

## Introduction

This tutorial presents the new CFD capabilities of CONTAM 3.0. These capabilities provide a means to couple the multizone capabilities of CONTAM with the CFD capabilities of CFD0. Two methods are presented here referred to as *interior-zone coupling* and *exterior-zone coupling*. *Interior-zone coupling* refers to the treatment of an interior zone of a multizone building with CFD, and *exterior-zone coupling* refers to the use of CFD0 to perform calculation in the exterior zone of a building. The *interior-zone coupling* is a fully coupled method while the *exterior-zone coupling* is a loose coupling between the two programs, i.e., the coupling requires that the two programs be run sequentially.

## CASE 1: Interior-Zone Coupling

This tutorial will provide you with a brief overview of how to create a CONTAM project using the combined multizone/CFD capabilities of CONTAM 3.0. This project is not meant to be representative of an actual building but to simply introduce you to the program features you will need to utilize this capability. There are actually two programs presented – CONTAM and the CFD0 Editor. The ContamW 3.0 interface is very similar to previous versions with some CFD-related additions, and the CFD0 Editor is a recently developed application used to define CFD zones and help you manage the *link* between the multizone and CFD regions of your project.

### Step 1 – Define a CONTAM Project (Demo\_CFD0.prj)

The case for this example is a five-zone office suite with a center hallway as shown in Figure 1. The hallway is a CFD zone and the rest of the zones are normal, well-mixed CONTAM zones. To keep the case simple, the airflow is isothermal, driven by wind pressure at Path 5, and there is no mechanical ventilation.

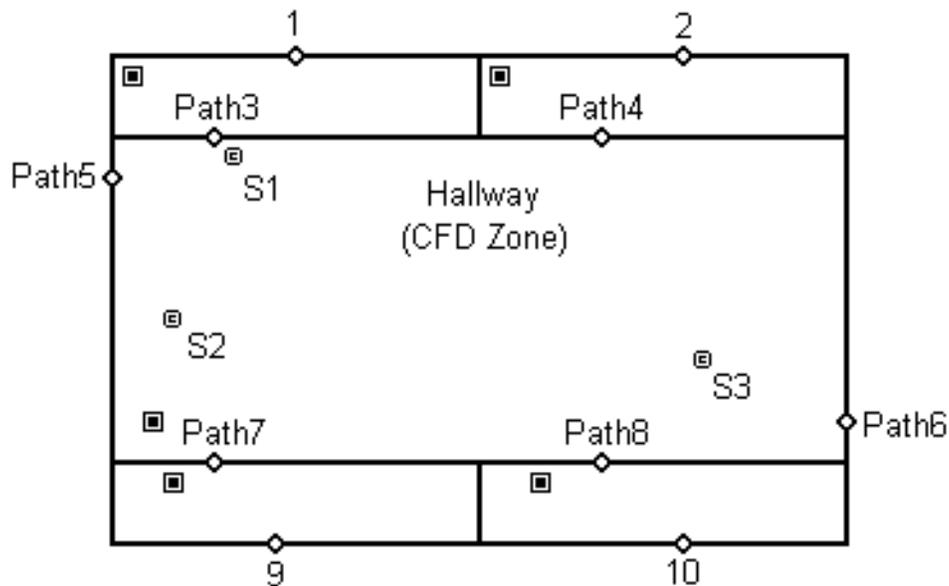


Figure 1 – CONTAM Sketch

## Define Zones

The Hallway is defined to be a CFD zone via the *Detailed Zone* page of the Zone Properties as shown in Figure 2. Set the Zone Detail property to *CFD Zone* and provide a *CFD Zone ID*. This ID will be utilized when naming CFD-related files that are generated by the CFD0 Editor and ContamX. These files will be discussed later in this tutorial.

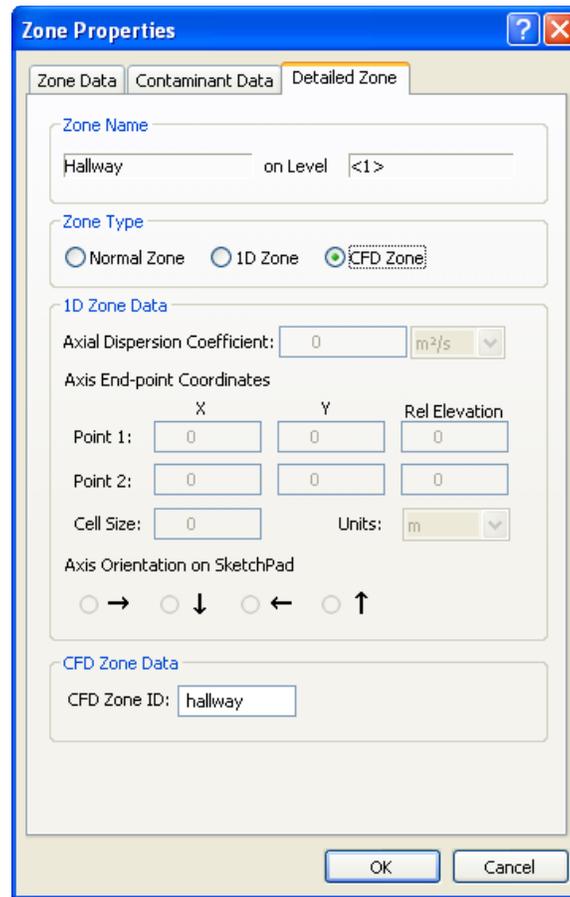


Figure 2 – CFD Zone properties

The surrounding four zones will all be normal, well-mixed zones with volumes of 75 m<sup>3</sup> and temperatures of 23 °C.

### NOTE - CFD Zones

#### Number of CFD zones

*CONTAM 3.0 only allows you to define one CFD zone per CONTAM project.*

#### Well-mixed zones

*All other zones must be well-mixed, i.e., 1D convection/diffusion zones are currently not allowed when performing a CFD calculation.*

### Define Airflow Paths

The leakage information and boundary condition of each path are provided in Table 1. All airflow paths in this example use the orifice airflow element type. *Interface paths* connect CFD zones with well-mixed zones. In this case Paths 3, 4, 5, 6, 7 and 8 connecting the hallway with the CONTAM zones are the interface paths. You define the interface path properties via the *CFD* tab of the Airflow Paths Properties dialog box shown in Figure 3.

Path Number	Relative Elevation [m]	Airflow Element Name	Opening Area [m <sup>2</sup> ]	Wind Pressure [Pa]	CFD Path ID	Boundary Condition
1, 2, 9, 10	0.5	OpenWindow	1	none	n/a	n/a
3	0.5	Path3	2	n/a	Path3	Linear
4	0.5	Path4	2	n/a	Path4	Linear
5	0.5	Path5	1	1.0	Path5	Stagnation
6	0.5	Path6	1	none	Path6	Linear
7	0.5	Path7	2	n/a	Path7	Linear
8	0.5	Path8	2	n/a	Path8	Linear

Table 1 – CONTAM airflow path properties

*NOTE - Interface path airflow elements*

*Each interface path must have a unique airflow element, i.e., it cannot share an airflow element with any other paths in the project. This is because the coupling method will modify the airflow element properties during the simulation to “transfer” boundary conditions between the multizone and CFD regimes during the coupling iterations.*

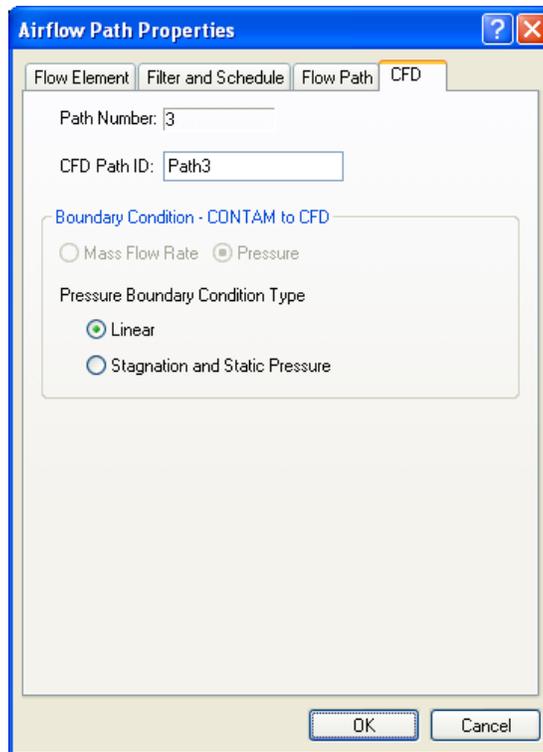


Figure 3 – CFD interface path properties

*NOTE – CFD Interface Path Properties**Path Number*

*Path index provided by ContamW. This index can change whenever paths are added or removed from the project file and the project file is saved.*

*CFD Path ID*

*A unique CFD path ID must be specified for each interface path.*

*Boundary Condition – CONTAM to CFD*

**Mass Flow Rate:** *CONTAM provides a mass flow rate boundary condition to CFD.*

**Pressure:** *CONTAM provides a pressure boundary condition to CFD.*

*Pressure Boundary Condition Type*

**Linear:** *When a pressure boundary condition is provided by CONTAM to CFD, the linear coefficient ( $C = 1.0$ ) and exponent ( $Exp = 1.0$ ) will be used for each interface cell in the CFD zone. This simple model should be used for large openings with potential two-way flow (recirculation) across the openings, where the “Stagnation and Static Pressure Model” normally cause numerical issues. This is the default model.*

