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IDENTIFICATION METHODS FOR MULTIPLE CELL SYSTEMS

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SYNOPSIS

A tracer gas technique for determining volumes and airflow rates in multi-cell systems with a single tracer gas is considered. Tracer gas is injected in all cells simultaneously according to a cetain pattern and the resulting tracer gas concentrations are recorded. We show how the volumes and flow rates can be identified from the measurements using the quadratic programming method. A characteristic of this method is that the unknown model parameters, i.e. the volumes and flows, can be determined subjected to given constraints. Accordingly we can utilize all known information about the flow system and make sure that a found solution is physically compatible with a flow system.

Different formulations of the mass balance relations are discussed and a new method to overcome the difficulties to calculate the derivatives of the tracer gas concentrations is proposed. The properties of the different formulations such as the sensitivity to noise and the significance of the sample period are exemplified by identifications on a simulated three cell system.

LIST OF SYMBOLS

A	the matrix $V^{-1}Q$	n by n
A	matrix of measured data, see (3.4)	mn by n_p
b	vector of measured data, see (3.5)	mn by 1
$c(t)$	tracer gas concentration vector	n by 1
$\dot{c}(t)$	derivatives of $c(t)$	n by 1
D	the matrix $A(\exp(AT_s)-I)^{-1}$	n by n
$E(x)$	expectation value of x	
G	matrix of constraints	n_g by n_p
g	vector of lower limits in the constraints	n_g by 1
I	identity matrix	
m	number of samples	
m_{int}	number of subintervals of the interval of integration	
n	number of cells in the flow system	
n_c	number of parameters in the LCP problem, see (3.22)	
n_g	number of constraints	
n_p	number of parameters	
$p(t)$	tracer gas injection vector	n by 1
Q	flow matrix	n by n
Q	the matrix A^TA	
q_{ij}	flow to cell i from cell j	
T_{int}	interval of integration	
T_s	sample period	
TC	building time constant (inverse of air exchange rate)	
t	time	
t_k	discrete time	
u	vector of Lagrange multipliers	n_g by 1
V	volume matrix	n_g by n
v	vector of Lagrange multipliers	n_p by 1
x	model parameter vector, see (3.1)	

1 INTRODUCTION

Following the ideas suggested by Jensen (1986,1987b) we consider an experiment where tracer gas is injected in all cells simultaneously using a certain pattern in time, so that the influence of different tracer gas inputs can be separated. Ideal mixing is assumed in each cell and the flows are assumed to be constant and without time delays.

A large system of equations can be stated based on the mass balance equations, measured tracer gas concentrations and tracer gas injections. As the model is stated in continuous time the system of eqautions is linear in the model parameters, i.e. the unknown flows and volumes which are to be identified. There are also linear constraints on the model parameters which must be fulfilled if the solution should be compatible with a flow system. Important constraints are that all flows and volumes must be non-negative. Because of these constraints the commonly used least square identification method is not so useful in this case.

So far the linear programming (LP) method has been used, see Jensen (1987b). This method permits constraints but, however, as the number of measurements (m) increases the demand for computer time and storage grows very fast (approx. as m^3 and m^2, respectively) and soon this may be a serious limitation. This is certainly true on a PC based system.

In this paper some alternative methods to state and solve the identification problem are proposed. Especially we show that quadratic programming (QP) has some attractive properties. The QP method has been used on a number of simulated test experiments with a three cell system and with different levels of measurement noise. It has proved to work well in these tests.

Like the LP method, the QP method makes use of the constraints of the model parameters to guarantee that the solution is a flow system. But, and this is the main advantage, the dimension of the QP problem does not depend on the number of measurements, but only on the number of model parameters and constraints. In spite of a slightly more complicated solution, the savings in computer time and storage may become most considerable when the number of measurements increases.

2 MODELS FOR FLOW SYSTEMS

In this chapter we shall derive some different variations of the mass balance relations which can be stated from measurement of a multi-cell flow system. These models will be used in the next chapter when we show how to compute the flows and volumes from given measurements.

Section 2.1 summarizes some basic facts about the mass balance equations for a flow system. This is a well-known model, see e.g. Sinden (1978) for a more detailed treatment. A difficulty with the mass balance is that it contains the time derivatives of the tracer gas concentrations. The following sections deal with different ways to overcome this problem. Since it is not suitable to use an ordinary discrete time model, we show how to calculate the derivatives from measurements both approximately and exactly with an iterative model, see Section 2.3. Another way to avoid the derivatives is to integrate the mass balance equations. In this case, however, a new problem is how to compute the integral of the tracer gas concentration. Again, this can be done approximately as well as exactly by a model based method. This is described in Section 2.4. Finally, in Section 2.5 we make a summing up of the models.

2.1 The mass balance of a flow system

Consider a flow system with n cells. Each cell can be connected to the other n-1 cells and to the exterior or the outside by flows through one-way passages, see Figure 2.1

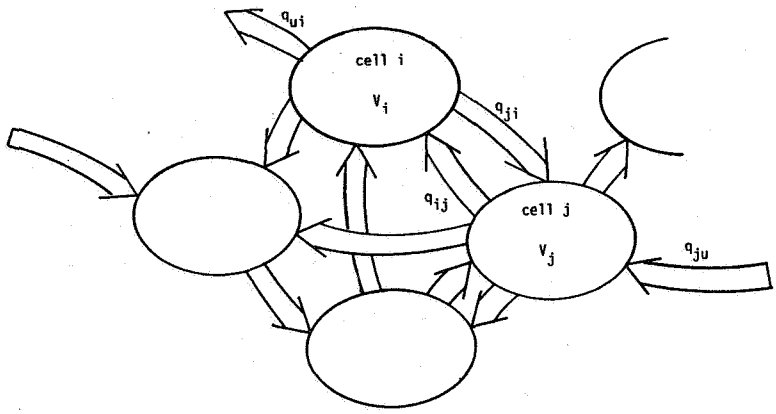

Figure 2.1 An example of a flow system

The parameters of the system are the volumes, denoted v_i, the flows to and from the outside, denoted q_{ui} and q_{iu} respectively and the interflows between the cells, where the flow to cell i from cell j is denoted q_{ij}. The number of parameters is n volumes, n inflows, n outflows and n(n-1) interflows or altogether n(n+2) parameters. Some of the flows may, of course, be equal to zero.

As the sum of flows into each cell must be equal to the sum of flows out from the cell, it follows that n flows are dependent of the other flows. Thus a general flow system with n cells has n(n+1) independent parameters.

Provided that all flows are constant and without time delays, and that the mixing in each cell is perfect the following mass balance equation holds for each cell i, i=1,n

$$v_i \dot{c}_i(t) = \sum_{j \neq i}^{n} q_{ij} c_j(t) - q_{ti} c_i(t) + p_i(t), \quad i=1,n \qquad (2.1)$$

where $c_i(t)$ denotes the tracer gas concentration in cell i at time t, $\dot{c}_i(t)$ denotes the time derivative of $c_i(t)$ and $p_i(t)$ denotes the tracer gas injection in cell i. q_{ti} denotes the total outflow from cell i.

