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Improvements to User-friendliness of a Computational Fluid Dynamics (CFD) Code for Simulation of Air Movement in Buildings

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Abstract

Starting from the basic governing equations for fluid flows, a three-dimensional computational fluid dynamics (CFD) code is described. The pre-processing and post-processing software was integrated with the CFD code to form a more user-friendly computer package. This new computer package has been used to carry out several simulations on air and smoke movement in atrium with balconies. It has been found that the pre-processing and post-processing software can greatly reduce the data preparation and analysis time. It can also reduce the likelihood of making errors in data entry. Some of the simulation results on air movement have been compared with results from a physical model at Melbourne University. Qualitatively, there appears to be good agreement between the simulation results and those from the physical model.

Nomenclature

C_1	empirical constant in generation/destruction term of ε-equation
C_2	empirical constant in generation/destruction term of ε-equation
C_3	empirical constant in buoyant term of ε-equation
C_D	empirical constant for eddy viscosity
g_i	gravitational constant in X_i-direction (m/s^2)
$\bar{k}$	mean turbulent kinetic energy (m^2/s^2)
$\bar{p}$	mean static pressure (N/m^2)
$\bar{S}_\theta$	mean volumetric heat source generation rate (W/m^3)
t	time (s)
$\bar{U}_i$	mean velocity component in X_i-direction (m/s)
$\bar{U}_j$	mean velocity component in X_j-direction (m/s)
X_i, X_j	distance in cartesian coordination (m)
$ß$	volumetric expansion coefficient ($°K^{-1}$)
$\bar{\varepsilon}$	mean dissipation rate of k (m^2/s^3)
$\bar{\Theta}$	mean temperature difference (°K)
κ	thermal diffusivity (m^2/s)
ν	kinematic molecular viscosity (m^2/s)
ν_t	eddy viscosity (m^2/s)
Π	total pressure (N/m^2)
ρ	fluid density (kg/m^3)
σ_k	empirical constant in diffusive term of k-equation
σ_ε	empirical constant in buoyant term of ε-equation
σ_θ	Prandtl number for heat transport

Introduction

With the advance in computer technology, new techniques that predict temperature distribution and air flow pattern have been developed in the past few years. These techniques are based on computational fluid dynamics (CFD) - the numerical solution of the equations which govern fluid flow. These equations are of partial-differential form, and represent the conservation or balance of physical quantities, such as mass, energy and momentum.

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Table 1 Modelled Equations for the Computer Code EXACT3

Description	Equations
Mass	$\frac{\partial \overline{U_i}}{\partial X_i} = 0$ (1)
Momentum	$\frac{\partial \overline{U_i}}{\partial t} + \overline{U_j}\frac{\partial \overline{U_i}}{\partial X_j} = -\frac{1}{\rho}\frac{\partial \Pi}{\partial X_j} + \frac{\partial}{\partial X_j}[(\nu + \nu_t)(\frac{\partial \overline{U_j}}{\partial X_i} + \frac{\partial \overline{U_i}}{\partial X_j})] - \beta g_i \bar{\theta}$; $\Pi = \bar{p} + \frac{2\rho\bar{k}}{3}$ (2)
Thermal Energy	$\frac{\partial \bar{\theta}}{\partial t} + \overline{U_i}\frac{\partial \bar{\theta}}{\partial X_i} = \frac{\partial}{\partial X_i}(\kappa + \frac{\nu_t}{\sigma_\theta})\frac{\partial \bar{\theta}}{\partial X_i} + \overline{S_\theta}$ (3)
Turbulence Kinetic Energy	$\frac{\partial \bar{k}}{\partial t} + \overline{U_j}\frac{\partial \bar{k}}{\partial X_j} = \frac{\partial}{\partial X_j}[(\nu + \frac{\nu_t}{\sigma_k})\frac{\partial \bar{k}}{\partial X_j}] + \nu_t(\frac{\partial \overline{U_i}}{\partial X_j} + \frac{\partial \overline{U_j}}{\partial X_i})\frac{\partial \overline{U_i}}{\partial X_j} + \beta g_i \frac{\nu_t}{\sigma_\theta}\frac{\partial \bar{\theta}}{\partial X_i} - \bar{\varepsilon}$ (4)
Dissipation Rate of Turbulence Kinetic Energy	$\frac{\partial \bar{\varepsilon}}{\partial t} + \overline{U_j}\frac{\partial \bar{\varepsilon}}{\partial X_j} = \frac{\partial}{\partial X_j}[(\nu + \frac{\nu_t}{\sigma_\varepsilon})\frac{\partial \bar{\varepsilon}}{\partial X_j}] + \frac{\bar{\varepsilon}}{\bar{k}}[C_1 \nu_t(\frac{\partial \overline{U_i}}{\partial X_j} + \frac{\partial \overline{U_j}}{\partial X_i})\frac{\partial \overline{U_i}}{\partial X_j}] - C_2\frac{\bar{\varepsilon}^2}{\bar{k}} + C_3\frac{\bar{\varepsilon}}{\bar{k}}\beta g_i\frac{\nu_t}{\sigma_\theta}\frac{\partial \bar{\theta}}{\partial X_i}$ (5)
Eddy Viscosity	$\nu_t = C_D\frac{\bar{k}^2}{\bar{\varepsilon}}$ (6)