**Stagnation and Static Pressure:** *When a pressure boundary condition is provided by CONTAM to CFD, a stagnation pressure is imposed for inflows to the CFD zone, and a static pressure is imposed for outflows from the CFD zone. Numerically, a static pressure is set for CFD outflows as follows: a linear coefficient with the order of  $10^3$  is used so that the CFD local pressure can be maintained as a difference of  $10^3$  from the external boundary pressure. This may cause numerical issues for large openings with two-way flows, where a slight change of dynamic pressure head could cause a huge airflow at the boundary. In such cases, a linear model should be used. When comparing a coupled simulation to a whole-CFD (all zones simulated by CFD) simulation, the flow coefficients and exponents in a coupled simulation are very important, which are normally unknown. Above all, a linear model brings more numerical stability while a stagnation and static pressure model is a means of setting CFD pressure boundary conditions.*

*The boundary conditions options will be enabled/disabled depending on the Coupling Method selected (see **NOTE – CFD Numerics in CONTAM** section presented later) and the type of airflow element of the interface path. The “CONTAM <-> CFD” and the “CONTAM -> CFD->CONTAM” coupling methods will set all BCs to their default values to provide the pressure-pressure BC exchange method which is the most stable of the three (pressure-pressure, pressure-flow, flow-pressure).*

### Contaminants and Sources

There are two contaminants defined in the project, CO and CO<sub>2</sub>, and three sources located within the Hallway zone – two CO sources and one CO<sub>2</sub> source. Table 2 provides contaminant source information. The source location within the zone will be defined later using the CFD0 Editor. The source/sink *Location* properties within ContamW are not relevant within a CFD zone.

*NOTE – Number of Contaminant Species and Sources*

*Number of contaminant species*

*You can define up to **Five** contaminant species for a coupled CONTAM+CFD simulation.*

*Number of contaminant sources*

*The number of sources you can define is limited by CONTAM itself, however you must provide a unique CFD Source ID for each source located within a CFD zone.*

*Constant Coefficient source/sink models only*

*Currently, only Constant Coefficient source sinks can be placed within a CFD zone, and only the Generation rate is taken into account, i.e., the removal rate is assumed to be zero during the simulation.*

Source Number	Species	Element Name	Generation Rate [g/hr]	CFD Source ID
1	CO	CO_Rate	500	S1
2	CO	CO_Rate	500	S2
3	CO <sub>2</sub>	CO <sub>2</sub> _Rate	500	S3

**Table 2 – CONTAM source properties**

## Step 2 – Define CONTAM Simulation Parameters

Access the Simulation Parameters via the **Simulation** → **Simulation Parameters...** menu command.

### CFD Numerics

Simulation parameters were added to CONTAM 3.0 to control the CFD calculation. Access the CFD Numerics shown in Figure 4. This tutorial implements the coupling method “CONTAM <-> CFD” with a *Convergence Factor for Airflow Coupling* set to 0.001. Parameters are explained in the following NOTE.

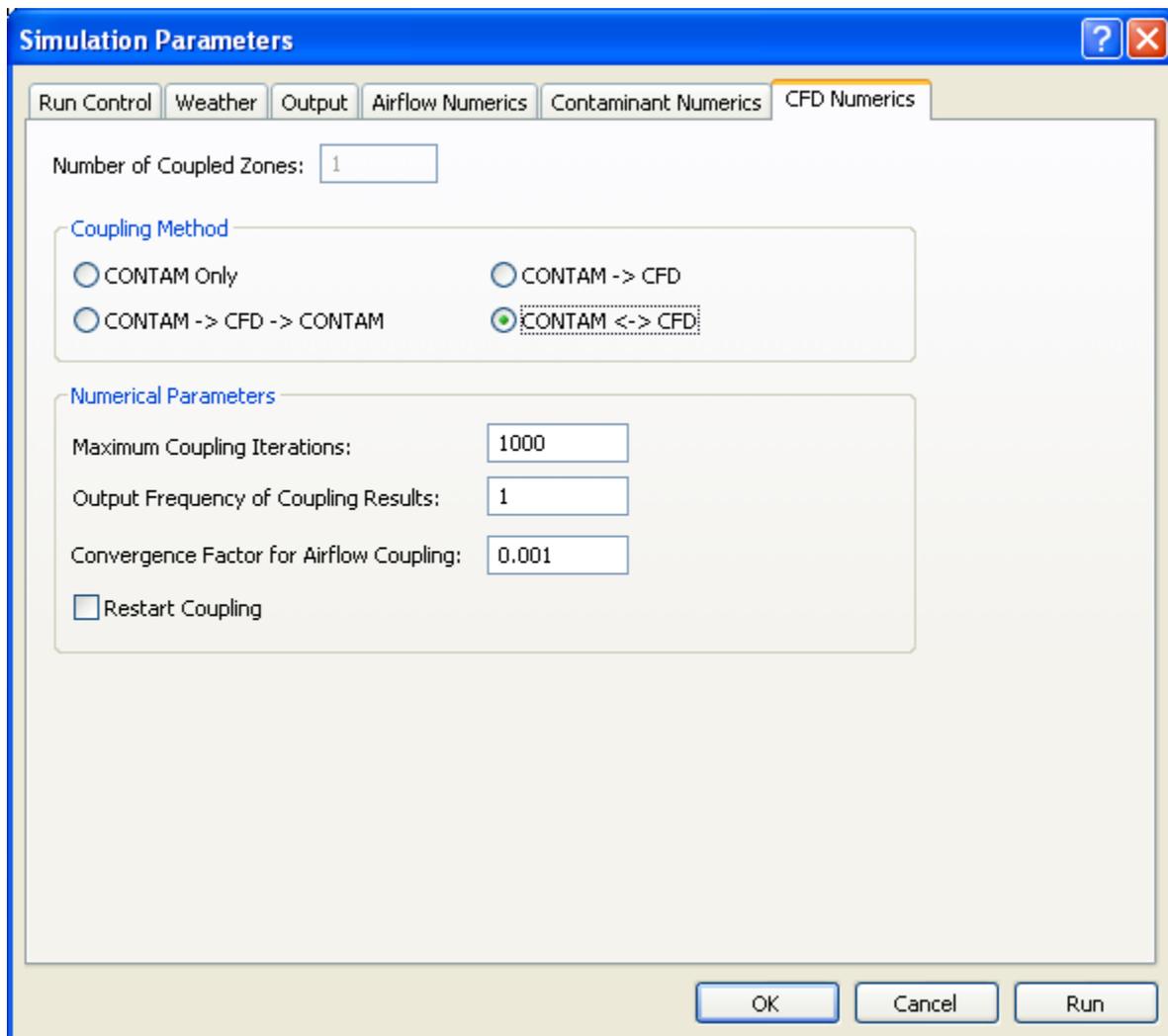


Figure 4 – CFD Numerics properties in ContamW

*NOTE – CFD Numerics in CONTAM**Number of Coupled Zones*

*The total number of CFD zones in the project. Only one zone is allowed in the current version.*

*Coupling Method*

**CONTAM only:** Perform only a multizone CONTAM simulation without CFD (i.e., no coupling). This is the default option.

**CONTAM -> CFD:** CONTAM runs first and then provides boundary conditions to the CFD simulation. No information is passed back from CFD to CONTAM.

**CONTAM -> CFD -> CONTAM:** CONTAM runs first, provides mass flow (airflow and contaminant mass flow) boundary conditions to CFD, CFD then runs, and provides contaminant concentration boundary conditions back to CONTAM. The airflow calculation information is exchanged between CONTAM and CFD only once, but the contaminant concentration information is exchanged iteratively between CONTAM and CFD until concentrations at the interface paths converge.

**CONTAM <-> CFD:** CONTAM runs first. CONTAM and CFD provide boundary conditions iteratively to each other during each time step until they either reach convergence with each other or the Maximum Coupling Iterations is exceeded.

*Numerical Parameters*

**Maximum Coupling Iterations:** When the coupling method of “CONTAM <-> CFD” is chosen, this is the maximum number of information exchange iterations between CONTAM and CFD for each time step.

**Output Frequency of Coupling Results:** When the coupling method of “CONTAM <-> CFD” is chosen, this controls how often the results of a coupled simulation are saved. The default is one, which means the information will be saved in a “\*.CMO” file at every information exchange iteration between CONTAM and CFD.

**Convergence Factor for Airflow Coupling:** The convergence criterion when the coupling method of “CONTAM <-> CFD” is chosen. The default value is 0.01.

**Restart Coupling:** Whenever a CFD airflow simulation is performed, a “\*.VAR” file will be saved in the same location as the PRJ file. The VAR file contains the airflow results of the last time step for which a CFD calculation was performed. Check this option to run a contaminant simulation using the steady airflow results contained in the VAR file.

**Output**

Set the CONTAMX Display Mode to the “Console window” option in order to view the CFD related simulation status. This option is available on the Output tab of the Simulation Parameters dialog box.

*NOTE – Save the CONTAM Project*

**Be sure to save a the CONTAM project file before you begin working with the CFDO Editor.**

### Step 3 – Setup CFD case in the *CFD0 Editor*

After setting up the CONTAM case, you should be sure to save the project file which for this case is “Demo\_CFD0.prj”. Now you will use the *CFD0 Editor* software to create a CFD input file for the CFD zone. CFD0 Editor provides a graphical user interface that enables you to coordinate the multizone and CFD aspects of your coupled simulation (see Figure 5).

