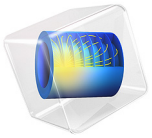

Adsorption and Desorption of Water in a Load Lock Vacuum System

Introduction

This model shows how to simulate the time-dependent adsorption and desorption of water in a vacuum system at low pressures. The water is introduced into the system when a gate valve to a load lock is opened and the subsequent migration and pumping of the water is modeled.

Model Definition

The model geometry is shown in Figure 1. The system consists of two chambers separated by a gate valve (not shown in the geometry). The lower cylindrical chamber is the load lock chamber. The upper spherical chamber is a high vacuum chamber, which is not vented during the sample loading process. The vacuum pump is located opposite the gate valve, and has a constant speed of 500 l/s.

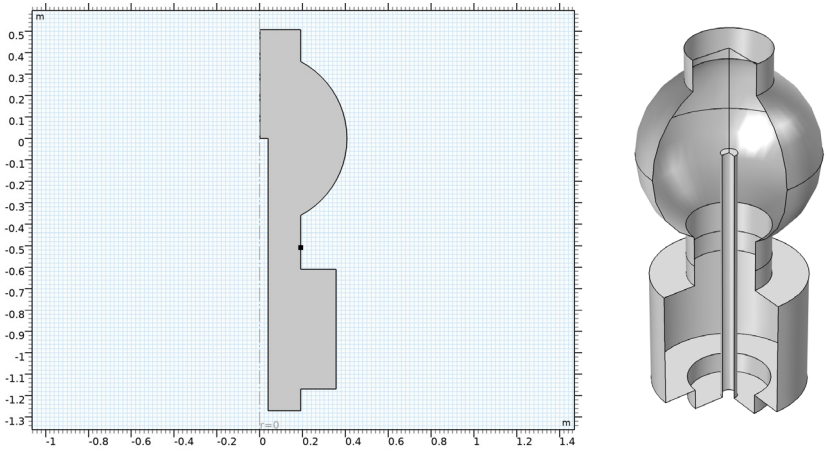

Figure 1: Axisymmetric model geometry, shown in 2D (left) and 3D (right).

WATER ADSORPTION AND DESORPTION

Several simplifying assumptions are made about the adsorption and desorption of the water vapor in this model:

- Multilayer adsorption of water is neglected, since only the chemisorbed layer bound directly to the surface of the chamber, is significant during the high vacuum stages of pump-down (Ref. 1). It is therefore assumed that a single, chemically adsorbed layer of water is present on the surfaces of the wall.

- The probability of water adsorption (also known as the sticking coefficient) is assumed to depend linearly on the occupancy of the surface sites. For a clean surface the maximum value of the sticking coefficient is assumed to be 0.1, consistent with the upper limits of the values reported in Ref. 1, and producing reasonable agreement with typical outgassing data reported in Ref. 2.
- The density of the water adsorption sites is assumed to be 1×10^{-4} mol/m^2. This corresponds to 6×10^{15} molecules/cm^2, consistent with typical outgassing data reported in Ref. 2.
- It is assumed that the water does not dissociate when adsorbing, so that the desorption process is first order (the desorption rate is therefore proportional to the molar concentration of adsorbed molecules, n_{ads}). Since the flow is isothermal, the desorption rate, D, is determined by a constant time constant, τ (D=n_{ads}/τ). τ is chosen as 200 s to produce reasonable agreement with the outgassing data reported in Ref. 2 and with the range of data reported in Ref. 1.
- At the start of the simulation, it is assumed that the walls of the load lock and the sample stage are both fully saturated with a single monolayer of adsorbed water and that there is no adsorbed water vapor on the surfaces of the high vacuum chamber.

COMSOL Multiphysics treats the adsorption and desorption of molecules in a molecular flow by specifying a sticking coefficient (S) and a molar desorption rate (D) such that:

$$\begin{aligned} J &= (1-S)G + DN_A \\ \frac{dn_{\text{ads}}}{dt} &= \frac{SG}{N_A} - D + \Gamma \end{aligned} \tag{1}$$

where J is the emitted molecular flux, G is the incident molecular flux, N_A is Avogadro's number and Γ is an additional surface source of molar flux (enabling, for example, the coupling of a diffusion problem to the interface in order to model the diffusion or permeation of gases through the walls of the system). An initial value is specified for n_{ads} on each surface.