Because of the characteristics of the governing equations, the methods are mesh-based (or grid-based) involving a large number of iterative calculations. Because of the iterative nature of the analysis and the large number of input variables (e.g. boundary conditions), this type of computer programme tends to be specialised and not very user-friendly. Most building designers are not familiar with the techniques and tend to shy away from them.

This paper presents the work on improvements to the user-friendliness of a CFD code EXACT3. Starting from the basic equations for fluid flows, the three-dimensional CFD code EXACT3 is described. Research and development work on pre-processing and post-processing software is presented. The pre-processing software is basically a menu-driven data input computer programme, which simplifies and facilitates input data preparation. The post-processing software helps sort the massive numerical data and displays the computed results in graphical form, which is more comprehensible to building designers.

Computer Code EXACT3

The turbulent flow field is governed by the conservation equations of mass, momentum and energy, and the equation of state. Applying Reynolds-averaging technique to these governing equations yields a set of differential equations involving temporal means of the relevant variables. Turbulence closure is through the two-equation k-ε turbulence model. Details of turbulence modelling can be found in (Lam et al. 1991). The modelled equations used for the computer code EXACT3 are summarised in Table 1.

EXACT3 stands EXplicit Algorithm for Continuous Turbulent fluid flows, first written by T. Kurabuchi at Tokyo University and later modified at the National Institute of Standards and Technology in U.S. (Kurabuchi et al. 1990). It is based on the two-equation k-ε turbulence model and finite difference numerical technique. It is a numerical programme for predicting three-dimensional indoor temperature and air distribution, including turbulent and thermal effect. Basic characteristics of EXACT3 are as follows:

(a) Turbulence Effect

Buoyancy extended k-ε turbulence model.

(b) Applicable Flows

Three-dimensional continuous non-isothermal and buoyant turbulent flow.

(c) Numerical Discretisation

Finite difference discretisation, and variables defined on staggered grid system.

(d) Iterative Procedure

Explicit time marching technique to obtain converged solution.

(e) Convective Term Approximation

Combination of both the upwind hybrid and central differencing scheme with arbitrary specification for switching parameter and location.

(f) Solution Procedure for Poisson Equation of Mass Continuity

Pressure Relaxation Method to speed up each time iteration.

(g) Boundary Condition

- Inflow and outflow in terms of velocity or pressure.
- Wall turbulence by wall-function method (Power Law).
- Heat flux, temperature and heat transfer coefficient for thermal and buoyant effect.

(h) Thermal Analysis

Volumetric heat sources are included.

(i) Obstacles

Permit the modelling of the effect of furniture and partitions on the flow field and provide a mean for modelling multi-room airflow.

The source code of EXACT3 was written in FORTRAN and can be run on UNIX and DOS operating systems.

Because of the characteristics of the governing equations (see Table 1), EXACT3 code is mesh-based involving a large amount of input variables such as boundary conditions and mesh dimensions. The voluminous numerical output also makes the analysis difficult and time-consuming. This means that this type of iterative programme tends to be specialised and not very user-friendly, and is not widely used in the design process by building designers. To overcome these shortcomings, pre-processing and post-processing facilities were developed to interact with EXACT3 code, to make it more user-friendly, and therefore more accessible by building professionals.