The steps for using the CFD0 Editor include:

1. Import the CONTAM PRJ file to obtain the building components that are relevant to the CFD calculation, i.e., the CFD zone, interface paths and sources contained within the CFD zone.
2. Define the domain and mesh of the CFD zone.
3. Manage the CFD boundaries, i.e., establish the location and sizes of the interface paths and source.
4. Define the CFD simulation parameters.
5. Generate CFD input files for CONTAM.
6. View CFD zone simulation results.

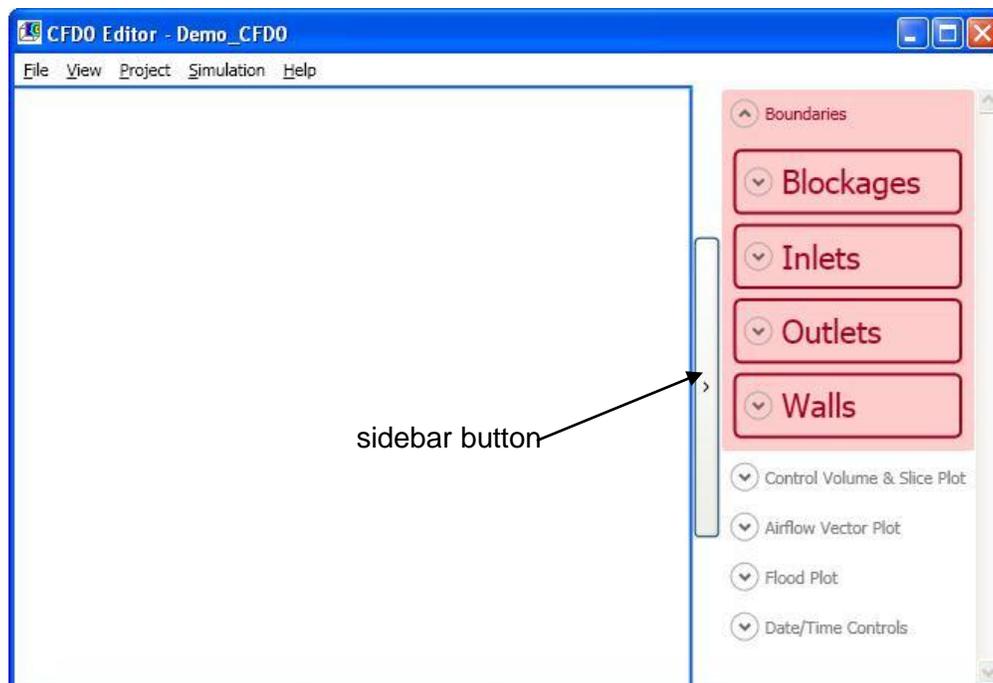


Figure 5 – CFD0 Editor

*NOTE – CFD0 Editor Controls*

*The Help menu provides a list of Keyboard Shortcuts for working with the CFD0 Editor.*

*A Show X, Y and Z axis*

*R Reset the view*

*Use the keyboard arrow keys or mouse to rotate the model. You can also use the following keyboard shortcuts to restrict the movement performed by arrow keys or mouse.*

*X,Y, Z Rotate about the associated axis*

*M Move closer or farther away (similar to zoom)*

*T Tilt camera left/right*

*P Pan the camera*

**Import CONTAM PRJ File**

Run the CFD0 Editor and import the CONTAM project via the **Project → Get Paths and Sources from CONTAM Project** menu command.

Select the file to import, “Demo\_CFD0.prj”. The CFD0 Editor will read the file and create a list of the *Interface Paths* and *Sources* with their CFD IDs. For each source defined in the PRJ file, the editor will prompt you to select whether the source should be considered a *Blockage* or *Wall* type. All of the sources in this project will be *Blockage* types. Once all the boundaries have been imported, they should appear in the *Blockages* and *Inlets* lists available in the sidebar that can be displayed by clicking the sidebar button located to the right of the CFD0 Editor window. There should be three blockages (S1, S2, S3) and six inlets (Path3 – Path8).

*NOTE – Blockage and Wall Source boundary types in CFD0 Editor*

*The size of a Blockage source should be non-zero in all three dimensions (X, Y, and Z). A Wall source can have a thickness of zero in one of the dimensions corresponding to the wall upon which it is located.*

**Define the CFD Domain**

The CFD domain describes the CFD zone of the project. The domain is made up of one or more regions containing control volumes or mesh. With this editor, you describe the regions via the *Control Volumes* dialog box shown in Figure 6 and accessed via the **Project → Edit Regions...** menu command. Select the *Add Region* button for each of the X, Y and Z Dimension tabs. The properties of each region are provided in Table 3

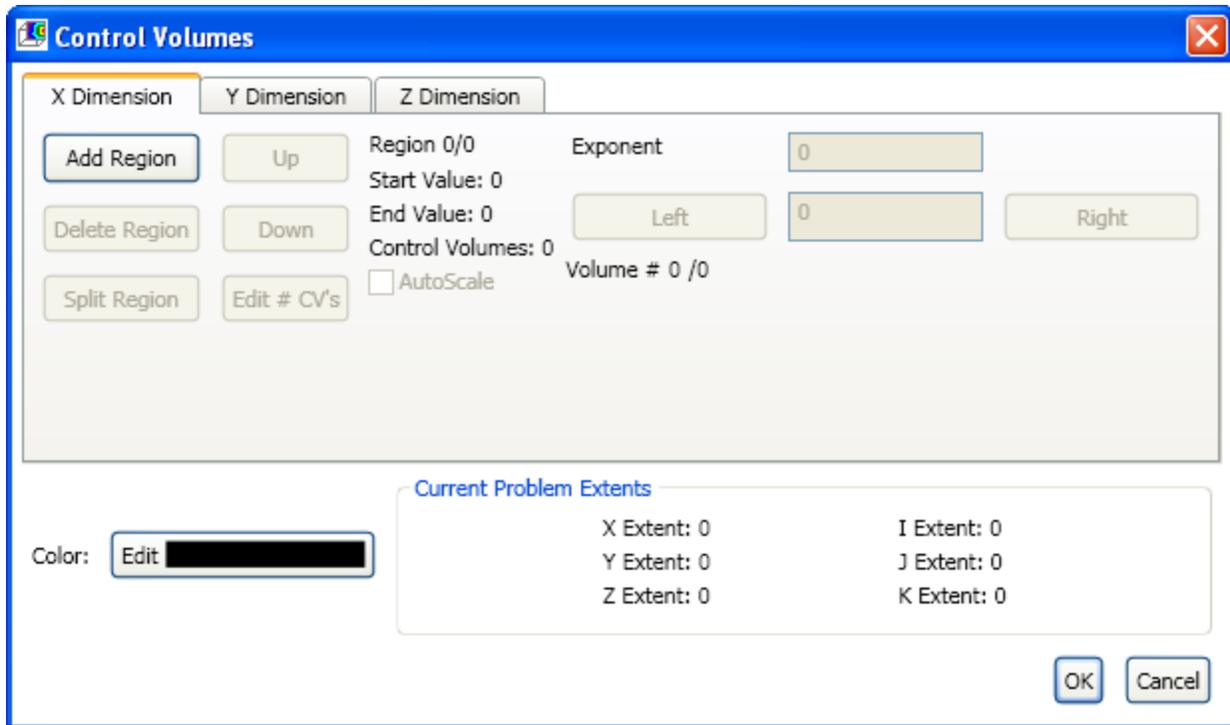


Figure 6 – Control Volume editing dialog of CFD0 Editor

*NOTE – Define a CFD Domain and Mesh*

*Add Region*

*Use the “Add Region” button in the X, Y, and Z Dimension tabs of the Control Volumes dialog box. Set the Start Value and End Value of the region and the number of Control Volumes (or grids) in each direction. The “Auto Scale” option will calculate the grid spacing based on the values you entered. You can add more regions as needed and navigate through them using the “Up” and “Down” buttons.*

*Dimensions*

*All dimensions are in units of meters.*

*Frame Properties*

*Use the Color control to adjust the appearance of the domain within the CFD0 Editor.*

The domain of this CFD zone consists of a single region of control volumes described in Table 3.

