Nov 20 2006

To the summary of the
bubble formation WITH gas I added those we have discussed in Chicago
before I left about the bubble formation WITHOUT gas.

Bubble formation ~~WITHOUT~~ hydrophobic gases

Bubble Height

Dear Bob,

I have attached a pdf file will all the figures. To the summary of the bubble formation WITH gas I added those we have discussed in Chicago before I left about the bubble formation WITHOUT gas.

Best wishes,
Roland

Roland Roth <Roland.Roth@mf.mpg.de>   hide details 11/20/06
reply-to   Roland Roth <Roland.Roth@mf.mpg.de>
to   Bob Eisenberg <beisenbe@rush.edu>
cc
wolfgang nonner <wnonner@chroma.med.miami.edu>,
Dirk Gillespie <dirk_gillespie@rsh.net>
date Nov 20, 2006 11:23 AM
subject Re: Bubble Gating Nov15.doc

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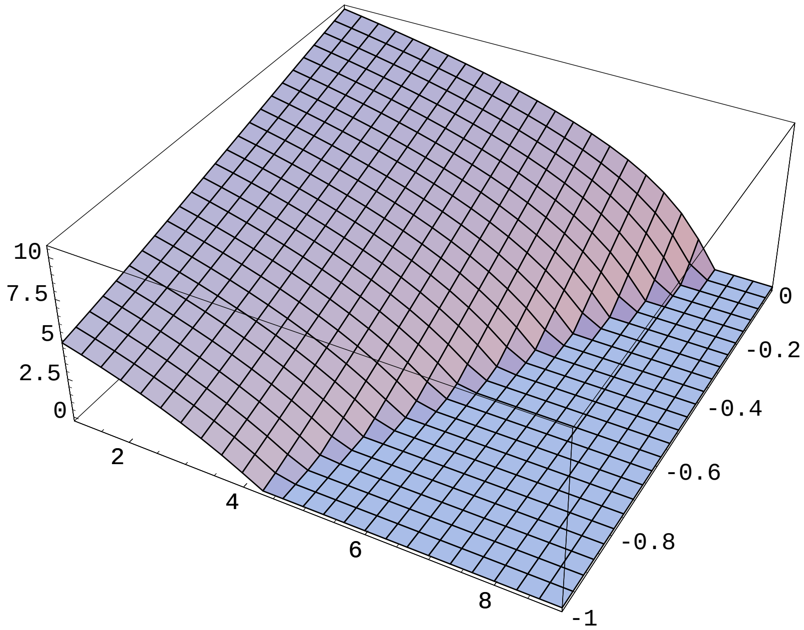
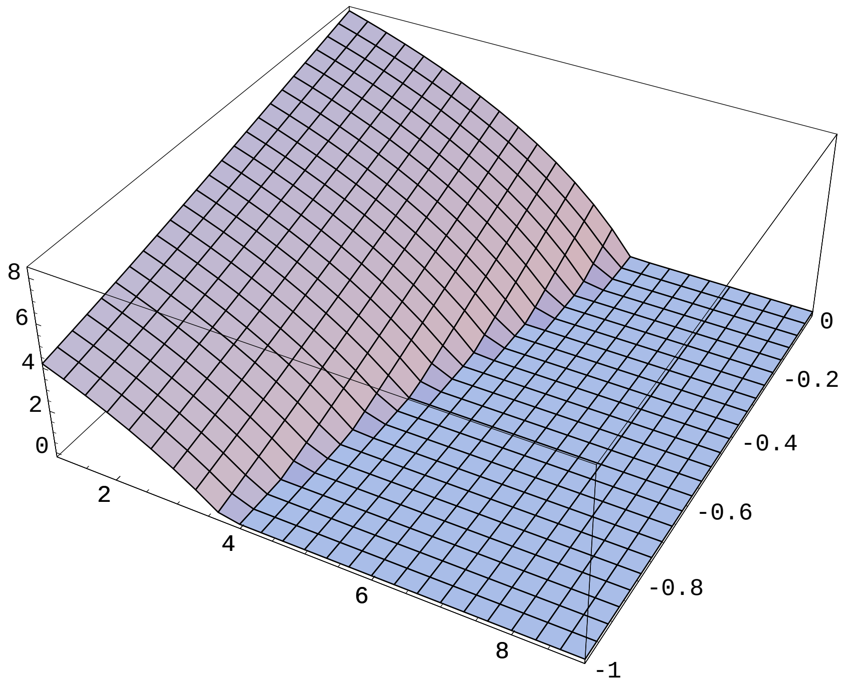


Out[4]= - SurfaceGraphics -

```
In[9]:= Plot3D[h[R, va], {R, 1, 9}, {va, 0, −1}]
```



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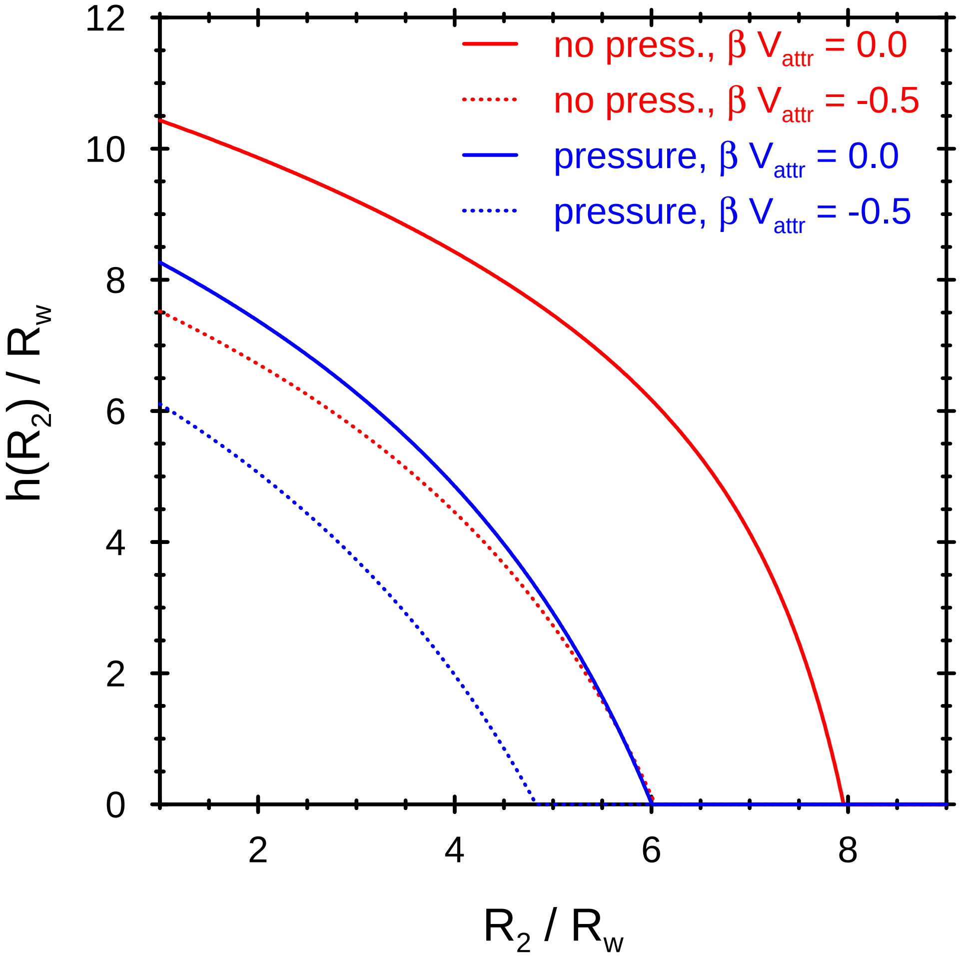