Table 2 Segment of Input Data File for EXACT3

```
atrium with balconies, air change=8
6010,20,50000000,1
59200,0.71,0.0,1.4,0.0001,0.02,10.0
0.09,1.44,1.92,1.00,1.00,1.30,0.90
0.0433,0.0433,0.0433,0.0433,0.0433,0.0433,0.0433,0.0433,0.0685,0.02,0.0685,
0.06895,0.1,0.1,0.0745,0.0745,0.0745,0.1299,0.1299,0.1299,0.1299,
0.1299,0.1299,0.105495,0.105495,0.105495,0.105495,0.11496,0.11496,0.1173,0.1,
0.1
0.2,0.2,0.2,0.2
0.25,0.25,0.24,0.24,0.26,0.26,0.11,0.11,0.07667,0.07667,
0.07667,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,
0.04,0.04,0.07667,0.07667,0.07667,0.04,0.04,0.04,0.04,0.04,
0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.07667,0.07667,0.07667,0.04,
0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,
0.07667,0.07667,0.07667,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,
0.04,0.04,0.04,0.04,0.07667,0.07667,0.07667,0.04,0.04,0.04,
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0.07667,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,0.04,
0.04,0.04,0.15,0.15,0.15,0.125,0.125,0.125,0.125,0.15,0.15,
0.15,0.125,0.125,0.125,0.125
3,3,3,3,3,3
128
 1, 2, 2, 3, 3, 3, 4, 0.296
 2, 2, 2, 3, 3, 3, 4, 0.0
 3, 2, 2, 3, 3, 3, 4, 0.0
 4, 2, 2, 3, 3, 3, 4, 0.000438
 5, 2, 2, 3, 3, 3, 4, 0.00000551
 .  .  .  .  .  .  .  .
 .  .  .  .  .  .  .  .
15, 3, 9, 3, 3,86,87, 0.0
15, 3, 8, 3, 3,88,87, 0.0
15, 9, 9, 3, 3,93,92, 0.0
15,27,30, 3, 3, 2, 20.73
16
 3, 7, 3, 3,97,104
 8,16, 3, 3,99,104
 .  .  .  .  .  .
 .  .  .  .  .  .
 3, 8, 3, 3,87,87
 9, 9, 3, 3,87,92
0
1
 1.31, 1, 4, 1,105, 2.0
```

The integrated package was developed with the following objectives in mind:

(a) universal applicability,
(b) high precision on data preparation, and
(c) economy and ease of use.

Pre-processing Code PREXACT3

To carry out iterative analysis of air movement, the FORTRAN-written EXACT3 code requires an input data file with a strict specification of format. Major difficulties involved in data preparation are:

(a) complexity of mesh generation,
(b) problems identification such as for obstacles location and boundary conditions,
(c) significance of data, especially those involved in numerical iteration,
(d) parameters adjustment to promote convergence and stability of iterative solution, and
(e) specification of input data format.

The user had to prepare a data file containing all the required input data in ASCII code. Table 2 shows a segment of such input data file. Typing in those numbers was time-consuming and error-prone. To facilitate the data input process, a pre-processing software, PREXACT3, was developed so that data could be entered in a manner familiar to most building designers.

PREXACT3 is basically a menu-driven software with pop-up menus similar to most wordprocessing and computer-aided design packages. Figure 1 shows a typical screen layout. After going through the

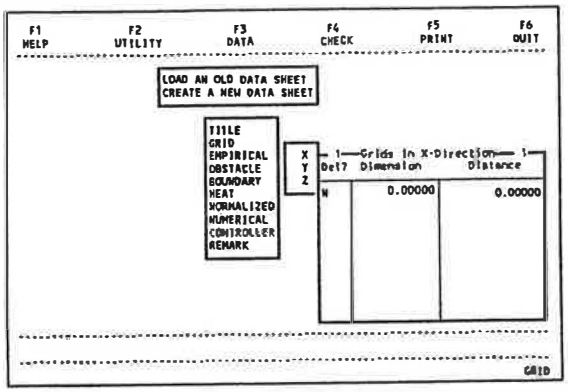


Figure 1 Typical Screen Layout for PREXACT3

menu-driven data entering process, PREXACT3 will then generate a data file in the special format required by the EXACT3 code. The transformation is automatic and is transparent to the user. Some basic features of PREXACT3 are as follows:

(a) Menu-driven user environment, with cursor and control keys similar to computer-aided design and wordprocessing packages.
(b) On-screen "help" information for operating the programme and interpreting the data significance.
(c) Automatically generating the normalized form of data adopted by EXACT3.
(d) Automatically numbering the mesh system and calculating its coordinations.
(e) Communication with DOS operating system without quitting PREXACT3.
(f) Printing support for comprehensible data report.
(g) Built-in function for checking range and format of data to eliminate error.
(h) A set of default values available for data which can be updated by users.
(i) Making note on the data file without interfering the simulation process of EXACT3.

