AIR MOVEMENT & VENTILATION CONTROL WITHIN BUILDINGS

12th AIVC Conference, Ottawa, Canada 24-27 September, 1991

POSTER 33

A New Approach for the Numerical Identification of Interzonal Airflows from Tracer Gas Measurements

Simone Guiti $Zad^{1\dagger}$

Helmut Jarausch¹

Willigert Raatschen²

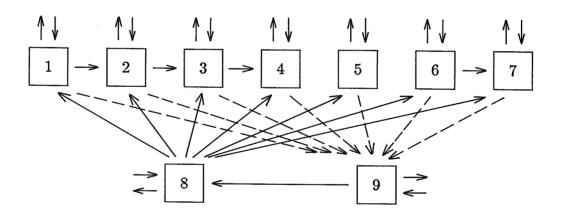
- Institut für Geometrie und Praktische Mathematik Technische Hochschule RWTH Aachen
 Templergraben 55
 D-W-5100 Aachen
- DORNIER GmbH
 Postfach 1420
 D-W-7990 Friederichshafen 1

0. Synopsis

This paper presents a new approach to determine the interzonal airflows of a multizone system using tracer gas measurements. In contrast to methods proposed earlier, the presented method does not use the mass balance as basis for the least squares problem but identifies the interzonal airflows as coefficients of the evolution equations for the concentrations. Therefore estimating the derivatives with respect to the time from measured data is avoided. Furthermore the concentration can be calculated arbitrary points in time. In addition, if exact intervals bounding the sampling error are available, interval arithmetic can be used to determine bounds for the interzonal airflows.

1. Introduction

For determining the unknown interzonal airflows of a multizone enclosure, it is modelled as an multizone system. To illustrate this, consider the following example, for which we want to thank J. B. Mattson, Lund University, Sweden. This model consists of 9 zones, where the zones 8 and 9 correspond to a main air supply and exhaust air ducts.



Later the method presented in this paper will be demonstrated on this example.

Using the mass-balance for each zone we get

$$V_i \, \dot{\tilde{c}}_i = \sum_{j=0, \, j\neq i}^n \tilde{q}_{ij} \, \tilde{c}_j \, - \sum_{j=0, \, j\neq i}^n \tilde{q}_{ji} \, \tilde{c}_i \, + \, \tilde{g}_i \quad , \qquad i=1,\cdots,n$$

where n is the number of zones, \tilde{q}_{ij} the interzonal airflow from zone j into zone i (index 0 for outdoor air), V_i the volume of zone i, \tilde{c}_j the concentration in zone j and \tilde{g}_i the injection (constant) into zone i.

With $c_i \equiv \tilde{c}_i - \tilde{c}_0$ we get

$$(1.1) V_i \dot{c}_i = \sum_{j=1, j \neq i}^n \tilde{q}_{ij} c_j - \sum_{j=1, j \neq i}^n \tilde{q}_{ji} c_i + \tilde{g}_i , i = 1, \dots, n$$

The system (1.1) will be used to compute the modelled concentrations at time t.

The problem of determining the interzonal airflows now leads to a nonlinear least squares problem, which is solved using the Gauss-Newton-method.

Having identified the unknown parameters, one can get information about the quality of these approximations using statistical considerations, i.e. the á-posteriori-covariance matrix.

It may be possible that the structure of the multizone system does not allow us to identify all parameters. In this case only certain fixed linear combinations are identifiable. We use a heuristic algorithm to find 'smallest' sets of dependent parameters.

Last, interval arithmetic is used to get bounds for the true values of the interzonal airflows.

2. The Identification Problem

Now we have to determine the interzonal airflows from the measured tracer gas concentrations. Let m be the number of sampling intervals, M the number of samples, $\bar{c}_i \in \mathbb{R}^n$ the measured concentrations and $c(t_i, Q) \in \mathbb{R}^n$ the modelled concentrations at time t_i $(0 \le i \le m)$, where the parameter-vector Q contains the unknown interzonal airflows. Thus the interzonal airflows can be determined by the requirements

$$c(t_i, Q) \approx \bar{c}_i$$
 , $i = 0, \cdots, m$

Under the assumption that the measurement errors and model uncertainties can be described by a Gaussian statistics, the least squares method gives an optimal estimator

