PREDICTION OF AIR FLOW DISTRIBUTION IN ROOMS AND ASSOCIATED POLLUTANT TRANSFERS BY THE SYSTEMIC APPROACH

S. Domenech[1], S. Drecourt[2], P. Floquet[1], J.C. Laborde[2], C. La

[1]Laboratoire de Génie Chimique - UMR CNRS 5503 INP-EN
18, Chemin de la Loge, F 31078 Toulouse Cedex 4, FRANCE
[2]Institut de Protection et de Sûreté Nucléaire, DPEA/SERAC
CEA/Saclay - F 91191 Gif-sur-Yvette Cedex, FRANCE

ABSTRACT

The general strategy adopted in the development of a computational tool performing the identification of parametric models based on the Residence Times Distribution (RTD) theory is exposed. Two main aspects of the modelling procedure are presented: the structural discrimination of the various solution schemes, and the parameters estimation step. The structural model determination is solved by a stochastic procedure based on a Simulated Annealing algorithm, while the parametric identification is solved by a nonlinear deterministic procedure. An application example is proposed for the description and the quantification of the air flow patterns and the associated pollutant transfers observed in a ventilated room.

KEYWORDS

Air flow pattern - Ventilation efficiency - Mixing ventilation - Modelling - Residence times distribution.

INTRODUCTION

In order to achieve a satisfactory level of hygiene and comfort in industrial premises, it is necessary to control the air flow distribution. Furthermore, to prevent and to detect chemical or radiological hazards, the validation of a proper ventilation system is required. Evaluating the performance of such systems, lies on the description of the air flow patterns. The research on air distribution in ventilated rooms traditionally involves full-scale experiments, scale-model experiments and Computational Fluid Dynamics (CFD) tools.

An intermediate approach between predictive numerical simulation and experimental determination of aerodynamic parameters constitutes the purpose of this paper. The solution retained here is the establishment of models based on the well known Residence Times Distribution theory, widely used in chemical engineering to model non-ideal flows and called the « systemic approach ».

Most of the time, the predictive approach based on CFD codes is difficult to use, particularly in the case of large and cluttered enclosures; this is mainly why the « systemic approach » has been retained. Furthermore, this approach leads to more integrated results, giving a physical significance to the flow model while not being too time consuming. At present, only codes performing the estimation of parameters for a fixed model structure given by the user are available (Olander et al., 1995). The originality of the strategy proposed is based on the fact that our code allows to perform simultaneously the generation of the model structures and the estimation of their optimal parameters.

This paper provides first an overview of the global strategy retained for the development of a computational package performing the identification of models based on the proposed approach. This identification procedure is performed in two steps: a structural identification of the models and a parametric identification loop for a given model structure in order to fit an experimental RTD curve. The various

modules implemented in the package are then detailed. Finally, an application example illustrates how these models can be applied to the safety analysis and the contamination monitoring in nuclear facilities.

POSITION OF THE PROBLEM

As illustrated by figure 1, an industrial ventilation system of a room is made up of blowing and exhaust networks; leaks or infiltrations can occur, the enclosure being in depression or in overpressure with respect to the adjacent rooms. The air flow patterns and the associated contaminant transfers subjected to the ventilation cannot be represented most of the time by ideal flows such as plug flow or perfect mixing. As a consequence, the distribution of airborne pollutants will not be homogeneous when an emission occurs somewhere.

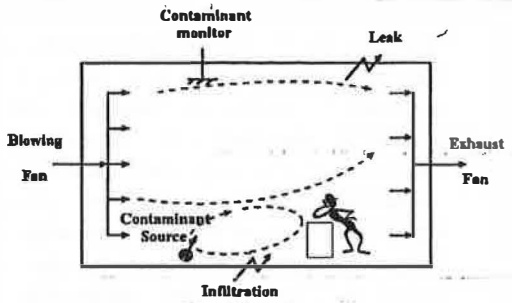


Figure 1: Position of the problem.

With the establishment of a flow model, the contaminant transfers after an accidental pollutant release or in standard working conditions can be evaluated. This model allows to predict the amount of contaminant that workers can inhale, the concentrations to be recorded by the contaminant monitors located somewhere in the indoor space, and then it allows to validate the pertinence of the monitors location.