Table 3 Key Functions Contained in Prexact3

Function Name	Function details
HELP	Give help information
UTILITY	Provide DOS utility programs
DATA	Prepare and format data file for EXACT3
CHECK	Check validity of data
PRINT	Send data to printer or text file
QUIT	Leave PREXACT3 and go back to DOS
TITLE	Prepare title of data sheet
GRID	Define flow domain and grid system
EMPIRICAL	Insert empirical parameter for turbulence model
OBSTACLE	Define obstacle location
BOUNDARY	Define boundary conditions
HEAT	Define heat generation sources
NORMALIZED	Define parameters for normalization
NUMERICAL	Prepare data to define numerical scheme
CONTROLLER	Prepare data to control sequence of EXACT3
REMARK	Make notes

Overlaying technique was used to minimise memory occupied by PREXACT3. A summary of its major functions is shown in Table 3.

Post-Processing Code POEXACT3

Table 4 shows a segment of a typical computer output from the EXACT3 code. It can be seen that the numerical format is very difficult to analyse. For building designers, it would be more attractive if the computer output is shown in graphical form. For instance, it would provide a quick feedback to an engineer designing an air extract system if the air movement for different designs could be shown graphically. To this end, a post-processing software called POEXACT3 was developed to make the data analysis more comprehensible and user-friendly.

POEXACT3 was written in standard C language with support from standard C libraries and has the following features:

(a) Integrating with graphic facility with menu-

Table 4 Segment of Computer Output Data File from EXACT3

```
RK21.DAT
79    90
TITLE
 25   4   38
0.10865  0.10865  0.10865  0.10865  0.112975 0.112975 0.1      0.1      0.112975  0.112975
0.1299   0.1299   0.1299   0.1299   0.1299   0.1299   0.11384  0.11384  0.11384   0.11384
0.11384  0.0827   0.1173   0.1      0.1
1.0      1.0      1.0      1.0
0.24     0.24     0.24     0.24     0.06     0.23     0.23     0.22333  0.22333   0.22333
0.22333  0.22333  0.22333  0.22333  0.22333  0.22333  0.22333  0.22333  0.22333   0.22333
0.22333  0.22333  0.22333  0.22333  0.22333  0.22333  0.22333  0.22333  0.125     0.125
0.125    0.15     0.15     0.15     0.125    0.125    0.125    0.125
  3  3  3  3  3  3
4
  3  4  3  3 30 37
  5 10  3  3 32 37
 11 16  3  3 35 37
 17 22  3  3 37 37

atrium with balconies, air change=8
   U-DISTRIBUTION ON  Y-Z PLAN I =   3    KSTP=     10200

              1              2              3              4              5
    1      .0000000       .0000000       .0000000       .0000000       .0000000
    2      .0000000       .0263974       .0263974       .0621223       .3141654
    3      .0000000       .0188551       .0263974       .0621223       .3141654
    4      .0000000       .0188551       .0263974       .0621223       .3141654

              6              7              8              9              10
    1      .0000000       .0000000       .0000000       .0000000       .0000000
    2      .0588353       .0192368       .0094351       .0056679       .0035126
    3      .0588353       .0192368       .0094351       .0056679       .0035126
    4      .0588353       .0192368       .0094351       .0056679       .0035126

             11             12             13             14             15
    1      .0000000       .0000000       .0000000       .0000000       .0000000
    .       .              .              .              .              .
    .       .              .              .              .              .
    .       .              .              .              .              .
```

