Exploring inhaled air-particle-vapor mixtures in the Human Respiratory System with Ansys Fluent® simulations

Part 4: Pre-Processing Ansys Fluent Solver Setup (Single Phase Flow, DPM, and Species Transport)

Yu Feng, Ph.D.

Developed by CBBL at Oklahoma State University

Edited by the Ansys Academic Development Team

education@ansys.com

Ansys Software Used

This tutorial segment uses Ansys Fluent®, the fluid simulation software.

Learning Goals

In this tutorial segment, we will cover:

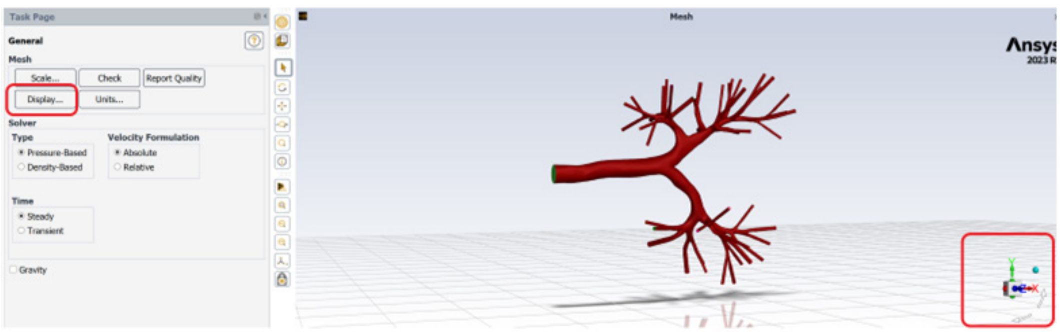
- Physics and Solver Settings in Ansys Fluent Solver
    - » Material Properties
    - » Boundary Conditions
- Solver Settings
- Simulation Setup

Open Ansys Fluent Software in Solution Mode

To read the CFD mesh:

File→Read→Mesh→Choose the .msh.h5 file generated in Ansys Fluent Meshing.

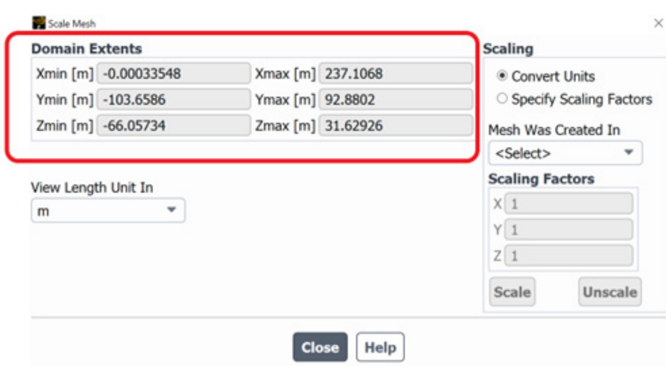
Domain→Mesh→ Display can be used to visualize the geometry



Note: Visualizing the geometry and the coordinates is necessary for the scale check in the next step and to set up the gravitational direction properly. This is to ensure that the geometric dimension and unit when the mesh is imported are correct.

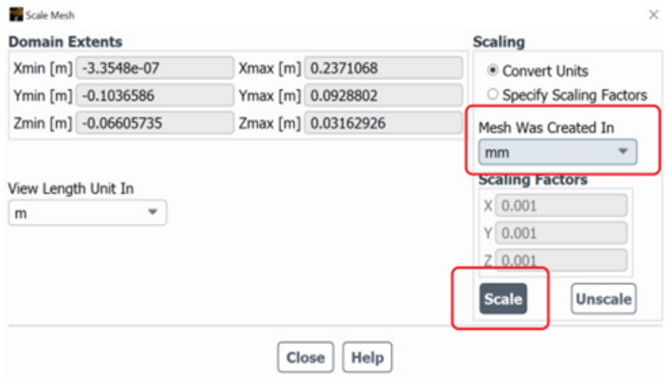
Check the scale of the geometry:

Domain→Mesh→Scale



You may initially observe that the distance along the x-direction (from head to foot) is approximately 240 meters, which is incorrect. The length of the trachea is typically around 100 millimeters. This discrepancy indicates that the unit used by the Ansys Fluent Solver to import this geometry is meters instead of the correct unit, which should be millimeters. Therefore, it is necessary to properly scale the geometry:

Domain→Mesh→Scale→Set "Mesh was created in" as "mm"→Click "Scale" (see the setup as shown in the snapshot below).



