

Analytical solutions for compartmental models of contaminant transport in enclosed spaces

Problem presented by

Simon Parker

DSTL

Executive Summary

Understanding the transport of hazardous airborne materials within buildings and other enclosed spaces is important for predicting and mitigating the impacts of deliberate terrorist releases of chemical and biological materials. Multizone models provide an approach to modelling the contamination levels in enclosed spaces but in certain cases they can be computationally expensive. Alternative methods are being explored at DSTL that involve the direct solution of the contaminant dynamics equation. The Study Group was asked to identify the limits to this alternative approach and to explore its extension.

Version 1.1

November 3, 2011

iii+24 pages

Report author

Tristram Armour (Industrial Mathematics KTN)

Contributors

Tristram Armour (Industrial Mathematics KTN)
Elif Başkaya (Karadeniz Technical University)
Stephen Cowley (University of Cambridge)
Ishak Cumhuri (Rize University)
Patricio Farrell (University of Oxford)
Dariusz Grala (CIAMSE & University of Warsaw)
Jens Gravesen (Technical University of Denmark)
Siân Jenkins (University of Bath)
James Kirkpatrick (University of Oxford)
Karin Mora (University of Bath)
Margarita Schlackow (University of Oxford)
Süleyman Sengül (Karadeniz Technical University)
Xiaoting Wang (University of Cambridge)
Dave Wood (University of Warwick)

ESGI80 was jointly organised by

The University of Cardiff
The Knowledge Transfer Network for Industrial Mathematics

and was supported by

The Engineering and Physical Sciences Research Council

Contents

1	Introduction	1
1.1	Background	1
1.2	Multizone models	1
1.3	Analytical solutions	3
1.4	Questions	4
2	Work	5
2.1	Diagonalisation	5
2.2	Alternative methods of calculating the exponential of a matrix	6
2.3	Total Exposure	8
2.4	Inverse problem - quadratic minimisation	10
2.5	Inverse problem: Control theory method	12
2.6	Transient growth	16
3	Conclusions	17
3.1	Multizone model with lags	17
3.2	Final comments	18
A	Results from special cases	19
A.1	Alternative model for finding the toxic load	19
A.2	Duct model	20
B	Tools and codes	23
B.1	EigTool	23
B.2	Schur-Parlett	23
	Bibliography	24

1 Introduction

1.1 Background

- (1.1.1) Understanding the transport of hazardous airborne materials within buildings and other enclosed spaces is important for predicting and mitigating the impacts of deliberate terrorist releases of chemical and biological materials. Because such materials may be acutely toxic or infectious it is important to understand how concentrations may change with time to understand the hazards that different scenarios may pose. It is also relevant to the study of accidental releases of industrial materials and the impact of environmental pollutants on indoor air quality.
- (1.1.2) A range of different numerical modelling approaches are regularly used to study these problems as well as experimental methods. Computational fluid dynamics (CFD) can be used for detailed studies of air and contaminant movement within enclosed spaces. However, CFD methods require highly detailed input data and have significant model creation and execution times. This can make them impractical for whole building studies in some cases.
- (1.1.3) Multizone models (CONTAM, COMIS) provide an alternative approach where the building is divided into a series of well-mixed volumes connected by paths through which air and contaminants can pass. These models have the advantage that they are quicker to execute than CFD models and typically require less input information. The contaminants are normally considered dilute in such approaches. Typical model size is of the order of 10-100 zones, although 1000 or more may be required in some cases.
- (1.1.4) Multizone models solve the air flow through the network (typically using a non-linear pressure solver) for a series of quasi-steady states. The contaminant dispersion resulting from the air flow solution and the contaminant initial and boundary conditions is then calculated. Whilst these models are well developed and have been validated for a range of studies, they rely on numerical methods which can become time consuming for large studies (e.g. Monte Carlo analysis). In addition, little insight is gained into the system behaviour using a numerical approach.

1.2 Multizone models

- (1.2.1) The transport of a dilute contaminant between a number of zones of fixed volumes can be considered as an example of a compartmental system and we describe it by a system of linear ordinary differential equations,

$$\dot{\mathbf{x}} = \mathbf{Ax} + \mathbf{Bu} \quad (1)$$

where \mathbf{x} is the vector of the contaminant concentrations (mass / volume) in each zone of the system, \mathbf{A} is the matrix of interzone and exhaust flows normalised by zone volumes (defined below) and $\mathbf{B}\mathbf{u}$ describes the mapping of external concentrations and internal source terms onto the system. In the general case, $\mathbf{B} = \mathbf{V}^{-1}$ and $\mathbf{u} = \mathbf{Q}_{ext}\mathbf{x}_{ext} + \mathbf{u}_{int}$, where \mathbf{Q}_{ext} is a matrix of flow rates into the building, \mathbf{x}_{ext} is the vector of external contaminant concentrations at the entry points into the building and $\mathbf{u}_{int} \equiv \mathbf{u}_{int}(t)$ is the source term of the contaminant within the building.

(1.2.2) \mathbf{A} is defined as follows:

$$\mathbf{A} = \mathbf{V}^{-1}\mathbf{Q} \tag{2}$$

where \mathbf{V} is a diagonal matrix where $V_{i,i}$ is the volume of zone i in $[\text{m}^3]$ and $V_{i,j} = 0$ for $i \neq j$.

$$\mathbf{Q} = \begin{bmatrix} Q_{1,1} & Q_{1,2} & \cdots & Q_{1,n} \\ Q_{2,1} & Q_{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & Q_{n-1,n} \\ Q_{n,1} & \cdots & Q_{n,n-1} & Q_{n,n} \end{bmatrix} \tag{3}$$

where $Q_{i,j}$ is the flow into zone i from zone j when $i \neq j$ and $Q_{j,j} = (-\sum_{i=1}^n Q_{i,j} - Q_{0,j})$ is the flow out of zone j , where $Q_{0,j}$ is the flow of air out of the system from zone j . Note that i and j take values from 1 to n and the index 0 represents the exterior to the building. All flow rates have units of $[\text{m}^3 \text{ s}^{-1}]$.

Figure 1 shows the general case of a multizone system with labelled volumes and flow rates.

(1.2.3) Note that since \mathbf{A} is diagonally dominant, we will have negative or zero eigenvalues in all systems.

(1.2.4) A complete description is given in reference [1]. In reality there will be no control over the external concentration or internal source terms. However, it may be possible to control the volumetric flow into the building. Since this is incorporated within the term \mathbf{u} some control over the input may be achieved, although it is likely that this would also change \mathbf{A} . One related application is the case where an airborne decontaminant is introduced into the building to remediate contaminated building surfaces. In that case one problem of interest would be how to control \mathbf{u} to achieve a certain \mathbf{x} .

(1.2.5) In standard multizone models this system of equations is integrated numerically to give concentrations based on the initial conditions. For a single scenario such a calculation is typically fast to carry out. However for some applications, such as the optimisation of detector placement or

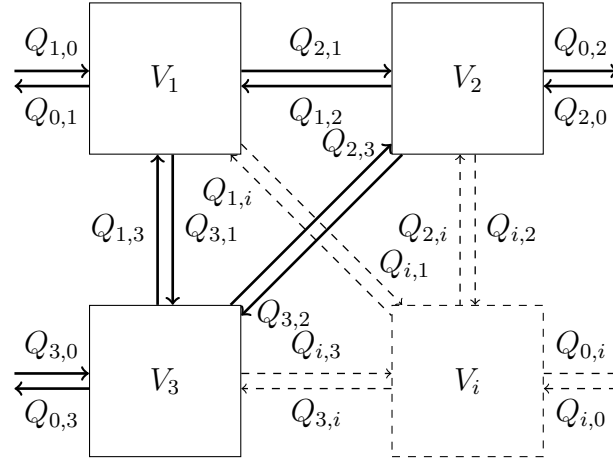


Figure 1: Ventilated and connected multizone system

the interpretation of sensor data, many thousands of individual simulations may need to be carried out. For large numbers of these repeated cases \mathbf{A} will be constant, with only variation in the initial concentration or source terms \mathbf{u} . In some cases there may be large differences in zone volumes, or secondary effects which introduce a wide range of timescales and require small timesteps over long periods to solve the stiff equations.