The total outflow for each cell i can be written as

$$q_{ti} = \sum_{j \neq i}^{n} q_{ji} + q_{ui}, \qquad i=1,n \qquad (2.2)$$

and the equally large total inflow can be written as

$$q_{it} = \sum_{j \neq i}^{n} q_{ij} + q_{iu}, \qquad i=1,n \qquad (2.3)$$

By using matrix notation, all the n mass balances in (2.1) can also be expressed in a compact form

$$V\,\dot{c}(t) = Q\,c(t) + p(t) \qquad (2.4)$$

Now, $\dot{c}(t)$, $c(t)$ and $p(t)$ are n by 1 vectors with the elements $\dot{c}_i(t)$, $c_i(t)$ and $p_i(t)$, i=1,n. V is an n by n diagonal volume matrix with entries equal to the volumes v_i. Q is an n by n flow matrix. The diagonal elements Q_{ii} are equal to $-q_{ti}$ and the off-diagonal elements Q_{ij}, $i\neq j$ are the interflows q_{ij}.

However, if a given model in the form (2.4) should be compatible with a flow system the matrices V and Q must have the following properties, (2.5)-(2.9). All the volumes and flows must be non-negative, that is

$$V_i \geq 0, \quad i=1,n \qquad (2.5)$$

$$Q_{ij} \geq 0, \quad i\neq j \qquad (2.6)$$

The total flows to/from each cell are positive. Consequently, the diagonal elements in the flow matrix must be negative

$$Q_{ij} < 0, \quad i=j \qquad (2.7)$$

From the equations (2.2) it follows that the sums of the rows of the flow matrix equal the negative value of the inflows from the outside. As all inflows must be non-negative it follows that

$$\sum_j Q_{ij} = -q_{iu} \leq 0, \quad i=1,n \qquad (2.8)$$

In the same way the equations (2.3) state that the sums of the columns of the flow matrix equal the negative value of the outflows to the outside. Hence, also the sums of columns must be non-positive

$$\sum_i Q_{ij} = -q_{uj} \leq 0, \quad j=1,n \qquad (2.9)$$

These five constraints on the volume and flow matrices will play an important role when we shall choose identification method.

2.2 The mass balance equations in discrete time

The most convenient way to work with a system of linear differential equations, as our mass balances (2.4), is to transform it to a system of difference equations. The difference equations only describe the variables at discrete sample instants. But provided that the inputs (i.e. the tracer gas injections) are constant during the sample periods, this is an exact description of the continuous time system at the sample instants.

It is very easy to make simulations with the difference equations, and the methods to identify discrete time models are very well established, see Jung (1987).

To obtain the mass balance in discrete time we shall first rewrite (2.4) in a more common form

$$\dot{c}(t) = A\,c(t) + B\,p(t) \qquad (2.10)$$

where A and B are the n by n matrices

$$A = V^{-1}Q \tag{2.11}$$

$$B = V^{-1} \tag{2.12}$$

The corresponding equation in discrete time is given by (see e.g. Åström (1985) for complete details or just integrate (2.10))

$$c(t_k+T_s) = Fc(t_k) + Gp(t_k) \tag{2.13}$$

where $c(t_k)$ och $p(t_k)$ are the sampled values of $c(t)$ and $p(t)$ at the discrete sample instants $t_k=t_o+kT_s$, $k=\ldots,-1,0,1,\ldots$. T_s is the sample period and F and G are n by n matrices given by

$$F=\exp(AT_s) \tag{2.14}$$

$$G=(\exp(AT_s)-I)A^{-1}B=(\exp(AT_s)-I)Q^{-1} \tag{2.15}$$

In our case, however, the discrete time model is not an appropriate model to identify. The reason is that the constraints on the flow matrix Q (2.8) and (2.9) will not be linear after transformation to discrete time, this is shown in detail in Jensen (1987a). As we cannot make use of all the constraints we can neither guarantee that an identified model will be compatible with a flow system. Of course, it may be compatible this is easy to check afterwards but generally, we will not find a flow system. Moreover, even if the identified model is a flow system, it is hard to compute the diagonal matrix V from (2.14) and (2.15) as F and G are filled matrices.

Since we cannot use the discrete time model we have to work with the original time continuous model (2.4). The next two sections will treat how to deal with the time derivative in this model.

Nevertheless, we will take advantage of the discrete time model in the following sections when computing the derivative and integral of the tracer gas concentration vector. It will also be used to simulate the test example in chapter 4.

2.3 Computing the time derivatives of the tracer gas concentration vector

The simplest but certainly not the most accurate method to estimate the time derivative is to use a difference approximation. There are several possibilities: forward, backward, forward/backward difference and so on. The most useful method, see Jensen (1986), turns out to be the ordinary forward difference

$$c(t) \approx (c(t_k+T_s) - c(t_k))/T_s \tag{2.16}$$

If the sampled signal $c(t_k)$ is measured without measurement noise then the approximation becomes better the smaller the sample period is chosen. But (2.16) is quite sensitive to noise and the error caused by noise increases as the sample period is reduced. The final choice of sampling period becomes a compromise between error from the approximation and error from the noise.

As already mentioned, the derivative can also be computed exactly from the discrete time model. To derive a formula for this, start from equation (2.13) and replace the matrices F and G with the expressions (2.14) and (2.15), respectively. After subtracting both sides by $c(t_k)$ we get

$$c(t_k+T_s)-c(t_k) = (\exp(AT_s)-I)c(t_k)+(\exp(AT_s)-I))Q^{-1}p(t_k) \qquad (2.17)$$

Multiply this equation from the left by D, where D denotes the n by n matrix

$$D = A(\exp(AT_s)-I)^{-1} \qquad (2.18)$$

After reduction we obtain

$$D(c(t_k+T_s)-c(t_k)) = A\ c(t_k) + B\ p(t_k) \qquad (2.19)$$

Comparing this equation with (2.10) we recognize that the left side in (2.19) equals c(t), i.e.

$$\dot{c}(t_k) = D(c(t_k+T_s) - c(t_k)) \qquad (2.20)$$

Notice that this formula is not an approximation but holds exactly the same assumptions as provided for the discrete time model. A comment is that theoretically the tracer gas injection p(t) thus must be constant between the sampling instants. In practice, however, a more convenient way is to inject the tracer gas by pulses. But these pulses must be sufficiently small and equally spread over the sampling period. The meaning of 'sufficiently small' in this context is possible to calculate, given a discrete time model.

A difficulty with (2.20) is that D depends on A, see (2.18). Since we want to identify the flow and volume matrices, $A(=V^{-1}Q)$ is unknown and so we cannot calculate the derivatives.

A solution of this problem is to start with $D=IT_s^{-1}$ as in the forward difference approximation and identify a preliminary model. With this model we can calculate a new matrix D and a new better approximation of $c(t_k)$. Then we can identify a new model and the process proceeds iteratively. The method will converge in a few steps if the sampling period is not too long compared with the time constants of the system, see examples in chapter 4.

