THE USE OF STATE VARIABLES IN THE MODELLING AND NUMERICAL SIMULATION OF POLLUTANTS DISPERSION

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Abstract: The paper presents a method based on „the matrix with partial derivatives of the state vector" (M_{pdx}) for numerical modelling and simulation of processes with distributed parameters, using the Taylor series. This method can also be used for modelling and numerical simulation of pollutants dispertion.
Keywords: partial derivative equation, state variables, Taylor series, numerical integration, pollutants .

1. INTRODUCTION

It is known that the usual analytical of linear processes with distributed parameters can be expresses using equations or equation systems with linear partial derivatives. The equation with linear partial derivatives (pde), to which this paper refers to is presented in the below:

$$a_{0000}\cdot c + a_{1000}\cdot\frac{\partial c}{\partial t} + a_{0100}\cdot\frac{\partial c}{\partial p} + a_{0010}\cdot\frac{\partial c}{\partial q} + a_{0001}\cdot\frac{\partial c}{\partial r} +$$
$$a_{2000}\cdot\frac{\partial^2 c}{\partial t^2} + a_{1100}\cdot\frac{\partial^2 c}{\partial t\cdot\partial p} + a_{0200}\cdot\frac{\partial^2 c}{\partial p^2} + a_{0110}\cdot\frac{\partial^2 c}{\partial p\cdot\partial q} +$$
$$a_{0020}\cdot\frac{\partial^2 c}{\partial^2 q} + a_{0011}\cdot\frac{\partial^2 c}{\partial q\cdot\partial r} + a_{0002}\cdot\frac{\partial^2 c}{\partial^2 r} + a_{1010}\cdot\frac{\partial^2 c}{\partial t\cdot\partial q} +$$
$$a_{0101}\cdot\frac{\partial^2 c}{\partial p\cdot\partial r} + a_{1001}\cdot\frac{\partial^2 c}{\partial t\cdot\partial r} = \varphi(t,p,q,r) \qquad (1)$$

All coefficients (...) are considered to be constant and φ(t,p,q,r), and c(t,p,q,r) and fulfill the continuity conditions in the Cauchy sense. The independent variables (t), (p),(q), and (r) could represent the time (t), respectively the spatial abscise (p), (q), and (r) in Cartesian system (Omatu., and Seinfeld, 1989; Farlow, 1982; Bellomo, and Preziosi, 1995).
The initial conditions (IC) are considered to be know and for boundary conditios (BC) and final condition (FC), as the case may be, other explanations could be added.

2. STATE VARIABLES, INITIAL CONDITIONS, BOUNDARY CONDITIONS AND FINAL CONDITIONS

Introducing the notation:

$$x_{TPQR} = \frac{\partial^{T+P+Q+R} c}{\partial t^T\cdot\partial p^P\cdot\partial q^Q\cdot\partial r^R} \qquad (2)$$

for the state variables and T=0,1,2,…, P=0,1,2,…, Q=0,1,2…., R=0,1,2,….., equation (1) can be rewritten as follow:

$$a_{0000}\cdot x_{0000}+a_{1000}\cdot x_{1000}+a_{0100}\cdot x_{0100}+a_{0010}\cdot x_{0010}+$$
$$a_{0001}\cdot x_{0001}+a_{2000}\cdot x_{2000}+a_{1100}\cdot x_{1100}+a_{0200}\cdot x_{0200}+$$
$$a_{0110}\cdot x_{0110}+a_{0020}\cdot x_{0020}+a_{0011}\cdot x_{0011}+a_{0002}\cdot x_{0002}+$$
$$a_{1010}\cdot x_{1010}+a_{0101}\cdot x_{0101}+a_{1001}\cdot x_{1001}=\varphi_{0000} \qquad (3)$$

The state vector values for initial conditions, boundary conditions and final conditions are presented in Tabel 1.