1.3 Analytical solutions

(1.3.1) The solution to (1) can be written as follows

$$\mathbf{x}(t) = e^{\mathbf{A}(t)}\mathbf{x}(0) + \int_0^t e^{\mathbf{A}(t-\mu)}\mathbf{B}(\mu)\mathbf{u}(\mu)d\mu \quad (4)$$

where t is the current time and μ is a variable of integration.

(1.3.2) In the case where the state transition matrix \mathbf{A} is diagonalisable the exponential term can be expressed as

$$e^{\mathbf{A}t} = \mathbf{S}e^{\mathbf{\Lambda}t}\mathbf{S}^{-1} \quad (5)$$

where \mathbf{S} is the matrix of eigenvectors and $\mathbf{\Lambda}$ is a matrix with the eigenvalues arranged on the diagonal.

(1.3.3) This explicit solution for the contaminant concentrations as well as the exposure (the integral of the concentration x for any zone) in the form of a sum of exponentials is particularly useful as it allows us to calculate the concentration at any future time (for a constant \mathbf{A}) without iteration. When screening a large number of scenarios this direct calculation can save time.

(1.3.4) Furthermore, in the special case where \mathbf{u} is constant in time, we have the following analytical solution.

$$\mathbf{x}(t) = \mathbf{S}e^{\mathbf{A}(t-\tau)}\mathbf{S}^{-1}\mathbf{x}(\tau) - \mathbf{S}\mathbf{A}^{-1}(\mathbf{I} - e^{\mathbf{A}(t-\tau)})\mathbf{S}^{-1}\mathbf{B}\mathbf{u} \quad (6)$$

(1.3.5) The eigenvectors and eigenvalues provide insight into the behaviour of the system such as the late phase decay rate and concentration ratio. The eigenvalue of the smallest magnitude controls the final decay rate of the system. The dependence of this eigenvalue on system properties is of interest. Complex eigenvalues appear to arise from recirculating flow paths and result in damped oscillations.

(1.3.6) However, it was recognised by DSTL that \mathbf{A} may not always be diagonalisable. For example, a collection of zones with identical volumes in series and with the same flow through each of them leads to a non-diagonalisable case. This is an important case, since a series of such zones can be used in the CONTAM multizone software to represent a length of duct work to improve the time resolution of the contaminant transport.

1.4 Questions

(1.4.1) These are the questions posed to the Study Group by DSTL:

- (a) Are there other cases where \mathbf{A} is not diagonalisable? Is it possible to characterise the types of systems that are diagonalisable and non-diagonalisable?
- (b) For the diagonalisable case is it possible to bound the values of the smallest magnitude eigenvalue based on the properties of the system matrix \mathbf{A} or related system properties such as the total exhaust flow and volume? We have seen examples where this value is both larger and smaller than the system flushing rate (the air change rate).
- (c) For the general case where \mathbf{A} is not diagonalisable it seems that it is possible to construct an analytical solution to state transition matrix $e^{\mathbf{A}t}$ using the Jordan canonical form. Is it possible to derive a useful analytical form for the concentration solution for any matrix \mathbf{A} ? Many authors warn against the use of the Jordan form for practical calculations - does this rule out this approach for the solution for any \mathbf{A} ? For the simpler cases is there a physical interpretation?
- (d) Is it possible to solve the inverse problem? In other words, if we have measurements of concentration (x_i) in one or more zones, can we establish any information about the source terms or external concentrations \mathbf{u} ?
- (e) What are the practical limits to using solutions of the form (5) for large systems? We have encountered numerical problems in calculating the concentration at short times when compared to iterative

schemes, for systems with around 300 zones for large condition numbers. Are there alternative approaches that can avoid these problems?

- (f) We have explored some results for a nested two-zone case where it can be shown that the exposure in each zone is the same as the external exposure. Can this be extended to more zones? Are there other systems which lead to special case solutions?
- (g) Is it possible to write down solutions for cases when the input function \mathbf{u} is not constant (e.g. periodic, linear ramp etc.)?
- (h) Can we calculate the total exposure, $\int_0^\infty x(t)dt$?
- (i) Can we calculate the toxic load, $\int_0^\infty x^p(t)dt$ where $p > 1$?
- (j) Can we find the maximum of $x(t)$?

2 Work

2.1 Diagonalisation

- (2.1.1) From a linear maths point of view, there are ways of finding out if a matrix A is diagonalisable or not. The minimal polynomial of A , $m(x)$, is defined as the polynomial of least degree that satisfies $m(A) = 0$. It can be shown that A is diagonalisable if and only if $m(x)$ is decomposable into distinct linear factors. To find the minimal polynomial of A , you start with the characteristic polynomial, $\chi(x) = \det(A - xI)$ which satisfies by definition, $\chi(A) = 0$. The minimal polynomial is either the characteristic polynomial or another polynomial that includes some of the factors from the characteristic polynomial.
- (2.1.2) What sort of models in the form lead to the case when A is not diagonalisable? It was recognised that A is not diagonalisable if we have zone layouts that introduce wave-like elements to the solution of x . Indeed, if the building contains a long air duct, or if there is a chain of identical rooms with the same air flow leads to a situation where A has repeated eigenvalues and in these cases we would have to find an alternative method to find e^{At} . Appendix A.2 works through the solution to a single duct case.
- (2.1.3) A further complication can arise when we model fast flowing air such as may be found in an air handling system. The small volume with a high flow rate compared to the large volumes and low flow rates inside the building will create a system with large and smaller eigenvalues which will lead to stiff systems for large multizone models. To treat the specific case of the time lag in air handling systems an extension to the multizone model described in Section 3.1 may be worth developing.

2.2 Alternative methods of calculating the exponential of a matrix

(2.2.1) The paper by Moler and Van Loan [2] gives a very good summary of methods for calculating the exponential of a matrix. They suggest methods which are likely to be most efficient for problems involving large matrices and repeated evaluation of e^{At} . The method investigated by the Study Group involves the Schur decomposition and the Cayley-Hamilton Theorem.

(2.2.2) The Schur decomposition turns a square matrix into an upper triangular matrix. Further transformations (laid out in [5]) turn the matrix into a block triangular structure.

$$\mathbf{A} = \mathbf{S} \begin{pmatrix} \mathbf{T}_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{T}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \dots & \mathbf{0} & \mathbf{T}_m \end{pmatrix} \mathbf{S}^{-1}, \quad (7)$$

where \mathbf{T}_i is triangular with eigenvalues close to each other and \mathbf{S} is well conditioned.

(2.2.3) If the triangular blocks \mathbf{T}_i are small, we may use the Caley-Hamilton theorem. Consider a $k \times k$ matrix A and the characteristic polynomial for tA :

$$\Delta_t(s) = \det(t\mathbf{A} - s\mathbf{I}). \quad (8)$$

We can write

$$\exp(s) = \Delta_t(s) Q_t(s) + R_t(s), \quad (9)$$

where Q_t is an analytic function and the remainder R_t is a polynomial of degree $k - 1$,

$$R_t(s) = \sum_{\ell=0}^{k-1} r_\ell(t) s^\ell. \quad (10)$$

(2.2.4) Caley-Hamilton's theorem that states that $\Delta_t(t\mathbf{A}) = \mathbf{0}$, implies that

$$\exp(t\mathbf{A}) = \Delta_t(t\mathbf{A}) Q_t(t\mathbf{A}) + R_t(t\mathbf{A}) = R_t(t\mathbf{A}) = \sum_{\ell=0}^{k-1} r_\ell(t) t^\ell \mathbf{A}^\ell. \quad (11)$$

(2.2.5) We want to determine the coefficients $r_\ell(t)$, especially in the case of nearly defective eigenvalues. We consider the case of a triangular matrix

$$\mathbf{T} = \lambda\mathbf{I} + \mathbf{E}, \quad (12)$$

where \mathbf{E} is triangular with small values in the diagonal. Since $\lambda\mathbf{I}$ and \mathbf{E} commute we have

$$\exp(t\mathbf{T}) = \exp(t\lambda\mathbf{I}) \exp(t\mathbf{E}) = \exp(t\lambda) \exp(t\mathbf{E}), \quad (13)$$

which is enough to determine $\exp(t\mathbf{E})$.