Set the gravity direction:

Task page→Check "Gravity"→Enter "9.81" in x-direction of "Gravitational Acceleration", the unit should be in m/s^2

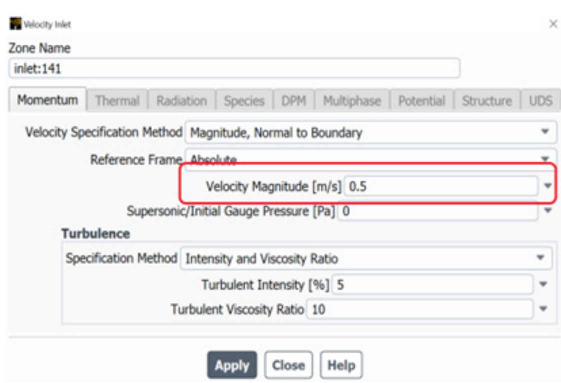
Steady-State Airflow Simulations

We will first run a steady-state airflow field simulation. We will follow the outline view menu and work from the top to the bottom to set up the laminar steady-state simulation for airflow first.

Models→Viscous→Laminar (since the inhalation flow rate is 6 L/min and the Reynolds number is around 500)

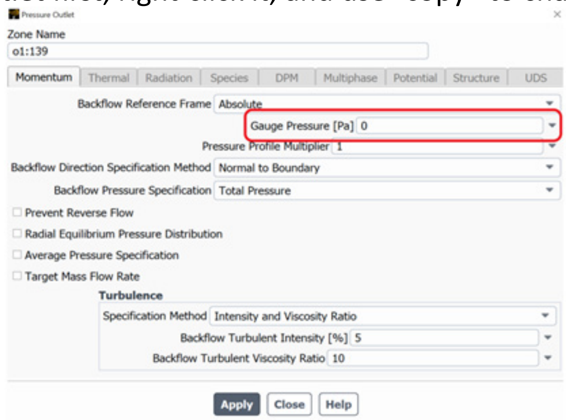
Materials→Fluid→Make sure the fluid material is "Air".

Boundary conditions→Inlet:141→Change the type to Velocity Inlet→Double click inlet: 141→Momentum→Velocity Magnitude→type "0.5" which is 0.5 m/s responding to 6 L/min

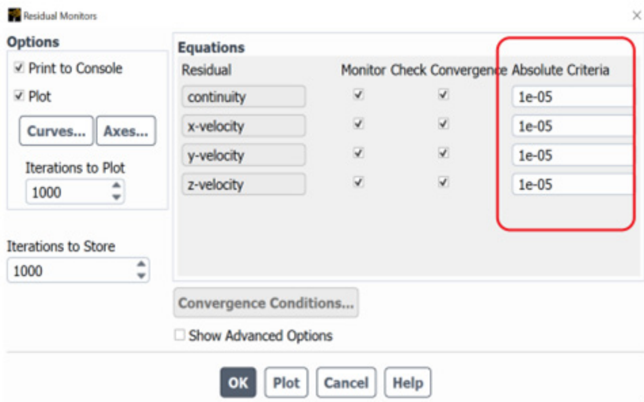


Boundary conditions→Outlet→change all outlet surfaces named “o**” type to “pressure outlet”→ Set “Gauge Pressure” to 0 for all outlets

Note: You can change one outlet first, right-click it, and use “copy” to change the rest.

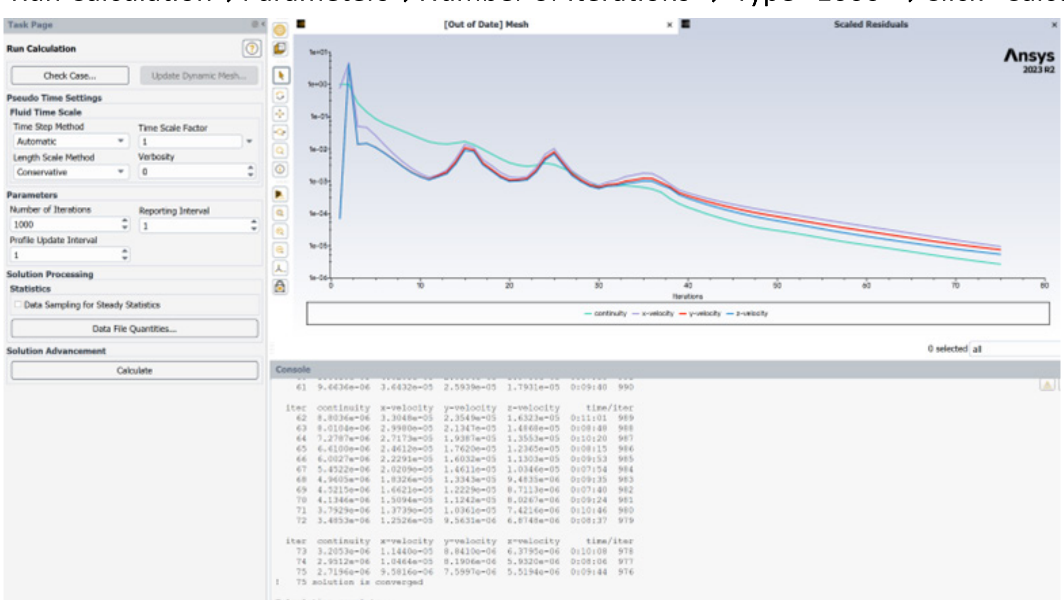


Solution→Monitors→Residual→Equations→Set all “Absolute Criteria” of residuals to 1e-5 instead of the default value 1e-3



Solution→Initialization→Hybrid Initialization→More Settings→Change “Number of Iterations” to 20→Click OK→Click “Initialize”

Solution→Run Calculation→Parameters→Number of Iterations → Type “1000”→Click “Calculate”



You can then monitor residuals in the GUI. It took approximately 80 iterations to converge.

