

## Adsorptive Gas Dryer Simulation Instructions

### OVERVIEW

PEDCO's Adsorptive Gas Dryer Simulation predicts the performance of an adsorptive desiccant dryer by solving the conservation equations of mass, energy, and momentum subject to the specified dryer geometry, operating conditions, and desiccant system.

#### DRYER TYPES

The software can be used to simulate performance of Thermal Swing Dryers (Open Loop Blower, Closed Loop Blower, Heated Purge, and Heat of Compression), Pressure Swing (Conventional, Vacuum Purge, and Single Tower), and Once Through.

#### GASES

Drying of Air, Argon, Carbon Dioxide, Ethane, Helium, Hydrogen, Methane, Nitrogen, Oxygen, and any mixture of up to four of these gases can be simulated. Based on the dryer type, the gas being dried and the gas used to regenerate the desiccant can be different.

#### DESICCANTS

	Drying Inlet Layer 1	Layer 2	Layer 3	Drying Outlet Layer 4
Type	Act Alumina	None	None	None
Diameter (inches)	Mixture			
Depth (%)	Gran Silica Gel	0	0	0
Shape Factor	Mol Sieve - 4A			
10% Aging Factor	Spher SG			
100% Aging Factor	Mol Sieve - 13X			
Tortuosity	None			

The program contains isotherms and property data for all the typical desiccants; activated alumina, 3A, 4A and 13X molecular sieve, granular silica gel, and spherical silica gel. Any desiccant diameter can be specified. Aging factors can be specified to study the impact of desiccant aging and contamination on dryer performance.

The user can also specify custom desiccant properties. The data must be provided in an Excel file in the same format that the standard desiccants are output on sheet "DesProp" of the Excel output file. Select Desiccant Type "User 1," "User 2," "User 3", or "User 4" and the program will later prompt the user for the location and name of the file containing the desiccant data.

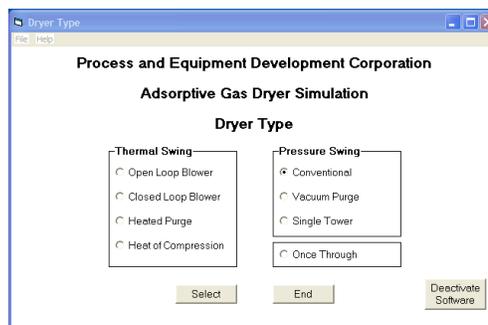
Sample desiccant input files are provided on the software CD specific to activated alumina, 4A molecular sieve, granular silica gel, and spherical silica gel that can be used as a template for creating a user specified desiccant input file.

Up to four layers of desiccant can be specified. The desiccant can be layered based on desiccant type, desiccant diameter, or aging factor for example to simulate a layer of contaminated desiccant near the inlet.

Within each layer a mixture of up to four desiccants can be specified. As with layering, the mixture can be of different desiccant types or the same desiccant type with different properties, e.g. bead diameter.

#### APPLICATIONS

Uses for the program are unlimited for the Desiccant Dryer Engineer. Just a few examples of its use include:



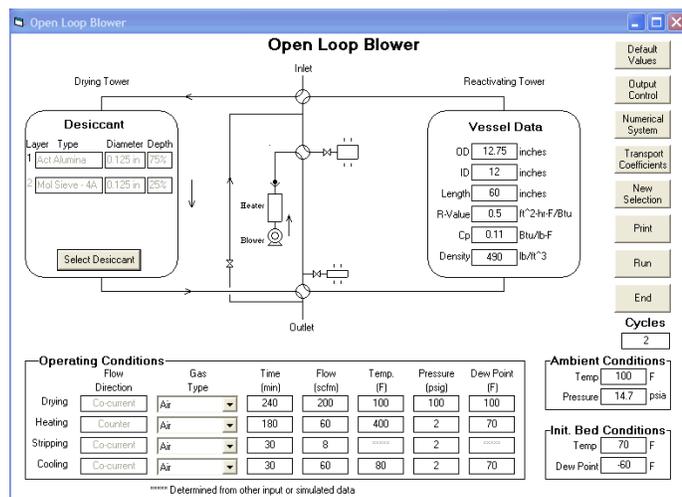
- Predict performance of an existing dryer operating at off-design conditions,
- Assist in development of an energy management system,
- Enable a better understanding of the inner workings of a desiccant dryer to optimize performance and design,
- Evaluate reactivation scheme options to intelligently conduct a cost-benefit analysis,
- Conduct a sensitivity analysis to determine purge air requirements for a pressure swing dryer as a function of required dew point, inlet temperature, inlet pressure, inlet relative humidity, desiccant type, desiccant diameter, etc.,
- Study the effects of desiccant particle size distribution on drying and reactivation performance,
- Study the effects of desiccant layering on drying and reactivation performance,
- Develop new energy efficient dryers,
- Create support documents for proposal presentation,
- Etc.