(2.2.6) First we do the simplest possible case, namely a 2×2 matrix:

$$\mathbf{T} = \begin{pmatrix} \lambda + \epsilon & c \\ 0 & \lambda - \epsilon \end{pmatrix} = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} + \begin{pmatrix} \epsilon & c \\ 0 & -\epsilon \end{pmatrix} \quad \text{and} \quad \mathbf{E} = \begin{pmatrix} \epsilon & c \\ 0 & -\epsilon \end{pmatrix} \quad (14)$$

(2.2.7) As $\Delta_t(t(\lambda \pm \epsilon)) = 0$, we have

$$\exp(-t\epsilon) = R_t(-t\epsilon) = r_0(t) - r_1(t)t\epsilon, \quad (15)$$

$$\exp(t\epsilon) = R_t(t\epsilon) = r_0(t) + r_1(t)t\epsilon. \quad (16)$$

(2.2.8) This gives us the linear equations

$$\begin{pmatrix} 1 & -t\epsilon \\ 1 & t\epsilon \end{pmatrix} \begin{pmatrix} r_0(t) \\ r_1(t) \end{pmatrix} = \begin{pmatrix} \exp(-t\epsilon) \\ \exp(t\epsilon) \end{pmatrix} \quad (17)$$

with the solution

$$\begin{pmatrix} r_0(t) \\ r_1(t) \end{pmatrix} = \frac{1}{2t\epsilon} \begin{pmatrix} t\epsilon & -t\epsilon \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \exp(-t\epsilon) \\ \exp(t\epsilon) \end{pmatrix}. \quad (18)$$

(2.2.9) That is,

$$r_0(t) = \frac{t\epsilon \exp(-t\epsilon) + t\epsilon \exp(t\epsilon)}{2t\epsilon} = \cosh(t\epsilon), \quad (19)$$

$$r_1(t) = \frac{\exp(t\epsilon) - \exp(-t\epsilon)}{2t\epsilon} = \frac{\sinh(t\epsilon)}{t\epsilon}. \quad (20)$$

Thus

$$\exp(t\mathbf{E}) = \cosh(t\epsilon)\mathbf{I} + \frac{\sinh(t\epsilon)}{t\epsilon}t\mathbf{E} \quad (21)$$

and, using that $\mathbf{T} = \lambda\mathbf{I} + \mathbf{E}$

$$\exp(t\mathbf{T}) = \exp(t\lambda) \left(\cosh(t\epsilon)\mathbf{I} + \frac{\sinh(t\epsilon)}{t\epsilon}t\mathbf{E} \right). \quad (22)$$

(2.2.10) When $\epsilon \rightarrow 0$ we obtain

$$\lim_{\epsilon \rightarrow 0} \exp(t\mathbf{T}) = \exp(t\lambda) (\mathbf{I} + t\mathbf{E}) = \exp(t\lambda) \begin{pmatrix} 1 & t\epsilon \\ 0 & 1 \end{pmatrix} = \exp(\lim_{\epsilon \rightarrow 0} t\mathbf{T}). \quad (23)$$

(2.2.11) Here we have a 3×3 example matrix

$$\mathbf{T} = \begin{pmatrix} \lambda + 2\epsilon & c_{12} & c_{13} \\ 0 & \lambda - \epsilon + \delta & c_{23} \\ 0 & 0 & \lambda - \epsilon - \delta \end{pmatrix} = \begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} + \begin{pmatrix} 2\epsilon & c_{12} & c_{13} \\ 0 & -\epsilon + \delta & c_{23} \\ 0 & 0 & -\epsilon - \delta \end{pmatrix}. \quad (24)$$

(2.2.12) We now have the linear equations

$$\begin{pmatrix} 1 & t(\lambda + 2\epsilon) & t^2(\lambda + 2\epsilon)^2 \\ 1 & t(\lambda - \epsilon + \delta) & t^2(\lambda - \epsilon + \delta)^2 \\ 1 & t(\lambda - \epsilon - \delta) & t^2(\lambda - \epsilon - \delta)^2 \end{pmatrix} \begin{pmatrix} r_0(t) \\ r_1(t) \\ r_2(t) \end{pmatrix} = \exp(t\lambda) \begin{pmatrix} \exp(2t\epsilon) \\ \exp(-t(\epsilon - \delta)) \\ \exp(-t(\epsilon + \delta)) \end{pmatrix}. \quad (25)$$

2.3 Total Exposure

(2.3.1) Recall our linear system,

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}(t), \quad (26)$$

where

$$\mathbf{A} = \mathbf{V}^{-1}\mathbf{Q}, \quad \mathbf{B} = \mathbf{V}^{-1}, \quad \mathbf{u} = \mathbf{Q}_{ext}\mathbf{x}_{ext} + \mathbf{u}_{int}. \quad (27)$$

When there is a single external concentration that impacts on the building \mathbf{x}_{ext} is a scalar and \mathbf{Q}_{ext} becomes a column vector which satisfies the following:

$$\mathbf{Q} \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} + \mathbf{Q}_{ext} = \mathbf{0}. \quad (28)$$

(2.3.2) We can see that

$$-\mathbf{A}^{-1}\mathbf{B} = -\mathbf{Q}^{-1} \quad (29)$$

and

$$-\mathbf{Q}^{-1}\mathbf{Q}_{ext} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}. \quad (30)$$

(2.3.3) The solution with initial condition $\mathbf{x}(0) = \mathbf{x}_0$ is

$$\mathbf{x}(t) = e^{\mathbf{A}t} \mathbf{x}_0 + e^{\mathbf{A}t} \int_0^t e^{-\mathbf{A}\tau} \mathbf{B} \mathbf{u}(\tau) d\tau \quad (31)$$

and we have

$$\int e^{\mathbf{A}t} dt = \mathbf{A}^{-1} e^{\mathbf{A}t}. \quad (32)$$

(2.3.4) As all the eigenvalues of \mathbf{A} are strictly negative, $\lim_{t \rightarrow \infty} e^{t\mathbf{A}} = 0$ implies that

$$\int_t^\infty e^{\mathbf{A}t} dt = -\mathbf{A}^{-1} e^{\mathbf{A}t}. \quad (33)$$

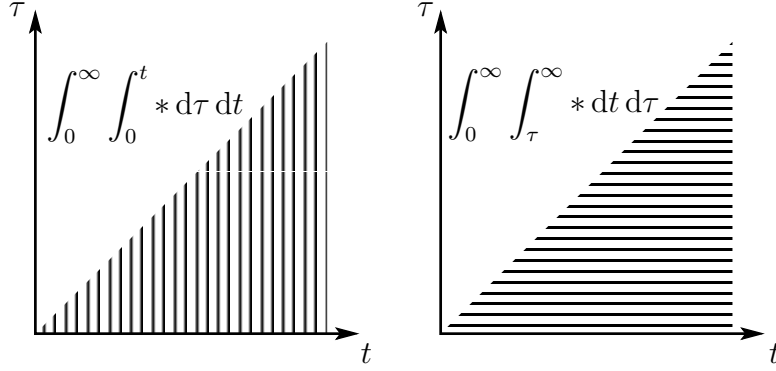


Figure 2: The two integration orders

Therefore

$$\int_0^\infty \mathbf{x}(t) dt = \int_0^\infty e^{\mathbf{A}t} \mathbf{x}_0 dt + \int_0^\infty e^{\mathbf{A}t} \int_0^t e^{-\mathbf{A}\tau} \mathbf{B} \mathbf{u}(\tau) d\tau dt.$$

We switch the integration order in the double integral, see Figure 2, and get

$$\begin{aligned} &= -\mathbf{A}^{-1} \mathbf{x}_0 + \int_0^\infty \left(\int_\tau^\infty e^{\mathbf{A}t} dt \right) e^{-\mathbf{A}\tau} \mathbf{B} \mathbf{u}(\tau) d\tau \\ &= -\mathbf{A}^{-1} \mathbf{x}_0 + \int_0^\infty -\mathbf{A}^{-1} e^{\mathbf{A}\tau} e^{-\mathbf{A}\tau} \mathbf{B} \mathbf{u}(\tau) d\tau \\ &= -\mathbf{A}^{-1} \mathbf{x}_0 - \mathbf{A}^{-1} \mathbf{B} \int_0^\infty \mathbf{u}(\tau) d\tau \\ &= -\mathbf{A}^{-1} \mathbf{x}_0 + \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \int_0^\infty \mathbf{x}_{ext}(\tau) d\tau - \mathbf{Q}^{-1} \int_0^\infty \begin{pmatrix} u_{int_1}(\tau) \\ \vdots \\ u_{int_n}(\tau) \end{pmatrix} d\tau. \end{aligned} \quad (34)$$

2.4 Inverse problem - quadratic minimisation

(2.4.1) Consider the equations presented in Section 2.3.

