1}$$

$$\frac{\partial F(y_{n+1})}{\partial y_{n+1}} = I - \Delta t \, J_{n+1}$$

6.b. Backward Euler - continuation

$$\left(I - \Delta t J_{n+1}^{[i-1]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f\left(t_{n+1}, y_{n+1}^{[i-1]}\right)$$

$$y_{n+1}^{[i]} = y_{n+1}^{[i-1]} + \Delta y_{n+1}^{[i]}$$

$$y_{n+1}^{[0]} = y_n \qquad or \qquad y_{n+1}^{[0]} = y_n + \frac{\Delta t_{n+1}}{\Delta t_n}\left(y_n - y_{n-1}\right)$$

At each iteration the following operations must be carried out:

1. **Function evaluation**
2. **Jacobian evaluation**
3. **Form a system of linear algebraic equations**
4. **Solve the system of linear algebraic equations**
5. **Update the solution**

6c. Modified Newton methods

$$\left(I - \Delta t J_{n+1}^{[i-1]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f(t_{n+1}, y_{n+1}^{[i-1]})$$

$$\left(I - \Delta t J_{n+1}^{[0]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f(t_{n+1}, y_{n+1}^{[i-1]})$$

$$\left(I - \Delta t J_{m}^{[j]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f(t_{n+1}, y_{n+1}^{[i-1]})$$

$$m \le n+1, \qquad j \ge 0$$

$$y_{n+1}^{[i]} = y_{n+1}^{[i-1]} + \Delta y_{n+1}^{[i]}$$

7. Other integration methods

Implementation: similar to that for the BE

- Trapezoidal Rules
- Second order RK method

Alexandrov et al. (1997)

Difficulty: load balancing when parallel computers are used

Rosenbrock methods

8. Numerical Results

Method	Computing time
QSSA-1	12.85
QSSA-2	11.72
Euler	15.11
Trapez.	15.94
RK-2	28.49

Better accuracy with the classical numerical methods