In this model the sticking coefficient S is given the following value:

$$S = S_0\left(1 - \frac{n_{\text{ads}}}{n_{\text{sites}}}\right) \tag{2}$$

where S_0 is the sticking coefficient with no site occupancy (assumed to be 0.1) and n_{sites} is the molar capacity of the surface sites on the system (assumed to be 1×10^{-4} mol/m^2). The model sets the desorption rate in the following manner:

$$D = \frac{n_{\text{ads}}}{\tau} \tag{3}$$

where τ is the time constant for desorption. Equation 3 assumes that the desorption process is first order, that is that there is no dissociation of the water on adsorption, or recombination required for desorption.

The wall boundary condition implements Equation 1 automatically when the **Adsorption/Desorption** wall type is selected. Equation 2 and Equation 3 are implemented with expressions typed into the boundary condition. S_0 (`sc`), n_{sites} (`nsites`) and τ (`tau`) are all parameters in the model with the names indicated in the brackets.

Results and Discussion

Figure 2 shows the evolution of the adsorbed molecules per unit area on the surface of the system, as the water vapor is pumped out. A redistribution of the molecules between the load lock and the high vacuum chamber is observed initially. After that the distribution of molecules appears qualitatively similar but the number of molecules adsorbed decreases progressively.

Figure 3 and Figure 4 show the pressure and the adsorbed molecules per unit area evolving over time as the water is pumped out. The results are shown for two points, one in the high vacuum system and the other in the load lock. The two curves are similar in form. Initially the pressure in the load lock is significantly higher than that in the high vacuum system. After approximately 0.3 hours (18 mins) the pressure in the two parts of the system converges and there is a smaller, time independent difference between the pressure measured in the two chambers. For the first three hours of pumping the pressure in the system drops slowly, but after that a more rapid decrease in the pressure occurs as the remainder of the water is pumped out. Using the load lock ensures that the pressure in the high vacuum part of the system remains below 7×10^{-7} Torr.

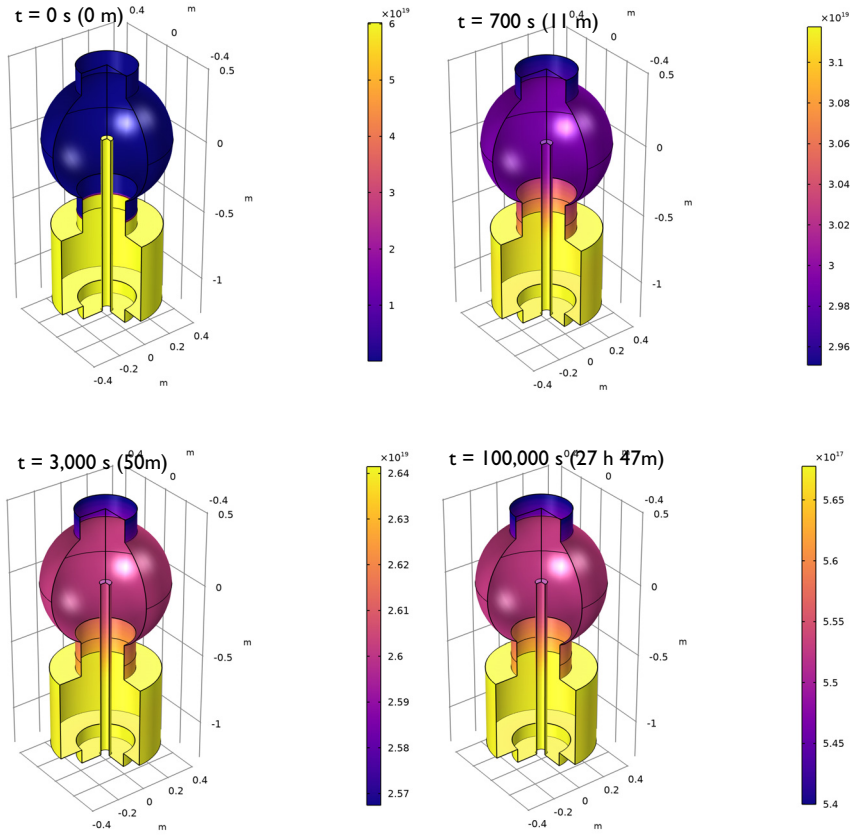

Figure 2: Molecules adsorbed per square meter on the surface of the chamber as a function of time.