(2.4.2) We now assume we have a series of observations/measurements y_i and want to determine a load $\mathbf{u}(t)$ that explains the observations. Observation i is the concentration in room k_i at time t_i , i.e., $y_i = x_{k_i}(t_i)$. So we need to calculate $\mathbf{x}(t_i)$ in order to check our guess $\mathbf{u}(t)$. We consider the case where $\mathbf{x}_0 = \mathbf{0}$ and $\mathbf{u} = \phi_j(t)\mathbf{e}_\ell$, \mathbf{e}_ℓ is the ℓ th standard basis vector, and

$$\phi_j(t) = \begin{cases} 1 & t \in [(j-1)\Delta, j\Delta], \\ 0 & t \notin [(j-1)\Delta, j\Delta]. \end{cases} \quad (35)$$

(2.4.3) We can now perform the integration in (4) and obtain

$$\mathbf{x}(i\Delta) = \mathbf{0}, \quad i < j, \quad (36)$$

$$\mathbf{x}(i\Delta) = (e^{\mathbf{A}\Delta} - \mathbf{I})\mathbf{A}^{-1}\mathbf{B}\mathbf{e}_\ell, \quad i = j, \quad (37)$$

$$\mathbf{x}(i\Delta) = e^{\mathbf{A}(i-j)\Delta}(e^{\mathbf{A}\Delta} - \mathbf{I})\mathbf{A}^{-1}\mathbf{B}\mathbf{e}_\ell, \quad i > j. \quad (38)$$

(2.4.4) We next consider the case $\mathbf{u} = \sum_{j=1}^k v_j \phi_j(t)\mathbf{e}_\ell$ and obtain

$$\begin{pmatrix} \mathbf{x}(\Delta) \\ \vdots \\ \mathbf{x}(k\Delta) \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{11}\mathbf{e}_\ell & \mathbf{C}_{12}\mathbf{e}_\ell & \dots & \mathbf{C}_{1k}\mathbf{e}_\ell \\ \mathbf{0} & \mathbf{C}_{22}\mathbf{e}_\ell & \dots & \mathbf{C}_{2k}\mathbf{e}_\ell \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \dots & \mathbf{0} & \mathbf{C}_{kk}\mathbf{e}_\ell \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_k \end{pmatrix} \quad (39)$$

where \mathbf{C}_{ij} is a $n \times n$ matrix

$$\mathbf{C}_{ij} = e^{\mathbf{A}(i-j)\Delta}(e^{\mathbf{A}\Delta} - \mathbf{I})\mathbf{A}^{-1}\mathbf{B}. \quad (40)$$

(2.4.5) Observe that $\mathbf{C}_{ij}\mathbf{e}_\ell$ is simply the ℓ th column in \mathbf{C}_{ij} and that we can obtain the matrices \mathbf{C}_{1j} by recursion

$$\mathbf{C}_{1,j+1} = e^{\mathbf{A}\Delta}\mathbf{C}_{1j}. \quad (41)$$

(2.4.6) It is worth noting that the eigenvalues for \mathbf{A} all lie in the left half plane so the exponential $e^{\mathbf{A}\Delta}$ has norm less than 1. That in turn implies that we do not amplify errors by the multiplication in (41). Let Π be the projection on to the observed rooms, i.e., Π is obtained from the unit matrix \mathbf{I} by removing the rows corresponding to the rooms without sensors. We then

have the following equation to determine the load $\mathbf{u} = \sum_{j=1}^k v_j \phi_j(t) \mathbf{e}_\ell$.

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix} = \begin{pmatrix} \Pi \mathbf{C}_{11} \mathbf{e}_\ell & \Pi \mathbf{C}_{12} \mathbf{e}_\ell & \dots & \Pi \mathbf{C}_{1k} \mathbf{e}_\ell \\ \mathbf{0} & \Pi \mathbf{C}_{22} \mathbf{e}_\ell & \dots & \Pi \mathbf{C}_{2k} \mathbf{e}_\ell \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \dots & \mathbf{0} & \Pi \mathbf{C}_{kk} \mathbf{e}_\ell \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_k \end{pmatrix} = \mathbf{C}_\ell \mathbf{v}. \quad (42)$$

(2.4.7) Observe that we can obtain \mathbf{C}_ℓ from the large matrix

$$\begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} & \dots & \mathbf{C}_{1k} \\ \mathbf{0} & \mathbf{C}_{22} & \dots & \mathbf{C}_{2k} \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \dots & \mathbf{0} & \mathbf{C}_{kk} \end{pmatrix} \quad (43)$$

by deleting some rows and columns.

(2.4.8) The least square solution to (42) is

$$\mathbf{v}_\ell = (\mathbf{C}_\ell^T \mathbf{C}_\ell)^{-1} \mathbf{C}_\ell^T \mathbf{y}, \quad (44)$$

and the error is

$$\epsilon_\ell = \|\mathbf{y} - \mathbf{C}_\ell \mathbf{v}_\ell\|. \quad (45)$$

(2.4.9) We have an error ϵ_ℓ for each $\ell = 0, \dots, n$ and the ℓ which gives the smallest error is our prediction for where the contaminant originates.

(2.4.10) We consider the situation where we for each time step $i\Delta$ have a set of measurements $\mathbf{y}_i = \Pi \mathbf{x}(i\Delta)$. We can now solve the least square problems (42) for $\ell = 0, \dots, n$ in each time step and thereby get both a prediction for origin of the contaminant, ℓ , and for the level of the contaminant, \mathbf{v}_ℓ .

(2.4.11) We can only have positive terms in $\mathbf{u}(t)$ so we should solve the following constrained optimisation problem.

$$\underset{v_i}{\text{minimise}} \|\mathbf{y} - \mathbf{C}_\ell \mathbf{v}_\ell\|^2 \quad (46)$$

such that

$$v_i \geq 0, \quad i = 1, \dots, k. \quad (47)$$

This is a standard problem, a quadratic functional with linear constraints, and is not much harder to solve than the unconstrained version.

2.5 Inverse problem: Control theory method

- (2.5.1) This is an alternative method to solving the inverse problem using a control theory result and data assimilation. Given $\mathbf{x}(T)$ at time $T > 0$, can we find $\mathbf{u}(t)$? The controllability Gramian is given by:

$$Q_T = \int_0^T e^{A\tau} B B^* e^{A^*\tau} d\tau \quad (48)$$

- (2.5.2) Given $\mathbf{x}(T)$, $T > 0$ and $\mathbf{x}(t_\delta)$, if $\det Q_T \neq 0$, then we can steer $\mathbf{x}(t_\delta)$ to $\mathbf{x}(T)$ in time T using the control

$$\mathbf{u}(t) = B^* e^{A^*(T-t)} Q_T^{-1} (\mathbf{x}(T) - e^{AT} \mathbf{x}(0)) \quad t \in [0, T] \quad (49)$$

and $Q_T = \int_0^T e^{A^*t} B^* B e^{At} dt$ is defined as the *Controllability Gramian* and $\cdot^* = \cdot^T$ [8].