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Number of Water Molecules

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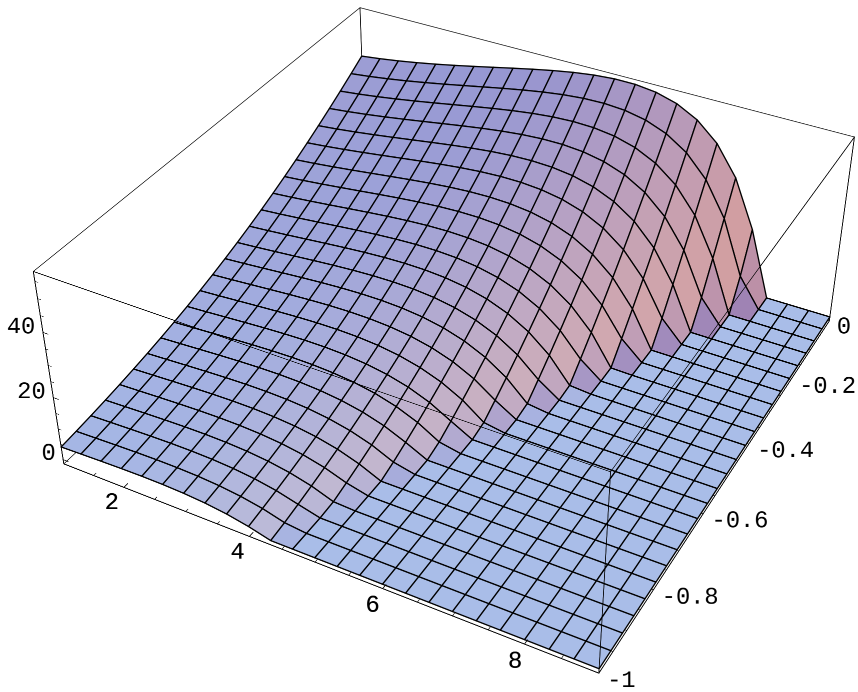
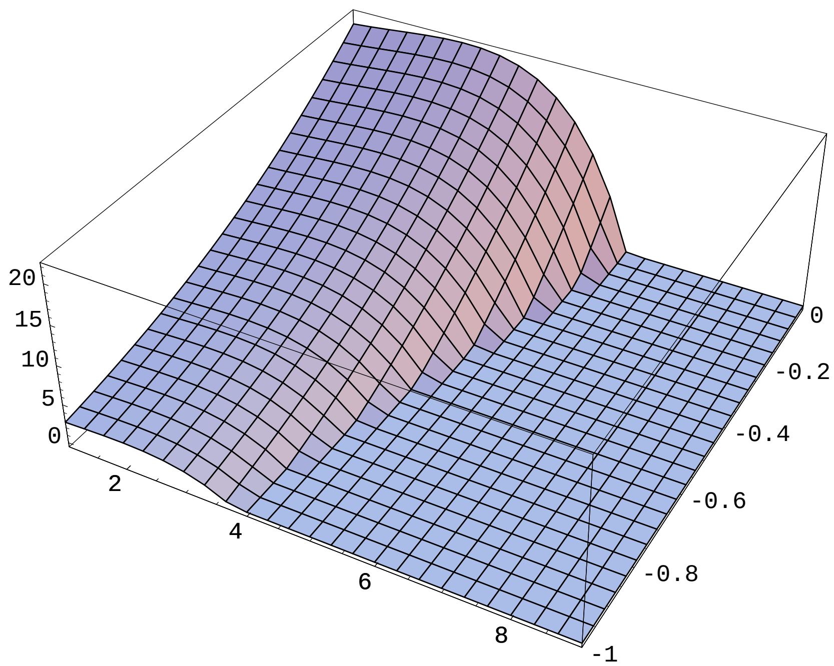



```
Out[5]= - SurfaceGraphics -

In[10]:= Plot3D[dn[R, va], {R, 1, 9}, {va, 0, -1}]
```



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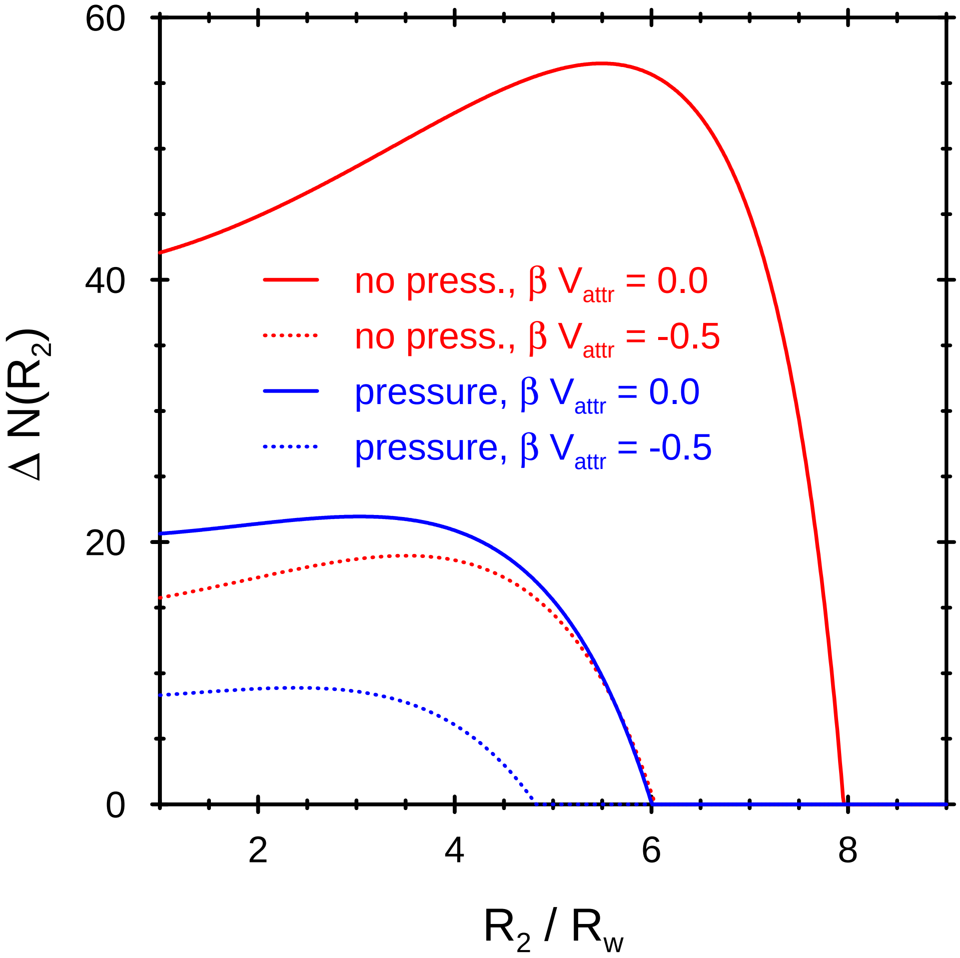