The best numerical method to calculate D from (2.18) is to use the following Taylor series expansion

$$T_sD=(AT_s)(\exp(AT_s)-I)^{-1}=I-(AT_s)/2+bn_1(AT_s)^2/2!-bn_2(AT_s)^4/4! +bn_3(AT_s)^6/6!-\ldots \qquad (2.21)$$

where bn_i, i=1,2,... denotes the Bernoulli numbers.

From (2.21) it is clear that the matrix D is approaching IT_s^{-1} as the sample period T_s decreases. As a limit, the formula (2.20) will turn into the forward difference (2.16) when T_s goes to zero.

The matrix D has the properties that the diagonal elements are a bit greater than 1 while the off-diagonal elements are rather small and negative. This results in a somewhat higher sensitivity to noise in the model based formula than in the forward difference formula. In both formulas the noise sensitivity increases as T_s decreases.

2.4 The integrated mass balance

A common way to suppress noise is to integrate. Integrating the mass balance (2.4) from the time t_k to t_k+T_{int} yields

$$V(c(t_k+T_{int}) - c(t_k))=Q\ C(t_k)+P(t_k) \tag{2.22}$$

where $C(t_k)$ and $P(t_k)$ denote the integrals of $c(t_k)$ and $p(t_k)$ respectively

$$C(t_k)=\int_0^{T_{int}} c(t_k+s)ds \tag{2.23}$$

$$P(t_k)=\int_0^{T_{int}} p(t_k+s)ds=T_{int}p(t_k) \tag{2.24}$$

The last equality in (2.24) makes use of the assumption that the tracer gas injection is constant during the interval of integration, T_{int}.

The integral $C(t_k)$ can be calculated approximately with the trapezoidal rule. Suppose that the interval of integration is subdivided in $m_{int}=T_{int}/T_s \geq 1$ equal subintervals, then the integral is approximated by

$$C(t_k)=T_s \sum_{i=0}^{m_{int}} f_i c(t_k+iT_s) \tag{2.25}$$

where the coefficients $f_0=f_{m_{int}}=1/2$ and the others $f_i=1$, i=1,n-1.

In this formula it is always advantageous to choose a short sampling period in order to use many measurements and reduce the noise corruption.

The integral $C(t_k)$ can also be determined exactly and this can be done in several different ways. Since the discrete time model is valid for every choice of the sample period as long as the input is constant, we can exchange T_s in (2.13) for the time argument s, where $0 \leq s \leq T_{int}$. This gives

$$c(t_k+s) = \exp(As)c(t_k) + (\exp(As)-I)A^{-1}B\ p(t_k) \tag{2.26}$$

and $C(t_k)$ can be computed by integration of this expression as stated in (2.23). Let us call this method A.

In this approach we use the values of the constant tracer gas injections and the values of the tracer gas concentrations in the beginning of the interval of integration in order to determine the tracer gas concentrations during the whole interval.

An alternate approach is to use the concentrations at the end of the interval instead of the values at the beginning of the interval. An equation expressing $c(t_k+s)$ as a function of $p(t_k)$ and $c(t_k+T_{int})$ can be derived in the following way. Multiply (2.13) from the left by $\exp(-AT_{int})$ and use the equation to express $c(t_k)$

$$c(t_k)=\exp(-AT_{int})c(t+T_{int})-\exp(-AT_{int})(\exp(AT_{int})-I)A^{-1}\,Bp(t_k) \quad (2.27)$$

Substitute $c(t_k)$ in (2.26) with (2.27). After reduction we obtain

$$c(t_k+s)=\exp(A(s-T_{int}))c(t+T_{int})+(\exp(A(s-T_{int}))-I)A^{-1}Bp(t_k) \quad (2.28)$$

Now the integral $C(t_k)$ can be computed by integration of (2.28) as well. This will be called method B.

With respect to noise reduction, however, it seems sensible to use the concentration at both the beginning and the end of the interval. This can be done in two ways. One is to integrate the mean value of $c(t_k+s)$ expresed by (2.26) and (2.28). Let us call this method C. The other way is to eliminate $p(t_k)$ from (2.26) by (2.28) and express $c(t_k+s)$ from the resulting equation, i.e., method D.

Now we have four possibilities A-D to calculate the integral $C(t_k)$ and all of them hold exactly, provided that $p(t_k)$ is constant during the interval of integration and, of course, that there are no measurement errors. In the presence of noise however, the four methods will behave quite different. (For example we can notice that (2.28) is an extrapolation backwards of a stable system, and this is an unstable process with respect to disturbances in the initial value. On the other hand, (2.26) is an extrapolation forward of a stable system and does not cause any problem.

In Hedin (1989) the noise sensibility of the four methods are calculated in a simple case. It is shown that method C, i.e., integrating the mean of $c(t_k+s)$ from (2.26) and (2.28), gives the best result provided the interval of integration is reasonably small compared to the time constants of the system.

Leaving methods A, B and D, we can perform the integration with method C. After simple calculations this gives

$$C(t_k)=\int_0^{T_{int}} c(t_k+s)ds=R\,c(t_k)+S\,c(t_k+T_{int})+T\,B\,p(t_k) \quad (2.29)$$

where R, S and T are n by n matrices given by

$$R=(\exp(AT_{int})-I)A^{-1}/2 \quad (2.30)$$

$$S=(I-\exp(-AT_{int}))A^{-1}/2 \quad (2.31)$$

$$T=((\exp(AT_{int})-\exp(-AT_{int})A^{-1}-2IT_{int})A^{-1}/2 \quad (2.32)$$

For the numerical calculations of R, S and T we can use the following Taylor series expansions

$$R=(IT_{int}+AT_{int}^2/2!+A^2T_{int}^3/3!+\ldots)/2 \quad (2.33)$$

$$S=(IT_{int}-AT_{int}^2/2!+A^2T_{int}^3/3!-\ldots)/2 \quad (2.34)$$

$$T=AT_{int}^3/3!+A^3T_{int}^5/5!+\ldots \quad (2.35)$$

The extension of (2.29) to the case with several subdivisions ($m_{int}>1$) of the interval of integration is easy to derive. Just exchange T_{int} for T_s in (2.29)-(2.35) and calculate the integral as the sum of integrals for each subdivision

$$C(t_k)=R\sum_{k=0}^{m_{int}-1} c(t_k)+S\sum_{k=0}^{m_{int}-1} c(t_{k+1})+T\ B\ p(t_k) \qquad (2.36)$$

Notice from the equations (2.33)-(2.35) that when the number of samples in each interval of integration is increasing, then the matrices R and S will approach $IT_s/2$ while T will approach $AT_s^3/3!$ (or almost zero, as T_s is a small number). Accordingly, the equations (2.29) and (2.36) will approach the simple trapezoidal rule as T_s becomes small.

Like the model based estimation of the derivative this model based estimation of the integral will be an iterative method as we do not know the matrix A in advance. As a first estimation of the integral it is natural to use the trapezoidal rule.

2.5 Summing up the models

In this chapter we have been engagaed with the problem of finding the relations between tracer gas injections and the resulting tracer gas concentrations in a multicell flow system.