(2.1)
$$Q = \arg\min_{Q} \sum_{i=0}^{m} \|c(t_i, Q) - \bar{c}_i\|_2$$

According to (1.1) the time evolution of the concentrations c(t,Q) can be modelled by

(2.2)
$$V \dot{c}(t,Q) = Q c(t,Q) + \tilde{g}$$
, $c(t_0,Q) = c_0$

With
$$V = diag(V_1, \dots, V_n)$$
, $\tilde{g} = (\tilde{g}_1, \dots, \tilde{g}_n)^T$, $g \equiv V^{-1}\tilde{g}$ and

$$Q = (q_{ij}) q_{ij} = \begin{cases} \tilde{q}_{ij} & \text{if } i \neq j \\ \sum_{z=0, z \neq i}^{n} \tilde{q}_{zi} & \text{if } i = j \end{cases}$$

we get

(2.3)
$$\dot{c}(t,Q) = V^{-1}Q c(t,Q) + g \equiv f(t,c,Q)$$
, $c(t_0,Q) = c_0$

There exist several methods to solve the linear differential equation (2.3), e.g.

- i) a closed formula for the exact solution
- ii) solving (2.3) with a numerical scheme

With the aid of the variation of constants formula we obtain the solution of (2.3) with $A \equiv V^{-1}Q$

(2.4)
$$c(t,Q) = \exp(At) c(t_0,Q) + A^{-1} (\exp(At) - I) g$$

where I is the identity-matrix in $\mathbb{R}^{n\times n}$. The concentrations can now be approximated using a Padé-Approximation to the exponential function. But this method needs $\mathcal{O}(n^3)$ operations to compute the solution and is therefore not efficient.

To integrate (2.3) numerically, we can use

- an explicit method of Runge-Kutta type, e.g. as given by Dormand and Prince (1980) with automatic step size control (see [1] page 171).
- an implicit method like the extrapolated lineary implicit Euler method combined with a dense output formula and automatic step size control. The advantage of this method is, that it is well suited for the (mildly) stiff equations (2.3) and with the aid of the dense output formula we can obtain the solution at each point of time within each integration step (see [2]).

Each of the proposed methods is able to approximate the solution of (2.3) at arbitrary points in time. Notice that c(t,Q) is piecewise continously differentiable with respect to time.

Since the initial values c_0 are not known we have to identify them as well. Putting $P = \begin{pmatrix} c_0 \\ Q \end{pmatrix} \in \mathbb{R}^n$, now (2.3) is replaced by

(2.5)
$$\dot{c}(t,P) = V^{-1} Q c(t,P) + g \qquad c(t_0,Q) = c_0 \dot{Q} = 0 \qquad Q(t_0) = Q$$

Problem (2.1) now reads

(2.1')
$$P = \arg\min_{P} \sum_{i=0}^{m} \|c(t_i, P) - \bar{c}_i\|_2$$

For this nonlinear least squares problem we have to evaluate $c(t_i, P)$, i.e. solve (2.5), so the whole technique is similar to the shooting technique for boundary value problems. Moreover, the nonlinear problem (2.1') is solved by iterating with the linearized problem — this technique is called the Gauss-Newton-Method. We linearize c(t, P) at \tilde{P} . We get with $c_p \equiv \frac{\partial c}{\partial P}$

(2.6)
$$c(t,P) \approx c(t,\tilde{P}) + c_p(t,\tilde{P})(P - \tilde{P})$$

Inserting (2.6) into (2.1') we get

$$\min_{P} \sum_{i=0}^{m} \left\| c_{p}(t_{i}, \tilde{P})(P - \tilde{P}) - \left(\bar{c}_{i} - c(t_{i}, \tilde{P}) \right) \right\|_{2}$$

With $\Delta P = (P - \tilde{P}) \in \mathbb{R}^N$ and

$$J = \begin{pmatrix} c_{p}(t_{0}, \tilde{P}) \\ \vdots \\ c_{p}(t_{m}, \tilde{P}) \end{pmatrix} \in \mathbb{R}^{M \times N}, \qquad b = \begin{pmatrix} c(t_{0}, P) - \bar{c}_{0} \\ \vdots \\ c(t_{m}, P) - \bar{c}_{m} \end{pmatrix} \in \mathbb{R}^{M}$$

where M is the number of samples and N is the number of the unknown parameters, we get the linearized least squares problem

$$\min_{\Delta P} \|J \Delta P - b\|_2$$

The solution P of (2.1') is now obtained with the aid of ΔP by iteration

$$(2.8) P^{k+1} = P^k + \Delta P$$

which terminates when $\|\Delta P\|_2$ is small enough. For this iteration we have to compute the Jacobian J.