Dimension	Start [m]	End [m]	Control Volumes
X	0	10	42
Y	0	3	24
Z	0	3	24

Table 3 – CFD control volumes

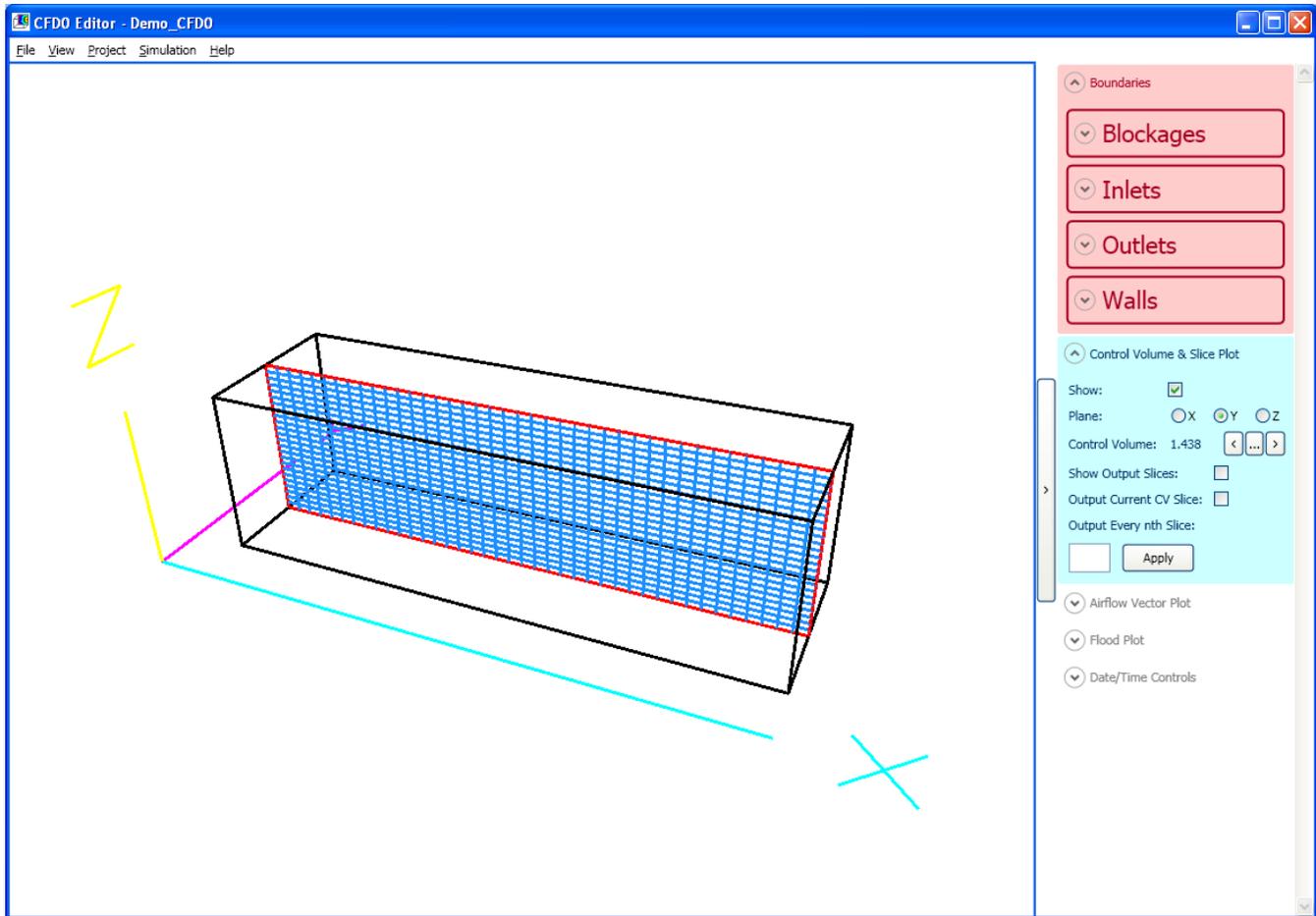


Figure 7 – CFD Domain (XZ plane) displayed in CFD0 Editor

Once you have defined a mesh, you can view it by displaying the *Sidebar*, the region to the right of the interface as shown in Figure 7, via the **View** → **Sidebar** menu command. Use the *Control Volume & Slice Plot* section of the *Sidebar* to turn the display on/off, control which axis of control volumes to display and to move the display along the axis normal to the plane being displayed.

*NOTE – Change Color and Frame of CFD Domain*

*In the CFD0 Editor GUI, the color and the frame of the CFD domain can be accessed by moving the mouse over the domain frame and pressing the Right Mouse Button. Click elsewhere on the screen to hide the dialog box. The Edit Region dialog can also be accessed from this pop-up dialog.*

### Manage CFD Boundaries

Boundaries refer to the *paths (Inlets and Outlets)* and *sources (Blockages and Walls)* associated with the CFD zone. All of the boundaries that were imported from the PRJ file should be listed in the *Boundaries* section of the sidebar. Select each boundary item in turn and click the “Edit” button (or double-click) to define the geometry of the boundaries by setting the *Start* and *End* locations in all three dimensions. Locations of the boundaries for this project are provided in Table 4 and Table 5. Once a boundary has been created, you can access its properties by right clicking on the item on the main screen of the editor.

Name	X (Start, End)	Y (Start, End)	Z (Start, End)
Path3	2.0, 3.0	3.0, 3.0	0.0, 2.0
Path4	7.0, 8.0	3.0, 3.0	0.0, 2.0
Path5	0.0, 0.0	2.5, 3.0	0.0, 2.0
Path6	10.0, 10.0	0.0, 0.5	0.0, 2.0
Path7	2.0, 3.0	0.0, 0.0	0.0, 2.0
Path8	7.0, 8.0	0.0, 0.0	0.0, 2.0

Table 4 – Inlet (coupled airflow path) coordinates in CFD0 Editor

Name	Block Type	X (Start, End)	Y (Start, End)	Z (Start, End)
S1	Solid	0.3, 0.4	2.45, 2.55	0.0, 0.1
S2	Solid	5.0, 5.1	0.3, 0.4	0.0, 0.1
S3	Solid	8.0, 8.1	2.0, 2.1	2.5, 2.6

Table 5 – Blockage (source) properties in CFD0 Editor

#### NOTE – Coupled paths and contaminant source properties

##### Location

*In a coupled simulation, the pressure/mass flow rate boundary condition of an opening and the source strength of a contaminant source are defined via ContamW. You only need to define the location of each path and source in the CFD0 Editor. You also need to provide heat generated (if any) from the blockage if the Energy calculation option is enabled via the Simulation Parameters of the CFD0 Editor.*

##### Blockage Type

*Use the Thermal property of a source blockage to define it to be either a fluid or solid type. The contaminant is generated from within every cell of a fluid blockage and from all the surfaces of a solid blockage. The fluid type is preferable.*

### Select Output Slices

You must select the CFD cells to be output by the CFD calculation. This is done via the *Control Volume & Slice Plot* controls in the sidebar. Check the “Show” and “Show Output Slices” check boxes. Select the Plane normal to the slices you want to output, enter a value in the “Output Every nth Slice” box and click the Apply button. For this case, all slices for all planes are output. The output planes should be displayed corresponding to the currently selected Plane button. Optionally, you can select to output the currently displayed control volume slice.

### Define CFD Simulation Parameters

Define the CFD calculation properties via the **Simulation → Simulation Parameters...** menu command. This will display the Simulation Parameters dialog box shown in Figure 8.

#### Run Control

The *Case Name* is automatically set when the CONTAM project is imported. It is the name of the PRJ file appended with the CFD Name of the CFD zone of the imported CONTAM project. For this case, uncheck the *Energy* box to treat the zone as isothermal. Set the *Airflow Convergence* criterion to 0.001 and leave the remaining values at their defaults.

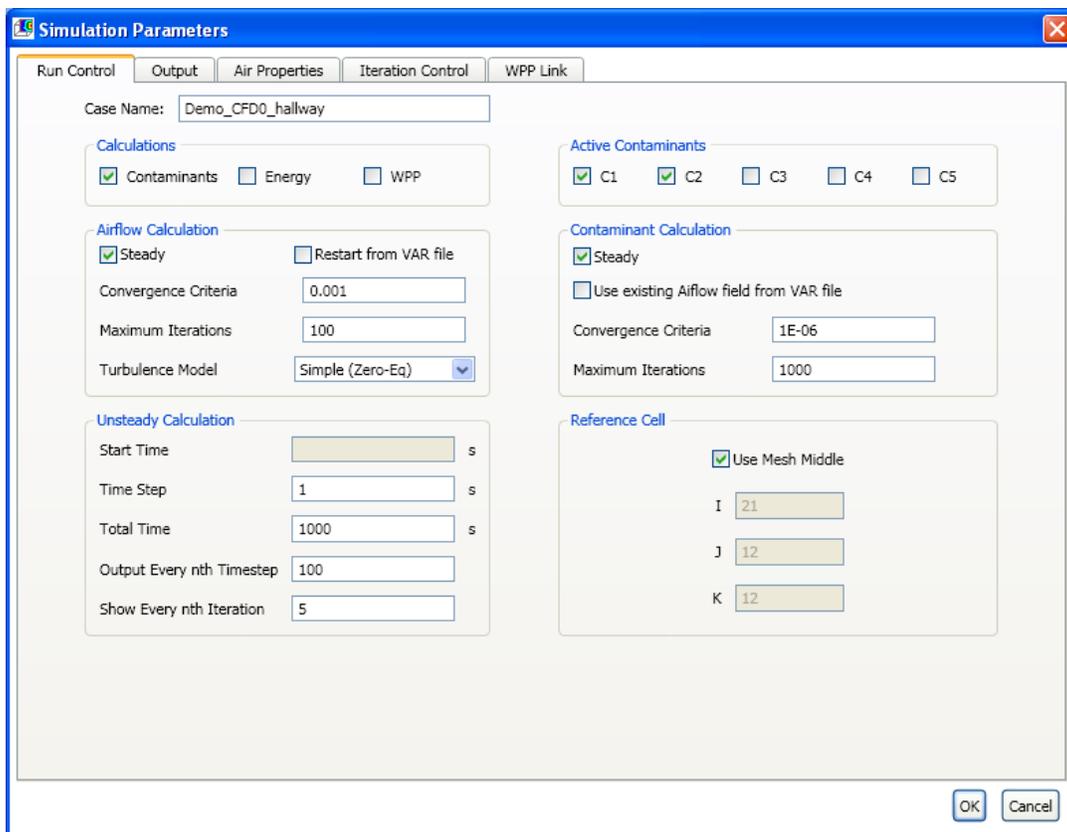


Figure 8 – Simulation Run Control parameters in CFDO Editor

*NOTE – Reference Cell and Monitoring Cell**Reference Cell*

*The pressure at this point in the CFD domain is used as a reference if there is no pressure boundary condition explicitly defined in the CFD simulation. For such a situation, the absolute value of pressure is not relevant, and only differences in pressure are meaningful.*

*Monitoring Cell (Simulation Parameters – Output)*

*The Monitoring Cell serves two purposes:*

- 1) The coupled simulation will set the Pressure and Contaminant Concentration of the CFD zone in CONTAM to the corresponding values at the monitoring point. These values can be used in the multizone regime as sensor input for a control network. These values will also be written to the multizone results file, i.e., the SIM file for the CFD zone.*
- 2) The values calculated at the monitoring point will be provided as the simulation status during a coupled simulation.*

*Location*

*Be sure neither the monitoring point nor the reference point is located inside a solid blockage.*

*Iteration Control*

Define the CFD0 Editor *Iteration Control* parameters as shown in Figure 9. Set the *Convection Scheme* to use the *Power Law* method for all parameters. The *False Time* and *Under-relaxation Factor* provide two different ways to stabilize the numerical iterations. A smaller *False Time Step* or *Under-relaxation Factor* will slow down and stabilize a calculation. The *False Time Step* is used only for steady-state calculations, allowing conservation equations to march with a different artificial time step so that all conservation equations reach steady state no matter what time step is used during the calculation. The *False Time Step* is useful when different conservation equations have different convergence characteristics. However, using *False Time Steps* may slow down the calculation after a certain number of iterations, at which point a change of *False Time Step* to a greater value may be necessary. This is done by enabling the option to *Change False Time After iteration* and providing a *New False Time Step*.