Figure 2 Atrium Air Movement Generated from EXACT3 Code

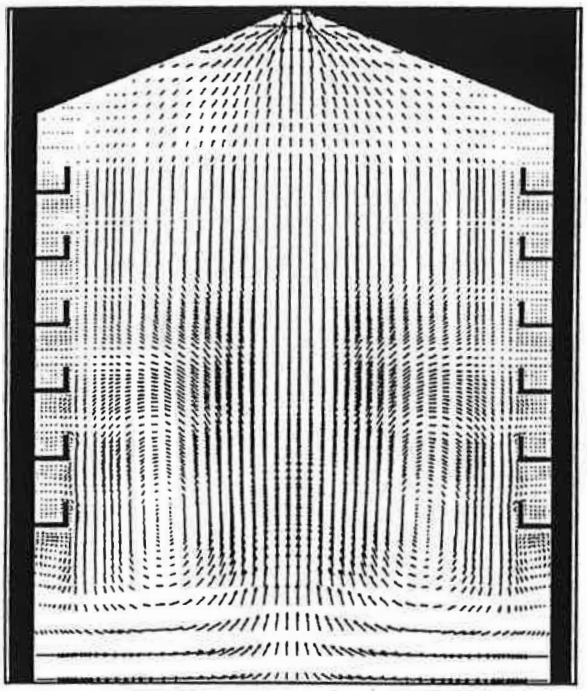
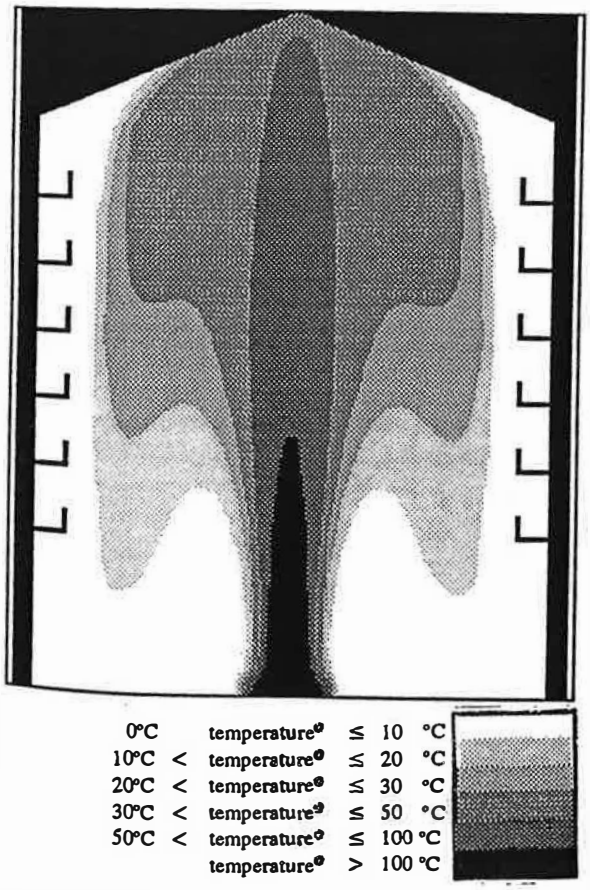
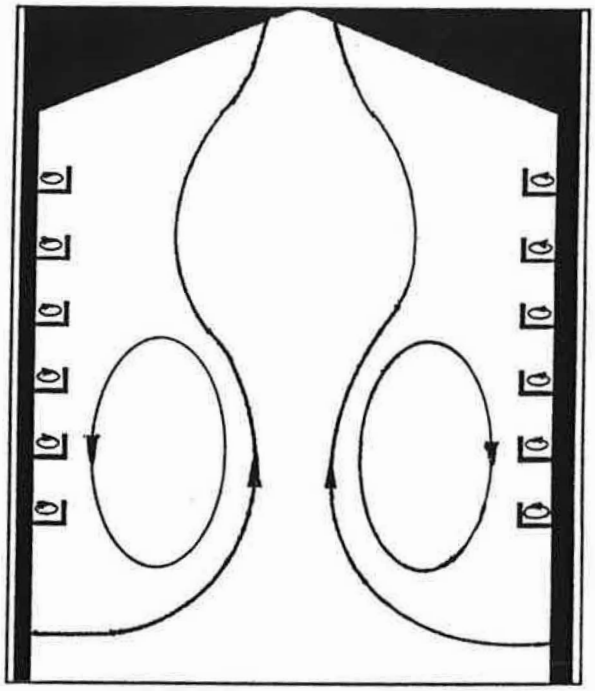


Figure 3 Atrium Temperature Distribution Generated from EXACT3 Code



@ *Temperature above ambient room temperature*

Figure 4 Atrium Air Movement from Physical Model at the University of Melbourne



driven environment.