The control, (49) is not necessarily unique in its ability to steer \mathbf{x}^0 to \mathbf{x}^1 in time $T > 0$. It minimises the energy $\int \|\mathbf{u}(t)\| dt$, over all possible $\mathbf{u}(t)$ that steer $\mathbf{x}(t)$ from \mathbf{x}^0 to \mathbf{x}^1 in time $T > 0$. Identifying $\tilde{\mathbf{u}}(t)$ would provide a possible control for determining the future progression of the contaminant throughout the building and also allow the identification of an interior or an exterior source for the contaminant.

- (2.5.3) In order for the control $\tilde{\mathbf{u}}(t)$ to be identified, both \mathbf{x}^0 and \mathbf{x}^1 need to have contaminant readings for every room in the building. However, due to practical constraints, detectors may not be placed in every room in the building. This means that \mathbf{x}^0 and \mathbf{x}^1 are incomplete data sets. This means that the missing entries need to be estimated in some way to allow $\tilde{\mathbf{u}}(t)$ to be identified. *Data assimilation* is a process which could be used to estimate the missing values.
- (2.5.4) Data assimilation requires a model for the physical process and a set of observations of the true physical system. The aim of the process is to find the least squares solution between the observations and the results of the model, given some initial estimate for the initial conditions. The result of the process provides an initial condition for the model which, when run, will produce a simulation of the model which will minimise the square error between the observations and the previous results of the model created using the estimated initial conditions.
- (2.5.5) Let time $t = 0$ denote the time the contaminant is first detected and let time $T > 0$ be another time in the future where contaminant levels are also known. Also, assume $\det Q_T \neq 0$ and that there are $n \in \mathbb{N}$ rooms in the building. The model for this problem is given by (4), where the control is given by (49), with $\mathbf{x}^0 = \mathbf{x}(0) \in \mathbb{R}^n$ and $\mathbf{x}^1 = \mathbf{x}(T) \in \mathbb{R}^n$. The model will provide complete sets of data to allow the identification of $\tilde{\mathbf{u}}(t) \in \mathbb{R}^n$.

- (2.5.6) Let $\mathbf{y} : \mathbb{R} \rightarrow \mathbb{R}^m$, $t \mapsto \mathbf{y}(t)$ denote an observation of the contaminant levels in the building at time t , where the i th element represents the concentration of the contaminant in the i th room at time t . This means that there are $m \in \mathbb{N}$ rooms with detectors in. Let $\mathbf{y}_i \in \mathbb{R}^m$ denote the i th observation of the contaminant levels in the building, where $\mathbf{y}_0 = \mathbf{y}(0)$ and $\mathbf{y}_N = \mathbf{y}(T)$. Also, denote $\mathbf{x}_i \in \mathbb{R}^n$ as the corresponding state of the model at the time of the i th observation. This means that $\mathbf{x}_0 = \mathbf{x}(0)$ and $\mathbf{x}_N = \mathbf{x}(T)$.
- (2.5.7) In order to generate the model states for comparison with the observations, estimates for $\mathbf{x}(0)$ and $\mathbf{x}(T)$ need to be made in order to simulate $\tilde{\mathbf{u}}(t)$, so $\mathbf{x}(t)$ can be simulated. Let $\mathbf{x}_b \in \mathbb{R}^n$ denote an estimate for $\mathbf{x}(0)$ and $\mathbf{x}_e \in \mathbb{R}^n$ denote an estimate for $\mathbf{x}(T)$. These estimates can be made based upon the observations at these points in time, $\mathbf{y}(0)$ and $\mathbf{y}(T)$ respectively.
- (2.5.8) As the observations \mathbf{y}_i are incomplete sets of data, in order to allow for the comparison of \mathbf{y}_i with \mathbf{x}_i , the matrix $H_i \in \mathbb{R}^{m \times n}$ is required to select only the elements of \mathbf{x}_i that are present in \mathbf{y}_i . This means that H_i is linear and due to the assumption that each detector remains in the same position for each reading, $H_i = H \forall i$ where H is constant. In control theory, H would normally be denoted by C .
- (2.5.9) Data assimilation also requires knowledge on the accuracy of the observations, the initial state estimate, $\mathbf{x}_b \in \mathbb{R}^n$ and the final state estimate, $\mathbf{x}_e \in \mathbb{R}^n$. The accuracy of the i th observation is represented by the i th covariance matrix $R_i \in \mathbb{R}^{m \times m}$. As the detectors used to take each observation remain the same over time, $R_i = R \forall i$, a constant covariance matrix. $G \in \mathbb{R}^{n \times n}$ (usually denoted by B) and $E \in \mathbb{R}^{n \times n}$ represent the covariance matrices for \mathbf{x}_b and \mathbf{x}_e respectively. The j, k th element of these matrices is determined by the covariance of the j th and k th elements of the vectors they correspond to. For example, $(R)_{j,k} = cov((\mathbf{y}_i)_j, (\mathbf{y}_i)_k) \forall i$. It is assumed though that each covariance matrix is a diagonal matrix by assuming that the cross-covariances are always zero. For example $(R)_{j,k} = cov((\mathbf{y}_i)_j, (\mathbf{y}_i)_k) = 0$ for $j \neq k$. More information on the definitions of the different variables and the ideas and derivation behind data assimilation can be found in [9].
- (2.5.10) The least squares solution for \mathbf{x}_b and \mathbf{x}_e are achieved through data assimilation by minimising the following cost functions with respect to $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{z} \in \mathbb{R}^n$ respectively

$$J_1(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_b)^T G^{-1} (\mathbf{x} - \mathbf{x}_b) + \sum_{i=0}^N (\mathbf{y}_i - H\mathbf{x}_i)^T R^{-1} (\mathbf{y}_i - H\mathbf{x}_i), \quad (50)$$

$$J_2(\mathbf{z}) = (\mathbf{z} - \mathbf{x}_e)^T E^{-1} (\mathbf{z} - \mathbf{x}_e) + \sum_{i=0}^N (\mathbf{y}_i - H\mathbf{z}_i)^T R^{-1} (\mathbf{y}_{N+1-i} - H\mathbf{z}_i), \quad (51)$$

where $\mathbf{z}_i = \mathbf{x}_{N+1-i}$.

- (2.5.11) These both need to be minimised simultaneously to find the best solutions. (50) and (51) are minimised when $\nabla J_1(\mathbf{x}) = 0$ and $\nabla J_2(\mathbf{z}) = 0$, where in this case

$$\nabla J_1(\mathbf{x}) = 2G^{-1}(\mathbf{x} - \mathbf{x}_b) + 2 \sum_{i=0}^N R^{-1}(\mathbf{y}_i - H\mathbf{x}_i), \quad (52)$$

$$\nabla J_2(\mathbf{z}) = 2E^{-1}(\mathbf{z} - \mathbf{x}_e) + 2 \sum_{i=0}^N R^{-1}(\mathbf{y}_{N+1-i} - H\mathbf{z}_i). \quad (53)$$

- (2.5.12) Data assimilation is usually used to find an improved estimate for the initial condition for the model of the system which best fits the observations of the true system. This is what minimising (50) aims to achieve for $\mathbf{x}(0)$. However, we wish to also find a better estimate for $\mathbf{x}(T)$ as well. Due to the control function $\tilde{\mathbf{u}}(t)$, $\mathbf{x}(t)$ is steered from the current estimate for $\mathbf{x}(0)$ to the current estimate for $\mathbf{x}(T)$. This means that any results from the model start and end with these estimates respectively. This means that we can view the results in reverse order as results from the model where the current estimate for $\mathbf{x}(T)$ was the initial condition. This way, the same form of data assimilation can be applied to find an improved estimate for $\mathbf{x}(T)$ as for finding an improved estimate for $\mathbf{x}(0)$.