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Open Probability

Nov 20 2006

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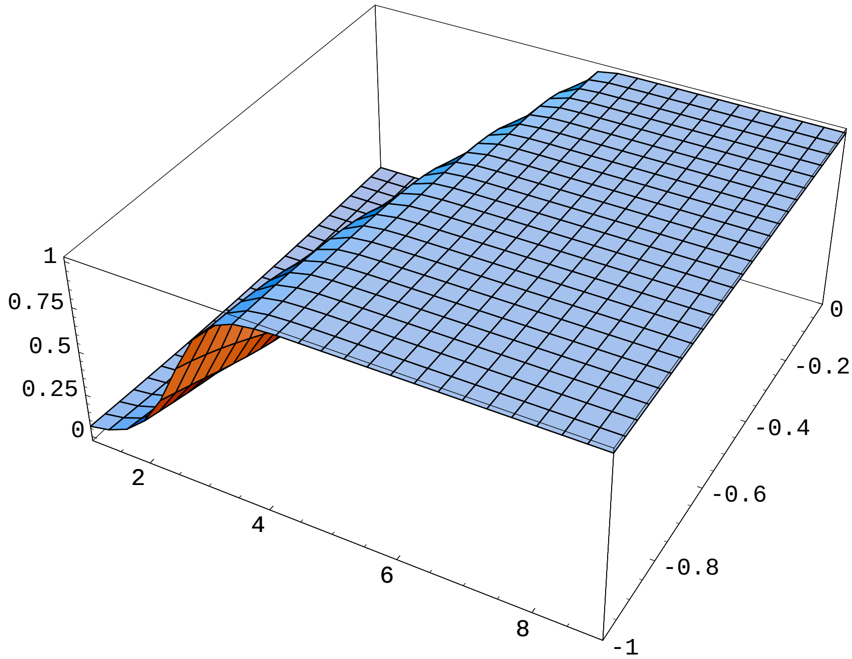
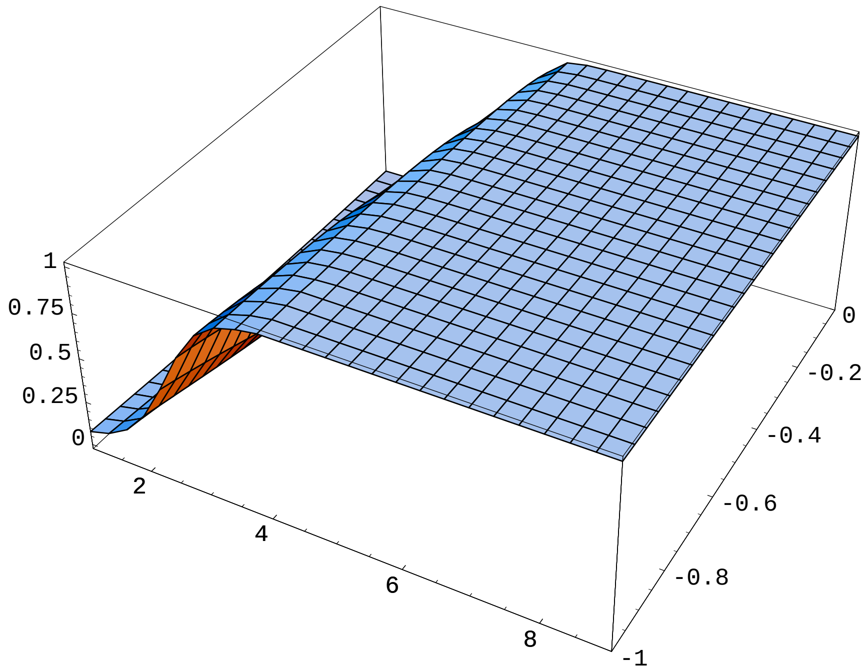


Out[6]= - SurfaceGraphics -

In[11]:= **Plot3D**[**po**[**R**, **va**], {**R**, **1**, **9**}, {**va**, **0**, **-1**}]



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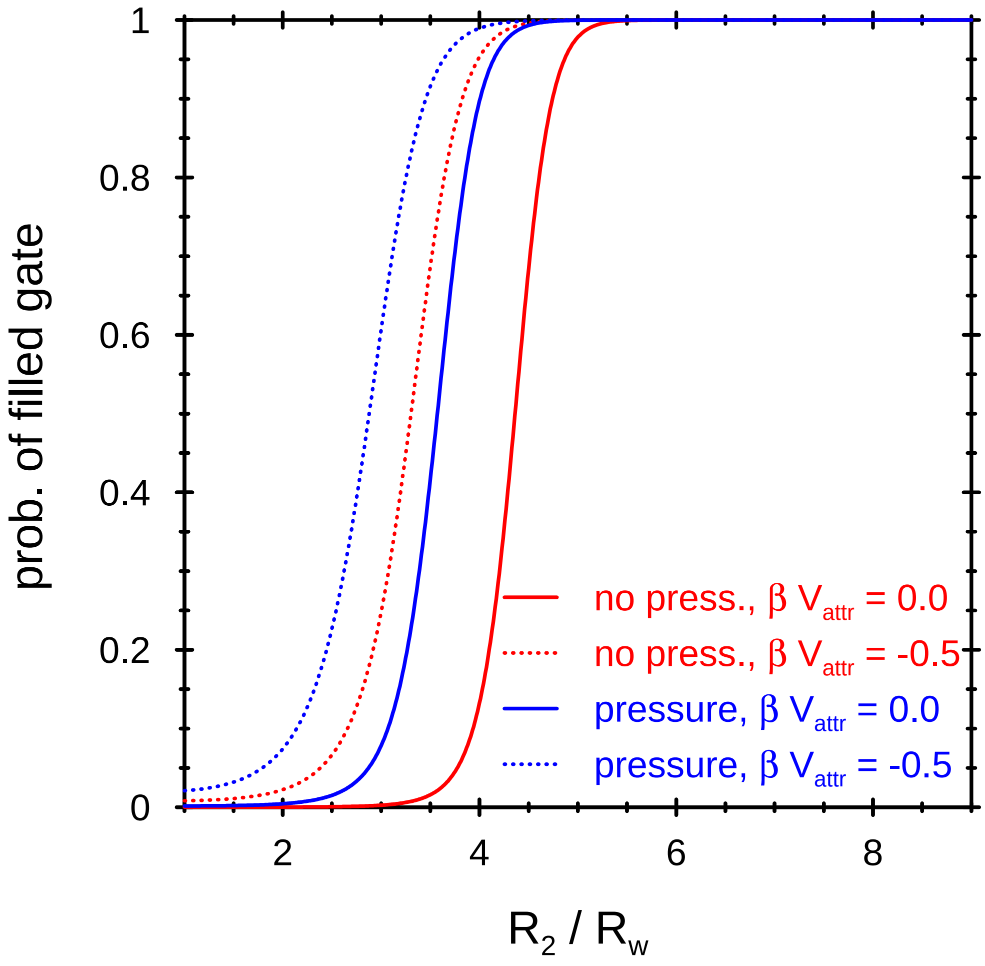