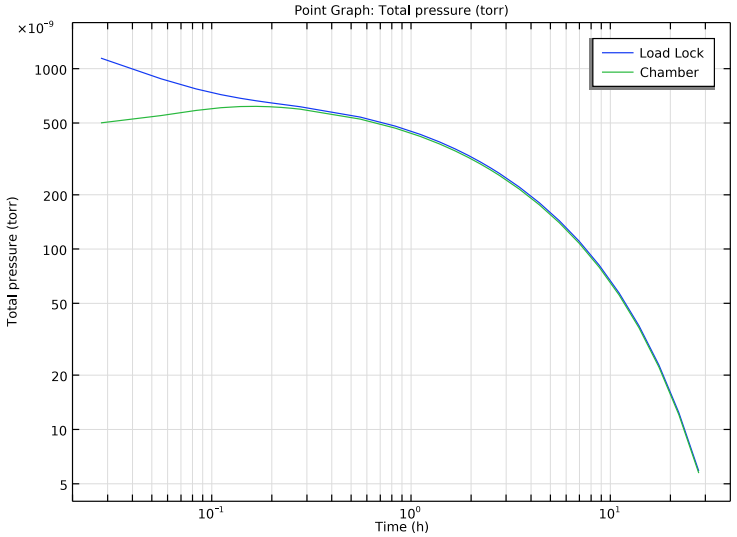

Figure 3: Pressure as a function of time at points in the load lock and high vacuum chambers.

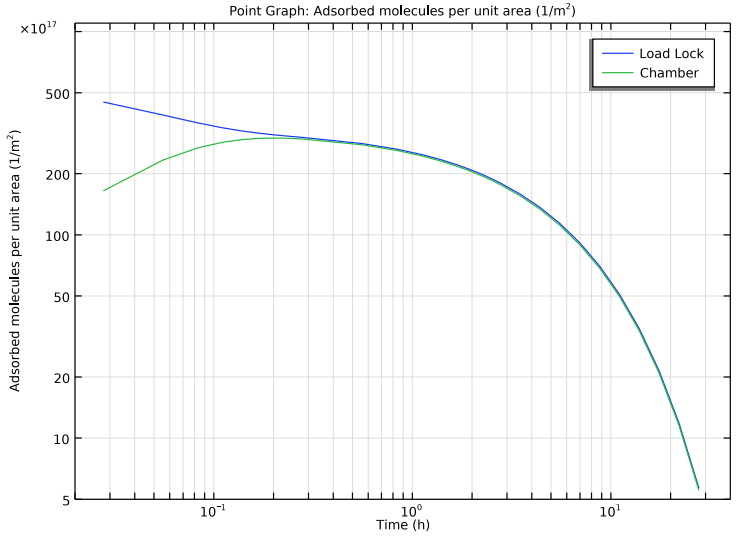

Figure 4: Adsorbed molecules per unit area at points in the load lock and high vacuum chambers.

Application Library path: `Molecular_Flow_Module/Industrial_Applications/water_adsorption_desorption`

References

1. J.F. O'Hanlon, *A User's Guide to Vacuum Technology*, John Wiley & Sons, 2003.

2. H.F. Dylla, "The Problem of Water in Vacuum Systems", *CERN Accelerator School*, Platja d'Aro, Spain, May 2006 (available at: http://cas.web.cern.ch/sites/cas.web.cern.ch/files/lectures/platjadaro-2006/dylla-2.pdf).

3. J.M. Lafferty, *Foundations of Vacuum Science and Technology*, John Wiley & Sons, 1998.

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Fluid Flow>Rarefied Flow>Free Molecular Flow (fmf)**.

3 Click **Add**.

4 In the **Incident molecular fluxes (1/(m²·s))** table, enter the following settings:

H2O

5 Click **Study**.

6 In the **Select Study** tree, select **General Studies>Time Dependent**.

7 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
nsites	1e-4[mol/m^2]	1E-4 mol/m²	Density of adsorption sites
tau	200[s]	200 s	Time constant for desorption
sc	0.1	0.1	Sticking coefficient

GEOMETRY 1

Circle 1 (c1)

1 In the **Geometry** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

3 In the **Radius** text field, type `16[in]`.

4 In the **Sector angle** text field, type `180`.

5 Locate the **Rotation Angle** section. In the **Rotation** text field, type `270`.

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `14[in]`.

4 In the **Height** text field, type `22[in]`.

5 Locate the **Position** section. In the **z** text field, type `-46[in]`.

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `7.5[in]`.

4 In the **Height** text field, type `70[in]`.

5 Locate the **Position** section. In the **z** text field, type `-50[in]`.

Point 1 (pt1)

1 In the **Geometry** toolbar, click **Point**.

2 In the **Settings** window for **Point**, locate the **Point** section.

3 In the **r** text field, type `7.5[in]`.

4 In the **z** text field, type `-20[in]`.

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 Select the objects **c1**, **r1**, and **r2** only.

3 In the **Settings** window for **Union**, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

Rectangle 3 (r3)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `1.5[in]`.

4 In the **Height** text field, type `50[in]`.

5 Locate the **Position** section. In the **z** text field, type `-50[in]`.

Compose 1 (co1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Compose**.