Theorem 1 Suppose that the partial derivatives of f in (2.3) with respect to c exist and are continous. Let $C \equiv \begin{pmatrix} c \\ Q \end{pmatrix}$.

Then the solution C(t,P) is differentiable with respect to P and the derivative is given by the matrix $\partial C/\partial P \equiv R(t,t_0)$, where R is the solution of the so called 'variational equation'

(2.9)
$$\dot{R}(t) = \begin{pmatrix} f_c(t, c, Q) \\ f_Q(t, c, Q) \end{pmatrix} \cdot R(t, t_0) , \qquad R(t_0) = E_n$$

where E_n is the identity-matrix in $\mathbb{R}^{n\times n}$ (see [1], pp 97). Notice that here we have $f_c(t,c,Q)=A$.

In our case, theorem 1 is not directly applicable since the right hand side of (2.3) is discontinuous at those points in time, where the injection \tilde{g} (a step function) has jumps. But one can show that the conclusion of theorem 1 stays valid.

The solution R of (2.9) can now be obtained by the same methods as the solution of (2.3). It is also possible to compute J by divided differences, but in this case it is necessary to freeze the step sizes, that means the step sizes used during the computation with the initial value \tilde{c} are memorized and reused during the computation with the initial value $\tilde{c} + \delta c$.

Differentiating the solution given by (2.4) one can give a closed form solution of the variational equation (2.9) by theorem 2.

Theorem 2 Let $A = (a_{ij}) \in \mathbb{R}^{n \times n}$ be regular and $t \geq 0$ Then

$$\frac{\partial}{\partial a_{ij}} exp(At) = \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{z=0}^{k-1} A^k B^{(ij)} A^{k-z-1} t^k$$

$$\frac{\partial}{\partial a_{ij}} A^{-1} (exp(At) - I) = \sum_{k=1}^{\infty} \frac{1}{(k+1)!} \sum_{z=0}^{k-1} A^z B^{(ij)} A^{k-z-1} t^{k+1}$$
where
$$B^{(ij)} = (b_{ls}^{ij}) \quad \text{with} \quad b_{ls}^{ij} = \begin{cases} 1 & \text{for } l = i \text{ and } s = j \\ 0 & \text{otherwise} \end{cases}$$

To solve the linear least squares problem (2.7) we first compute the QR-factorization of J such that J=QR, where $Q\in\mathbb{R}^{M\times M}$ is an orthogonal matrix and $R=(R_1,0)^T\in\mathbb{R}^{M\times N}$ is a triangular matrix. Then we have

$$||J \Delta P - b||_2^2 = ||Q R \Delta P - b||_2^2 = ||R_1 \Delta P - b_1||_2^2 + ||b_2||_2^2$$
with $Q^T b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$ and $b_1 \in \mathbb{R}^N$

Thus (2.7) is reduced to the much smaller problem

(2.10)
$$\min_{\Delta P} \|R_1 \ \Delta P - b_1\|_2$$

which can be tackled by the singular value decomposition. For this one computes orthogonal matrices $U, \mathcal{V} \in \mathbb{R}^{N \times N}$ and a diagonal matrix $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_N)$ such that $R_1 = U \Sigma \mathcal{V}^T$.

Using this factorization, the solution of (2.10) can be expressed as:

$$(2.11) \Delta P = \mathcal{V} \; \Sigma_r^+ \; U^T b_1$$

The pseudo inverse Σ_r^+ of Σ is given by $\Sigma_r^+ = \operatorname{diag}(\sigma_1^{-1}, \cdots, \sigma_r^{-1}, 0, \cdots)$, where r denotes the numerical rank of R_1 , which is equal to the numerical rank of J (see [3], p. 242). Thus the use of the singular value decomposition aids in determining the numerical rank of R_1 . This is combined with a trust region algorithm for the nonlinear problem (2.1) (see [9]). In principle the numerical rank is determined such that the solution ΔP of (2.10) is bounded by R_T – the trust region radius. For more difficult problems — characterized by a given amount of nonlinearity in relation to the minimal value in (2.1) — we have to include a Levenberg-Marquardt regularization technique, as well (see [9], pp 218–228). The relation of the numerical rank r to the size of the step ΔP follows from (2.11)

$$\|\Delta P\| = \sum_{i=1}^{r} (U_i^T b_1) / \sigma_i$$

3. Statistical Considerations

Once one has calculated the solution of (2.1) by iterating (2.7), it is desirable to give error estimates for the solution. For this we consider the last iteration.