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Close Probability

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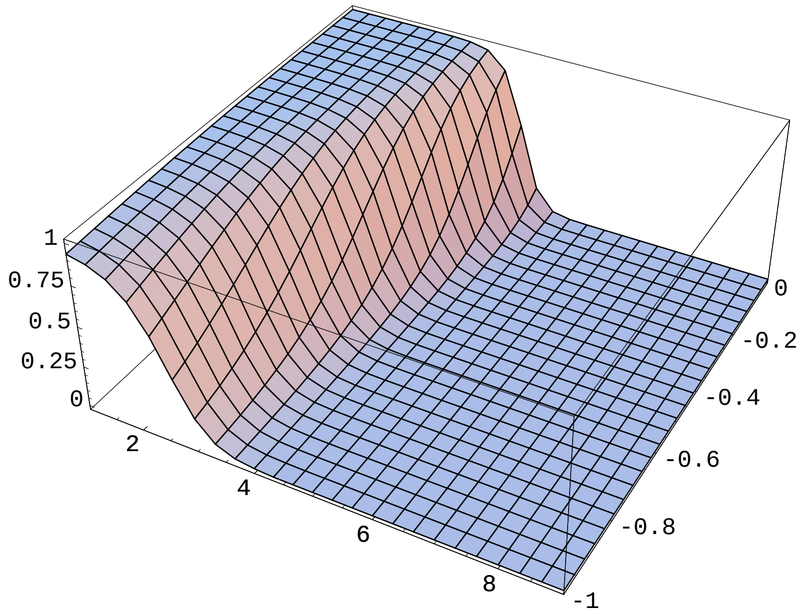
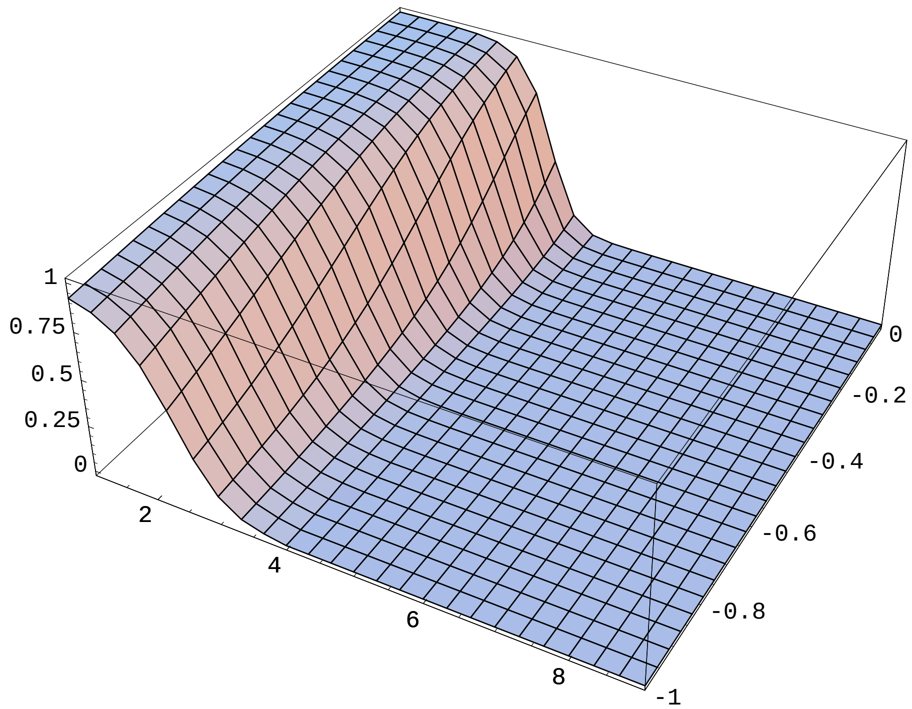


Out[7]= - SurfaceGraphics -

```
In[12]:= Plot3D[pc[R, va], {R, 1, 9}, {va, 0, -1}]
```



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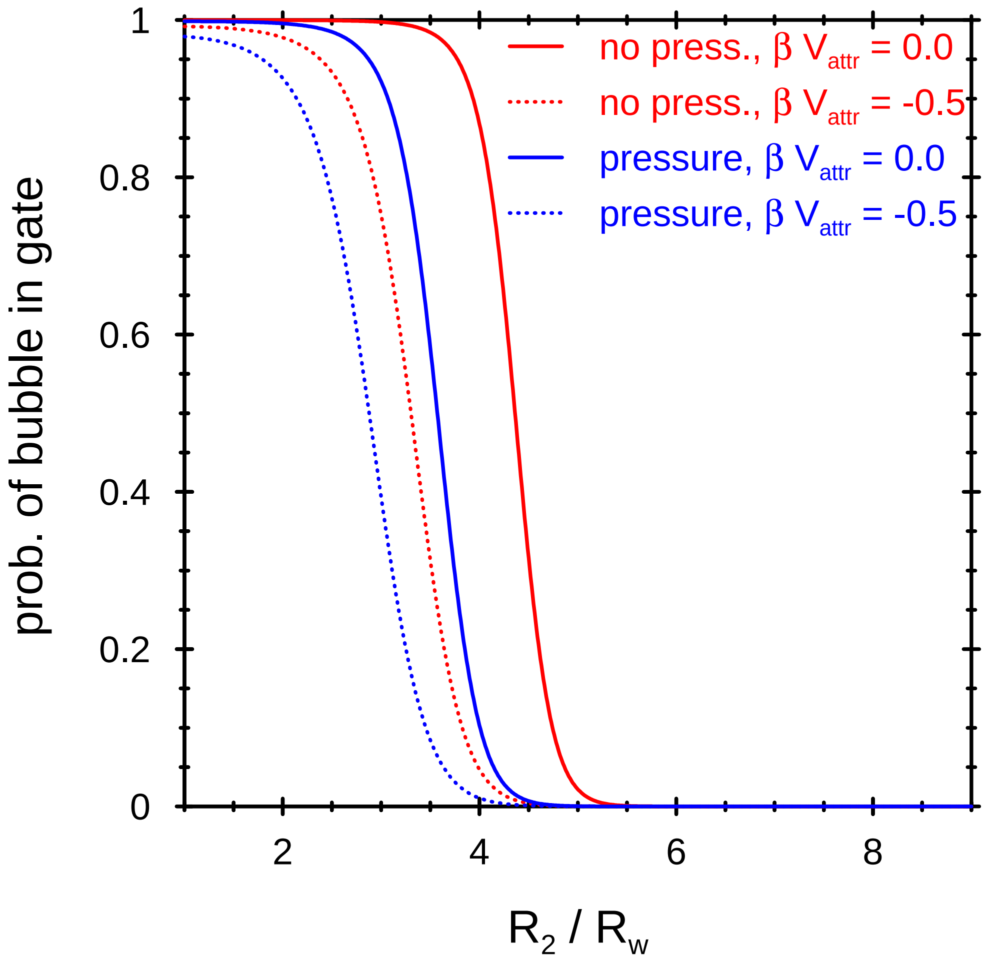