The fundamental model is the mass balance equations (2.4)

$$V\,\dot{c}(t) = Q\,c(t) + p(t)$$

To express the time derivative we have used two formulations of the mass balance equations

Formulation 1 forward difference of $\dot{c}(t_k)$

$$V(c(t_k+T_s)-c(t_k))/T_s=Q\ c(t_k)+p(t_k) \qquad (2.37)$$

Formulation 2 model based estimation of $\dot{c}(t_k)$

$$V\ D(c(t_k+T_s)-c(t_k))=Q\ c(t_k)+p(t_k) \qquad (2.38)$$

An alternative, where we avoid the time derivative, is to integrate the mass balance equation. To obtain the integral $C(t_k)$ of $c(t_k)$ we have also used two formulations

Formulation 3 integrated mass balance with the trapezoidal rule

$$V(c(t_k+T_{int})-c(t_k))=Q(c(t_k)+c(t_k+T_{int}))/2+T_{int}p(t_k) \qquad (2.39)$$

Formulation 4 integrated mass balance with model based integration of $c(t_k)$

$$V(c(t_k+T_{int})-c(t_k))=Q(R\ c(t_k)+S\ c(t_k+T_{int})+TBp(t_k))+T_{int}p(t_k) \qquad (2.40)$$

If we have m samples with measurements of $p(t_k)$ and $c(t_k)$, k=1,m, then the different formulations can be stated m-1 times. The measurements are normally recorded at a constant sampling rate, but this is no demand.

3 IDENTIFICATION OF MULTI-CELL FLOW SYSTEMS

In this chapter we address the identification problem: Given measured values of the tracer gas injections, $p(t_k)$, and the tracer gas concentrations $c(t_k)$ in a multi-cell flow system, how could the volumes and flow rates be determined?

The chapter is organized as follows. In Section 3.1 we show how to state the measured data as an overdetermined system of equations.

Next, in Section 3.2, we show how this system of equations can be formulated as an quadratic programming problem.

Finally, this QP problem is formulated as a linear complementary problem (LCP) with Kuhn-Tucker conditions. The LCP problem is then solved with Lemke's algorithm, see Section 3.3.

3.1 Formulation of the QP problem

First of all we notice that all four formulations of the mass balance (2.37)-(2.40) have the same structure as the original mass balance (2.4). Therefore, it is sufficient to show how to perform the identification by using model (2.4) as if the measured data consist of $c(t_k)$, $\dot{c}(t_k)$ and $p(t_k)$, k=1,m. When we actually use one of the other four formulations, we only have to modify the input data set to the identification routine. For example, when using formulation 1 $\dot{c}(t_k)$ should be exchanged for $(c(t_k+T_s)-c(t_k))/T_s$ and so on.

Secondly, we observe that the mass balances are not quite adapted to identification since the known tracer gas concentrations and injections are mixed with the unknown flows and volumes. Consequently, our first task will be to rearrange the mass balance equations into the common form Ax=b, where A is a matrix and b a vector which contains all known measurements while x is a model parameter vector which contains all the unknown flows and volumes that we want to identify.

Since all flows are not independent of one another, the model parameter vector can be chosen in many ways, but comparing with (2.4) the following may be a natural choice

$$\begin{aligned} x = (&V_1, -Q_{11}, Q_{12}, \dots, Q_{1n} \\ &V_2, Q_{21}, -Q_{22}, \dots, Q_{2n}, \\ &\dots \\ &V_n, Q_{n1}, Q_{n2}, \dots, -Q_{nn})^T \end{aligned} \qquad (3.1)$$

The vector x has a dimension of n_p*1, where $n_p=n(n+1)$ equals the number of unknown parameters.

Remember that $Q_{ii}<0$ (equation (2.6)). By using a minus sign on these elements in (3.1) all model parameters are made non-negative. Do also note that the in and outflows to/from the outside are not included in the model parameter vector, but they can easily be calculated with (2.8) and (2.9), respectively.

Now, order the measured data in the following way: First form an m by (n+1) matrix A_i for each cell, i=1,n. Let the rows k=1,m in A_i contain the following measured data set from the k:th sample

$$(A_i)_{\text{row } k} = (\dot{c}_i(t_k), -c_1(t_k), \dots, c_i(t_k), \dots, -c_n(t_k)), \quad k=1,m \qquad (3.2)$$

Similarly, set up an m by 1 vector b_i for each cell, i=1,n. Let its elements be given by

$$(b_i)_{\text{row } k} = p_i(t_k) \ , \ k=1,m \tag{3.3}$$

Now we can form an mn by n_p block matrix A (do not confuse with the n by n matrix $A=V^{-1}Q$), and an $n_p$mn by 1 block vector b with

$$A=\begin{bmatrix} A_1 & 0 & \dots & 0 \\ 0 & A_2 & \dots & 0 \\ 0 & 0 & \dots & A_n \end{bmatrix} \tag{3.4}$$

$$b=\begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} \tag{3.5}$$

With this notation all mn mass balances can easily be written as

$$A\ x = b \tag{3.6}$$

As there are $n_p=n(n+1)$ unknown model parameters we need at least m=n+1 samples in order to identify the model parameters. If m>n+1, and this is the common case, the system of equations (3.6) will be overdetermined and cannot be exactly satisfied. Instead, our object becomes to find a solution x that minimizes the norm ||r|| where r=Ax-b. Depending on which norm we use, the problem can be solved by different methods.

Up to now the linear or l_1 norm has been used. This leads to a linear programming (LP) problem, see Jensen (1987b). But the computations are greatly simplified if we instead use the Euclidean or l_2 norm

$$||r||_{l_2} = \sqrt{\sum_i r_i^2} \tag{3.7}$$

The problem can now be stated as a quadratic programming problem. Disregarding the constraints (2.5)-(2.9) the problem can be stated

$$\text{Minimize} \quad ||r||_{l_2} \qquad \text{where } r = A\ x - b \tag{3.8}$$

The least square solution to (3.7) is given by the well-known normal equations

$$A^TA\ x = A^Tb \tag{3.9}$$

and x can be solved as

$$x = (A^TA)^{-1}\ A^Tb \tag{3.10}$$

Notice that matrix A has the dimension $mn*n_p$, while matrix A^TA has the dimension n_p*n_p and thus it is not dependent of the number of samples, m. As it is desired to use many samples in order to reduce the influence of measurement errors, this is an important quality. This is also a reason to prefer the QP solution to the LP solution, which deals with the system of equations in its original form (3.6). However, as we do not use the constraints it is not sure that the solution will correspond to a flow system. For example, it may happen that a row sum of the identified flow matrix is positive and thus one inflow would be negative, which is physically impossible. Furthermore, it is unwise not to use all the information that is known about the solution as this can help us to

find a better solution. The appropriate solution is therefore to minimize $\|r\|_{12}$ as above, but to do it subjected to the constraints which we know must be fulfilled. This will be done with the QP approach in the next two sections.

Before we discuss how to formulate the QP problem we shall do some remarks about the normal equations and the choice of pattern for the tracer gas injection.