The vector b_1 of (2.7) coincides with the measured data \bar{c} up to the bias $c(\cdot, P)$. Therefore the components b_1^i $(1 \le i \le N)$ of the vector b_1 can be viewed as statistical independent random variables with mean value \tilde{b}_1^i and variance σ , which equals the variance of the measured data \bar{c}_i .

Then one gets for the expected value:

$$E(b_1^i) = \tilde{b}_1^i$$
 , $i = 1, \dots, N$

and for the covariances of b_1^i

$$cov(b_1^i,b_1^j) \ = \ E\big((b_1^i-\tilde{b}_1^i)(b_1^j-\tilde{b}_1^j)\big) \ = \ \left\{ \begin{matrix} \sigma^2 & \text{if } i=j \\ 0 & \text{otherwise} \end{matrix} \right.$$

Under these assumptions the solution ΔP of (2.7) can be viewed as random variable too and because ΔP is given by $\mathcal{V} \Sigma_r^+ U^T b_1$ we obtain the expected value of ΔP

$$E(\Delta P) = \mathcal{V} \ \Sigma_r^+ \ U^T \tilde{b}_1$$

Thus we have for the covariance matrix (see [10], p 182)

$$E((\Delta P - E(\Delta P))(\Delta P - E(\Delta P))^{T}) = \sigma^{2} \mathcal{V}(\Sigma_{r}^{+})^{2} \mathcal{V}^{T} \equiv C$$

From this we also get the correlation coefficients $cor(\Delta P_i, \Delta P_j)$ for the solution, which indicate how much the computed parameter ΔP_i depends on the computed parameter ΔP_i . We have

$$cor(\Delta P_i, \Delta P_j) = \frac{C_{i,j}}{\sqrt{C_{i,i}C_{j,j}}}$$
, $i, j = 1, \dots, N$

4. Singular Jacobian

Sometimes it is known in advance or detected in previous runs that the Jacobian J in (2.7) is singular. This may have different reasons

- there exists no connexion between some zones
- some combinations of parameters cannot be identified numerically because some zones are hardly influenced by the given injections into other zones.

In this case it is interesting to know which parameters or combinations of parameters lie in the kernel of J and thus cannot be identified. We get the (numerical) null space from the singular value decomposition of R_1

(3.1)
$$\operatorname{null} J = \operatorname{span} \{V_{r+1}, \dots, V_N\}$$

But, to draw conclusions on which parameters are identifiable and on the experimental settings, we need a special type of basis for the kernel where each basis vector has as many zero components as possible. The remaining (hopefully) few nonzero components can be interpreted as coefficients of those linear combinations of parameters that cannot be identified — at least by the current experimental settings.

It is well known that computing a 'sparsest null space basis' cannot be done efficiently. Therefore one has to resort to heuristic algorithms which compute a nearly optimal basis. In our case we propose the following simple algorithm. Let k denote the dimension of the null space (here k=N-r), and z^1,\ldots,z^k a basis for it. We start with $z^j=V_{r+j},\ 1\leq i\leq k$. We now try to replace each of these basis vectors z^j by a vector with fewer nonzero components. We describe the first step only, the same technique is applied to the remaining vectors — theoretically by renumbering the vectors z^j . For ease of presentation let us rename z^1 to z.

We need some more notation. Let us define the 'indicator vector' χ

$$\chi_i = \begin{cases} 1 & \text{if } z_i = 0 \text{ (or should be 0)} \\ 0 & \text{if } z_i \text{ may be nonzero} \end{cases}$$

and

$$Z = (z^2, z^3, \dots, z^k)$$
 $\alpha = \begin{pmatrix} \alpha_2 \\ \vdots \\ \alpha_k \end{pmatrix} \qquad \alpha_j \in \mathbb{R}$
 $X = \operatorname{diag}(\chi_1, \dots, \chi_N)$

Note that in this notation the new basis vector \tilde{z} has the representation $z + Z\alpha$.