You can write the case and data files: File→Write→Case and Data

Note: The steady-state airflow simulation case and data are saved and named “Airway After Setup Steady-State Airflow.cas.h5” and “Airway After Setup Steady-State Airflow.dat.h5”

The post-processing of the steady-state airflow field will be covered in the next segment (Part 5)

Particle Transport Simulations using Discrete Phase Model (DPM)

Since we will run particle transport in transient style, we need first to change the simulation to transient simulation.

Open “Airway After Setup Steady-State Airflow.cas.h5” and “Airway After Setup Steady-State Airflow.dat.h5”

Read “Airway After Setup Steady-State Airflow.dat.h5”

Note: Since we will apply a one-way Euler-Lagrange model (one-way DPM) in this tutorial, which means that the airflow field will not be influenced by the presence of particles, we can read the steady-state airflow field and do not need to update the airflow field during the DPM simulation. The one-way coupled DPM is based on the assumption that the particle volume fraction is low (dilute particle suspension). For dense particle suspension, two-way coupled DPM needs to be employed (Feng et a., 2021).

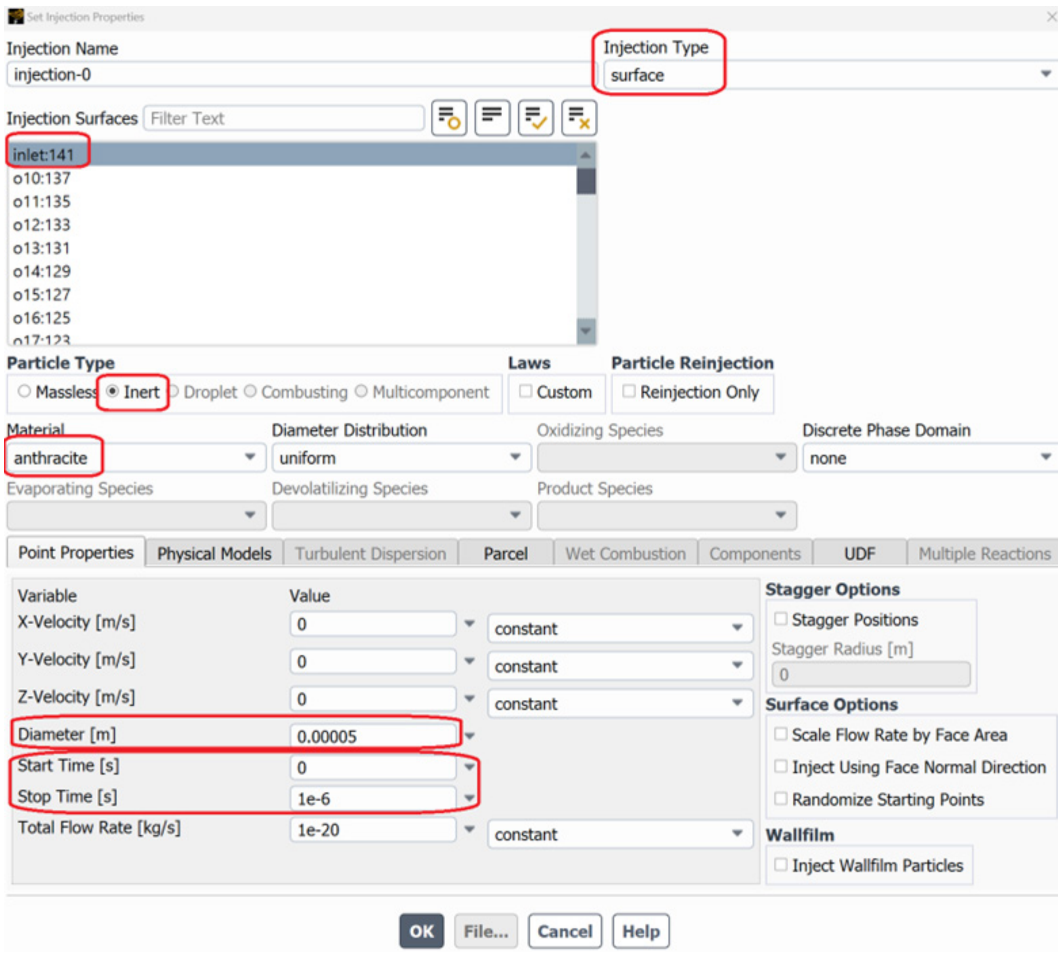
Task Page → General → Time → Change to “Transient”

Enable DPM Model and Define Particle Injection

Model→Discrete Phase→Max. Number of Steps→Change it to 5000

Model→Discrete Phase →Physical Models→We do not enable any of the forces listed in this tab in this tutorial for simplicity, but you may need to enable some of them based on ROMA and Eq. (6) discussed in Part 2. Without enabling those forces listed in this tab, only drag force and gravity will be considered.