The least square solution with the normal equations which is the basis for the QP approach does not have the best of reputations from a numerical point of view. This is certainly true when the tracer gas concentrations are highly correlated to each other. The matrix A^TA will then be near singular and the problem will be ill-conditioned. But even when A^TA is calculated, some numerical precision will be lost which cannot be recovered.

To obtain correct result in single precision, it is therefore necessary to form and solve the normal equations in double precision. Because of these reasons, other least square solutions as e.g. QR decomposition, is often preferred to the simpler normal equations. But their solutions will be more complicated when constraints are involved.

Fortunately, when identifying a flow system the demands for accuracy are low. Since the measurement error of the tracer gas injections and concentrations hardly can be lower than some per cent, i.e., uncertainty in the second or third digit, then the normal equations seem to be accurate enough.

However, it should be stressed that it is very important that the tracer gas concentrations are not too similar to each other. Accordingly, the choice of input sequence of the tracer gas injection is very important. The Pseudo Random Binary Signal (PRBS) sequence is frequently used in process identification, see Jung (1987) and may be a good choice. Characteistic for this is that the same sequence, but with different time delays, can be used for all inputs. The mutually correlation between the inputs will be as low (i.e., negative) as possible. To be able to choose suitable parameters to the PRBS sequence, it is necessary to have a feeling of the values of the searched parameters. Preferably, the amplitude should be bigger, the bigger the volumes are, and the period should be of the same magnitude as the time constants according to some rules.

3.2 The QP problem with constraints

We shall now write the overdetermined system of equations (3.6) and its constraints in the standard formulation for a quadratic problem. The constraints (2.5)-(2.7) can simply be written as

$$x \geq x_o \tag{3.11}$$

where x_o is an n_p by 1 vector which elements all are zero. The 2n inequalities (2.8) and (2.9) are linear in the model parameter vector and in matrix notation they are written (after multiplying with -1)

$$G\,x \geq g \tag{3.12}$$

where G is a 2n by n_p matrix and g is a 2n by 1 vector. Each row in G describes one sum of rows or columns of the flow matrix and it consists of n elements with the value +1 or -1 while all other elements are zero. The vector g is the minimal permitted value, or just the lower limit, of the sum. In (2.8)-(2.9) we suppose that the lower limit is zero but, of course, if we e.g. know the value of an exhaust flow then the correspond-

ing lower limit should be set to this value.

It is also easy to extend the number of linear constraints. Every new constraint is written as an extra row of G and g. The row elements in G define a linear combination of model parameters and the corresponding row in g is its lower limit. For example, if we know that

$$v_1 + v_2 \geq v_{min}$$

this is written as

$$(G)_{new\ row} = (\ 1\ \ 0\ \ 0 \ldots\ \ 1\ \ 0\ \ 0 \ldots 0\ )$$

$$(g)_{new\ row} = v_{min}$$

where the two '1' are placed in the same locations as v_1 and v_2 have in x^T.

Inequalities which contain an upper limit must be converted by multiplying with -1. For example

$$v_1 + v_2 \leq v_{max}$$

is written as

$$-v_1 - v_2 \geq -v_{max}$$

and can then be treated in the same way as above.

Equality constraints are expressed by two inequalities. For example

$$v_1 + v_2 = v_{sum}$$

is written as

$$v_1 + v_2 \geq v_{sum}$$

$$-v_1 - v_2 \geq -v_{sum}$$

To fix a model parameter x_i to zero, it is sufficient to use the inequality $-x_i \geq 0$ since the inequality $x_i \geq 0$ already is given by (3.11).

An alternative to fix parameters is, of course, to replace the parameter by its value in the mass balances. This will decrease the size of the problem instead of increasing it but, on the other hand, it requires more programming since it is not so easily described.

As seen, the rows of G have no restrictions such as they must be linear independent. But, naturally, there must not be any contradictory demands. In that case a solution does not exist.

Assuming that besides (2.8)-(2.9) we use n_e extra inequality constraints, then G and g have the dimensions of n_g by n_p and n_g by 1 respectively, where $n_g = 2n+n_e$.

Finally, we shall rewrite (3.8) so it fits to the standard form of quadratic programming

$$r^T r = (b-Ax)^T(b-Ax) = b^Tb - b^TAx - x^TA^Tb + x^TA^TAx \qquad (3.13)$$

The first term is constant and can be disregarded in the minimizing. The two following terms are equal and can be expressed by a single term.

Introduce the n_p by 1 vector $c=-2A^Tb$ and the n_p by n_p matrix $Q=A^TA$ (not to be confused with the n by n flow matrix Q).

Now the QP problem can be stated in its standard form

$$\text{minimize: } f(x)=c^Tx+x^TQx \tag{3.14}$$

subject to

$$\begin{aligned} G\,x &\geq g \\ x &\geq 0 \end{aligned}$$

The main difficulty when solving this QP problem is to know which constraints are binding and which are non-binding in the optimal solution. If we had known all the binding constraints, these constraints could be replaced by equality constraints and the other could be rejected. In this case the solution had been given by the well-known method of Lagrange multipliers. From the computational point of view this had only led to a minor expansion of the normal equations.

Kuhn and Tucker have developed an extension to the method of Lagrange multipliers to deal with inequality constraints (see Appendix for a short description). Using this the QP problem above can be transformed into an algebraical problem which is easier to deal with.

3.3 The solution of the QP problem

In the QP problem (3.14) all constraints are linear and as $Q=A^TA$ is positive definite it follows that the object function is convex. Thus there are no local minima and the Kuhn-Tucker conditions point out the global one.

As we have two constraints in (3.14) there will be two sets, u and v, of Lagrange multipliers. According to the Kuhn-Tucker condition (A.2)-(A.5), the solution (x,u,v) must satisfy the following system of equations

$$\begin{aligned} c^T + x^T(Q+Q^T) - u^TG - v^T &= 0 \qquad (3.15)\\ Gx-g &\geq 0 \\ x &\geq 0 \\ u^T(Gx-g) &= 0 \\ v^Tx &= 0 \\ u &\geq 0 \\ v &\geq 0 \end{aligned}$$

where u is an n_g by 1 vector of Lagrange multipliers for the n_g inequality constraints and v is an n_p by 1 vector of Lagrange multipliers for the n_p constraints that the model parameter vector is non-negative.

If we introduce an n_g by 1 slack vector $s \geq 0$ then we can write the first inequalities as an equality

$$G\,x - g = s \tag{3.16}$$

The system of equations (3.15) can now be written

$$\begin{bmatrix} v \\ s \end{bmatrix} = \begin{bmatrix} Q+Q^T & -G^T \\ G & 0 \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} + \begin{bmatrix} c \\ -g \end{bmatrix} \tag{3.17}$$

subject to

$$v^T x + s^T u = 0$$

$$v \geq 0 \ , \ s \geq 0 \ , \ x \geq 0 \ , \ u \geq 0$$

This can be written more compact by introducing the following symbols

$$M = \begin{bmatrix} Q+Q^T & -G^T \\ G & 0 \end{bmatrix} \tag{3.18}$$

$$w = \begin{bmatrix} v \\ s \end{bmatrix} \tag{3.19}$$

$$z = \begin{bmatrix} x \\ u \end{bmatrix} \tag{3.20}$$

$$q = \begin{bmatrix} c \\ -g \end{bmatrix} \tag{3.21}$$

where M is an n_c by n_c matrix with $n_c = n_p + n_g$ and w, z and q are three n_c by 1 vectors. The solution of the QP problem will now be given by the solution of the following problem, called

The linear complementary pivot problem:

Find the vectors w and z so that

$$w = M z + q \tag{3.22}$$

subject to

$$w^T z = 0$$

$$w \geq 0 \ , \ z \geq 0$$

This problem has been fully studied in the econometric literature during the last 25 years. The basic method to solve (3.22) is called Lemke's complementary pivot algorithm. This is an iterative method and provided certain assumptions it will always find a solution, if there exists one. Such an assumption that is applicable to our problem is that the matris M is positive semi-definite.