General principles of the approach

In a first step, the approach proposed is based on the experimental determination of the RTD curve, obtained generally from the response of the ventilated room to a tracer release (helium for instance). Then, a model is built up and consists in a combination of elementary systems representing ideal flows: piston (or plug flow reactor PFR), perfect mixing zone (or continuous stirred tank reactor CSTR), by-pass and recycling. Each elementary system is characterized by specific parameters, such as the mean residence time or the volume. The adjustment of the model is derived from the comparison of the simulated response of the model from a stimulus, with the experimental response. The parameters of the various candidate structures are optimized in order to fit the experimental curve.

In steady state conditions, the response of the ventilated room to a general input stimulus can be deduced from the RTD curve through the following convolution integral:

$$C_{out}(t) = \int_0^t C_{int}(t-t').E(t')\,dt' \qquad (1)$$

where C_{out} (t) = response of the system (generally, tracer concentration at the ventilated room exhaust)

C_{int} (t) = imput stimulus

E(t') = RTD curve

A lot of items can be deduced from such curves; the most common one is the mean residence time τ:

$$\tau = \frac{\int_0^\infty t.C_{out}(t)\,dt}{\int_0^\infty C_{out}(t)\,dt} - \frac{\int_0^\infty t.C_{int}(t)\,dt}{\int_0^\infty C_{int}(t)\,dt} \qquad (2)$$

General solving strategy

The solving strategy implemented in the computational package includes three modules: the simulation module, the parameter estimation module, and the structural evolution module. The problem is solved through a two levels procedure, as illustrated in figure 2: an inner-level performing the parametric identification for a given structure, and an upper-level performing the structural identification. Only these two modules are presented in the next parts; the simulation module allowing the response calculation of a given model to any kind of stimulus is not described here because it is a commercial solver (LSODI).

The objective function (criterion 1) to be minimized here (j(p)) is given by the following equation :

$$j(p) = \frac{1}{n_t} \sum_i \left[y_{exp}(t_i) - y_{mod}(t_i) \right]^2 \qquad (3)$$

where n_t = number of experimental sample points

y_{exp} = experimental response

y_{mod} = simulated model response

p = vector of the model parameters

t_i = time

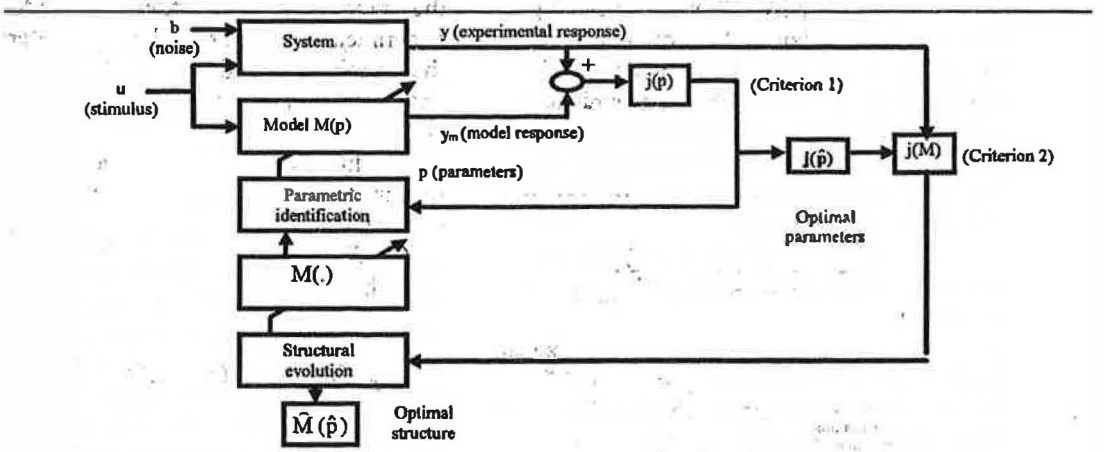


Figure 2: Structure of the general identification strategy.

PARAMETRIC IDENTIFICATION MODULE

This module solves the slave problem; it consists in a constrained nonlinear least squares problem solved with a Successive Quadratic Procedure (SQP) which determines an optimal set of continuous parameters in order to fit the simulated response to the experimental curve (Powell, 1988). The set of parameters is related to the volume of the elementary unit (PFR, CSTR) and the fluid flow rate circulating in the branches of the oriented graph describing the model.