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Bubble formation WITH hydrophobic gases

This is a summary of my calculations of bubble formation with hydrophobic gases in the system. The geometry is the same as in the earlier calculation, characterized by the gate height $H = 18$Åand one fixed radius $R_1 = 13$Å. The second radius, R_2 of the cone can vary. Beside water there is a small amount of a hydrophobic gas dissolved. The parameters are: diameter of the gas $\sigma = 3.36$Åand the concentration is 10^-7M. Note that if I choose a higher concentration, the bubble can not form at all, i.e. the gate is *always* open – I tried also 10^-6M and could not find a bubble at all in the present geometry.
Here I compare the scenario of bubble formation with and without additional hydrostatic pressure (40MPa).

Bubble Height

First I show some results for the bubble height. The three dimensional plots are in the same format as before:
The top plot shows the bubble height $h(R_2, V_{attr}/(k_B T))$ for a system without hydrostatic pressure, the bottom plot shows the bubble height for a system with 40MPa hydrostatic pressure.
Note the bubble height without hydrostatic pressure is large and one can find a bubble even for large values of R_2. This indicates that bubbles form easier with the hydrophobic gas dissolved in the water. If hydrostatic pressure is applied, the bubble height reduces again.
This can also be seen in the cut on the next page.

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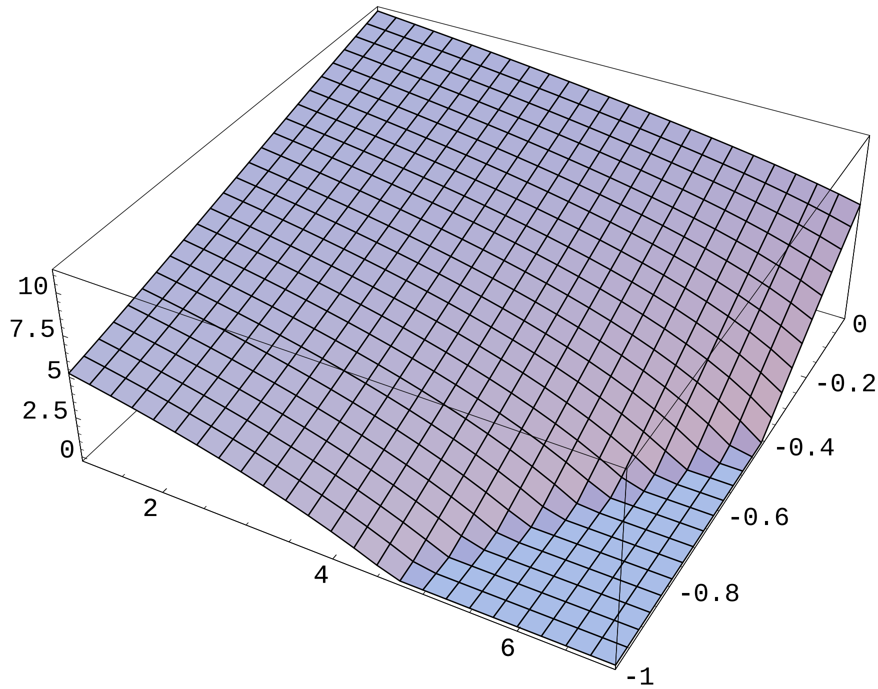
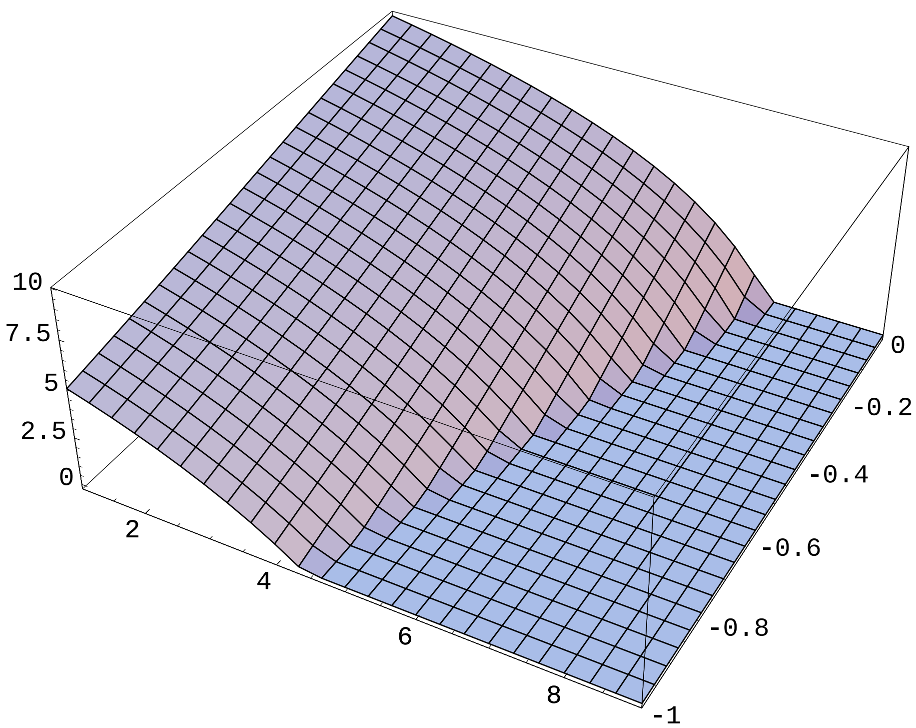


Out[18]= - SurfaceGraphics -

```
In[20]:= Plot3D[h[R, va], {R, 1, 9}, {va, 0, -1}]
```