*NOTE – Iteration Control Parameters*

*For most of cases, the default values of the control parameters should work well. Sometimes, you may need to change either of the Convergence Factors or Maximum Iterations if the CFD calculation appears to be non-convergent.*

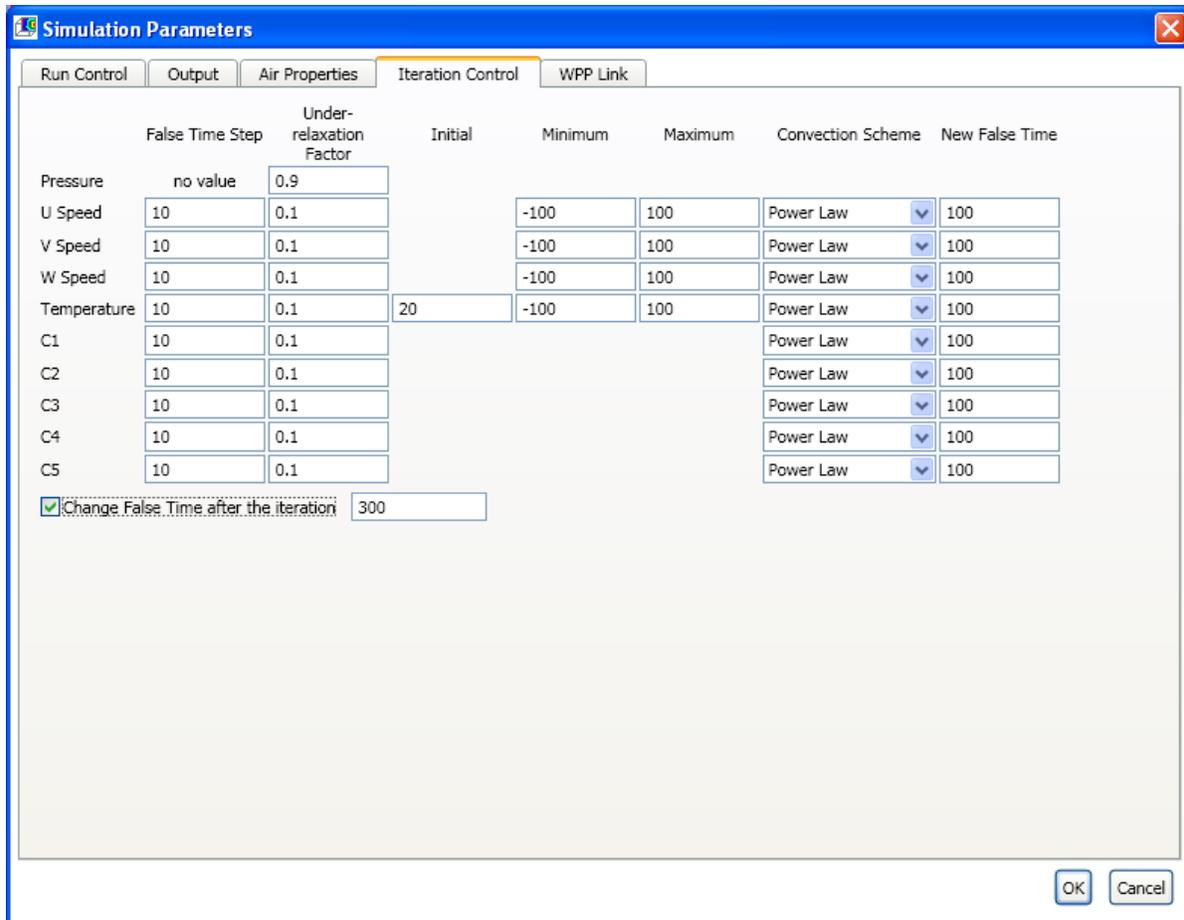


Figure 9 – Variable Iteration Control parameters in the CFD0 Editor

### Generate CFD Input Files for CONTAM

If you have not already done so, save the CFD0 project via the **File → Save Project As...** menu command and give it the name “Demo\_CFD0” and the file will be saved with the “CFD0” file extension.

When all of the CFD-related information has been set and the CFD0 project has been saved, you need to generate the input file needed by ContamX to perform the CFD-related calculations. Use the **Project → Generate CFD File for CONTAM** menu command. This will create a file having the same name as the *Case Name* with a “.cfd” file extension. The *Case Name* is generated by the CFD0 Editor and provided by the *Simulation Parameters* dialog box. The CFD file is a text file that can be viewed and edited with a text editor.

## Step 4 – Run Coupled Simulation with CONTAM

### Simulation Method

Once you have created the CFD input file for CONTAM, return to ContamW and set the CONTAM *Run Control* parameters accessible via the **Simulation → Set Simulation Parameters...** menu item and shown in Figure 10. Set the *Simulation Method* to perform a steady-state airflow and contaminant calculation. On the *Output* tab set the *CONTAMX Display Mode* to the *Console Window* option in order to monitor the progress of the CFD and coupled simulation.

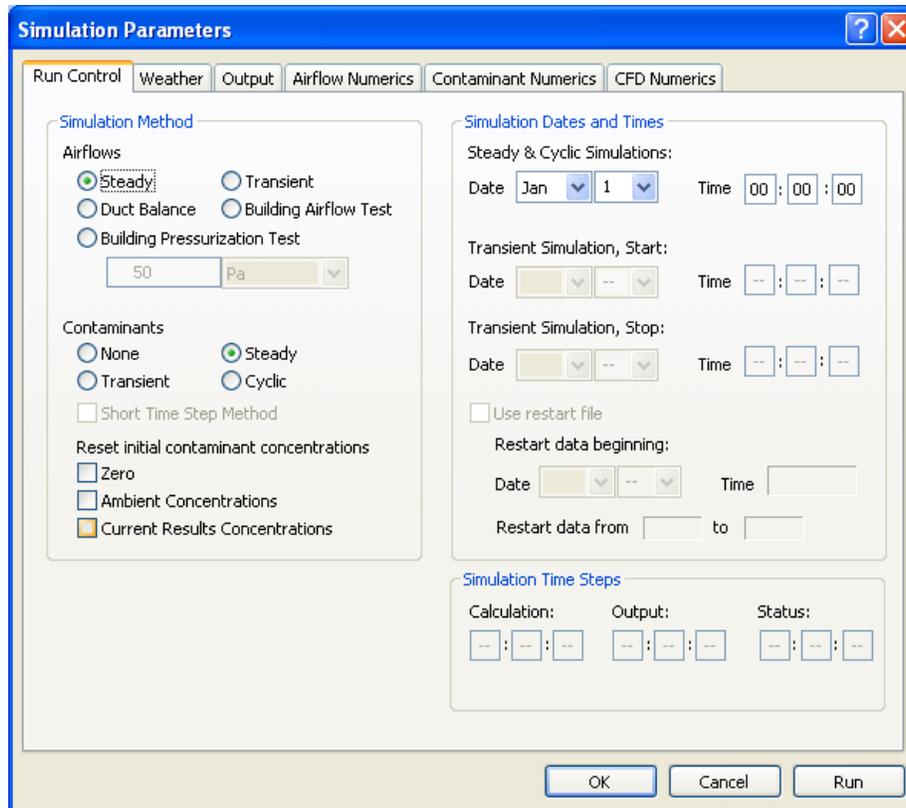
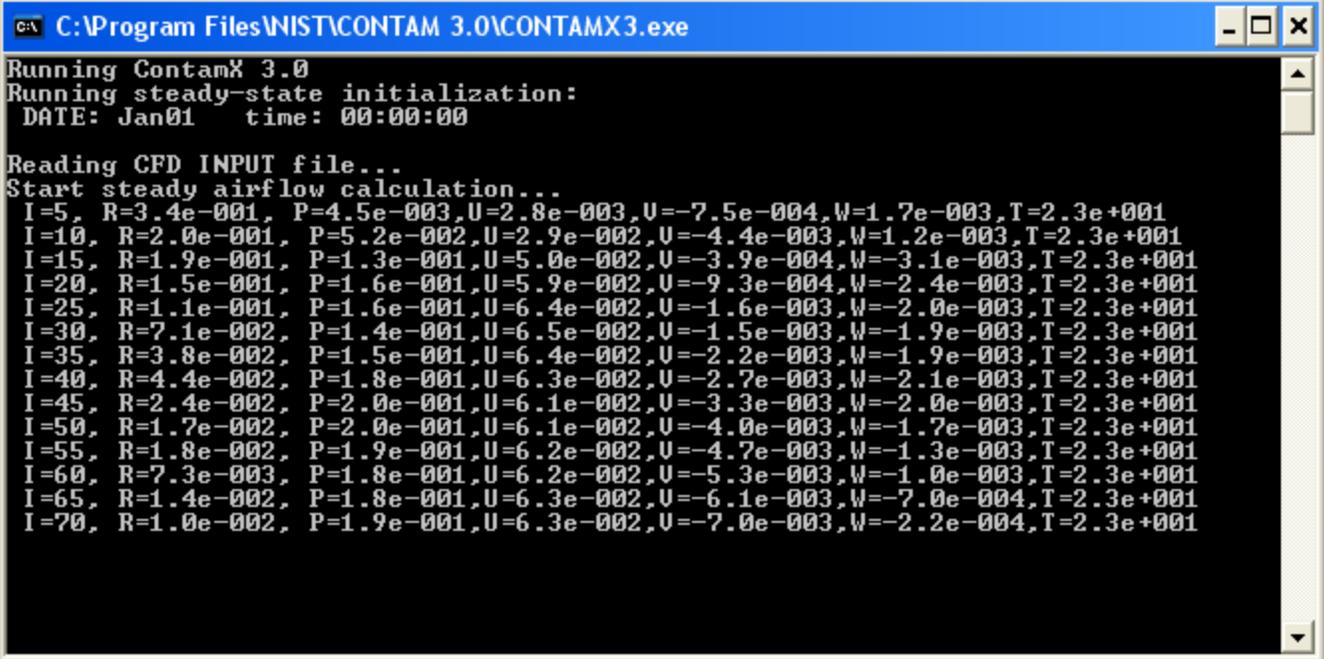