The constraints include equality constraints related to mass balances at each node of the flow diagram and inequalities constraints corresponding to identifiability conditions given by the structural identification loop.

STRUCTURAL IDENTIFICATION MODULE

This module resolves the master problem and proposes the structures of the candidate models to the slave problem. The generation of the structures consists in the choice of the elementary ideal flow models and the determination of their connections. To tackle the combinatorial aspect of the problem, a stochastic procedure is retained

through a classical simulated annealing algorithm (SA) as introduced by Kirkpatrick et al. (1983). Furthermore, it avoids the procedure blocking on local minima paths, with occasionally accepting solutions that increase the objective function value.

The simulated annealing procedure mimics the physical annealing of solids : the slow cooling of a molten substance, that redistributes the arrangement of the crystals. In a rapid cooling or quenching, the final result would be a metastable structure with higher internal energy. The rearrangements of the crystals follow probabilistic rules.

In the annealing of solids, the goal is to reach given atomic configurations that minimize internal energy. In SA, the goal is to generate feasible solutions of the optimization problem that minimize the objective function. The detailed analogy between statistical physical mechanisms and the SA procedure can be found in Kirkpatrick et al. (1983).

Table 1 presents the simulated annealing algorithm implemented in our software.

Table 1 The SA algorithm

```
Select an initial structure M = M°.
Select initial value for the SA-temperature
Tsa°.
Select length of cooling stage Nsa.
Do while the search can evolve:
    Do Nsa times:
        Generate a new structure M'
        neighbour of M,
        Estimate the set of continuous
        parameter of M',
        Accept or reject the new
        configuration according to the
        Metropolis method:
            If M' accepted: M = M'
            If M' rejected: cycle keeping M
            unchanged
    Decrease Tsa according to the SA-
    cooling schedule.
Final structure : M.
```

The various steps of the algorithm are described below.

Objective function

The objective function retained in the structural identification module (criterion 2) is:

$$j(M) = j(M, \hat{p}) + \rho \dim(p) \qquad (4)$$

where $j(M, \hat{p})$ = optimal function given by the slave module for the structure M

ρ = wheighting factor

$\dim(p)$ = number of parameters included in the structure M

This objective function allows the procedure to find a compromise between the simplicity of the model and the adequation between the experimental curve and the simulated one.

Initial structure (M°)

Two options are offered to choose the initial structure: this structure can be synthesized through a pure random procedure or can be given by the user.

Initial annealing temperature (Tsa°)

The initial value of this control parameter, which can be expressed in our case in the dimension of the objective function, is determined according to each particular problem treated. Particular attention is required to set this parameter which seems to be the most sensible for the SA procedure.

SA-temperature stage

The SA-temperature stage is characterized by the number Nsa of structures generated keeping the SA-temperature constant; a value from 10 to 20 has been retained.

SA-cooling schedule

The SA-cooling schedule of the parameter Tsa retained is the classical geometrical cooling schedule:

$$Tsa_{i+1} = \alpha . Tsa_i$$

where the multiplicative factor α is set to 0.95.

Rule of acceptance of the structures tested

The probability p of acceptance of a structure is the Metropolis one :

$$p = 1 \qquad \text{if } \Delta j < 0$$

or

$$p = \exp\left(\frac{-\Delta j}{Tsa_i}\right) \qquad \text{if } \Delta j \geq 0$$

where Δj is the difference between the objective function of the new structure tested with the current structure retained. This expression allows the procedure to escape from local minima. This criterion of acceptance has provided good performances through the resolution of various combinatorial problems.

Termination conditions

The procedure stops when the current SA-temperature is lower than a specified temperature or when a steady state is detected. For a given SA-temperature stage k, a steady state is reached if no-evolution of the objective function greater than the tolerance *Tol* is detected on the n previous levels of temperature; this can be expressed by the following condition:

$$\forall i = k-1,\ldots,k-n \qquad \left| j_{Tsa_k} - j_{Tsa_i} \right| \leq Tol$$

Generation of neighbour structures

The structures are coded through an oriented graph corresponding to the fluid flow diagram and with the description of the elementary systems composing the branches of the structures. The generation of neighbour structures is carried out through probabilistic mechanisms consisting in adding or suppressing an unitary ideal flow model.