Create particle injection through the inlet: Model→Discrete Phase→Injection→Create→The window shown in the snapshot below will pop up, please follow the setup in the snapshot to set a particle injection through inlet.



Note: The setup for this injection is for spherical particles with diameter equal to 5 µm and injection between t=0s and t=1e-6 s.

Define the drag la Model→Discrete Phase →Injection→injection-0→Physical Models→For simplicity, we choose " spherical" in Drag Law.

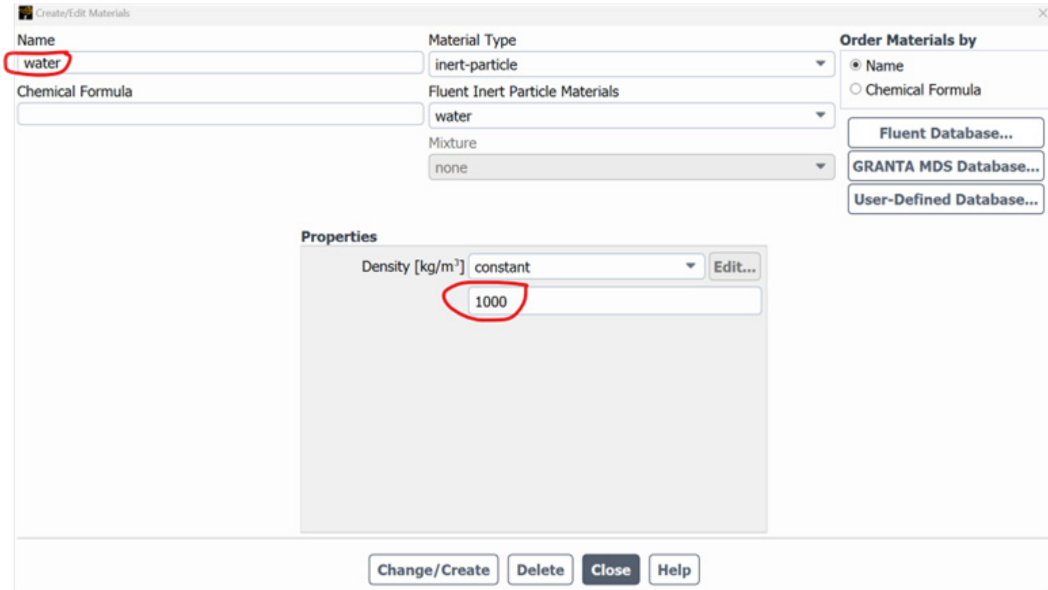
Note: It is worth mentioning that the Cunningham factor may need to be enabled for small particles. If you need to do so, please either choose "Stokes Cunningham" in Drag Law or use UDF "DEFINE_DPM_DRAG".

Click "OK".

Now you may see the Discrete Phase model status changed from "off" to "on". We can now define the inert particle material properties.

Define Particle Material Properties

Materials→inert Particle→double click “anthracite”→change the name to “water” and change the density for the particles to “1000”→Click “Change/Create”→click “Close” (see snapshot below).



Note: The reason we need to change the particle density to water density is based on the assumption that the particle diameter is aerodynamic diameter.

Note: (1) Particle time step can be precisely controlled using UDF “DEFINE_DPM_STEP” (can be hooked in Discrete Phase Model→UDF→DPM Time Step), which is not covered in this tutorial. (2) For particle injection setup, it is highly recommended to use “file” injection with a .inj file. This will allow the researcher to fully control how many particles will be inhaled. The particle number density must be sufficiently high to reach particle number density independent” of the particle deposition pattern. Details can be found in Feng et al. (2021).