From considerations of space we will not describe Lemke's complementary pivot algorithm in this paper but we refer to the main report Hedin (1989) or rather, to the literature of mathematical programming, e.g. Balinsky and Cottle (1978) which also includes a number of further references. To mention something about the solution of (3.22), we can observe that from the constraints it follows that at least one of the two elements w_i or z_i is equal to zero for i=1,n. The solution thus consists

of at most n_g non-zero elements in z and w. As there as well are n_g equations in (3.22), the system of equations may be possible to solve.

There are computer routines published which perform Lemke's algorithm. We have used one of them written by Ravindran (1972). This is a quite uncomplicated program. The complete program listing is covered in about a single sheet of paper. It has newly been revised to be up to date and has proved to work well.

4 NUMERICAL EXPERIMENTS

In this chapter we shall test the identification method and its different formulations. Only a few of the simulated identifications will be discussed in this paper. To make it easier to compare the results with prior works, we shall use the same flow system, pattern of tracer gas injection and initial conditions as in Jensen (1987b).

4.1 A simple testsystem

The simulated flow system consists of three cells with volumes and flows as shown in Figure 4.1.

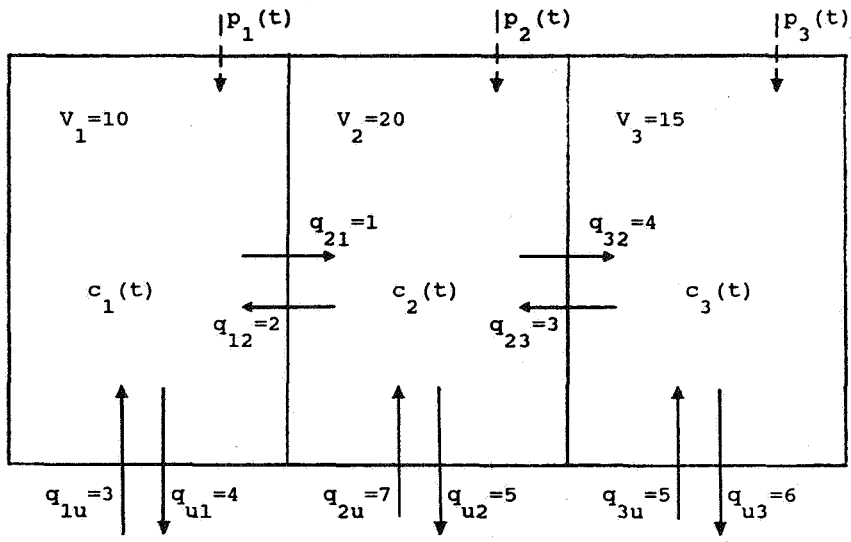

Figure 4.1 The simulated flow system. Units are arbitrary.

The volume and flow matrices are given by

$$V = \begin{bmatrix} 10 & 0 & 0 \\ 0 & 20 & 0 \\ 0 & 0 & 15 \end{bmatrix} \quad \text{and} \quad Q = \begin{bmatrix} -5 & 2 & 0 \\ 1 & -11 & 3 \\ 0 & 4 & -9 \end{bmatrix}$$

The three time constants $TC_i = v_i/q_{it}$ are 2.00, 1.82 and 1.67 time units, respectively.

The flow system has been simulated with the discrete time model (2.13) The initial values were $c(0)=(0.8, 1.1, 1.2)^T$ and the tracer gas injection in each cell has been varied as a very simple pseudo random binary sequence. Figure 4.2 shows the tracer gas injections and the resulting tracer gas concentrations during the first 30 time units. (In most cases we will only use the first 15 time units).

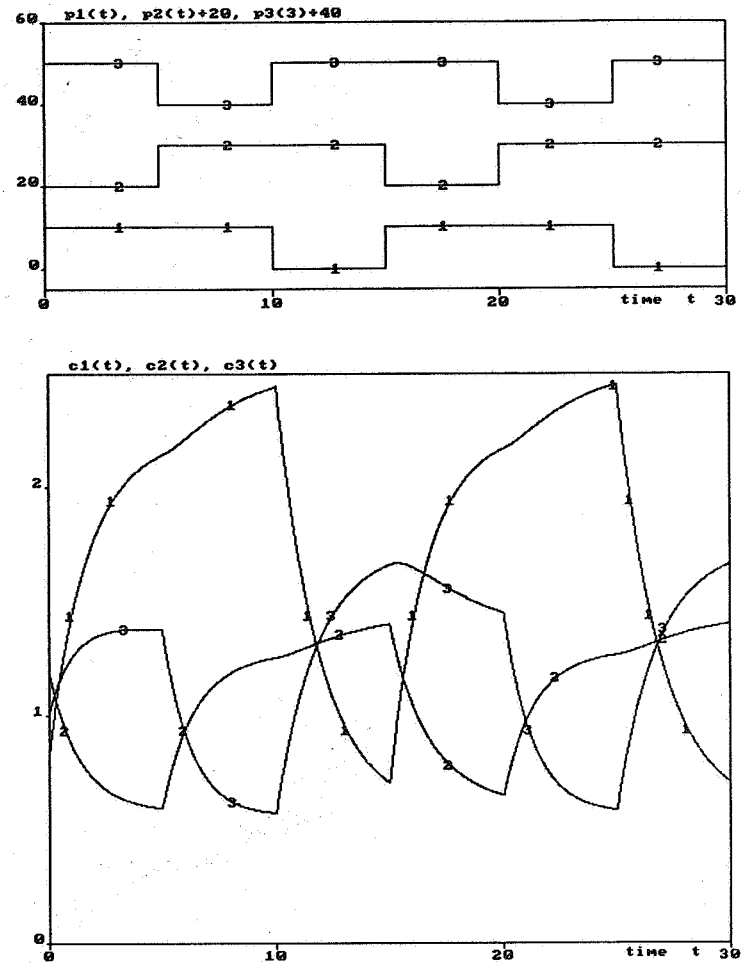

Figure 4.2 Tracer gas injections $p_1(t)$-$p_3(t)$ and the resulting tracer gas concentrations $c_1(t)$-$c_3(t)$ in the simulated three cell system. No measurement noise.