We now proceed as follows

Loop over the following steps and the inner loop until we escape the inner loop because the maximum number of iterations is exceeded.

- Increase the number of components in z, that should equal 0, by 1. For this select an index l at random for which $\chi_l = 0$ and set $\chi_l = 1$, i.e. z_l should become 0, now.
- * Solve the least squares problem $e = \min ||X(z + Z\alpha)||_2$.

Note that multiplication by X is 'shooting operator' which kills all components which are allowed to take nonzero values. If e is tiny, we have succeeded in finding the replacement vector $\tilde{z} = z + Z\alpha$ with just that vector α for which the minimum is attained.

• Set $e_o = e$.

Iterate the following step until we escape or the maximum number of iterations is exceeded.

• (Exchange step)

Select indices i and j for which $\chi_i = 0$, $\chi_j = 1$ and set $\chi_i = 1$, $\chi_j = 0$. Perform step (\star) and escape if e is tiny. Otherwise proceed as in 'simulated annealing' (see [12] for an introduction).

Accept this exchange if $e^{(e_o - e)/T} > \gamma$.

Here γ is some constant $\gamma < 1$, $\gamma \approx 1$ and T > 0 is the simulated temperature which is driven to 0 gradually. Note that a step with $e < e_o$ is always accepted. Set $e_o = e$.

Otherwise undo this exchange step.

5. Calculation of Intervals for the Parameters

Interval arithmetic gives a possibility of computing bounds for the parameters, if there exist bounds for the measurements. Analogous to calculating with real numbers, one can calculate with intervals using the following arithmetic

Let $\star \in \{+, -, *, /\}$, $I_1 = [a, b]$ and $I_2 = [c, d]$ then we define $I_1 \star I_2 = \{x \star y \mid x \in I_1 \land y \in I_2\}$ where I_1/I_2 is defined only if $0 \notin I_2$.

This can be extended to vectors and matrices (see [4,6]).

Now we want to compute intervals bounding all parameters. For this the solution of the interval version of (2.3) is needed

(5.1)
$$\dot{c}(t,P) = A c(t,P) + g \quad , \qquad c(t_0,P) = c_0$$

where now A is an interval matrix, c(t,p) and c_0 are interval vectors. The interval differential equation (5.1) can now be solved by an algorithm due to R. Lohner[7]. This gives the interval solution c(t,P) for a given parameter interval P. The parameter interval has again to be determined by solving (now an interval) nonlinear least squares problem. Similarly as in (2.1), given an interval vector \bar{c}_i of measurements, an interval vector P containing all solutions of

(5.2)
$$\arg\min_{\tilde{P}} \sum_{i=0}^{m} \|c(t_i, \tilde{P}) - \tilde{c}_i\|_2 \quad \text{for all} \quad \tilde{c}_i \in \bar{c}_i$$

has to be determined. This can again be reduced to a sequence of linear interval least squares problems. Let ΔP be the interval vector containing all solutions of

(5.3)
$$\arg\min_{\widetilde{\Delta P}} \|J|\widetilde{\Delta P} - b\|_2$$

where J is an interval extension of the Jacobian in (2.7) and b is an ordinary vector given by

$$b = \begin{pmatrix} c(t_0, \breve{P}) - \breve{c}_0 \\ \vdots \\ c(t_m, \breve{P}) - \breve{c}_m \end{pmatrix}$$

where \check{P} denotes the midpoint of the interval vector P and \check{c}_i denote the midpoints of the interval vectors \bar{c}_i , $0 \le i \le m$. Therefore the solution ΔP of (5.3) is an interval vector and can be obtained using an algorithm due to Neumaier[5].

The solution of (5.2) is again obtained by iteration

$$P^{k+1} = P^k + \Delta P^k$$

and this iteration terminates when $P^{k+1} \subset P^k$.

Numerical Example

We used the experimental setting of [11]. We were able to get the same results as quoted in [11] using 8 iterations. The results agreed within 3% in most cases and up to 12% in a few cases.