Figure 10 – ContamW Simulation Run Control Parameters

### Run Simulation

Run the simulation via the **Simulation → Run Simulation** menu command or pressing the *Run* button on the *Simulation Parameters* dialog box. A console window will display the simulation status as illustrated in Figure 11. This status will also be written to a file having the same name as the case with a “.bal” file extension, and coupling progress will be written to a file having the .CMO extension.



```
C:\Program Files\NIST\CONTAM 3.0\CONTAMX3.exe
Running ContamX 3.0
Running steady-state initialization:
DATE: Jan01 time: 00:00:00
Reading CFD INPUT file...
Start steady airflow calculation...
I=5, R=3.4e-001, P=4.5e-003, U=2.8e-003, V=-7.5e-004, W=1.7e-003, T=2.3e+001
I=10, R=2.0e-001, P=5.2e-002, U=2.9e-002, V=-4.4e-003, W=1.2e-003, T=2.3e+001
I=15, R=1.9e-001, P=1.3e-001, U=5.0e-002, V=-3.9e-004, W=-3.1e-003, T=2.3e+001
I=20, R=1.5e-001, P=1.6e-001, U=5.9e-002, V=-9.3e-004, W=-2.4e-003, T=2.3e+001
I=25, R=1.1e-001, P=1.6e-001, U=6.4e-002, V=-1.6e-003, W=-2.0e-003, T=2.3e+001
I=30, R=7.1e-002, P=1.4e-001, U=6.5e-002, V=-1.5e-003, W=-1.9e-003, T=2.3e+001
I=35, R=3.8e-002, P=1.5e-001, U=6.4e-002, V=-2.2e-003, W=-1.9e-003, T=2.3e+001
I=40, R=4.4e-002, P=1.8e-001, U=6.3e-002, V=-2.7e-003, W=-2.1e-003, T=2.3e+001
I=45, R=2.4e-002, P=2.0e-001, U=6.1e-002, V=-3.3e-003, W=-2.0e-003, T=2.3e+001
I=50, R=1.7e-002, P=2.0e-001, U=6.1e-002, V=-4.0e-003, W=-1.7e-003, T=2.3e+001
I=55, R=1.8e-002, P=1.9e-001, U=6.2e-002, V=-4.7e-003, W=-1.3e-003, T=2.3e+001
I=60, R=7.3e-003, P=1.8e-001, U=6.2e-002, V=-5.3e-003, W=-1.0e-003, T=2.3e+001
I=65, R=1.4e-002, P=1.8e-001, U=6.3e-002, V=-6.1e-003, W=-7.0e-004, T=2.3e+001
I=70, R=1.0e-002, P=1.9e-001, U=6.3e-002, V=-7.0e-003, W=-2.2e-004, T=2.3e+001
```

Figure 11 – Console display of coupled CONTAM+CFD simulation status

### Step 5 – Results

Simulation results are written to the .SIM file as with a normal CONTAM simulation, but the coupled simulation also creates output files that contains the detailed results of the CFD Zone. These files will have the same name as the *Case Name* having a .OUT extension and another file will have a .DAT extension. The SIM file can be viewed as usual via the ContamW interface. However, the zone pressure and contaminant concentration of the CFD zone will be the values at the monitoring point defined in CFD0 simulation parameters.

The OUT file can be viewed via the CFD0 Editor by using the **Project → Open Results File...** menu command. You will be prompted to select a .OUT file. CFD0 Editor enables you to view airflow vectors, airflow contours and concentration contours. Figure 12 shows an example of a contour plot of contaminant concentration within the CFD zone. The .DAT file can be viewed using Tecplot.

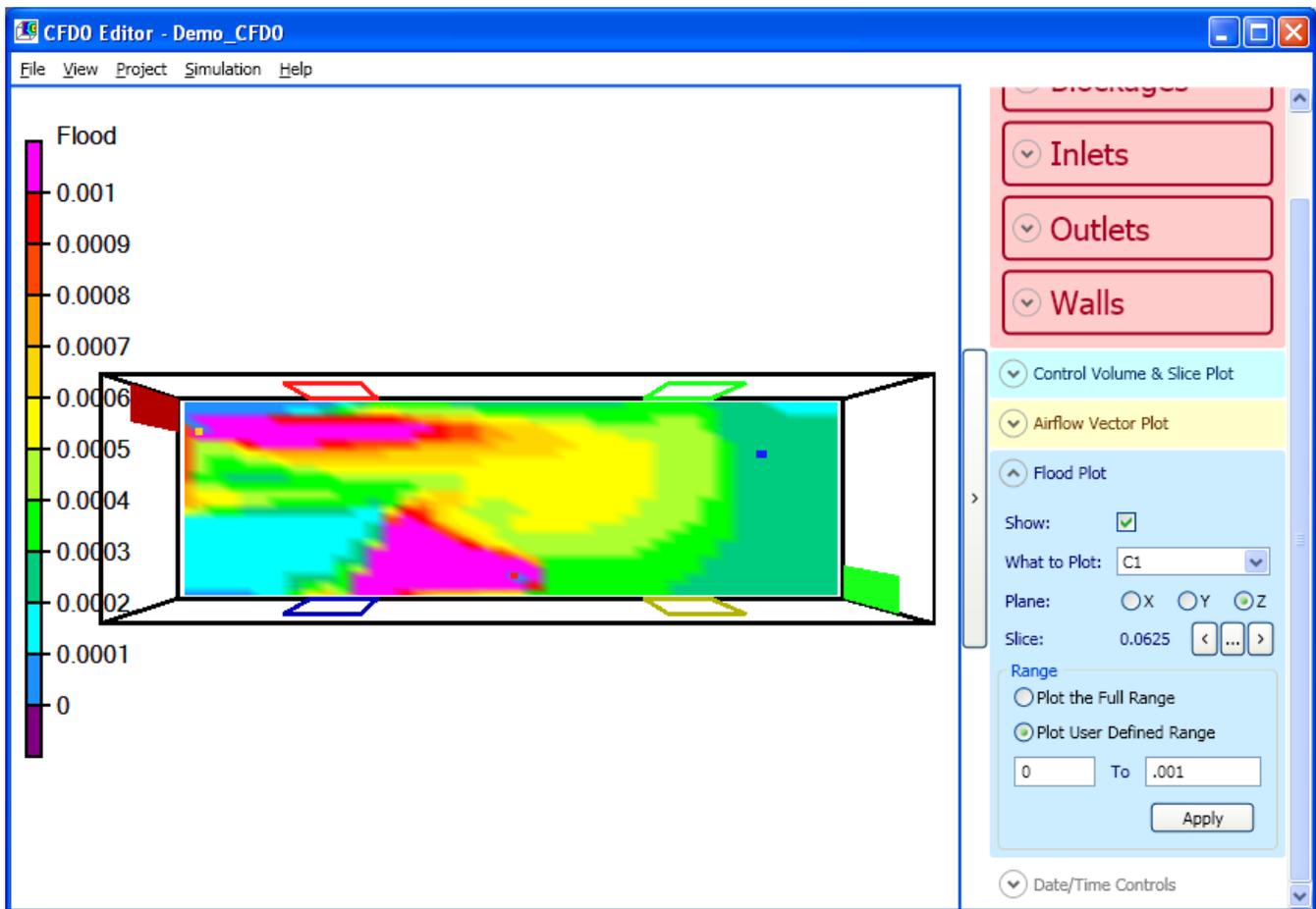


Figure 12 – Contaminant concentration results in CFD0 Editor

## Conclusion

This case of the tutorial presented the *interior-zone coupling* between CONTAM 3.0 and the CFD Editor. The case is a simple 3-D office suite with multiple zones naturally ventilated at steady state. You can modify this case to perform transient simulations or add a control network. To learn more about coupled multizone and CFD and the zero-equation turbulence model please refer to the references provided in the following bibliography.