Set DPM Boundary Conditions

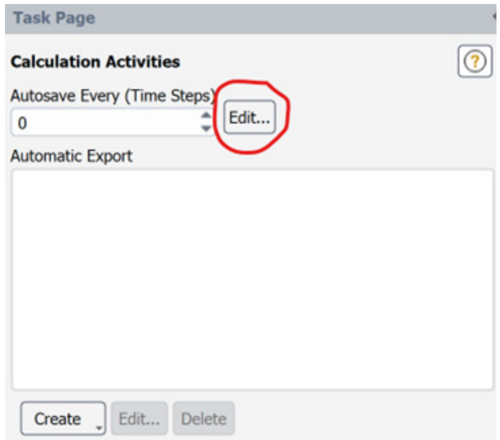
Boundary Conditions→Inlet→Click “inlet:141”→Click “DPM” tab→Choose “escape” in “Discrete Phase BC Type”→Click “Apply”

Boundary Conditions→Outlet→Click “DPM” tab→Choose “escape” in “Discrete Phase BC Type”→Click “Apply”

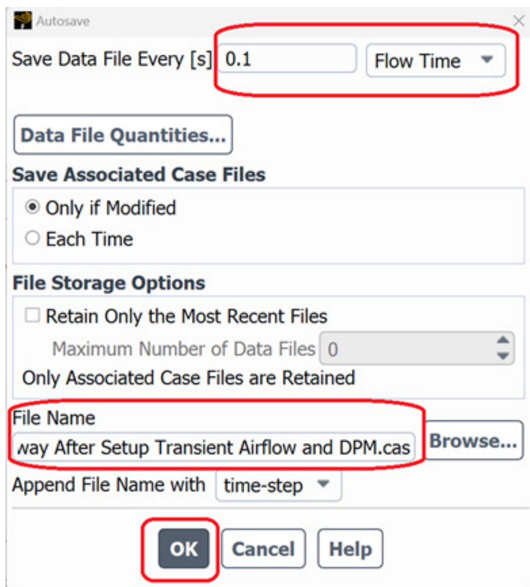
Boundary Conditions→Wall→Click “wall:51”→Click “DPM” tab→Choose “trap” in “Discrete Phase BC Type”→Click “Apply”

Save Transient Simulation Data

Outline View→Solution→Calculation Activities→Autosave→Calculation Activities→Click "Edit" (see the snapshot below)



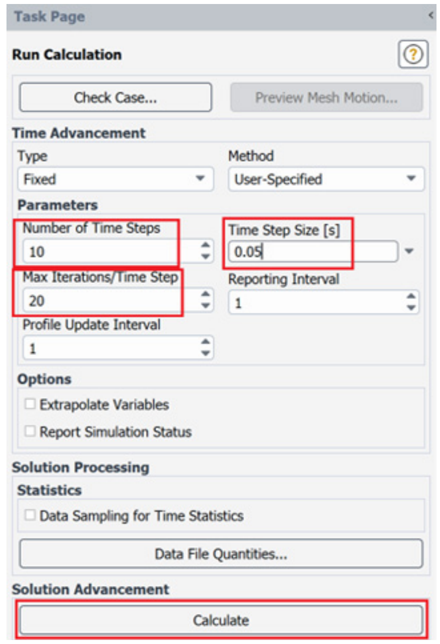
A new "Autosave" window will pop up (see snapshot below). Please follow the setup shown in the snapshot below, and click OK. The setup is to save the data every 0.1 s.



Note: Make sure the file name in "Autosave" window has the correct working directory with the .cas file.

Run Simulation

Outline View→Solution→Run Calculation→Follow the setup shown in the snapshot below and click "Calculate".



You should then have five .dat files at different flow time stations (t=0.1, 0.2, 0.3, 0.4, 0.5 s) named "Airway After Setup Transient Airflow and DPM-1-***.dat". It will also save a new case named "Airway After Setup Transient Airflow and DPM-1.cas".

Gas Species Advection and Diffusion Simulation using User-Defined Scalar (UDS)

In this section, we will work on a transient simulation case to simulate the transport and absorption of inhaled gas/vapor species as a second continuous phase, other than air. The gas/vapor species mass fraction will be modeled using a user-defined scalar (UDS) and the scalar transport equation (Feng et al., 2021) (also see Eq. (10) in Part 2).

To be more specific, the UDS will be created in this section, representing the nondimensionalized mass fraction of nicotine vapor (Sperry et al., 2023). The nicotine vapor (assuming no condensation) is assumed to be in excess air during transport. The binary diffusivity of nicotine in great excess of the air at body temperature (i.e., 37 °C or 310.15 K) can be then given as 0.695e-5 m^2/s (Sperry et al., 2023)

Open Ansys Fluent

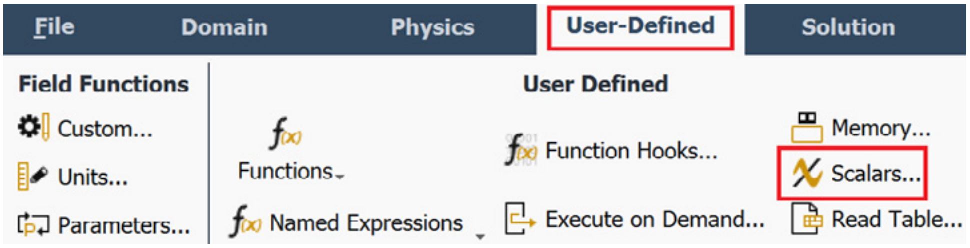
File→Read→Case and Data → Choose "Airway After Setup Steady-State Airflow.cas.h5". This step will allow us to start from the steady-state airflow simulation setup and result.