2 Select the objects **r3** and **uni1** only.

3 In the **Settings** window for **Compose**, locate the **Compose** section.

4 In the **Set formula** text field, type `uni1-r3`.

5 Click **Build Selected**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.

FREE MOLECULAR FLOW (FMF)

Molecular Flow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Free Molecular Flow (fmf)** click **Molecular Flow 1**.

2 In the **Settings** window for **Molecular Flow**, locate the **Molecular Weight of Species** section.

3 In the $M_{n,H2O}$ text field, type `0.018[kg/mol]`.

Wall 1

1 In the **Model Builder** window, click **Wall 1**.

2 In the **Settings** window for **Wall**, locate the **Wall Type** section.

3 From the **Wall type** list, choose **Adsorption/Desorption**.

4 Locate the **Adsorption/Desorption** section. In the S_{H2O} text field, type `sc*(1-fmf.n_ads_H2O/nsites)`.

5 In the D_{H2O} text field, type `fmf.n_ads_H2O/tau`.

6 In the $n_{ads,0,H2O}$ text field, type `0`.

Wall 2

1 Right-click **Component 1 (comp1)>Free Molecular Flow (fmf)>Wall 1** and choose **Duplicate**.

2 Select Boundaries 2, 5–10, and 13 only.

3 In the **Settings** window for **Wall**, locate the **Adsorption/Desorption** section.

4 In the $n_{ads,0,H2O}$ text field, type `nsites`.

Vacuum Pump 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Vacuum Pump**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Vacuum Pump**, locate the **Vacuum Pump** section.

4 From the **Specify pump flux** list, choose **Pump speed**.

MESH 1

Edge 1

1 In the **Mesh** toolbar, click **Edge**.

2 In the **Settings** window for **Edge**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

Size

1 In the **Model Builder** window, click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra fine**.

4 Click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,100,1000) range(2000,1000,10000) 1e4*10^{range(0,0.1,1)}`.

Use several ranges for the time steps, to obtain good resolution on different time scales.

Reduce the relative and absolute solver tolerance by an order of magnitude. This is recommended as the number of adsorbed molecules varies over several orders of magnitude.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `0.0001`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute Tolerance** section.

4 From the **Tolerance method** list, choose **Manual**.

5 In the **Absolute tolerance** text field, type `0.00001`.

6 In the **Study** toolbar, click **Compute**.

RESULTS

Adsorbed Molecules

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Adsorbed Molecules` in the **Label** text field.

Surface 1

1 Right-click **Adsorbed Molecules** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Free Molecular Flow>Adsorbed/Deposited species>fmf.N_ads_H2O - Adsorbed molecules per unit area - 1/m²**.

3 Locate the **Coloring and Style** section. Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Thermal>Plasma** in the tree.

5 Click **OK**.

6 In the **Adsorbed Molecules** toolbar, click **Plot**.

Compare the resulting plot with Figure 2 at different time steps.

Pressure vs. Time

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Pressure vs. Time` in the **Label** text field.

3 Locate the **Axis** section. Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0.02`.

5 In the **x maximum** text field, type `40`.

6 In the **y minimum** text field, type `4e-9`.

7 In the **y maximum** text field, type `1.8e-6`.

8 Select the **x-axis log scale** check box.

9 Select the **y-axis log scale** check box.

Point Graph 1

1 Right-click **Pressure vs. Time** and choose **Point Graph**.

2 Select Points 13 and 15 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `fmf.ptot`.

5 In the **Unit** field, type `torr`.

6 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

7 In the **Expression** text field, type `t`.

8 From the **Unit** list, choose **h**.

9 Click to expand the **Legends** section. Select the **Show legends** check box.

10 From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
`Load Lock`
`Chamber`

Pressure vs. Time

1 In the **Model Builder** window, click **Pressure vs. Time**.

2 In the **Pressure vs. Time** toolbar, click **Plot**.

Compare the resulting plot with Figure 3.

Adsorbed Molecules vs. Time

1 Right-click **Pressure vs. Time** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Adsorbed Molecules vs. Time` in the **Label** text field.

3 Locate the **Axis** section. In the **y minimum** text field, type `5e17`.

4 In the **y maximum** text field, type `1.1E20`.

Point Graph 1

1 In the **Model Builder** window, expand the **Adsorbed Molecules vs. Time** node, then click **Point Graph 1**.

2 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Free Molecular Flow>Adsorbed/Deposited species>fmf.N_ads_H2O - Adsorbed molecules per unit area - 1/m²**.

3 In the **Adsorbed Molecules vs. Time** toolbar, click **Plot**.

Compare the resulting plot with Figure 4.