Insight into the inner workings of a desiccant dryer NOT ATTAINABLE BY ANY OTHER METHOD is possible by studying the output from this simulation.

### DATA INPUT

After the dryer type is selected, the program displays a form showing a flow diagram for the specified dryer. This form contains unit system specified (English or SI) operating conditions, ambient conditions, dryer geometry, and initial bed conditions. Buttons on the flow diagram form can be clicked to display additional forms for entering desiccant properties, transport coefficients, numerical system specifications, output control parameters, etc. Default values based on dryer type, cycle timing, and number of cycles can be used if desired.

Four levels of input data error trapping are performed to assure a valid data set is provided prior to running the simulation.



### SOLUTION ALGORITHM

This program solves the system of non-linear partial-differential conservation equations of mass, momentum, and energy describing the physics of adsorption. Constitutive relations such as the ideal gas law, desiccant isotherms, correlations for molecular diffusivity in a desiccant particle, etc are utilized. The system of differential equations is solved using a finite-difference technique. The system of non-linear algebraic equations created by discretizing the differential equations is solved using the Newton-Raphson method.

### OUTPUT

Simulated data is output to an Excel spreadsheet. Output data includes:

- Dryer outlet Dew Point and Temperature as a function of Time,
- Desiccant Bed Temperature, Loading, and Dew Point distributions as a function of Time (output in tabular and plotted formats),
- Water Loading Distribution in a Desiccant Particle as a function of Bed Position and Time,
- Desiccant and Gas Properties, and
- Transport Coefficients - Gas-to-Vessel Heat Transfer Coefficient, Gas-to-Desiccant Mass Transfer Coefficient, Desiccant Bead Effective Diffusivity, etc.

The capabilities of Excel can be utilized to manipulate and plot data in a format most suitable for the objectives of the immediate project.

#### **MINIMUM SYSTEM REQUIREMENT**

- Computer - PC with Pentium 350 MHz (Recommend as fast as possible)
- Memory - 128 MB of RAM
- Hard-drive Space - 6 MB
- Video Display - 800 X 600
- Operating System - Windows 98 or later, some limits with Windows 98
- Support Application – Excel 97/Office 97 or later

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## SOFTWARE INSTALLATION

### FROM CD

- Insert CD
- With AUTORUN activated – installation will begin automatically. Follow on-screen instructions.
- Without AUTORUN activated – START > SETTINGS > CONTROL PANEL > ADD/REMOVE PROGRAM > INSTALL or CD OR FLOPPY > EXECUTE FILE setup.exe > follow on-screen instructions. (There may be slight deviations from this procedure depending on your operating system.)

### FROM SELF EXTRACTING (.EXE) EMAILED FILE

- Save the file PedcoAds#.##.exe to your hard drive.
- Use Windows Explorer and navigate to PedcoAds#.##.exe and double click.
- The self-extracting executable will unzip the files and launch the software installation.
- Follow the on-screen instructions to install the Adsorptive Gas Dryer Simulation software.