- (2.5.13) The algorithm for minimising (50) and (51) would begin by initially choosing $\mathbf{x} = \mathbf{x}_b$ for minimising (50) and $\mathbf{z} = \mathbf{x}_e$ for minimising (51). The Newton method is a possible method which could be used to identify \mathbf{x} and \mathbf{z} that satisfy (52) and (53) respectively. For example, denote the current best estimate for $\mathbf{x}(0)$ by $\mathbf{x}^{(k)}$ and the next best estimate by $\mathbf{x}^{(k+1)}$ and the current best guess for $\mathbf{x}(T)$ by $\mathbf{z}^{(k)}$ and the next best estimate by $\mathbf{z}^{(k+1)}$. Then

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - [\nabla J_1(\mathbf{x}^{(k)})]_{\mathbf{x}} \nabla J_1(\mathbf{x}^{(k)}), \quad (54)$$

$$\mathbf{z}^{(k+1)} = \mathbf{z}^{(k)} - [\nabla J_2(\mathbf{z}^{(k)})]_{\mathbf{z}} \nabla J_2(\mathbf{z}^{(k)}). \quad (55)$$

- (2.5.14) Algorithm

- (a) Estimate $\mathbf{x}(0)$ and $\mathbf{x}(T)$ based on observations $\mathbf{y}(0)$ and $\mathbf{y}(T)$ respectively and denote these \mathbf{x}_b and \mathbf{x}_e respectively.
- (b) Set $\mathbf{x}^{(k)} = \mathbf{x}_b$ and $\mathbf{z}^{(k)} = \mathbf{x}_e$ for $k = 0$.
- (c) Calculate $\tilde{\mathbf{u}}(t)$ steering from $\mathbf{x}^{(k)}$ to $\mathbf{z}^{(k)}$ in time $T > 0$, using (49). Check that $\det Q_T \neq 0$.
- (d) Calculate $\mathbf{x}(t)$ using (4) at the time of each observation \mathbf{y}_i using $\tilde{\mathbf{u}}(t)$ found in the previous step.
- (e) Minimise $J_1(\mathbf{x}^{(k)})$ to find $\mathbf{x}^{(k+1)}$.

- (f) Calculate $\nabla J_1(\mathbf{x}^{(k+1)})$ and $\nabla J_2(\mathbf{z}^{(k)})$ to see if they've been minimised. If not, continue. Otherwise, stop.
- (g) Calculate $\tilde{\mathbf{u}}(t)$ steering from $\mathbf{x}^{(k+1)}$ to $\mathbf{z}^{(k)}$ in time $T > 0$, using (49). Check that $\det Q_T \neq 0$.
- (h) Calculate $\mathbf{x}(t)$ at the time of each observation \mathbf{y}_i using $\tilde{\mathbf{u}}(t)$ found in the previous step.
- (i) Minimise $J_2(\mathbf{z}^{(k)})$ to find $\mathbf{z}^{(k+1)}$.
- (j) Calculate $\nabla J_1(\mathbf{x}^{(k+1)})$ and $\nabla J_2(\mathbf{z}^{(k+1)})$ to see if they've been minimised. If not, continue. Otherwise stop.
- (k) Add 1 to k and repeat steps 3 to 10 until $J_1(\mathbf{x})$ and $J_2(\mathbf{z})$ are minimised for some \mathbf{x} and \mathbf{z} .

This would find a better estimate for \mathbf{x}_b and \mathbf{x}_e . These can then be used to create $\tilde{\mathbf{u}}(t)$. One disadvantage to this method is that there is no constraint on making each concentration of contaminant in the system positive. There is also a need to estimate covariance matrices and the initial states for the system.

- (2.5.15) The second part of the inverse problem involved identifying whether the contaminant originated from an interior or an exterior source. The control function was proposed to be constructed from the following function

$$\mathbf{u}(t) = Q_{ext}\mathbf{x}_{ext}(t) + \mathbf{u}_{int}(t). \quad (56)$$

The equation (4), together with (49), can be written using (56) as

$$\begin{aligned} \mathbf{x}(t) &= e^{At}\mathbf{x}_0 + e^{At} \int_0^t e^{-A\tau} B [Q_{ext}\mathbf{x}_{ext}(\tau) + \mathbf{u}_{int}(\tau)] d\tau, \\ &= e^{At}\mathbf{y}_0 + e^{At} \int_0^t e^{-A\tau} B Q_{ext}\mathbf{x}_{ext}(\tau) d\tau + e^{At}\mathbf{z}_0 + e^{At} \int_0^t e^{-A\tau} B \mathbf{u}_{int}(\tau) d\tau, \\ &= \mathbf{y}(t) + \mathbf{z}(t), \end{aligned}$$

where

$$\mathbf{y}(t) = e^{At}\mathbf{y}_0 + e^{At} \int_0^t e^{-A\tau} B Q_{ext}\mathbf{x}_{ext}(\tau) d\tau, \quad (57)$$

$$\mathbf{z}(t) = e^{At}\mathbf{z}_0 + e^{At} \int_0^t e^{-A\tau} B \mathbf{u}_{int}(\tau) d\tau. \quad (58)$$

- (2.5.16) The proportion of each element of $\mathbf{x}(t)$ assigned to each element of $\mathbf{y}(t)$ and $\mathbf{z}(t)$ would be fixed over time and be based on the probability of the contaminant in the room having an interior or an exterior source. Room i has a probability of $0 \leq \alpha_i \leq 1$ that any contaminant which began entering the building in this compartment was from an external source and a probability of $1 - \alpha_i$ of coming from an internal source. Hence

$$\begin{aligned} (\mathbf{y})_i(t) &= \alpha_i(\mathbf{x})_i(t), \\ (\mathbf{z})_i(t) &= (1 - \alpha_i)(\mathbf{x})_i(t). \end{aligned}$$

For example, suppose room j has no exterior flows, then $\alpha_j = 0$.

(2.5.17) If $\det Q_T \neq 0$, then possible control functions to steer (57) from $\mathbf{y}(0)$ to $\mathbf{y}(T)$ and to steer (58) from $\mathbf{z}(0)$ to $\mathbf{z}(T)$ in time $T > 0$ are given by

$$\tilde{\mathbf{x}}_{ext}(t) = (Q_{ext}B)^* e^{A^*(T-t)} Q_T^{-1} (\mathbf{y}(T) - e^{AT} \mathbf{y}(0)), \quad (59)$$

$$\tilde{\mathbf{u}}_{int}(t) = B^* e^{A^*(T-t)} Q_T^{-1} (\mathbf{z}(T) - e^{AT} \mathbf{z}(0)), \quad (60)$$

such that $\tilde{\mathbf{u}}(t) = Q_{ext} \tilde{\mathbf{x}}_{ext}(t) + \tilde{\mathbf{u}}_{int}(t)$ where $\tilde{\mathbf{u}}(t)$ is a possible control that steers (4) from $\mathbf{x}(0)$ to $\mathbf{x}(T)$.

2.6 Transient growth

(2.6.1) We can find upper and lower bounds for the maximum of $x(t)$ for a given u . For some time t , the solution for $t > T$,

$$x(t) = e^{At} x(0) + e^{At} \int_0^T e^{-A\mu} B(\mu) u(\mu) d\mu \quad (61)$$

$$= e^{At} y. \quad (62)$$

(2.6.2) Define the following

$$\|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|} \quad (63)$$

and

$$G(t) = \sup_{x(0) \neq 0} \frac{\|x(t)\|}{\|x(0)\|} = \|e^{At}\|. \quad (64)$$

(2.6.3) Suppose A is diagonalisable, with eigenvalues $\lambda_1, \dots, \lambda_n$ where λ_1 is the eigenvalue with the smallest magnitude and λ_n is the eigenvalue with the largest magnitude. Note that $Re(\lambda_1)$ is the spectral abscissa $\alpha(\mathbf{A})$ since all eigenvalues are negative. Then $\exists F$ s.t. $A = F\Lambda F^{-1}$, where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$. Let v_j be the eigenvector associated with the j -th eigenvalue. Then

$$e^{At} v_j = e^{\lambda_j t} v_j. \quad (65)$$

Note that

$$\frac{\|e^{At} v_j\|}{\|v_j\|} = |e^{\lambda_j t}| = e^{Re(\lambda_j) t} \quad (66)$$

and so we have the following lower bound, $G(t) \geq e^{\alpha(\mathbf{A})t}$, [7].