The measurements of the tracer gas concentrations can also be simulated with a random noise. The standard deviation, std, of the noise will be chosen to 0.01, 0.02, 0.05 or 0.10. Setting for example 1 unit equal to 100 ppm NO_2 means that std=0.01 corresponds to a measurement error of 1 ppm. As the standard deviations of $c_1(t)$, $c_2(t)$ and $c_3(t)$ are about 0.59, 0.26 and 0.40 respectively, we can expect the parameters to be best estimated in cell 1 according to the different signal to noise ratios.

4.2 The criterion for the best model

There is no obvious criterion to compare different parameter estimations. The loss functions or norms $||r||$, which are minimized by the QP routine do not help us as they cannot be compared. Especially we cannot compare a LP with a QP solution by the norms. But, since the true parameters are known it will be natural to compare any norm of the error Δx of the model parameter vector

$$||\Delta x|| = ||\hat{x} - x|| \qquad (4.1)$$

where $\hat{x}$ denotes the estimated parameters and x the true parameters. A minor modification from this has been done as the n parameters q_{ii} have been exchanged by the 2n calculated in and outflows (q_{iu} and q_{ui}). The underlying idea was to calculate the estimation error on the primary physically parameters.

Depending on the norm chosen we will calculate the mean absolute error (linear norm), maximum absolute error (maximum norm) and mean error and standard deviation. (The two last mentioned come from the Eucledian norm after the splitting $E(\Delta x^2) = E^2(\Delta x) + Var(\Delta x)$).

A weakness of the norm (4.1) is that it only takes the absolute errors into account. This will lead to a quite too large influence on the absolute norms from the big volumes. An alternative is to work with the norm of the relative error

$$||(\hat{x} - x)/x|| \qquad (4.2)$$

Also the norms of the relative errors will be calculated. Two of the model parameters, q_{13} and q_{31}, are equal to zero. These parameters will of course be excluded when the norms of (4.2) are calculated.

4.3 Simulated experiments

If there is no noise, then the model parameters can be determined exactly with the model based formulations 2 and 4. The number of iterations that is required will depend on how good the start solution is. The lesser the sample period is, the better the start solution will be.

In the presence of noise, however, we can no longer suppose to find the correct model parameters. How large the estimation error will be depends not only on the noise level but also on the formulation used and the choice of sample period. For the two integrated formulations it will also depend on the choice of interval of integration. Tables 4.1 and 4.2 show the estimated parameters of the test system determined from the simulated experiment in Figure 4.2, but at different noise levels. The formulations 2 and 4, respectively, are used to express the mass balance equations. At the lower noise levels, the advantages over the non-iterative formulations 1 and 3 (not shown in this paper) are considerably but at the higher noise levels the differences are small and for std=0.1, the non-iterative formulations even give a somewhat better result. The latter means that, at this noise level, the estimation of the matrices D and R, S, T respectively, cannot be improved from the simple initial values.

Usually, a straightforward way to obtain better parameter estimations is to use more measurements. Table 4.3 shows the estimated parameters at the lower noise level, std=0.01, when the sample period is reduced from T_s=1 to 0.5, 0.2 and 0.1. However, the estimations get worse. Neither is it possible to improve the estimations significantly by lengthening the total experiment time. These unexpected results are due to the bias of the estimation. In the main report, see Hedin (1989), the expected bias is calculated in some simplified cases. It is shown that the bias is increasing when the sample period is decreasing. It is also shown that the bias is considerably higher in the estimation of the volumes than in the estimation of the flows. Another finding is that the bias in the estimation of the flows will not be lower, but higher, if the volumes are known and fixed to their correct values. This surprising result is also confirmed by simulated experiments.

A way to obtain better estimations that work, is to use formulation 3 or 4 with a sample period that is shorter than the interval of integration. Table 4.4 shows the estimations for formulation 4 when the interval

Table 4.1

Experiment		A0	A0	A0	A0
length		15.0	15.0	15.0	15.0
sampling period		1.0	1.0	1.0	1.0
noise st.dev.		0.01	0.02	0.05	0.10
Parameters	**true**	**estimated**	**estimated**	**estimated**	**estimated**
q11	-5.00	-5.02	-5.03	-5.08	-5.18
q12	2.00	1.99	1.99	1.98	1.97
q13	0.00	0.00	0.00	0.00	0.00
q21	1.00	1.02	1.02	0.91	0.61
q22	-11.00	-11.05	-11.06	-10.96	-10.52
q23	3.00	3.01	3.01	3.01	2.94
q31	0.00	0.00	0.00	0.00	0.10
q32	4.00	4.02	4.03	3.95	3.55
q33	-9.00	-9.02	-9.02	-8.99	-8.87
q1u	3.00	3.02	3.05	3.11	3.21
q2u	7.00	7.02	7.03	7.04	6.98
q3u	5.00	4.99	5.00	5.04	5.22
qu1	4.00	4.00	4.01	4.17	4.48
qu2	5.00	5.03	5.05	5.03	5.00
qu3	6.00	6.01	6.01	5.98	5.93
V1	10.00	9.93	9.86	9.60	9.08
V2	20.00	20.05	19.76	17.17	10.90
V3	15.00	14.81	14.49	12.91	9.32

Estimation errors	abs	rel%	abs	rel%	abs	rel%	abs	rel%
mean error	-0.01	0	-0.05	0	-0.34	-3	-1.05	-10
standard dev	0.06	1	0.15	1	0.88	6	2.67	19
max abs err	0.19	2	0.51	3	2.83	14	9.10	45
mean abs err	0.03	1	0.08	1	0.39	4	1.18	13

Table 4.2

Experiment		A0	A0	A0	A0
length		15.0	15.0	15.0	15.0
sampling period		1.0	1.0	1.0	1.0
noise st.dev.		0.01	0.02	0.05	0.10
Parameters	**true**	**estimated**	**estimated**	**estimated**	**estimated**
q11	-5.00	-5.01	-5.03	-5.07	-5.14
q12	2.00	1.99	1.98	1.95	1.89
q13	0.00	0.00	0.00	0.00	0.00
q21	1.00	1.03	1.05	0.97	0.63
q22	-11.00	-11.05	-11.10	-11.14	-10.56
q23	3.00	2.99	3.01	3.10	3.01
q31	0.00	0.00	0.00	0.00	0.04
q32	4.00	4.02	4.04	4.01	3.71
q33	-9.00	-9.02	-9.03	-9.04	-8.88
q1u	3.00	3.02	3.05	3.12	3.25
q2u	7.00	7.03	7.05	7.06	6.91
q3u	5.00	4.99	4.99	5.02	5.13
qu1	4.00	3.98	3.98	4.10	4.47
qu2	5.00	5.04	5.08	5.17	4.96
qu3	6.00	6.02	6.03	5.93	5.86
V1	10.00	9.94	9.87	9.65	9.29
V2	20.00	20.07	19.74	16.83	10.07
V3	15.00	14.81	14.48	12.91	9.59