In addition we computed the correlation coefficients and variances. All initial values could be identified with a variance of about 1%. The variances of the interzonal airflows differ widely. We got the following results (the notation $i \rightarrow i$ denotes the sum of all outflows from zone i)

interzonal airflow between zones	variance[%]
$1 \rightarrow 9, 2 \rightarrow 9, 3 \rightarrow 9, 4 \rightarrow 9, 5 \rightarrow 9, 6 \rightarrow 9, 7 \rightarrow 9, 8 \rightarrow 8, 9 \rightarrow 8, 9 \rightarrow 9$	0 - 0.7
1→1	1.7
$1 \rightarrow 2, \ 2 \rightarrow 2, \ 2 \rightarrow 3, \ 3 \rightarrow 3, \ 3 \rightarrow 4, \ 4 \rightarrow 4, \ 5 \rightarrow 5, \ 6 \rightarrow 6$	2.5 - 9
$6\rightarrow7, 7\rightarrow7, 8\rightarrow7$	14 - 18
8→1	86
$8\rightarrow 2, 8\rightarrow 4, 8\rightarrow 5, 8\rightarrow 6$	109 - 280
8→3	550

Furthermore the correlation coefficients between the initial concentrations and all the other parameters are quite small (about 10^{-3}) except the correlations of initial concentrations of connected zones which amount to 0.1 (approximately). Quite high correlations were found for the the following pairs of airflows $(9\rightarrow 8, 1\rightarrow 9)$, $(1\rightarrow 9, 2\rightarrow 9)$, $(4\rightarrow 9, 9\rightarrow 9)$ which amount to 0.914, 0.956, 0.916, respectively.

Summary and Conclusions

We have presented a new technique for estimating the interzonal airflows from tracer gas measurements. We set up a system of differential equations for the time evolution of the concentrations in each zone. The interzonal airflows enter these differential equations as coefficients. These unknown coefficients as well as the unknown initial concentrations are numerically identified by solving a (nonlinear) least squares problem where one function evaluation amounts to solving these differential equations with given initial values and coefficients. With the aid of the Jacobian of this 'function' we are able to estimate variances for and correlations between the unknown quantities. Furthermore, studying the (numerical) null space of this Jacobian shows unidentifiable interzonal airflows (or combinations) and gives hints on possible optimizations of the experimental settings. If rigorous bounds (intervals) for the measured data are available there is also a technique for computing rigorous bounds for the interzonal airflows (intervals), provided the applicability of the underlying model is out of question.

References

- [1] Hairer, E., Nørsett, S.P. and Wanner, G. Solving ordinary differential equations I, Nonstiff problems Springer, Berlin 1987
- [2] Hairer, E. and Ostermann, A. Dense output for extrapolation methods report Universitè de Genéve, 1988
- [3] Golub, G.H. und van Loan, Ch.F. Matrix computations, second edition The John Hopkins University Press, Baltimore and London 1990
- [4] Moore, R. Intervallanalyse
 R. Oldenbourg Verlag, München, Wien 1969
- [5] Neumaier, A. Solving linear least squares problems by interval arithmetic Freiburger Intervallberichte, 1987
- [6] Neumaier, A. Intervalmethods for systems of equations Cambridge University Press, Cambridge, 1990
- [7] Lohner, R. Enclosing the solution of ordinary initial and boundary value problems
 in E. Kaucher, U.Kulisch and Ch. Ullrich (eds) 'Computerarithmetic',
 Teubner, Stuttgart, 1987
- [8] Louis, A.K. Inverse und schlecht gestellte Probleme Teubner Studienbücher Mathematik, Stuttgart 1989
- [9] Dennis, J.E. jr. and Schnabel, R.B. Numerical methods for unconstrained optimization and nonlinear equations Prentice Hall Series in Computational Mathematics, Englewood Cliffs 1983
- [10] Stoer, J. and Bulirsch, R. Einführung in die Numerische Mathematik Band I und II Springer Verlag, Heidelberg, Berlin, 1983
- [11] Mattson, J.B. An Experiment for Airflow determination by Quadratic Programming Air Infiltration Review, Vol 11(4), 1990
- [12] Press, W.H., Flannery, B.P., Teukolsky, S.A. and Vetterling, W.T. Numerical Recipes Cambridge University Press, Cambridge, 1986
- [13] GuitiZad,S. Zur numerischen Identifizierung von Luftaustauschraten in Gebäuden
 Diplomarbeit am Institut für Geometrie und Praktische Mathematik, RWTH Aachen, 1991