### FROM ZIPPED (.ZIP) EMAILED FILE (A ZIP UTILITY IS REQUIRED FOR THIS OPTION)

- Save the file PedcoAds#.##.zip to your hard drive.
- Use Windows Explorer and navigate to PedcoAds#.##.zip and double click.
- The default Zip utility will launch, unzip the files, and initiate installation of the Adsorptive Gas Dryer Simulation. If the software installation does not launch automatically, use Windows Explorer and navigate to the folder where the files were stored. Double click on setup.exe.

## OPERATING INSTRUCTIONS

1. Launch Application – START > PROGRAMS > Pedco > AdsDryerSimVers#.##
2. Select Dryer Type – Click desired dryer type. Available types are Open Loop Blower, Closed Loop Blower, Heated Process Gas, Heat of Compression, Conventional Pressure Swing, Vacuum Pressure Swing, Single Tower Pressure Swing, and Once Through. CLICK SELECT.

*It is also possible to input data from a previous simulation run by going to File > Open (on the pull-down menu) and select the Excel file containing the desired data.*

The DEACTIVATION BUTTON is provided if the user decides to use the software on a different computer. After the current program is DEACTIVATED as proven by presenting the DEACTIVATION CODE to PEDCO, a new authorization code will be provided. A NEW AUTHORIZATION CODE WILL NOT BE PROVIDED WITHOUT THE DEACTIVATION CODE.

3. Specify Regeneration Stages and Flow Directions (*Open Loop Blower, Closed Loop Blower, Heated Process Gas, and Heat of Compression dryers only*) – Specify flow configurations (relative to drying) for each of the Heating, Stripping, and Cooling Stages. Stripping utilizes dried air to remove water and cool while the desiccant bed is hot. If a stage is not included (Stripping or Cooling) select None.

For a Closed Loop Blower dryer, the Heating Stage also requires specifying Closed Loop (heating outlet recycled back to blower inlet through a cooler) or Open Loop (blower inlet from ambient and heated air outlet exhausted to the ambient).

For a Heated Process Gas dryer, the reactivation gas can be exhausted to atmosphere or returned to the dryer inlet. If the reactivation gas is returned to the dryer inlet, this gas will be mixed with the inlet gas and the mixture temperature and dew point will be used for the drying bed inlet.

For a Heat of Compression dryer, the Cooling Stage requires specifying the source of the cooling gas (wet or dry gas) and the return location of the cooling gas (dryer inlet or outlet). Mixing calculations are made as required depending on the source and return location of the cooling gas. A second stage heating can also be specified that uses Stripping Gas flowing through an external heater.

CLICK SELECT.

NOTES:

Default Values – Input forms requiring numerical data have a Default Values Command Button to populate the form with reasonable values.

Print – Input forms requiring numerical data have a Print Command Button to output the current form to the computers default printer.

Tool Tip – Tool Tips provide expanded explanations for the necessary input data.

New Selection – While a Dryer Flow Diagram is displayed, a new data input session can be started at any time by CLICKING NEW SELECTION. THIS WILL ERASE ALL CURRENT INPUT DATA.

Error Trapping – The program uses four phases of error trapping for input data.

- Phase 1 – When data is entered, the value is checked to determine if the value is *unusually* low or high (warning is issued that can be bypassed) or *unacceptably* low or high (requires change to the value).
- Phase 2 – When OK or RUN is clicked, the current form is checked to assure a value has been entered for all input data for that form.
- Phase 3 – When RUN is clicked on the Flow Diagram Form, the other forms (Output Controls, Numerical System, Transport Coefficients, and Desiccant) are checked to assure values have been entered for data on the specific form. If values have not been entered you are prompted to use the Default Values. If you select NO, you will be returned to the specific form requiring data input.
- Phase 4 – At the beginning of program execution, relationships between input data are checked.

Examples include:

- i. Vessel Outside Diameter  $\geq$  Vessel Inside Diameter
- ii. Operating temperatures within the temperature window for the isotherm of the specified desiccant
- iii. Gas velocity will not cause fluidization of the desiccant in an upflow arrangement.

If an error occurs, you are notified. On acknowledgement, you are returned to the invalid data. If a warning is indicated, as in the case of excessively high velocity, you are given the option to proceed or change the data.