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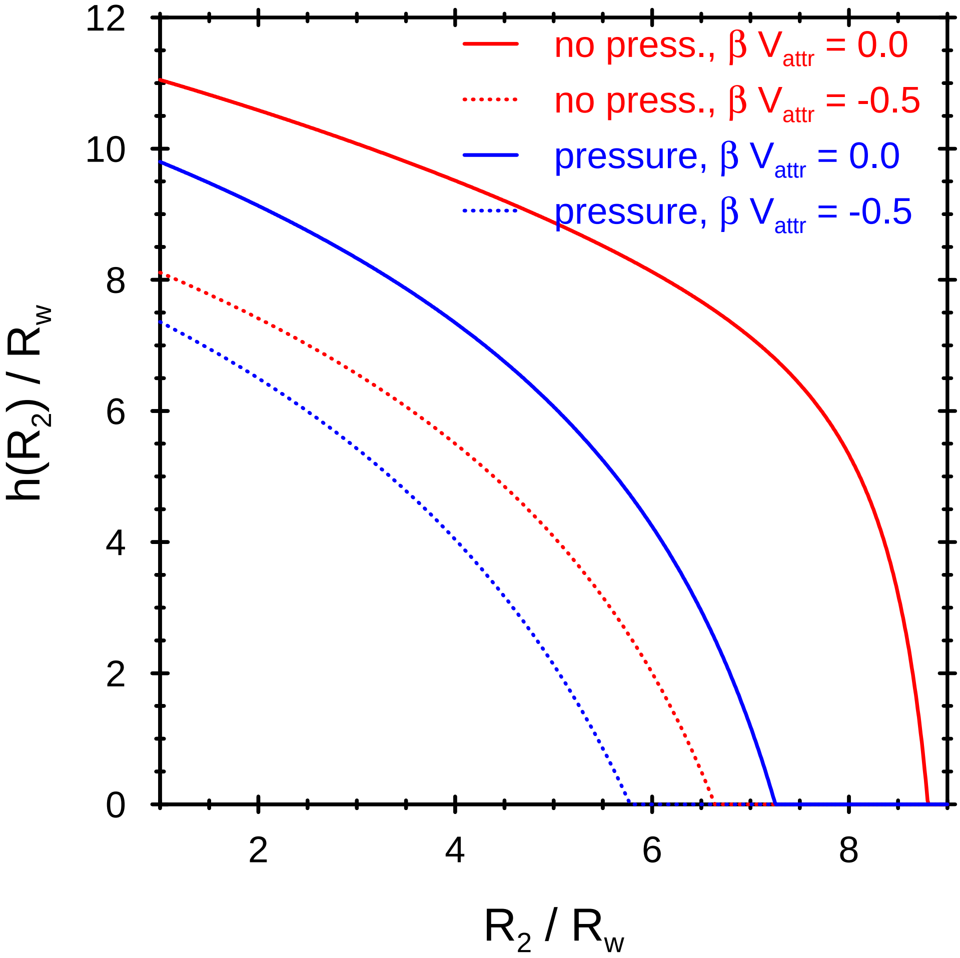

Number of Water Molecules

On the next two pages you find the number of water molecules removed from the gate, when the bubble forms. Now the bubble is filled with particles of the hydrophobic gas.

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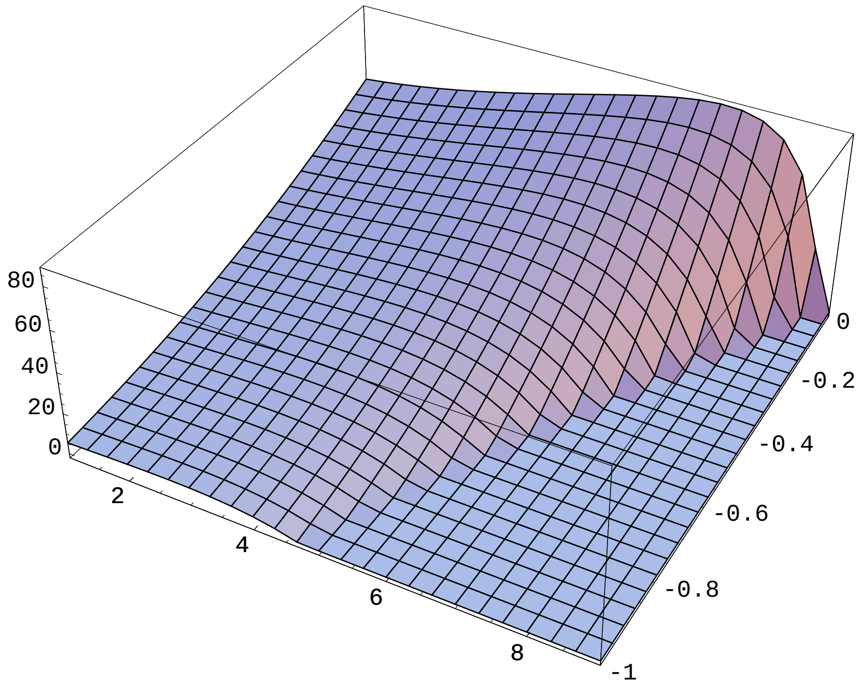
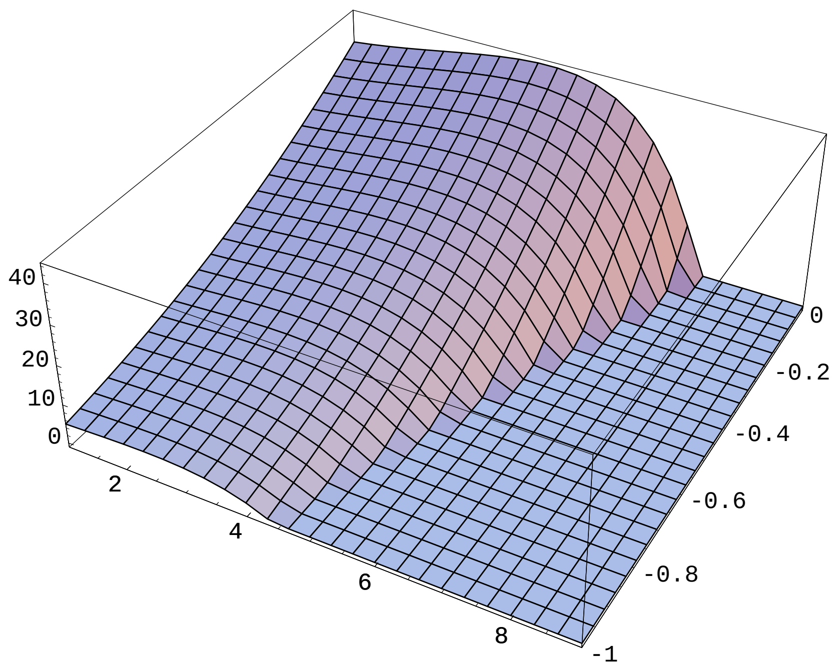