Tabel 1.

x_{IC}	x_{BC}	x_{FC}
$x(t_0,p,q,r)$	$x(t,p_0,q,r)$; $x(t,p,q_0,r)$ $x(t,p_f,q,r)$; $x(t,p,q_f,r)$	$x(t_f,p,q,r)$

3. THE COMPLETE METHOD OF THE TAYLOR SERIES FOR THE APPROXIMATION OF THE VECTOR (x_k). THE DEFINITION OF THE MATRIX M_{pdx}

The method is based on the iterative use of the Taylor series, included in a table structure.
For the case presented here, having the temporal variable (t) and three spatial variables (p), (q), and (r), the table structure will be denoted with (M_{pdx}) and it will be called „the matrix with partial derivatives of the state vector" (Colosi, 2006) . The table structure has the form below:

$$\mathbf{M}_{pdx} = \begin{array}{c|cc} & 1\text{xM} & \\ n & \mathbf{x} & \mathbf{x}_{PQR} \\ \text{x} & & \\ N & \mathbf{x}_T & \mathbf{x}_{TPQR} \end{array} \qquad (4)$$

Under more explicit x, $x_{PQR,}$ x_T, and x_{TPQR} terms the matrix become:

$$\mathbf{M}_{pdx} = \begin{array}{c|cc} & 1\text{xM} & \\ n & x_{0000} & \mathbf{x}_{0PQR} \\ \text{x} & x_{1000} & \mathbf{x}_{1PQR} \\ N & \ldots & \ldots \\ & x_{n-1,000} & \mathbf{x}_{n-1,PQR} \\ & x_{n,000} & \mathbf{x}_{n,PQR} \\ & x_{n+1,000} & \mathbf{x}_{n+1,PQR} \\ & \ldots & \ldots \\ & x_{n-2+N,000} & \mathbf{x}_{n-2+N,PQR} \\ & x_{n-1+N,000} & \mathbf{x}_{n-1+N,PQR} \end{array} \qquad (5)$$

Notations used:

- **x**(nx1) is the state vector corresponding to the variable with respect to which the numerical integration was made. Next, we consider this variable to be the (t) time variable;
- $\mathbf{x}_{PQR}$ (nxM) is made of a number of (M) state vectors which have been multiplied and partially derived with respect to (p), (q) and (r);
- $\mathbf{x}_T$(Nx1) is a state vector containing the partial derivatives of the state x vector elements in respect to time;
- $\mathbf{x}_{TPQR}$(NxM) is a matrix which was derived from the $\mathbf{x}_{PQR}$(nxM) , whose elements are partial derivatives with respect to time (p), (q), and (r);
- n is the order of the equation as well as the number of the state variables;
- N is the partial derivative number of the state vector in respect to time. Usually (N≥n).

The defined $\mathbf{M}_{pdx}$[(n+N)x(1+M)] matrix will be calculated using the iterative calculus. The calculation includes different stages according to each (Δt) integration step, as follows:

3.1 The Stage of the Rregressive Sequence (k-1).

Consists in the calculation of $M_{pdx,k-1}$ (matrix of the state vector partial derivatives).

$$\mathbf{M}_{pdx,k-1} = \begin{array}{|c|c|} \hline \mathbf{x}_{k-1} & \mathbf{x}_{PQR,k-1} \\ \hline \mathbf{x}_{T,k-1} & \mathbf{x}_{TPQR,k-1} \\ \hline \end{array} \qquad (6)$$

Which could also correspond to the start of the calculation, i.e. $t_0=t_{k-1}$. Knowing that $\mathbf{x}_{k-1} = \mathbf{x}(t_{k-1},p,q,r)$, we can calculate the elements of the matrix by means of partial and multiple derivatives.

$$\mathbf{x}_{PQR,k-1} = \mathbf{x}_{PQR}(t_{k-1},p,q,r) \qquad (7)$$

3.2 The Stage of the Current Sequence (k).

In this stage, the vector (x_k) and the matrix ($x_{PQR,k}$) are approximated by (trunk) Taylor series . Formally they are representd by:

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \sum_{T=1} \frac{\Delta t^T}{T!} \mathbf{x}_{T,k-1} \qquad (8)$$

respectively:

$$\mathbf{x}_{PQR,k} = \mathbf{x}_{PQR,k-1} + \sum_{T=1} \frac{\Delta t^T}{T!} \mathbf{x}_{TPQR,k-1} \qquad (9)$$

thus, showing that for the two (k-1) and (k) sequences we have the (t_{k-1}) and $t_k=t_{k-1}+\Delta t$, where the (Δt) integration step is considered to be short enough. At the end of this sequence we operate the change from the (k) sequence to (k-1) sequence and we start the stage of (k-1) regressive sequence.

4. EXAMPLE FOR A DISPERSION OF INDUSTRIAL POLLUTANTS

To check the above mentioned modelling and numerical simulation method the following cases are used.