4. Specify Vessel Data, Operating Conditions, Simulated Cycles, Ambient Conditions, and Initial Conditions – Enter the desiccant vessel geometric data, thermophysical properties, and insulation R-value (0.5 is a good R value for natural convection, i.e. no insulation). Specify the number of cycles to be simulated, ambient conditions, and initial conditions. *By Double-Clicking the Initial Condition Heading on the Flow Diagram, it is possible to select initial bed temperature and concentration/dew point distributions from final conditions of a previous run. Specify the Excel file containing the desired distribution from the dialogue box.*

Specify the gas type, time, flow rate, temperature, pressure, and dew point for the inlet gas for each stage of the cycle. Where necessary, based on the dryer type, etc, the program will determine the gas type and/or inlet conditions from other input or simulated data. This will be apparent since the operator will be unable to enter data into these fields.

The choices for gas type are Air, Argon, Carbon Dioxide, Ethane, Helium, Hydrogen, Methane, Oxygen, Nitrogen, and Mixture. If a gas “Mixture” is selected, as soon as another data field is clicked, a form will be displayed allowing a mixture of up to four of the nine gases to be entered. A Gas Mixture form will be displayed for Drying Gas, Heating Gas, or Cooling Gas if the specified dryer type allows these gases to be different. The gas type and mole fraction for each component must be entered. For a dryer type where a specific stage gas cannot be independently selected, the mixture data for the Drying Gas will be used. For example, if a pressure swing dryer is selected and a Drying Gas Mixture is specified, the program will use the Drying Gas Mixture for the Stripping Gas Mixture.

5. Specify the Desiccant System – CLICK SELECT DESICCANT on Flow Diagram Form – Select the desiccant in each layer starting with the drying inlet end of the desiccant bed. If no property data is specified for the specific layer, after the desiccant is selected, the default values for the specific desiccant type will be entered automatically. If any property data had been previously entered, the property data will not be updated. To select default property data for selected desiccants, CLICK DEFAULTS FOR SELECTED DESICCANT. After the desiccant system has been specified, CLICK OK.

If a desiccant “Mixture” is selected, as soon as another data field is clicked, a form will be displayed allowing a mixture of up to four desiccants to be selected for the specified layer. A mixture may be desired as a result of a mix of desiccant types, a mix of diameters to simulate a particle sized distribution, etc.

There is no restriction regarding mixture from one layer to another. For example, Layer 1 could have a desiccant mixture and Layer 2 could have a single desiccant specified.

6. Specify Output Control Frequency - CLICK OUTPUT CONTROL on Flow Diagram Form – Select the frequency for outputting Detailed Data, Plotted Data, Heat and Material Balances, and Temperature and Concentration Distribution. After the program output is discussed later, the significance of this data will be more apparent. It is best to select the defaults initially.

There are two check boxes on this form – Plot Data Continuously and Output Iteration Counter. Output Iteration Counter would only be used to debug a numerical problem and should not be set. It will slow the program execution drastically.

Plot Data Continuously is a nice feature to see plotted data as it is available. For pressure swing dryers it should be set. However if execution speed is a concern for heated dryers (they run much faster than pressure swing), you should leave this unchecked and the data will be plotted at the end. For typical heated dryer conditions, plotting data continuously will double execution time (4 minutes instead of 2 minutes on a 1.6 GHz computer).

Note: A pressure swing simulation using the default conditions requires approximately 1 hour of run time on a 1.6 GHz computer.

After the output control data has been specified, CLICK OK.

7. Numerical System - CLICK NUMERICAL SYSTEM on Flow Diagram Form – The discretization process involves dividing the desiccant bed into a finite number of grids and a representative desiccant particle in

each of these grids into a finite number of shells. Additionally, the time is divided into discreet time steps. As the number of bed grids and particle shells approaches infinity and the time step approaches zero, the finite difference solution approaches the exact solution of the equation set - unfortunately, the computational time also increases greatly. Fortunately, accurate solutions are obtained with grid systems between 120 and 480, bed shells between 1 and 10, and time steps between 0.125 and 5 minutes. The defaults will provide a good starting point for the dryer type selected and should be used until the Engineer is more comfortable with the impact of modifying these values. After the numerical system has been specified, CLICK OK.