Out[22]= - SurfaceGraphics -

In[24]:= **Plot3D[dn[R, va], {R, 1, 9}, {va, 0, -1}]**



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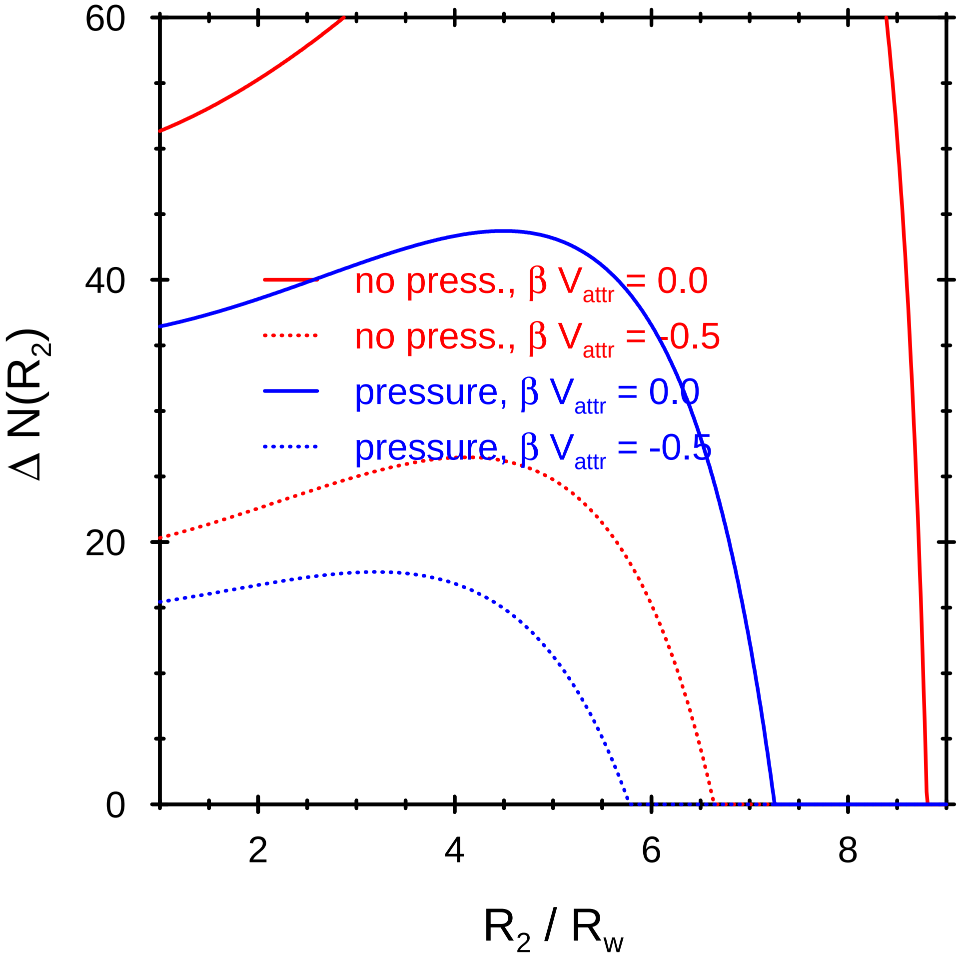

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Open Probability

This is the open probability, i.e. the probability to find a conducting channel.

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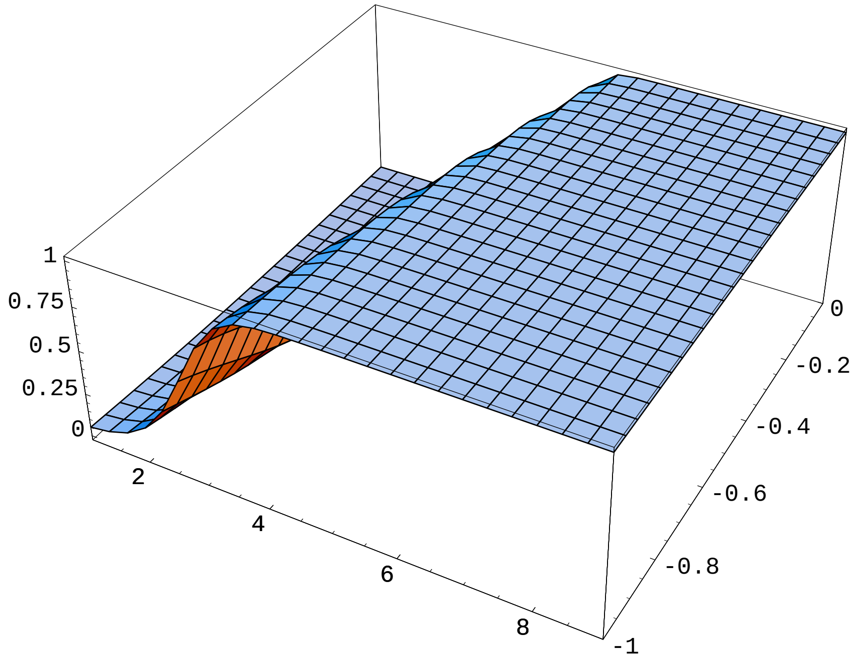
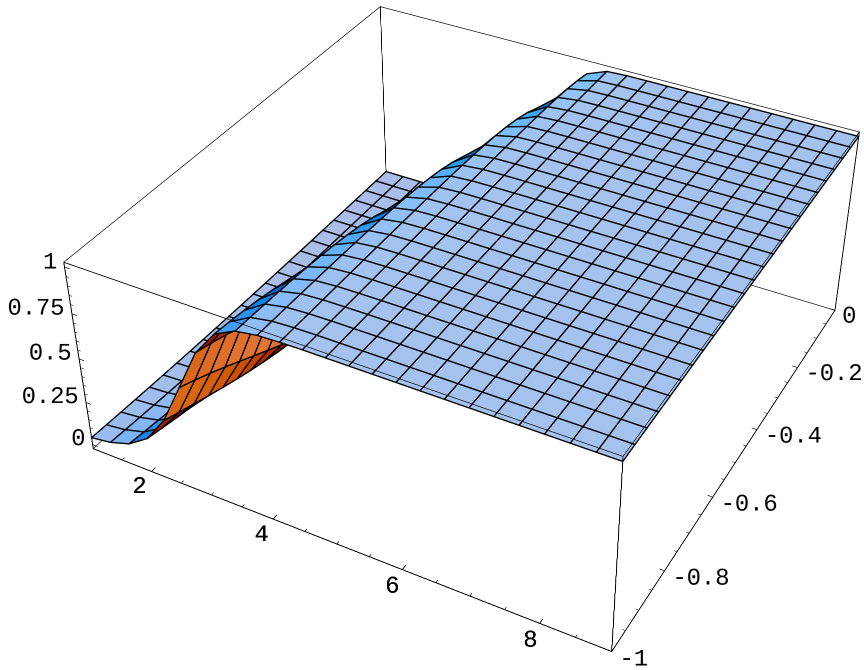



```
Out[26]= - SurfaceGraphics -

In[28]:= Plot3D[po[R, va], {R, 1, 9}, {va, 0, -1}]
```