Estimation errors	abs	rel%	abs	rel%	abs	rel%	abs	rel%
mean error	0.00	0	-0.04	0	-0.34	-2	-1.08	-9
standard dev	0.06	1	0.16	2	0.96	6	2.82	19
max abs err	0.19	3	0.52	5	3.17	16	9.93	50
mean abs err	0.04	1	0.08	1	0.42	4	1.20	13

Table 4.3

Experiment		A0	A0	A0
length		15.0	15.0	15.0
sampling period		0.5	0.2	0.1
noise st.dev.		0.01	0.01	0.01
Parameters	**true**	**estimated**	**estimated**	**estimated**
q11	-5.00	-5.04	-5.05	-5.16
q12	2.00	2.05	2.09	2.31
q13	0.00	0.00	0.00	0.00
q21	1.00	1.02	0.85	0.58
q22	-11.00	-11.00	-11.06	-11.07
q23	3.00	2.97	3.21	3.57
q31	0.00	0.01	0.20	0.51
q32	4.00	3.98	3.55	2.83
q33	-9.00	-9.00	-8.96	-8.90
q1u	3.00	2.99	2.96	2.85
q2u	7.00	7.01	7.00	6.93
q3u	5.00	5.01	5.21	5.56
qu1	4.00	4.01	4.00	4.07
qu2	5.00	4.97	5.41	5.93
qu3	6.00	6.03	5.75	5.33
V1	10.00	9.82	9.46	8.39
V2	20.00	19.64	15.84	10.13
V3	15.00	14.84	13.03	10.03

Estimation errors	abs	rel%	abs	rel%	abs	rel%
mean error	-0.04	0	-0.43	-4	-1.07	-9
standard dev	0.11	1	1.17	9	2.82	23
max abs err	0.36	3	4.16	21	9.87	49
mean abs err	0.06	1	0.58	7	1.46	20

Table 4.4

Experiment		A0	A0	A0
length		15.0	15.0	15.0
sampling period		0.5/1.0	0.2/1.0	0.1/1.0
noise st.dev.		0.01	0.01	0.01
Parameters	**true**	**estimated**	**estimated**	**estimated**
q11	-5.00	-5.03	-5.02	-5.02
q12	2.00	2.03	2.02	2.03
q13	0.00	0.00	0.00	0.00
q21	1.00	1.03	1.01	1.02
q22	-11.00	-11.04	-11.00	-11.02
q23	3.00	3.00	2.98	2.97
q31	0.00	0.01	0.00	0.00
q32	4.00	4.04	4.02	4.01
q33	-9.00	-9.05	-9.02	-9.02
q1u	3.00	3.00	3.00	2.99
q2u	7.00	7.01	7.02	7.03
q3u	5.00	5.00	5.00	5.00
qu1	4.00	3.99	4.01	4.00
qu2	5.00	4.97	4.96	4.97
qu3	6.00	6.05	6.05	6.05
V1	10.00	9.89	9.93	9.93
V2	20.00	20.12	19.94	20.03
V3	15.00	14.92	14.90	14.92

Estimation errors	abs	rel%	abs	rel%	abs	rel%
mean error	0.00	0	-0.01	0	0.00	0
standard dev	0.05	1	0.04	1	0.04	1
max abs err	0.12	3	0.10	1	0.08	2
mean abs err	0.03	1	0.03	1	0.03	1

of integration is 1.0 and the sample period is 0.5, 0.2 and 0.1. In this case the bias is not affected while the random error is reduced when more measurements are used.

4.4 Comparison with linear programming

Most of the shown identifications have also been solved with the linear programming method. This has been easy to do as Lemke's algorithm can also solve the LP problem, (see Hedin (1989)). The conclusions of these identifications are that the differences between the QP and LP solutions are surprisingly small. This is true, no matter what criterion is used, linear, maximum or Eucledian. Even the bias seems to be approximately the same. The great difference is instead the execution time required to solve the QP and LP problems. As mentioned earlier the dimension of the LP problem will depend on the number of measurements. Stated as a complementary problem the dimension of the LP problem will be $n_c = n_g+n_p+2mn = 2n+n(n+1)+2mn$ while the dimension of the corresponding QP problem will be only $n_c = n_g+n_p$. The following table shows the cpu time when one of the problems is solved with the QP and LP methods, respectively.

	QP method		LP method	
m	n_c	cpu time (s)	n_c	cpu time (s)
15	18	0.05	108	59
30	18	0.05	198	377
75	18	0.05	378	4383

When the number of measurements is increasing, then the cpu time for the LP solution is increasing exponentially. The exponent has been calculated to 2.676. Taking the first case m=15 as a reference, this means

$$\text{cpu time } (m) = \text{cpu time } (15)\ (m/15)^{2.676} \qquad (4.3)$$

In other cases the exponent has been calculated to 2.6 - 2.9. This is somewhat lower than 3 which is the expected value from a theoretical point of view.

4.5 Concluding remarks

One of the objects of this paper was to see if the QP solution is competitive with the LP solution. The conclusion is that it certainly is competitive.

In contrast to the LP method, the QP method is fast enough to be used in real-time applications even on a PC based system. Thus it is possible, and advisable, to incorporate the identification procedure into the computer programs which control the tracer gas injections and measurements. Now the identification can be done on-line and the estimated parameters can be followed. The advantages of knowing the latest model is obvious. It will give an immediate check that an experiment in progress is sufficiently informative so the parameters can be determined. It will also indicate when an experiment can be completed. A possibility may also be to let the computer adapt the tracer gas injections to the actual flow system.

Other advantages of the QP method that may be mentioned is that it is possible to estimate the error of the determined parameters. This is done

by means of the covariance matrix. Further, it is easy to include different weights of the measurements. This is done by computing Q as A^TWA, where W is a weight matrix. It is also easy to track slowly time varying parameters. This is done by computing $Q=A^TA$ as a filtered sum of inputs

$$Q(t_k+T_s) = f\ Q(t_k) + (1-f)(A_{t_k}{}^T A_{t_k})$$

where f, the 'forgetting factor', is a measure of how fast old data are forgotten. It usually has a value close below one. A lower value gives a faster tracking but a higher sensitivity to noise.

APPENDIX

Kuhn and Tucker have made an extension to the method of Lagrange multipliers to deal with minimizing problems with inequality constraints. Consider the following problem

Minimize f(x) (A.1)
subject to

$$g_j(x) \geq 0\ ,\quad j=1,n_g$$

According to the Kuhn-Tucker conditions, every optimal solution (x,u) must fulfill the following necessary conditions

$$\nabla f(x) - \sum_j u_j\ \nabla g_j(x) = 0 \qquad (A.2)$$

$$g_j(x) \geq 0\ ,\quad j=1,n_g \qquad (A.3)$$

$$u_j g_j(x) = 0\ ,\quad j=1,n_g \qquad (A.4)$$

$$u_j \geq 0\ ,\quad j=1,n_g \qquad (A.5)$$

If all constraints are linear and the object function f(x) is convex, then these conditions will also be sufficient for (x,u) to be the optimal solution. In this case, there are no local minima and the conditions (A.2)-(A.5) point out the global one.

For a detailed treatment of the Kuhn-Tucker conditions, see any textbook in quadratic programming as e.g. Van de Panne (1975).

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