

## Inlet System Design Considerations for Polar and Reactive Compounds

Sample inlets are vital part of mass spectrometer system design, particularly if the sample includes polar or reactive compounds. Quantitative analysis of these compounds could be affected by adsorption and absorption processes. Adsorption can be divided into two distinctly different mechanisms, physisorption which are long range attractive forces (dipole-dipole or van der Waals forces) between an adsorbate and substrate, and chemisorption which are short range intermolecular forces that involve some form of chemical bonding with the substrate. Absorption is a process where a component once reaching a surface is soluble in the substrate material and can further diffuse into and through the bulk matrix. This discussion will focus on adsorption processes although the potential for absorption should never be ignored.

When analyzing pure gases, adsorbate molecules that are in the initial growth layer are held there by the attractive forces discussed above, generally in the 5-20 kJ/mol range in the case of physical adsorption, and 50-150 kJ/mol for chemisorption. There are a number of models, illustrated in Figure 1, for layer growth that are strongly influenced by the nature of the substrate-adsorbate interaction. In any case, the intermolecular attractive forces associated with subsequent layers (after the initial) are represented by the heat of condensation. Therefore, these layers are often referred to as condensate. In the case of mixture analysis the situation is much more complex, both at the initial layer to substrate boundary and subsequent growth layers. However, in all cases the energy necessary to keep a surface “clean” or free of adsorbate molecules is a sum of all intermolecular binding energies between the substrate and various adsorbate molecules.

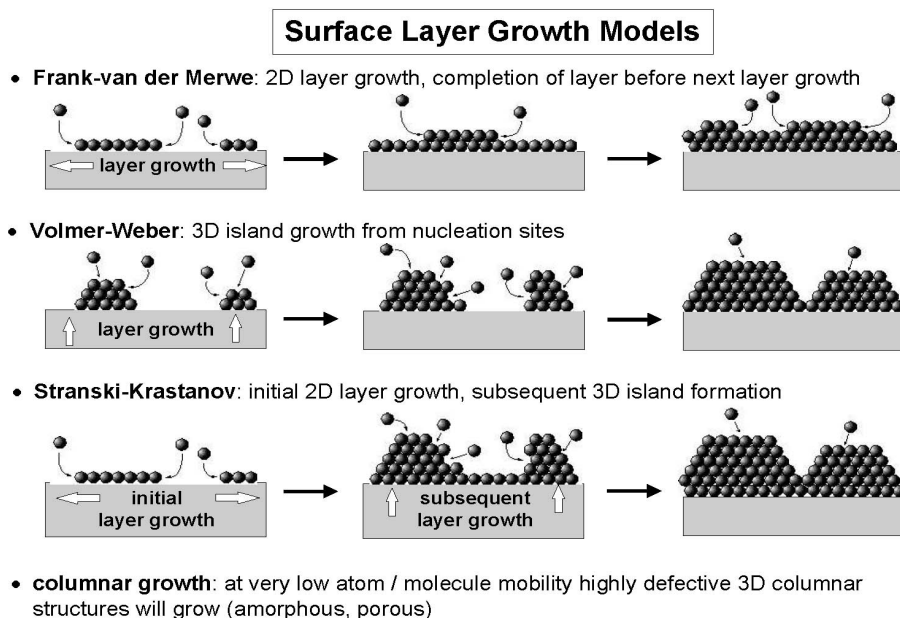
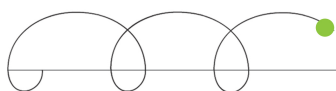


Figure 1



There are essentially 5 areas of inlet system design that can be used to minimize both adsorption and absorption processes and therefore improve mass transport characteristics:

- Material Selection
- Surface Treatment
- Surface Area
- Sample Flow Rate
- Temperature

It is interesting to consider the role of temperature with regard to minimizing the affect of adsorption on the analytical results. In this regard, consider the “average residence time” - the average time a molecule remains on a surface at a temperature “T” in the sample inlet. This parameter is the product of the Boltzmann distribution of the number of molecules having sufficient energy to overcome the intermolecular bonding forces and the frequency at which they oscillate perpendicularly to the surface. The equation for average residence time is as follows:

$$t = t_0 \times \exp(E_{des}/RT)$$

This equation can be used to calculate the average time a molecule is held at a surface by a range of intermolecular binding energies as a function of surface temperature. Table 1 shows selected data from this calculation expressed in seconds. Inspection of this data in the range of chemisorbed

T ° C	T K	4.19 kJ/mol	41.9 kJ/mol	100 kJ/mol	210 kJ/mol	419 kJ/mol
25	298	5.43E+00	2.20E+07	2.20E+07	6.70E+36	
100	373	3.86E-13	7.38E-08	1.01E+01	2.57E+16	4.77E+45
200	473	2.90E-13	4.24E-09	1.11E-02	1.55E+10	1.87E+33
300	573	2.41E-13	6.60E-10	1.31E-04	1.39E+06	1.58E+25
400	673	2.11E-13	1.79E-10	5.78E-06	1.99E+03	3.32E+19
500	773	1.92E-13	6.80E-11	6.80E-11	1.60E+01	2.00E+15

Table 1

molecules, around 100 kJ/mol, illustrates the importance of inlet system surface temperatures. At 100 kJ/mol binding energy, a surface temperature of 100 C results in an average residence time of 10 seconds, whereas at 200 C the average residence time decreases to 10 msec. Note that  $3.15 \times 10^7$  seconds is equal to 1 year. These differences indicate the time necessary to reach a stable measurement condition either when switching streams or when analyzing a single stream with changing composition.

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