## Bibliography

Axley, J.W. and D.H. Chung, *Zone Resistance in Embedded CFD Modeling*, in *RoomVent 2004*. 2004: University of Coimbra - Portugal.

Axley, J.W. and D.H. Chung, *POWBAMO Mechanical Power Balances for Multi-zone Building Airflow Analysis*. *International Journal of Ventilation*, 2005. **4**(2).

Chen, Q. and W. Xu (1998). *A zero-equation turbulence model for indoor airflow simulation*. *Energy and Buildings* **28**: 137-144.

Srebric, J., Chen, Q., and Glicksman, L.R. 1999. *Validation of a zero-equation turbulence model for complex indoor airflows*, *ASHRAE Transactions*, 105(2), 414-427.

Wang, L. and Q. Chen, *Theoretical and Numerical Studies of Coupling Multizone and CFD Models for Building Air Distribution Simulations*. *Indoor Air*, 2007. **17**: p. 348-361.

Wang, L. and Q. Chen, *Validation of a Coupled Multizone and CFD Program for Building Airflow and Contaminant Transport Simulations*. *HVAC&R Research*, 2007. **13**(2): p. 267-281.

Wang, L., *Applications of a Coupled Multizone and CFD Model to Calculate Airflow and Contaminant Dispersion in Built Environment for Emergency Management*. *HVAC&R Research*, 2008.

Wang, L. and Q. Chen, *Evaluation of some assumptions used in multizone airflow network models*. *Building and Environment*, 2008. **43**: p. 1671-1677.

Zhai, Z., et al., *Evaluation of various turbulence models in predicting airflow and turbulence in enclosed environments by CFD: part-1: summary of prevalent turbulence models*. *HVAC&R Research*, 2007. **13**(6): p. 853-870.

Zhang, Z., et al., *Evaluation of various turbulence models in predicting airflow and turbulence in enclosed environments by CFD: part-2: comparison with experimental data from literature*. *HVAC&R Research*, 2007. **13**(6): p. 871-886.

## CASE 2: Exterior-Zone Coupling

This tutorial utilizes a case study to present the tools and methods required to implement the *exterior-zone coupling* between CFD0 and CONTAM. CFD simulations of external airflows around a building are performed for various wind directions. These simulations are then used to generate wind pressure coefficient profiles for use within CONTAM. These coefficients are specific to each envelope flow path as opposed to the surface-averaged coefficients as presented in Chapter 24 of (ASHRAE 2009). This external coupling method was presented in the journal article (Wang 2010) which provides insight into the applications of this method. Further details of the coupled CFD/multizone modeling capabilities including CFD0 input and output files are provided in Dr. Wang's Thesis (Wang 2007). The following is an outline of the method.

1. Create CFD0 case with *CFD0 Editor* program
  - Define simulation region and flow inlet boundaries
  - Define building blockages
  - Define mesh
  - Set WPP simulation parameters
2. Run *CFD0* simulation
3. Create CONTAM case with *ContamW* program
  - Define external airflow paths and their locations / coordinates
  - Generate path location data (.PLD) file
4. Generate CONTAM wind pressure coefficient library (.LB2) file
  - Review CFD0 simulation results
  - Run *WPCTranslator.exe* program to generate an .LB2 file from the WDB file
5. Associate wind pressure profiles with associated CONTAM airflow paths
  - Import .LB2 file into CONTAM .PRJ file
  - Edit paths to select corresponding wind pressure coefficient profiles
6. Run CONTAM simulations
  - Verify wind pressures via Wind Pressure view
  - Set steady state wind direction or use .WTH file to set wind speed and direction for transient simulations

## Demonstration Case

This case is based on that which was presented by (Holmes and Morawska 2006). It consists of a rectangular one-story house with a low-sloped roof. Two CONTAM .PRJ files are available: *demo-cfd-wpp-sc.prj* implements the wind pressure coefficient profiles presented in (Swami and Chandra 1987) and *demo-cfd-wpp.prj* that is based on the external coupling method presented herein. All of the files associated with this case are provided in their final form.

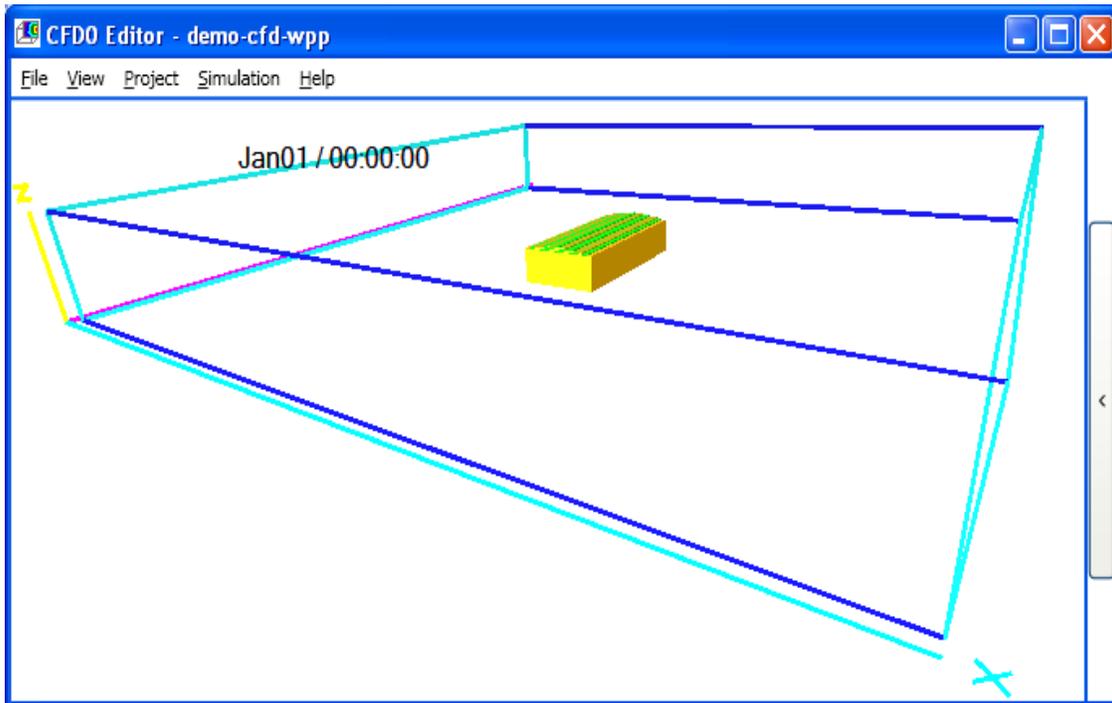


Figure 13 - CFDO Editor display of simulation region and blockage representation of the building

1. Create CFDO case with the *CFDO Editor* (see *demo-cfd-wpp.cfd0*). Note that the .CFDO file is a text file that can be viewed and edited with a text editor (but should be edited with caution).
  - a. Create a large region (via the **Project** → **Edit Regions...** menu item) that includes the entire external flow field of interest. In this case the region is 70 m x 70 m x 9 m in the X, Y and Z dimensions, respectively.
  - b. Create Inlet type boundaries on all four sides of the region (named North, South, East and West in the example).
  - c. Create a Blockage type boundary named "REFBLOCK" corresponding to the bottom rectangular portion of the building envelope. A Blockage named "REFBLOCK" is required by the *WPCTranslator* program that will create a set of wind pressure coefficient profiles from the results of the external CFD calculation.
  - d. Add roof Blockages to approximate a sloped roof (named Roof-1, 2, 3, 4 and 5 in the example).
  - e. Sub-divide the regions to define the mesh. The mesh boundaries should align with the house blockages in order for the *WPCTranslator* to properly identify the locations of the CONTAM airflow paths on the building surface. This alignment can be verified by close examination of the

mesh via the *Control Volume & Slice Plot* tool provided in the Side Bar of the *CFD0 Editor* as shown below.