8. Transport Coefficients - CLICK TRANSPORT COEFFICIENTS on Flow Diagram Form. Gas-to-Vessel Heat Transfer Coefficients and Gas-to-Desiccant Mass Transfer Coefficients are calculated using the correlations shown on the Transport Coefficients form. These correlations are obtained from published literature and/or are based on experimental data obtained by testing at Process & Equipment Development Corporation. Unless there is good reason to use other values, the default values should be selected, CLICK OK.
9. Program Execution - CLICK RUN. If the program has not been Purchased and Authorized it is for Demonstration Purposes Only and its execution capabilities are limited. A form will appear showing you its capability and indicate the process for Authorization.

## OUTPUT DATA

Simulated output is directed to an Excel workbook. The program will generate a *model number type* name for the Excel file and save it initially in the folder C:\Pedco\ADS\Temp. If the folder doesn't exist, it will be created. The program will NOT save the file at the end of the simulation. It is advised to resave the file in another folder after the simulation is complete.

The file name generated by the simulation includes the dryer parameters and operating conditions that are typically changed. However, the name is not always unique, and at times it will be necessary to provide additional differentiation when the output file is saved, e.g. trailing 'A', 'B', etc.

The file name is composed of up to 8 parts (based on the dryer type and reactivation configuration) as indicated below. The file name CL-DR-200-100-100-240-DB12-60-NS120-3-1-DES-AA100-HT-60-OS-400-2-180-ST8-S-2-30-CL60-S-80-2-30.xls is used for example.

1. Dryer type - 'CL-'
  - a. 'CL-' - Closed Loop Blower Purge
  - b. 'HP-' - Heated Purge
  - c. 'OL-' - Open Loop Blower Purge
  - d. 'HC-' - Heat of Compression
  - e. 'OT-' - Once Through
  - f. 'PS-' - Conventional Pressure Swing
  - g. 'ST-' - Single Tower Pressure Swing
  - h. 'VP-' - Vacuum Purge Pressure Swing
2. Drying conditions - 'DR-200-100-100-240-'
 

Flow rate - 200 scfm, Temperature - 100°F, Pressure - 100 psig, Time - 240 minutes
3. Heating conditions - 'HT-60-OS-400-2-180-'
 

Flow rate - 60 scfm, Flow configuration - Open Loop, Same direction as drying, Temperature - 400°F, Pressure - 2 psig, Time - 180 minutes

Flow configuration

  - a. 'CO' - Closed Loop Heating, Opposite (counter-current) to drying (Closed Loop Blower only)
  - b. 'CS' - Closed Loop Heating, Same (co-current) as drying (Closed Loop Blower only)
  - c. 'OO' - Open Loop Heating, Opposite (counter-current) to drying (Closed Loop Blower only)

- d. 'OS' – Open Loop Heating, Same (co-current) as drying (Closed Loop Blower only)
  - e. 'O' – Opposite (counter-current) to drying
  - f. 'S' – Same (co-current) as drying
4. Desiccant bed – 'DB12-60-'  
Bed diameter – 12 inches, Effective bed depth – 60 inches
  5. Numerical system – 'NS120-3-1-'  
Number of bed grids – 120, Number of bead shells – 3, Time step – 1 minute
  6. Desiccant system – 'DES-AA100-'  
Desiccant type – activated alumina, Desiccant depth – 100%  
  
Desiccant type
    - a. 'AA' – Activated alumina
    - b. 'MS3' – Molecular sieve – type 3A
    - c. 'MS4' – Molecular sieve – type 4A
    - d. 'MS13X' – Molecular sieve – type 13X
    - e. 'SGG' – Granular silica gel
    - f. 'SGS' – Spherical silica gel
    - g. 'SGWR' – Spherical silica gel, water resistant
    - h. 'USER1' – User specified desiccant #1
    - i. 'USER2' – User specified desiccant #2
    - j. 'USER3' – User specified desiccant #3
    - k. 'USER4' – User specified desiccant #4
    - l. 'MIX' – mixture of desiccants
  7. Stripping conditions – 'ST8-S-2-30-'  
Flow rate - 8 scfm, Flow direction – Same (co-current) as drying, Pressure - 2 psig, Time - 30 minutes  
  