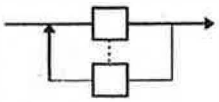
The originality of the proposed formulation lies in the representation of the various structures to ensure their identifiability and distinguishability. This is solved:

- by introducing supplementary constraints into the parametric identification step for a given structure,
- by rearranging the proposed structure in an unique hierarchical decomposition.

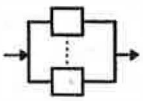
All the structures are decomposed in an unique hierarchical way through the complex following building blocks:

- linear cascade

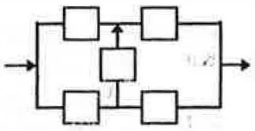
- recycling loops



- Parallel distribution



- Intermediate distribution



Each box composing these blocks can involve a complex structure built on the same principle or an unitary ideal model. This decomposition is made in a hierarchical way in order to obtain all elementary ideal flow models. At each level of decomposition the building blocks are ordered respecting the following order: linear cascade, recycling, parallel distribution, intermediate distribution, PFR, CSTR, by-pass. This coding strategy allows to generate the most common possible schemes and thus to explore a large solution space.

To respect the constraints on distinguishability and simplicity, the following rules are adopted:

- only one PFR is allowed in a straight branch,
- in a cascade branch, in parallel distribution and in recycling loops, blocks presenting the same structure are ranked in a decreasing mean residence time; this is carried out by injecting

blocks presenting the same structure are ranked in a decreasing mean residence time; this is carried out by injecting supplementary inequality constraints in the parametric identification step,

- constraints on bounds are also considered for all the parameters, in order to retain significant models, and to reduce the complexity of the final scheme proposed.

Finally, to ensure global identifiability, a general constraint is added on the global mean residence time. Knowing global flow rate entering in the studied system, it constitutes a constraint on the sum of the volume of the elementary systems (PFR and CSTR) which must be equal to the real global volume accessible to the fluid. A particular accuracy is required on this constraint to guide the performance of the whole identification procedure.

TEST EXAMPLE

The whole identification procedure has been first tested on a theoretical example. This test example is built with the step response of the model given in figure 3. The parameters (volumes V and flowrates F) used to generate the theoretical experimental response are in arbitrary units:

$V_{CSTR1} = 5$, $V_{CSTR2} = 10$
$F_1 = 0.6$, $F_2 = 0.4$

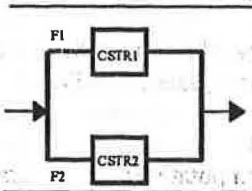


Figure 3: Structure of the illustrative example.

The identification is performed for various conditions. First, two initial structures are proposed: initialization 1 corresponds to a cascade of 3 CSTR while initialization 2 corresponds to an unique CSTR model. The presence of a fictitious noise is then simulated by adding a random variable to the initial response; this noise follows a gaussian distribution characterized by its standard deviation σ. Various values of the penalty factor ρ are also tested.

The results ares summarized in table 2.

Table 2: Results obtained on the test example.

Initial structure	σ (noise)	ρ (penalty factor)	Number of structures tested	Optimal structure reached (n° structure)
1	0	1.e-5	80	yes (19)
1	0	1.e-8	70	yes (28)
1	0	1.e-8	60	yes (30)
1	0	1.e-8	60	yes
1	0	1.e-8	100	yes
2	0	1.e-8	110	yes (10)
2	0	1.e-5	197	yes (25)
2	0	1.e-5	93	yes(14)
2	0	1.e-5	119	yes(15)
2	0	1.e-4	120	yes(4)
2	0.01	1.e-5	118	yes(43)
2	0.01	1.e-3	60	yes(5)

It can be noted that the optimal structure is found in all test configurations, providing a great robustness to the identification procedure for the test case; this remains true in the presence of noise on the signal.

APPLICATION TO VENTILATED PREMISES

This computational tool has been tested from a ventilated laboratory enclosure available at the Nuclear Safety and Protection Institute. The enclosure MELANIE is a 100 m^3 ventilated cell where it is possible to obtain different air flow patterns and residence times distributions by configuring the ventilation system in various ways. Helium stimulus corresponding to pulse release is realized into the inlet duct; the helium concentration has been monitored at the exhaust duct.

Figure 4 gives the experimental and the simulated responses of the model proposed by the identification procedure,

the structure of which is given in figure 5. All the concentrations are normalized and given in arbitrary units.