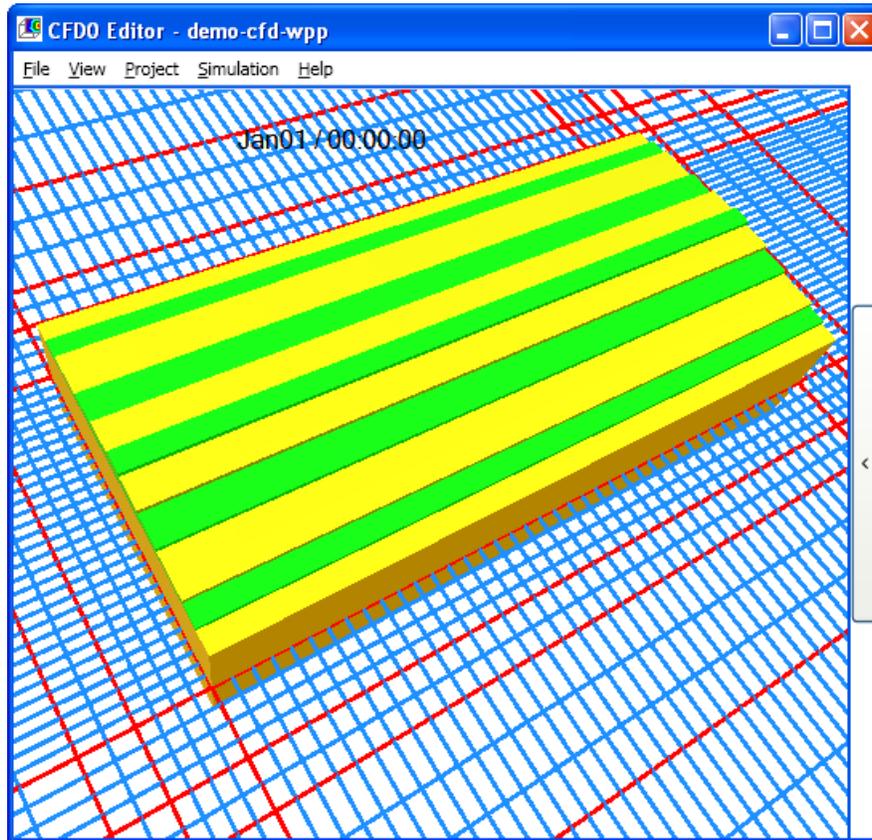


Figure 14 - CFD0 Editor display of z-plane control volumes

- f. Set WPP simulation parameters (via the **Simulation** → **Simulation Parameters...** menu item)
  - i. Run Control – Define the case name “demo-cfd-wpp”. This will be the name of all the output files having various extensions associated with them. Check the WPP box. Set the Reference Cell to ensure that it is not located within a blockage.
  - ii. Output – Set the monitoring cell to ensure that it is not located within a blockage.
  - iii. Iteration Control – Relaxation parameters of CFD0 are defaulted for indoor airflow calculations. These parameters are not generally acceptable for external flow modeling. Adjust the relaxation factors as follows: Pressure 0.2; U, V & W to 0.8. These factors may not provide absolute convergence and may need to be adjusted if maximum iterations are exceeded. In such cases, the BAL file should be reviewed for residual behavior and the “steadiness” of the properties of the monitoring points.
  - iv. WPP Link – Set the wind velocity profile parameters and wind angle data.
2. Run CFD0 simulation
  - a. This can be done directly from within CFD0 Editor via the **Simulation** → **Run CFD0** menu item.
  - b. You can also generate a .CFD file via the **Project** → **Generate CFD File for CONTAM** menu item, and then run *CFD0.exe* via by dragging and dropping the .CFD file onto the executable via Windows Explorer.

- c. Review simulation convergence behavior to ensure that “reasonable” results have been obtained. You can also review the results obtained for the first wind angle via the *CFD0 Editor* (shown in following figure) and review results in more detail by opening the .DAT file with Tecplot. If the results for any of the wind angles are non-convergent, you can delete the associated .VAR files, adjust the iteration parameters, and rerun the WPP simulation. The calculation will only be performed for those cases for which the associated .VAR files are missing.

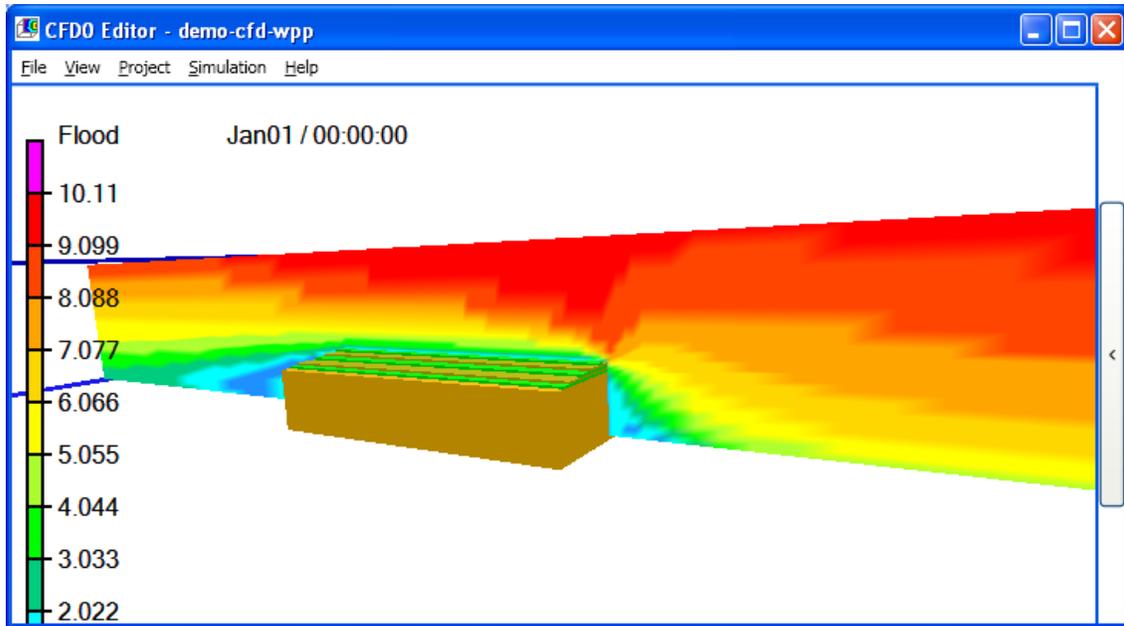


Figure 15 - CFD0 Editor display of velocity results for 0 degree wind angle

- 3. Run ContamW and open *demo-cfd-wpp.prj*
  - a. Note coordinates of the envelope airflow paths

path#	X	Y	Z
1	2.500	15.500	1.500
2	4.500	15.500	1.500
4	0.000	15.000	1.000
5	7.400	14.000	1.500
8	7.400	10.000	1.500
9	0.000	11.700	1.500
11	0.000	9.000	1.500
12	7.400	7.500	1.500
14	0.000	7.500	1.500
16	7.400	6.000	1.500
23	0.000	4.000	1.500
26	7.400	2.000	1.500
28	1.500	0.000	1.500
29	4.200	0.000	1.500
30	6.000	0.000	1.500

- b. Generate a path location data (.PLD) file
    - i. From the main menu choose **Weather → Create WPC**
    - ii. Set the origin of Coordinate Transformation Data to correspond to the location of REFBLOCK in the CFD0 case (31.3, 27.25, 0 for this case).

- iii. Click the **Generate PLD File** button

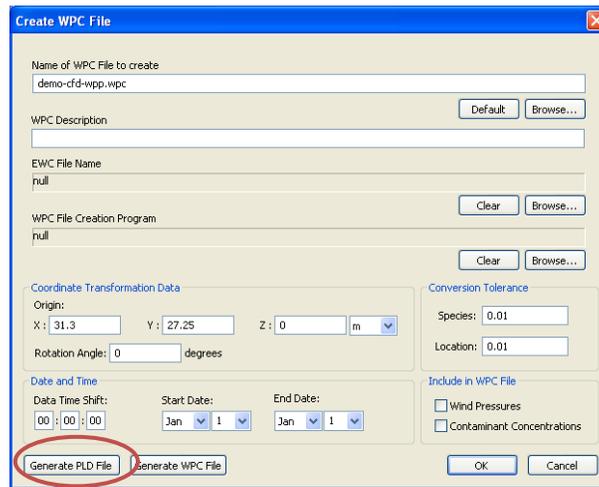


Figure 16 - ContamW Create WPC File dialog box

4. Use the *WPCTranslator.exe* program to generate a CONTAM wind pressure profile library file ***demo-cfd-wpp.lb2***.
  - a. Run the *WPCTranslator.exe* console application.
  - b. Respond to the prompts as follows:
    - i. Create WPC link from CFD0/FDS or ewc link from CFD0? CFD0=1; EWC=2; FDS=3:  
Type **1** then **Enter**
    - ii. Create WPC link file=1, or ambient contaminant link file=2:  
Type **1** then **Enter**
5. Set wind pressure profiles for envelope flow paths in ContamW
  - a. Run ContamW and open ***demo-cfd-wpp.prj***.
  - b. Import the .LB2 library file via the **Data → Wind Pressure Profiles...** menu item.
  - c. Edit the airflow path properties of each envelope flow path to set the Variable Pressure Data on the Wind Pressure. Select the Profile Name for the profile associated with the current path from the list of available profiles. NOTE that the path names generated by the WPCTranslator do not necessarily correspond to the numbers of the airflow paths in CONTAM (or the .PLD file). You must ensure that you make your selections based on the location information as provide in the .PLD file.
6. Run CONTAM simulations
  - a. Set the Wind Pressure Display of the Weather properties to check the wind pressure data via the SketchPad. Use the Wind Pressure view mode.
  - b. A CONTAM weather (.WTH) file is provided that sets the wind direction to 15 degree intervals every hour for a single day. You can run a transient simulation with this file to see the wind pressure vary as the wind direction varies through 360 degrees over 24 hours. You can do the same with the ***demo-cfd-wpp-sc.prj*** case and compare the wind pressures and air change rates for both cases.

## References

ASHRAE (2009). Fundamentals Handbook. Atlanta.

Holmes, N. S. and L. Morawska (2006). "A review of dispersion modeling and its application to the dispersion of particles: An overview of different dispersion models available." Atmospheric Environment **40**: 5902-5928.

Swami, M. V. and S. Chandra (1987). Procedures for Calculating Natural Ventilation Airflow Rates in Buildings. Atlanta, ASHRAE.

Wang, L. (2007). Coupling of Multizone and CFD Programs for Building Airflow and Contaminant Transport Simulations. Lafayette, Purdue University. **PhD**.

Wang, L. (2010). "Using CFD Capabilities of CONTAM 3.0 for Simulating Airflow and Contaminant Transport in and around Buildings." HVAC&R Research **16**(6).