(2.6.4) For the upper bound [7]

$$\|e^{At}\| = \|e^{F\Lambda F^{-1}t}\| = \|F e^{\Lambda t} F^{-1}\| \tag{67}$$

$$= \|F\| \|F^{-1}\| \|e^{\Lambda t}\| \tag{68}$$

$$\leq \|F\| \|F^{-1}\| e^{\alpha(\mathbf{A})t}. \tag{69}$$

(2.6.5) When A is not diagonalisable, we can look at pseudospectra to find lower bounds for $G_{max} = \max_t G(t)$. Let $\epsilon > 0$, define $R(z) = (zI - A)^{-1}$ and

$$C_\epsilon = \{z : \|R\| \geq \frac{1}{\epsilon}\}. \tag{70}$$

Then define $\beta(z) = \{\max Re(z) : z \in C_\epsilon\}$. Hille-Yosida theorem states that,

$$G_{max} \geq \sup_{\epsilon > 0} \frac{\beta(\epsilon)}{\epsilon}. \tag{71}$$

3 Conclusions

3.1 Multizone model with lags

(3.1.1) A possible multizone model extension is to deal with the disparate timescales introduced by air handling systems by using delay differential equations. Take the following example zone layout:

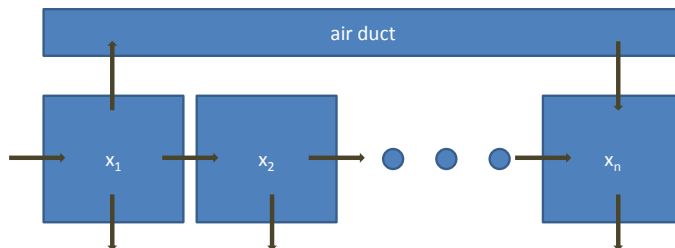


Figure 3: Multizone model with lag

- (3.1.2) Suppose we say that the air takes τ seconds to get from zone 1 to zone n . We have the following set of delay differential equations

$$\frac{dx_1}{dt} = Q_{10}x_0 - Q_{01}x_1 + Q_{21}x_1 - \alpha x_1(t) \quad (72)$$

$$\frac{dx_j}{dt} = Q_{j,j-1}x_{j-1} - Q_{0j}x_j + Q_{j+1,j}x_j \quad (73)$$

$$\frac{dx_n}{dt} = Q_{n,n-1}x_{n-1} - Q_{0n}x_n + \alpha x_n(t - \tau_n). \quad (74)$$

- (3.1.3) Taking all lags in the system into account, the linear system has the following form

$$\frac{dx}{dt} = Ax(t) + \sum_j B_j x(t - \tau_j) \quad (75)$$

$$\frac{dx}{dt} = Ax(t) - \sum_j B_j \tau_j \frac{dx}{dt}(t) + \dots \quad (76)$$

If the delays are small (with respect to evacuation time of the building) we find that

$$\frac{dx}{dt} = Ax(t) - \sum_j B_j \tau_j \frac{dx}{dt}(t) \quad (77)$$

$$\frac{dx}{dt} = (I + B_j \tau_j)^{-1} Ax \quad (78)$$

$$\frac{dx}{dt} = A'x. \quad (79)$$

- (3.1.4) Note that this is equivalent to the original problem except that A' is not diagonally dominant.

3.2 Final comments

- (3.2.1) The Study Group went some way to answer many of the questions posed by DSTL. We have identified the types of systems when \mathbf{A} is not diagonalisable. For other cases when DSTL were having trouble with certain large systems, the disparate timescales in the system led to a stiff system. The Study Group suggested two methods to solving these kinds of problems. One way would be to use a suitable preconditioner (or equivalently, a suitable matrix decomposition) for \mathbf{A} . The other, is to reformulate the problem using delay differential equations.

- (3.2.2) The inverse problem was tackled in two different ways. One is based on a result from control theory and data assimilation, the other, leads to a single minimisation problem of a quadratic functional. Further testing is required to see which method would be more suitable for DSTL.
- (3.2.3) A neat result was obtained related to the total exposure, $\int_0^\infty x(t)dt$, when the contaminant's source is from outside the building. Under the model assumptions, the total exposure is the same in all zones.
- (3.2.4) An alternative model was developed that could lead to a way of calculating the toxic load, $\int_0^\infty x^p(t)dt$ for $p > 1$. This is described briefly in Appendix A.1.
- (3.2.5) Finally, a method of finding the lower bound for the transient growth of the system was described in Section 2.6. A upper bound and a lower bound can be obtained when \mathbf{A} is diagonalisable.

A Results from special cases

A.1 Alternative model for finding the toxic load

- (A.1.1) Consider a steady state flow which carries some contaminant by pure advection, i.e., no diffusion. The concentration outside is a function of time only, $c = f(t)$, and it is carried through the area of interest along the stream lines, see Figure 4.

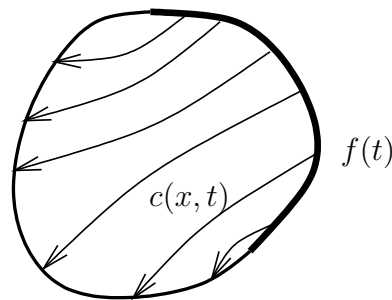


Figure 4: The streamlines of the flow through the area of interest.

- (A.1.2) We assume we know the flow and denote the velocity by $\mathbf{u}(x)$. Furthermore, we assume we have an incompressible flow, so $\nabla \cdot \mathbf{u} = 0$. Then the concentration $c(x, t)$ of the contaminant is given by the equation

$$c_t + \mathbf{u} \cdot \nabla c = 0. \tag{80}$$

- (A.1.3) We now consider a point x on one of the streamlines and let s denote arclength along the streamline. Assuming the concentration is zero at time $t = 0$ and for $t \rightarrow \infty$ we have

$$\begin{aligned} \frac{d}{ds} \int_0^\infty c(x, t) dt &= \int_0^\infty \frac{d}{ds} c(x, t) dt = \int_0^\infty \nabla c(x, t) dt \\ &= \int_0^\infty c_t(x, t) dt = 0. \end{aligned} \quad (81)$$

(A.1.4) So the total exposure is constant along the streamlines and is in particular equal to the total exposure at a point outside that area of interest. That is,

$$\int_0^\infty c(x, t) dt = \int_0^\infty f(t) dt. \quad (82)$$

(A.1.5) The moments $c(x, t)^m$ satisfies the same equation

$$(c^m)_t + \mathbf{u} \cdot \nabla(c^m) = 0. \quad (83)$$

Thus

$$\int_0^\infty c(x, t)^m dt = \int_0^\infty f(t)^m dt. \quad (84)$$

(A.1.6) The time integrated average in some area Ω satisfies

$$\begin{aligned} \int_0^\infty \frac{1}{\text{Vol}(\Omega)} \int_\Omega c(x, t)^m dV dt &= \frac{1}{\text{Vol}(\Omega)} \int_\Omega \int_0^\infty c(x, t)^m dt dV \\ &= \frac{1}{\text{Vol}(\Omega)} \int_\Omega \int_0^\infty f(t)^m dt dV = \int_0^\infty f(t)^m dt. \end{aligned} \quad (85)$$

(A.1.7) So the average of the moments is constant, but the moments of the average is in general not constant

$$\int_0^\infty \left(\frac{1}{\text{Vol}(\Omega)} \int_\Omega c(x, t) dV \right)^m dt \neq \int_0^\infty f(t)^m dt. \quad (86)$$

A.2 Duct model

(A.2.1) We consider a model, where we have n rooms. The air is flowing in one direction with the same flow rate q between each pair of compartments. The volume v in each room is constant. That is, our matrices are of the following form

$$V = \begin{pmatrix} v & 0 & \dots & 0 \\ 0 & v & \dots & 0 \\ & & \ddots & \\ 0 & 0 & \dots & v \end{pmatrix}$$

$$Q = \begin{pmatrix} -q & 0 & \dots & 0 \\ q & -q & \dots & 0 \\ & \ddots & \ddots & \\ 0 & \dots & q & -q \end{pmatrix}.$$

(A.2.2) The matrix $A = V^{-1}Q$ is not diagonalisable. However, using one modified Jordan block, we can easily analytically compute the solution of the equation

$$x(t) = e^{At}x(0) + e^{At} \int_0^t e^{-A\tau} B(\tau)u(\tau)d\tau,$$

where in our case we have $x(0) = 0$, $B = V^{-1}$ and $u = qx_0e_1$. Here e_1 is the first canonical basis vector and x_0 is the concentration of the inflowing contaminant from outside into the first room.