Outline View→General→Task Page→ Change to "Transient" in "Time"

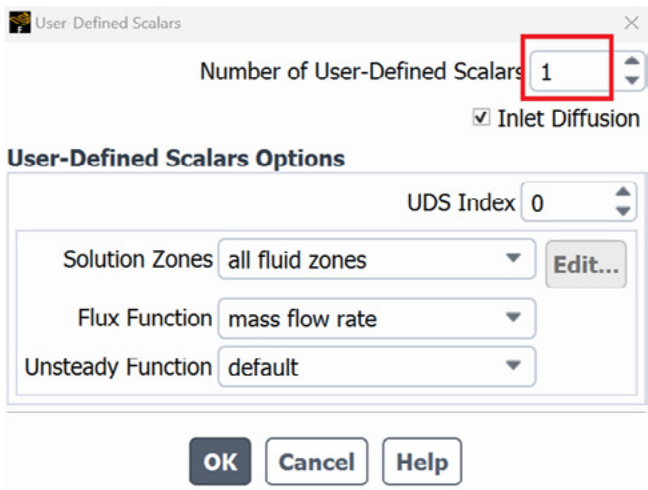
Note: The gas/vapor simulation in this section can be also integrated into the DPM simulation case, and the simulation of air, gas/vapor, and particles can be conducted simultaneously. However, for the simplicity purpose of this tutorial, we start from "Airway After Setup Steady-State Airflow.cas.h5" instead of "Airway After Setup Transient Airflow and DPM-1.cas".

Enable Scalar Transport Equation and UDS

Enable UDS that governed by Eq. (10) in Part 2: User-Defined→Scalars (see snapshot below)



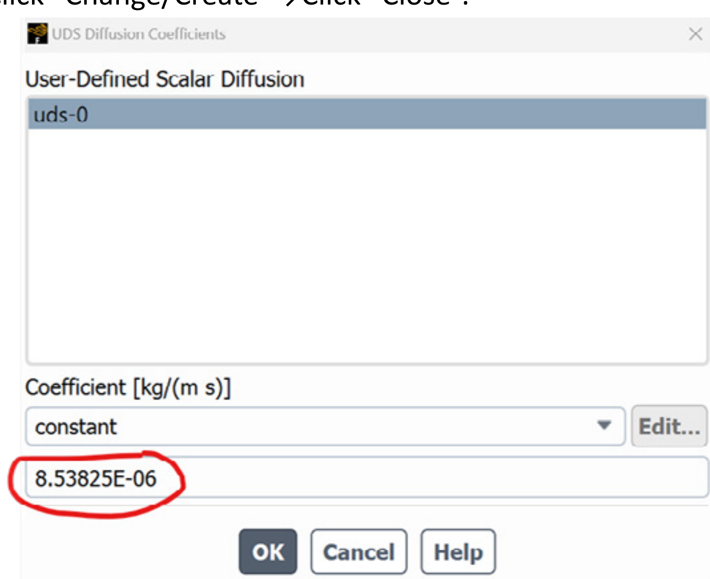
In the new window popped up (see snapshot below), choose “1” in Number of User-Defined Scalars→Click “OK”. There will be an additional advection-diffusion scalar transport equation added to the governing equation system. The variable is UDS-0, which represents the nondimensionalized mass fraction of nicotine vapor ranging from 0 to 1.



Define the Binary Diffusion Coefficient of UDS-0 in Great Excess of Air

Outline View→Setup→Materials→Fluid→Air→Click “Edit” to the right of “UDS Diffusivity [kg/(m s)]”

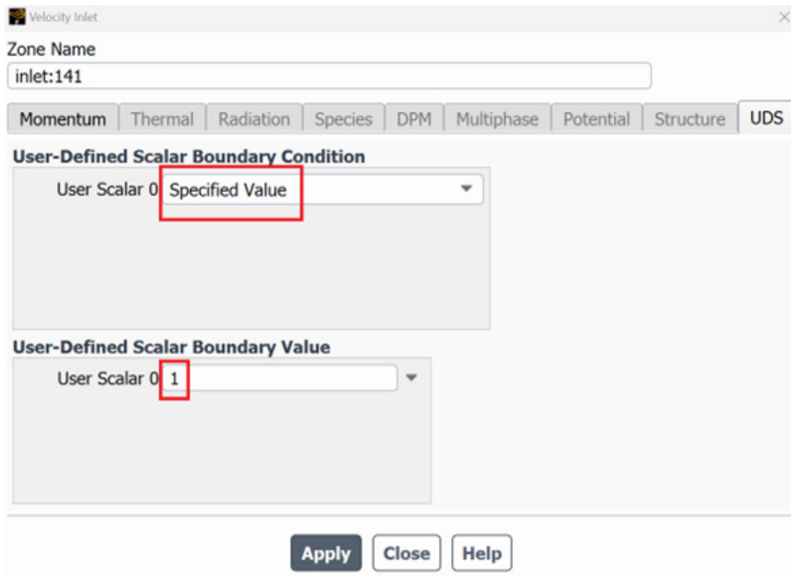
Type “8.53825E-06” in the blank in the UDS Diffusion Coefficients window pop up (see the snapshot below)→Click “OK”→Click “Change/Create”→Click “Close”.