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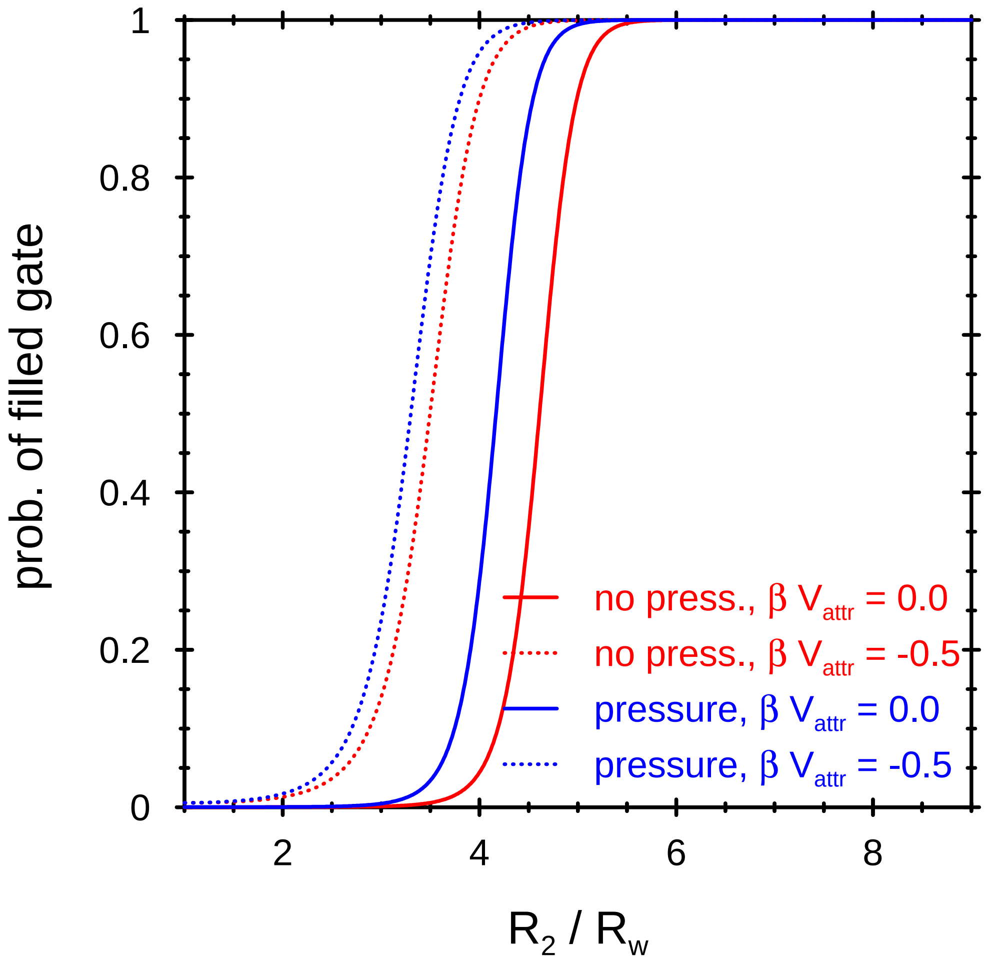

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Close Probability

This is the close probability, i.e. the probability of finding a bubble in the gate. Note that the effect of the hydrophobic gas shift the probability curve a little bit towards larger values of R_2 compared to a system without the hydrophobic gas. This means that a bubble forms easier in the sense that for a configuration of the gate in which it is unlikely to find a bubble without the hydrophobic gas, it is more likely to find one if we add the gas. If one increases the concentration of the gas then the probability curve moves towards even larger values of R_2 until at a sufficiently high concentration one can find a bubble independent of the configuration of the gate.

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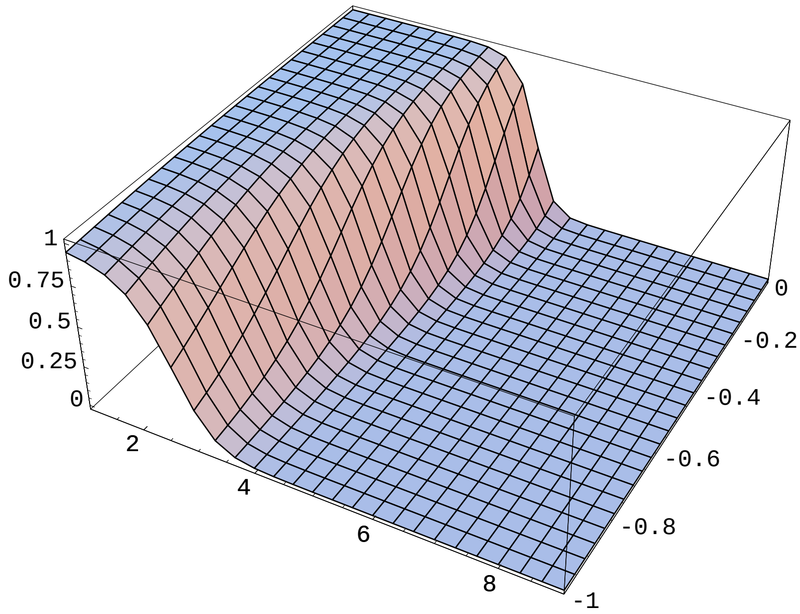
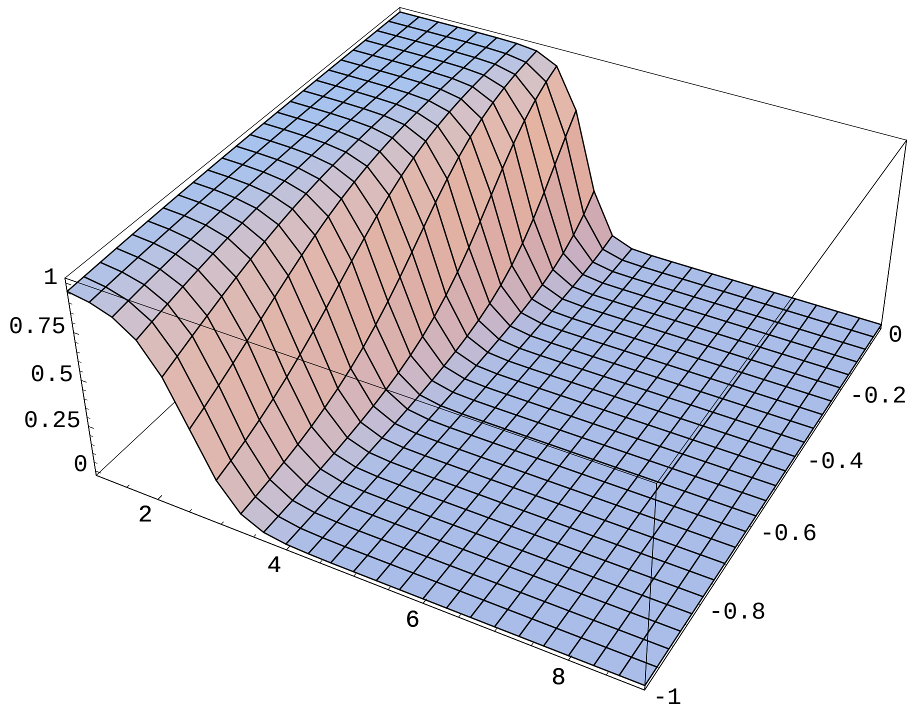



```
Out[30]=  - SurfaceGraphics -

In[32]:=  Plot3D[pc[R, va], {R, 1, 9}, {va, 0, -1}]
```



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