4.1 The Analytical Solution.

The analytical solution necessary for the start of the analytical calculations and for the cumulative relative error in percent (crep) is the following:

$$c_{AN}=A\cdot\varepsilon^{-(\frac{t-t_g}{\sigma_t})^2}\cdot\varepsilon^{-(\frac{p-p_g}{\sigma_p})^2}\cdot\varepsilon^{-(\frac{q-q_g}{\sigma_q})^2}\cdot\varepsilon^{-(\frac{r-r_g}{\sigma_r})^2}\cdot k_u\cdot u \quad (10)$$

4.2 The Coefficients of the Analytical Solution

They are:
A=1;
σ_t=0.5; σ_p=0.5; σ_q=0.5; σ_r=0.8
a_{0000}=1; a_{1000}=T1+T2; a_{0100}=P1+P2; a_{0010}=Q1+Q2;
a_{0001}=R1+R2;a_{2000}=T1*T2;a_{1100}=(T1+T2)*(P1+P2);
a_{1010}=(T1+T2)*(Q1+Q2);a_{1001}=(T1+T2)*(R1+R2);
a_{0200}=P1*P2;a_{0110}=(P1+P2)*(Q1+Q2);
a_{0101}=(P1+P2)*(R1+R2);a_{0020}=Q1*Q2; (11)
a_{0011}=(Q1+Q2)*(R1+R2); a_{0002}=R1*R2;
and
T1=0.1; T2=0.2; P1=0.15; P2=0.25; Q1=0.15; Q2=0.25; R1=0.04; R2=0.06;

4.3 Cases Considered.

We consider three usual cases described by the following values.

First case:
t_0 = 0; t_f = 1; t=0:0.05…1; r_g =0; r_0 =0; r_f =0.5 ; r=0:0.05…0.5; q_0=0;q_f= 0 ; q=q_f; p_0=0; p_f= 0; p = p_f
(the results are represented in figure 1.)

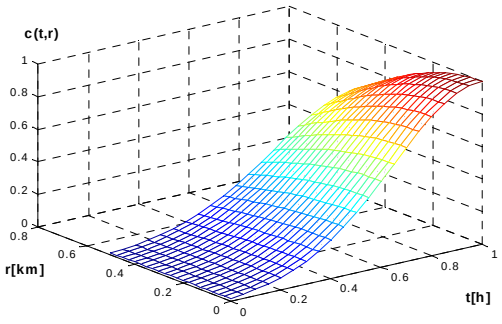

Fig. 1. The variation of c[μg/m^3] for p=0[km],q=0[km], r=0-0.5[km] and t=0-1[h].

Second case:
t_0 = 0; t_f = 1; t=0:0.05…1; q_0 =0; q_f =0; q= q_f;
p_0 = 0 ; p_f=2; p=0:0.1…2; p_g = 0; r_0=0; r_f = 0;r = r_f
(the results are represented in figure 2.)

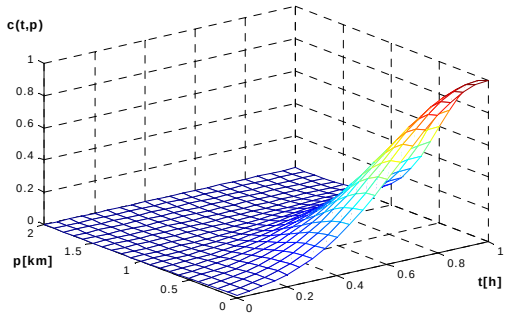

Fig. 2. The variation of c[μg/m^3] for q=0[km],r=0[km], p=0-2[km] and t=0-1[h].

Third case:
t_0 = 0; t_f = 1; t=0:0.05…1; p_0 =0; p_f =0 ;p=p_f; q_g = 0; q_0 = 0 ; q_f=2; q=0:0.1…2; r_0=0; r_f = 0.1; r = r_f ;(the results are represented in figure 3.)
The time and space's constants are: T_1=0.1; T_2=0.2; P_1=0.15; P_2=0.25; Q_1=0.15;Q_2=0.25; R_1=0.04; R_2=0.06 ; k_u=1; u=1 for all the cases studied.

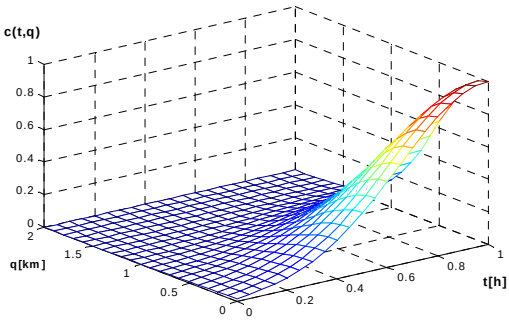

Fig. 3. The variation of c[μg/m^3] for p=0[km],r=0[km], q=0-2[km] and t=0-1[h].