Note: Please notice that UDS Diffusion Coefficient is kg/ (m s) instead of the diffusivity unit m^2/s, which means the value should be $\rho_{a\text{-}g}\ D_{a\text{-}g,s}$ instead of $D_{a\text{-}g,s}$.

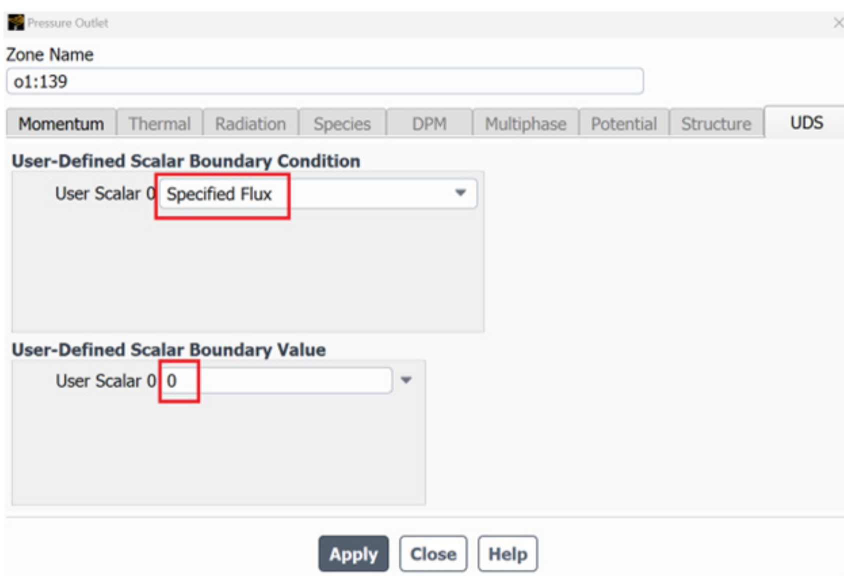
Define UDS Boundary Conditions

Boundary Conditions→Inlet→Follow the setup shown in the snapshot below.



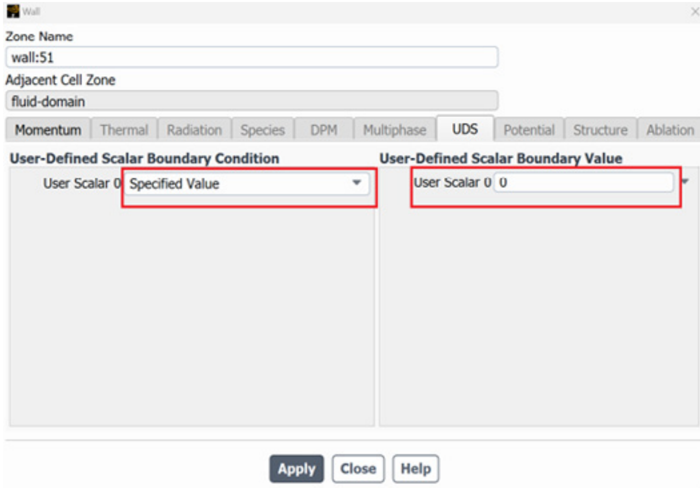
Note: Since UDS-0 is the nondimensionalized mass fraction, we can set the specified value equal to 1 at the inlet.

Boundary Conditions→Outlet→Follow the setup shown in the snapshot below to set up all outlets UDS boundary conditions.



Note: Zero specified flux indicate zero mass fraction gradient at outlets, which is reasonable.

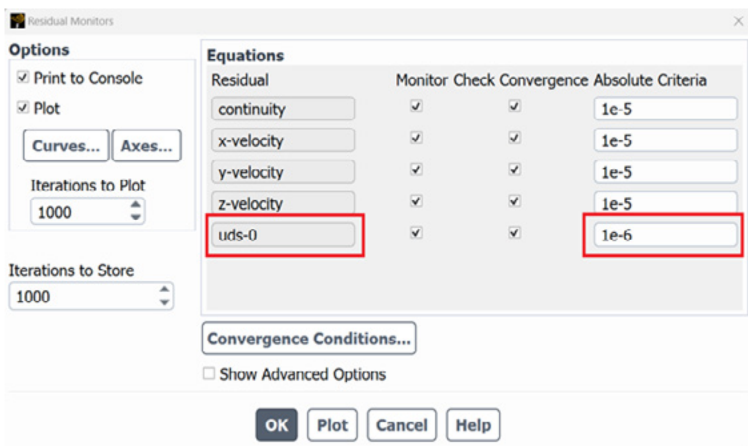
Boundary Conditions→Wall→Follow the setup shown in the snapshot below to set up the wall boundary condition for UDS.