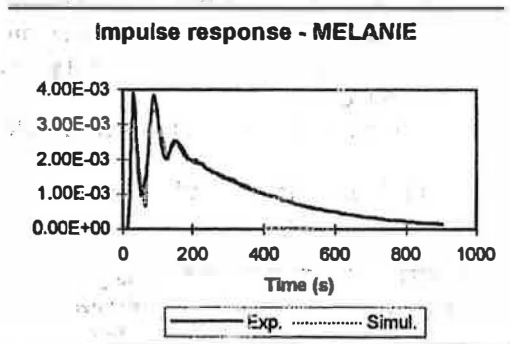


Figure 4: Example of identification.

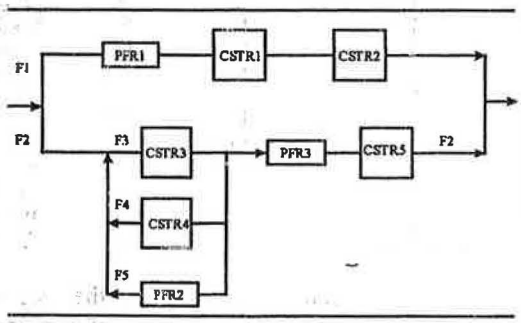


Figure 5: Structure of the model proposed.

For the proposed structure, the set of continuous parameters found is:

$$\begin{cases} V_{CSTR1} = 0.202\ m^3 \\ V_{CSTR2} = 0.399\ m^3 \\ V_{CSTR3} = 16.311\ m^3 \\ V_{CSTR4} = 24.401\ m^3 \\ V_{CSTR5} = 10.205\ m^3 \end{cases} \quad \begin{cases} V_{PFR1} = 0.522\ m^3 \\ V_{PFR2} = 30.641\ m^3 \\ V_{PFR3} = 17.289\ m^3 \end{cases} \quad \begin{cases} F1 = 0.0295\ m^3.s^{-1} \\ F2 = 0.275\ m^3.s^{-1} \\ F3 = 1.161\ m^3.s^{-1} \\ F4 = 0.388\ m^3.s^{-1} \\ F5 = 0.498\ m^3.s^{-1} \end{cases}$$

The adjustment of the experimental curve by the simulated response of the model is quite acceptable. The fluid flow pattern proposed can be decomposed into two main flows. A first one with a short mean residence time corresponding to the first peak and a second one with recycling loops corresponding to the oscillatory curve and to the major volume of the cell. Physically, the first flow can be neglected. The model obtained gives a good evaluation of the performance of the ventilation system, the major difficulty being of giving a physical signification to the flow model. In our case, the ventilation design involves a non homogeneous air change in the room.

With such a model, the evolution of the pollutant concentrations and the equilibrium concentrations can be followed in the various compartments when an accidental emission occurs somewhere. This kind of information is very important in order to optimize the worker protection and the location of the contamination monitors. Figure 6 gives the concentrations in the CSTR4 and in the extraction duct after a step-up release of pollutant, in the zone corresponding to the CSTR4. Contamination can reach an equilibrium concentration higher in the CSTR4 than in the global extraction duct. This kind of information constitutes an interesting information for safety surveys.

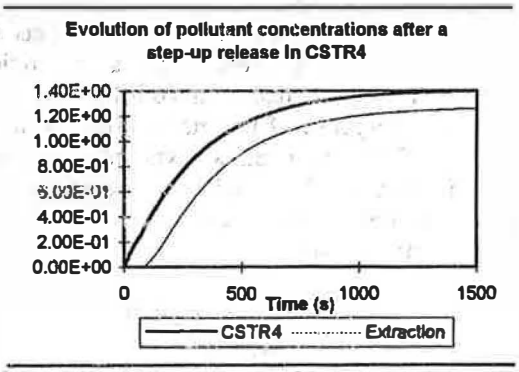


Figure 6: Evolution of concentrations after a step-up release in CSTR4.

CONCLUSIONS

The computational package presented in this paper constitutes an useful tool to study the operation of the ventilation system in geometrically complex existing premises and to predict the associated airborne pollutant transfers. The tool is still in validation on laboratory and industrial facilities. Furthermore, the structural identification module can be improved by implementing a new procedure based on genetic programming.

Useful applications of this automated modelling tool are possible not only in industrial ventilation but also in more classical chemical engineering fields (reactors diagnostic and design, fluidized beds, waste water treatment plants...) which commonly use the analysis of residence times distribution curves.

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