Flow configuration
    - a. 'O' – Opposite (counter-current) to drying
    - b. 'S' – Same (co-current) as drying
  8. Cooling conditions – 'CL60-S-80-2-30-'  
Flow rate - 60 scfm, Flow direction – Same (co-current) as drying, Temperature - 80°F, Pressure - 20 psig, Time - 30 minutes  
  
Flow configuration
    - a. 'O' – Opposite (counter-current) to drying
    - b. 'S' – Same (co-current) as drying

For Heat of Compression dryers, the following system is used to indicate the cooling configuration. The first character indicates the source of the cooling gas; Wet (W) or Dry (D). The second character indicates the cooling gas flow direction relative to the drying gas; counter-current or opposite (O) or co-current or same (S). The third character indicates the return point for the cooling gas; Dryer Inlet (I) or Dryer Outlet (O).

- a. 'DSO' – 'D' dry gas, 'S' same (co-current) direction as drying, 'O' with gas returned to dryer outlet
- b. 'DOO' – 'D' dry gas, 'O' opposite (counter-current) direction as drying, 'O' with gas returned to dryer outlet
- c. 'WSI' – 'W' wet gas, 'S' same (co-current) direction as drying, 'I' with gas returned to dryer inlet
- d. 'WSO' – 'W' wet gas, 'S' same (co-current) direction as drying, 'O' with gas returned to dryer outlet

- e. 'WOI' – 'W' wet gas, 'O' opposite (counter-current) direction as drying, 'I' with gas returned to dryer inlet
- f. 'WOO' – 'W' wet gas, 'O' opposite (counter-current) direction as drying, 'O' with gas returned to dryer outlet

There are eight worksheets in the workbook with data as indicated below.

1. Input – All input data. The program obtains input data from this sheet if input from an existing Excel file is specified.
2. Input - SI – Same as sheet 'Input' but data is displayed in SI units.
3. DesProp – Isotherms and property data for all specified desiccants for the specific run. Isotherms are for new desiccant, i.e. an aging factor of 0 is used.
4. Gas Prop – Gas properties for all cycle stages are listed. This includes molecular weight, viscosity, thermal conductivity, specific heat, Prantl number, density at atmospheric pressure, diffusivity at atmospheric pressure, and Schmidt number.
5. DepVarVsTime – Dew Point, Loading, and Temperature data at 5 bed locations (Drying Inlet,  $\frac{1}{4}$  through the bed,  $\frac{1}{2}$  through the bed,  $\frac{3}{4}$  through the bed, and Drying Outlet) at Cycle Frequency and Time Frequency specified on form Output Control.
6. Detailed Output – Data as a function of Bed Position and Time determined from Cycle Frequency, Time Frequency, and Distance Frequency specified on form Output Control. Data includes - Dew Point, Water Concentration, Bed Temperature, Vessel Temperature, Pressure, Average Desiccant Loading, Gas-to-Vessel Heat Transfer Coefficient, Gas-to-Desiccant Mass Transfer Coefficient, Desiccant Particle Effective Diffusivity, Desiccant Bead Dew Point Distribution, and Desiccant Bead Loading Distribution.
7. Plots – Data from sheet DepVarVsTime in plotted format. This is the most visually informative output to evaluate dryer performance.
8. Heat & Mtl Balance – Heat and Material Balances as a function of Time determined from Cycle Frequency and Time Frequency specified on form Output Control
9. Temp & Conc Dist – Temperature and Concentration at each Grid and Shell at the end of a cycle. Output Frequency is specified by Cycle Frequency on form Output Control.
10. Temp & Conc Dist - SI – Same as sheet 'Temp & Conc Dist' but data is displayed in SI units.