(A.2.3) In order to compute the concentration $x(t)$, we need to look at the matrix exponential e^{At} . We find

$$e^{At} = e^{-\frac{qt}{v}} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ \frac{qt}{v} & 1 & \dots & 0 & 0 \\ & \ddots & \ddots & & \\ \frac{(\frac{qt}{v})^{n-1}}{(n-1)!} & \frac{(\frac{qt}{v})^{n-2}}{(n-2)!} & \dots & \frac{qt}{v} & 1 \end{pmatrix}.$$

Similarly, we have

$$e^{-At} = e^{\frac{qt}{v}} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ \frac{-qt}{v} & 1 & \dots & 0 & 0 \\ & \ddots & \ddots & & \\ \frac{(-qt/v)^{n-1}}{(n-1)!} & \frac{(-qt/v)^{n-2}}{(n-2)!} & \dots & \frac{-qt}{v} & 1 \end{pmatrix}.$$

So that we can write,

$$x(t) = \frac{qx_0}{v} e^{At} \int_0^t e^{-A\tau} e_1 d\tau.$$

(A.2.4) Substituting $\mu = -\frac{q}{v}\tau$, the integral reduces to

$$\begin{aligned} x(t) &= -x_0 e^{At} \int_0^{-\frac{qt}{v}} e^{-\mu} \left(1, \mu, \frac{\mu^2}{2!}, \dots, \frac{\mu^{n-1}}{(n-1)!} \right)^T d\mu \\ &= x_0 e^{At} \left(1 - \Gamma\left(1, -\frac{qt}{v}\right), \dots, 1 - \frac{\Gamma\left(n, -\frac{qt}{v}\right)}{(n-1)!} \right)^T d\mu, \end{aligned}$$

where $\Gamma(m, -\frac{qt}{v})$ for $m = 1, \dots, n$ denotes the incomplete Gamma function. Note that for an integer m , we have

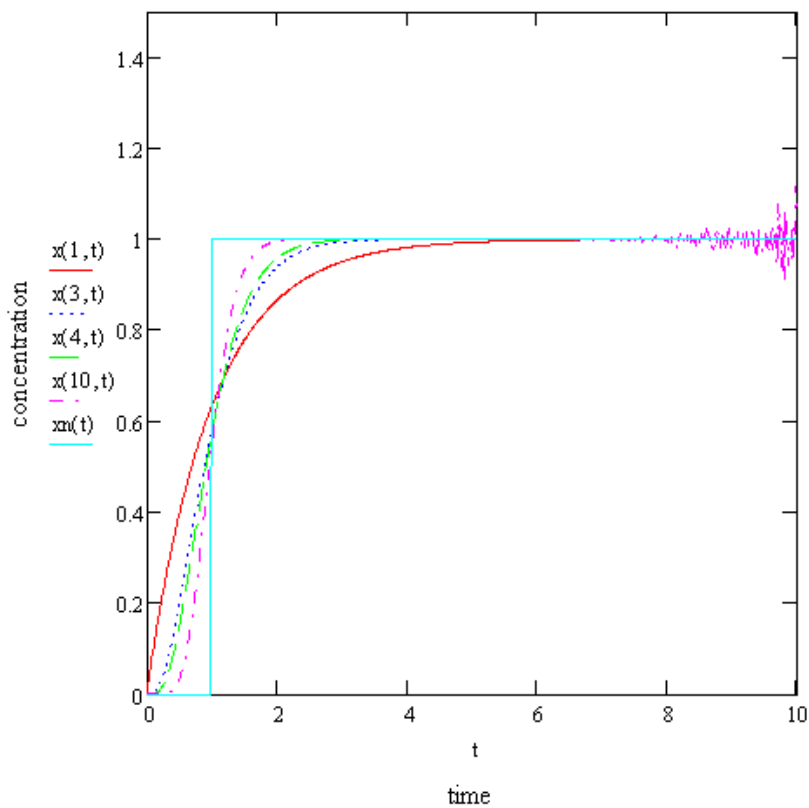
$$\Gamma\left(m, -\frac{qt}{v}\right) = (m-1)! e^{\frac{qt}{v}} \sum_{k=0}^{m-1} \frac{\left(-\frac{qt}{v}\right)^k}{k!}.$$

(A.2.5) Using the eigenvalue form for e^{At} we can then write the contaminant-concentration in the last room, i.e. the n th component of $x(t)$ as

$$x_n(t) = x_0 \sum_{m=1}^n \frac{\left(\frac{qt}{v}\right)^{n-m}}{(n-m)!} \left(\sum_{k=0}^{m-1} \frac{\left(\frac{qt}{v}\right)^k}{k!} - e^{-\frac{qt}{v}} \right)$$

This function starts at 0 and as time progresses it tends to the value of x_0 , which is what we expect to see.

(A.2.6) Note that in a general case when A is not diagonalisable, i.e. its minimal polynomial is not expressible as a product of distinct linear factors, you can write it as a matrix-product PJP^{-1} , where J is in Jordan block form, i.e. it consists of Jordan blocks on the diagonal and P is the transition matrix. Each Jordan block is a matrix with one eigenvalue on the diagonal, and ones on the superdiagonal. The size of the blocks corresponds to the multiplicity of the eigenvalues. Each exponentiation of the Jordan matrix has the advantage that the operations stay within the Jordan blocks. Then an explicit expression for $x(t)$ can be obtained similarly to the diagonalisable case, after expressing the e^{Jt} in terms of the eigenvalues and a polynomial matrix, similarly as we have done for e^{At} with the only difference, that the matrix is now upper triangular. The evaluation is then analogous to the diagonalisable case, but we integrate over the product of an exponential function and a polynomial (as done above).



Concentration in the last room x_n for $n = 1, 3, 4, 10$ rooms as well as the expected concentration x_n

B Tools and codes

B.1 EigTool

(B.1.1) Pseudospectra software -available at:

<http://www.comlab.ox.ac.uk/projects/pseudospectra/eigtool/>

B.2 Schur-Parlett

(B.2.1) Nick Higham's MATLAB code for the Schur-Parlett method:

<http://www.maths.manchester.ac.uk/~higham/NAMF/>

Bibliography

- [1] *State-space methods for calculating concentration dynamics in multizone buildings*, S Parker, V Bowman. Building and Environment (2011).
- [2] *Nineteen dubious ways to compute the exponential of a matrix*, C Moler, C Van Loan. Society for Industrial and Applied Mathematics (2003).
- [3] *Transient growth and why we should care about it* R Bale, R Govindarajan. Resonance (May 2010).
- [4] *Computing the matrix exponential - The Cayley-Hamilton Method* D Rowell. Lecture notes (2004)
- [5] *A Schur-Parlett algorithm for computing matrix functions* P Davies, N Higham. MIMS (2003)
- [6] *Spectra and pseudospectra: The behaviour of nonnormal matrices and operators* L Trefethen, M Embree. Bulletin of the American Mathematical Society (2007)
- [7] *Pseudospectra of linear operators* L Trefethen. SIAM Review (1997)
- [8] *MA30046 Lecture Notes, University of Bath*[online] H Logemann, 2008.
- [9] *Data Assimilation Concepts and Methods*[online] European Centre for Medium-Range Weather Forecasts. Reading. F Bouttier, P Courtier, 1999.
Available from:

http://www.ecmwf.int/newsevents/training/lecture_notes/pdf_files/ASSIM/Ass_cons.pdf
- [10] *Numerical Methods for Conservation Laws*. 5th ed. Berlin:Birkhäuser Verlag. R LeVeque, 1992.