4.4 Value of n,N,M.

Values for the n, N and M are: n=2; N=3 ; M=6.

4.5 The Cumulative Relative Error Percents.

The accuracy of the numerical integration was approximated through the cumulative relative error percents defined by:

$$crepc = 100\cdot\frac{\sum_{t_0}^{t_f}|\Delta x_{0..0}|}{\sum_{t_0}^{t_f}|x_{AN\,0..0}|} \quad (12)$$

where:
$|\Delta x_{0..0}| = |c_{AN} - x_{0..0}|$ (difference between numerical and analytical solution in absolute values);

$|x_{AN0..0}| = |c_{AN}|$ corresponds to the analytical value adding that $(\sum_{t_0}^{t_f})$ is the iterative sum up of calculus sequences from t_0 to t_f . The integration step is 0.001 and the cumulative relative error percents is less then 0.02 percents . The following tabel shows some values of crepc.

Table 2

t	0.2	0.4	0.6	0.8	1
c(t,p)	0.046	0.142	0.317	0.512	0.600
crepc	$5*10^{-5}$	$5*10^{-5}$	$5*10^{-5}$	$1*10^{-4}$	$1*10^{-4}$
c(t,q)	0.049	0.152	0.339	0.547	0.641
crepc	$5*10^{-5}$	$5*10^{-5}$	$5*10^{-5}$	$1*10^{-4}$	$1*10^{-4}$
c(t,r)	0.052	0.161	0.357	0.577	0.676
crepc	$5*10^{-5}$	$5*10^{-5}$	$5*10^{-5}$	$1*10^{-4}$	$1*10^{-4}$

5. CONCLUSIONS

This paper presents a possible numerical modelling and simulation variant with second order partial derivative equations, which depend on four independent variable . One of them (t), represents time and the other (p), (q), and (r), are usually considered spatial Cartesian coordinates.

The paper defines and uses the „ matrix with partial derivatives of state vector" (M_{pdx}), associated to the Taylor series, dedicated to modelling and numerical simulation of a large category of partial differential equations.

For the proposed variant we operate with time constants T_1 and T_2 and length constants P_1, P_2 ,Q_1 ,Q_2, R_1 , and R_2 . These constants are usually used in thermo-energetical and chemical engineering.

Choosing those constants conveniently we can obtain a lot of geometry for dispersion pollutants.

In this paper three examples which can approximate the following situations are considered:

- the source of the pollutants is a power plant stack;
- the origin of the Cartesian system is on the top of stack, which is the source of pollutants;
-the pollutants dispersion is considered during 1 hour and:
- on 0.1 km upper stack (p=0; q=0; r=0-0.5) (Fig. 1).
-on 2km horizontal (p=0-2km, q=0km and r=0) (Fig. 2);
- on 2km horizontal (q=0-2km, p=0km and r=0km) (Fig. 3);

For the validation of the method and to determine the performance of numerical integration the constants in (11) have been used .

Table 2 shows a cumulative relative error of c (crep c) equal with $5*10^{-5}$-10^{-4} percents, which demonstrates the numerical integration performance and validity.

The commonly used method of modelling air pollutant dispersion is represented by a differential equation, which expresses the rate of change of pollutant concentration in terms of average wind speed and turbulent diffusion. Mathematically, this process is derived from the mass conservation principle, (Mastoraks, 2004). The basic diffusion equation used in air quality modelling is given by:

$$\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \frac{\partial^2 C}{\partial^2 x} + D_y \frac{\partial^2 C}{\partial^2 y} + D_z \frac{\partial^2 C}{\partial^2 z} + w; \quad (13)$$

where:

- C represents the concentration in atmospheric pollution (μg /m^3);
- D_x,D_y, and D_z represent the diffusion coefficients (m^2/s);
- u represents the wind speed (m/s);
-w represents the mass of species due to chemical reactions(kg/m^3s);

Equation (13) can be obtained from (1) by setting the coefficients to particular values.

This preliminary approximated work for pollutants dispersion can be completed with details regarding meteorological and terrain factors.

Also, the work will be used for numerical modelling and simulation control system in reduced pollutants industrial processes.

The accuracy of the numerical integration that was approximated through the (crepc), can be controlled and improved if N and M are chosen accordingly.

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