The residence time of molecule is an important parameter to evaluate in order to understand the binding ability of an absorbent. It is calculated using residence auto correlation function C*R*(*t*):



where *θi*(0) = 1 when the molecule i is found in the region of interest (could be the molecules in the first monolayer of a surface, or within the structure of a porous adsorbent at time *t* = 0 or a chosen initial time *t0*). N is the total number of molecules in the region of interest (the first monolayer of adsorbent surface) considered at *t0*. Here *θi*(t0 + t) takes the value of 1 (unity) if the water molecule *i*, which is within the region of interest at the time origin t0, still exists in that region at time t0 + t. Otherwise *θi*(t0 + t) equals 0.

In other words, if an appended molecule continuously remains in the region of interest as the time ‘*t*’ progresses, then *θi*(t0 +*t*) = 1; and *θi*(t0 +*t*) = 0 when the molecule exit the region of interest. The *θi*(t0 +*t*) remains equal to 0 even if the molecule eventually returns inside the region.

The angular brackets denote averaging over various time origins with the aim of improving statistics as well as taking into account different areas of the trajectory. Therefore C(t) gives the average number of water molecules that still remain in the region of interest after a time t. The residence time (*τs*) is evaluated by fitting an exponential form, as shown in following equation, to the C*R*(*t*) values.



**Implementation algorithm**

1) Suppose we want to calculate the (average) residence time of a particular type of molecule in its first monolayer adjacent to the adsorbent surface. Then the first step is to count the all the molecules of this type in its first layer in contact with the adsorbent surface. Furthermore, label (or name or identify) all such molecules of this type in the first layer by index “*i*”. Let us assume the total number of such molecules in this layer is . The first time we count and identify all these molecules in the first layer on adsorbent surface is *t0*.

2) Now increment the time in the MD simulation by one time unit. Track all the (N) molecules identified at time *t0*. For each molecule that is still within the first layer dimensions we put *θi*(t0 +t)=1 (for that molecule). If it not within the layer then *θi*(t0 + t) = 0. For each molecule implement the product *θi*(t0).*θi*(t0 + t). The result of the product for each molecule will be zero or one depending on whether the molecule is still within the first layer of not.

3) Do this step for all N molecules initially found in the first layer of the adsorbent. Sum of all such N products gives us the number of molecules still within the first layer of the adsorbent. Divide this by the total number of initial molecules in the first layer. Thus we have evaluated C*R*(*t*) value for time (t0 +t).

4) Increment time of the MD program by another subsequent unit (t0 +t). Repeat the step 2) and 3). Evaluate C*R*(*t*) value for time (t0 +t). Do the above step (2) and (3) for the desired number of time increments.

5) Step 1) to 4) are repeated for different initial times (the angular brackets represent that summation and averaging).

6) Plot C*R*(*t*) versus time t graph. Calculate average residence or permanence time τs by fitting the equation .