(b) Transforming three-dimensional computed numerical output into graphical form for presentation.

(c) Analysing different distributions (e.g. velocity, temperature) side by side with the multi-tasking feature of UNIX system.

(d) Enlarging or displaying part of the flow region under investigation.

(e) Printing support by transforming the graphics to a RGB-formatted file for further external processing.

Figures 2 and 3 show the graphical output from POEXACT3 for velocity and temperature distributions inside an atrium with balconies. Fire, represented by a heat source of 0.5 MW/m^2 for an area of 3 m x 3 m, was assumed present in the middle of the ground floor (see Case Study below for details). From this type of graphical output, a designer can very quickly get an overall view of the indoor air movement and temperature distribution.

Case Study

The pre-processing and post-processing software was integrated with the EXACT3 code. A case study was carried out to demonstrate the ease of use of the modified CFD code.

The case considered is an open type seven-storey atrium with balconies on both sides. The atrium is

mechanically-ventilated with the extraction fans at the apex of the roof. Analysis on smoke movement is carried out to demonstrate the post-processing tool, visualising both the velocity vector and temperature profile of the air/smoke layer. Parameters used in the simulation are as follows:

Ventilation rate	:	8 air change per hour
Reynolds number	:	59,200
Prandtl number	:	0.71
Archimedes number	:	0.0
Supply air velocity	:	0.37 m/s
Extraction velocity	:	1.78 m/s
Fire heat output	:	0.5 MW/m^2 for an area of 3 m x 3 m in the middle of the ground floor

Values for the empirical constants of the turbulence model (shown in Table 1) were taken from (Launder and Spalding 1974; Rodi 1982); and are as follows:

C_D	=	0.09	C_1	=	1.44
C_2	=	1.92	C_3	=	1.00
σ_k	=	1.0	σ_ϵ	=	1.3
σ_θ	=	0.9			

Velocity boundary values near solid surfaces were approximated by a 1/7th power law type velocity profile. The no-slip type boundary condition was used for the wall boundary condition for the turbulent kinetic energy. The wall boundary condition for the turbulent energy dissipation rate was derived from the logarithmic law condition.

The input data file for EXACT3 calculation was prepared by the pre-processing programme PREXACT3. The simulation was conducted on a Hewlett Packard HP-S700 workstation. Maximum error in the continuity was estimated to be $1x10^{-4}$, and each simulation took approximately 8 hours and 12,000 iterations.

Some of the simulated results for velocity and temperature are shown in Figures 2 and 3 respectively. It has been found that the pre-processing software speeds up the data input and edit process. And, more importantly, it enables a user to input and check the data in a sequential and systematic way, reducing the likelihood of introducing incorrect data input.

To see how well EXACT3 simulate airflow field, simulated air movement was compared qualitatively with air movement predicted by a physical model. The 50:1 scale model was constructed in the Department of Architecture and Building at the University of Melbourne. Water was supplied at the ground floor of the model and extracted out at the top. Air movement was observed through the dye distribution in water. Details about the physical model and its study can be found in (Kas 1987).

Air movement predicted by the water model is shown in Figure 4. It can be seen from Figures 2 and 4 that results from both the computer simulation and the physical model show eddy formation within the atrium and inside the balconies. Inside this ventilated balcony-approached atrium, a large eddy is formed adjacent to the balconies and a small local eddy is formed inside each balcony. The large eddy interacts with small local eddy inside the balconies. The interaction will determine whether hot air/smoke can penetrate inside the balconies. It has also been observed that the large eddy will create downdrafts along the balcony wall.

Conclusions

With the advance in computer simulation, CFD can be a useful design tool for building designers. Pre-processing and post-processing software was developed and integrated with the CFD code, EXACT3. It has been found that the pre-processing software not only speeds up the data input process, but also reduces the likelihood of making errors. The post-processing software transforms the massive numerical computed output to graphical form, which enable users to get an overall view of the results more readily.

Case study on an atrium with balconies was carried out. It has been found that qualitatively, there is good agreement between computer simulated results from the CFD code and measured results from a physical model.

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