Note: The setup is to reflect the Dirichlet boundary condition, which means the absorption rate is infinitely high for nicotine vapor on the airway wall (Feng et al., 2021) (also see Part 2).

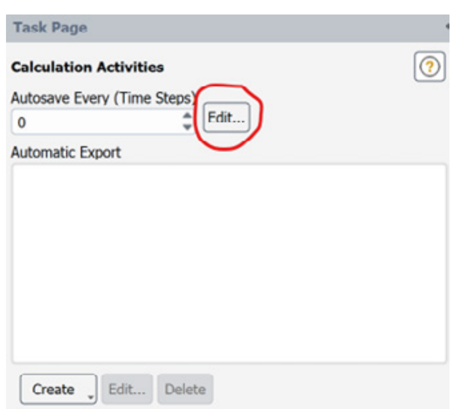
Setup Convergence Criterion for the UDS Scalar Transport Equation

Outline View→Solution →Monitors--<Residual→Set the convergence criterion for uds-0 as 1e-6.

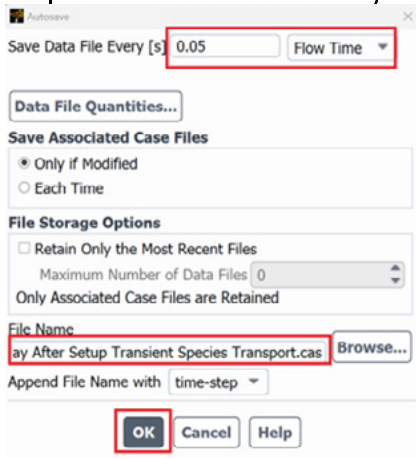


Save Transient Simulation Data

Outline View→Solution→Calculation Activities→Autosave→Calculation Activities→Click "Edit" (see the snapshot below)



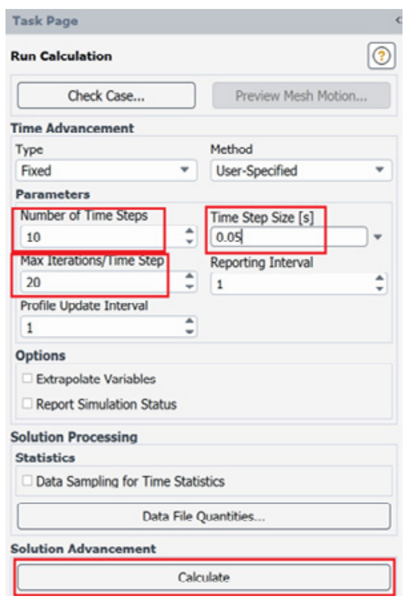
A new “Autosave” window will pop up (see snapshot below). Please follow the setup shown in the snapshot below, and click OK. The setup is to save the data every 0.05 s.



Note: Make sure the file name in “Autosave” window has the correct working directory with the .cas file.

Run Simulation

Outline View→Solution→Run Calculation→Follow the setup shown in the snapshot below and click “Calculate”.



You should then have Ten .dat files at different flow time stations (t=0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, and 0.5 s) named “Airway After Setup Transient Species Transport-1-***.dat”. It will also save a new case named “Airway After Setup Transient Species Transport-1.cas”.

References:

Feng, Y., Zhao, J., Hayati, H., Sperry, T., Yi, H. (2021). Tutorial: Understanding the transport, deposition, and translocation of particles in human respiratory systems using Computational Fluid-Particle Dynamics and Physiologically Based Toxicokinetic models. Journal of Aerosol Science, 151, 105672

Sperry, T., Feng, Y. , Zhao, J., Song, C., Shi, Z. (2023). Prediction of the transport, deposition, and absorption of multicomponent E-cigarette aerosols in a subject-specific mouth-to-G10 human respiratory system. Journal of Aerosol Science. 170, 106157

Use and Reproduction

The content used in this resource may only be used or reproduced for teaching purposes; and any commercial use is strictly prohibited.

Document Information

This tutorial segment is part of a set of teaching resources to help introduce students to topics related to fluids.

Ansys Education Resources

To access more undergraduate education resources, including lecture presentations with notes, exercises with worked solutions, microprojects, real life examples and more, visit www.ansys.com/education-resources.

Feedback

Here at Ansys, we rely on your feedback to ensure the educational content we create is up-to-date and fits your teaching needs.

Please click the link here out a short survey (~7 minutes) to help us continue to support academics around the world utilizing Ansys tools in the classroom.

ANSYS, Inc.
Southepointe
2600 Ansys Drive
Canonsburg, PA 15317
U.S.A.
724.746.3304
ansysinfo@ansys.com