Unit steps of an ALD half cycle

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ALD is based on exposing the substrate sequentially to saturative surface reactions with two or more reactants. The elemental step of the ALD deposition method is called the half cycle i.e. the pulse and purge step of one precursor. While in the open literature, the ALD deposition has vigorously been studied from the surface chemistry point of view, the fundamental unit steps from an engineering point of view are much less studied subjects.

In this presentation I will discuss the unit steps that an ALD reactor has to perform in order to approach the ideal ALD half cycle, namely a square wave partial pressure pulse followed by perfect purging of the reactor. In my analysis, I divided the pulse step into five unit steps:
1. Evaporation of the precursor in the source vessel.
2. Transport of the precursor gas to the reaction chamber by forced convection and diffusion.
3. Spreading of the precursor gas in the reaction chamber space by forced convection and diffusion.
4. Diffusion of the precursor gas through the boundary layer above the substrate.
5. Surface reaction of the precursor molecules with the substrate.

The purge step was divided into three unit steps:
1. Diffusion of the reaction by-products through the boundary layer above the substrate.
2. Transport of the surplus precursor and the reaction by-products from the free gas volume of the reactor by forced convection and diffusion and finally.
3. Thermal desorption of the physisorbed or reversibly chemisorbed precursor molecules from the surfaces of the gas inlet conduits and the reaction chamber.

Each unit step is discussed and analyzed theoretically and including some experimental results from real life systems. Based on the analysis of the different unit steps, it is concluded that the most important factors determining the productivity of an ALD process are generally the mass supply rate of the precursor from the source to the reactor and the fluid dynamic design of the reactor.