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Modeling the Precursor Utilization in Atomic Layer Deposition on Nanostructured Materials in Fluidized Bed Reactors

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Atomic layer deposition (ALD) carried out in fluidized bed reactors (FBRs) is a promising technology for coating and decorating nanostructured materials such as nanoporous micron-sized particles and nanoparticles. Such technology boasts the potential for attaining production schemes relevant to the industrial scale, owing to the inherent scalability of FBRs, while retaining the capability of ALD to tune surfaces at the nanoscale. Nevertheless, the economic and environmental feasibility of its actual scale-up strongly depends on the efficiency with which the ALD precursors are used. Residual gas analysis has shown how the use of FBRs, at low pressures, enables complete precursor utilization at high surface conversion for a wide range of particle substrates and ALD systems. However, a thorough dynamic analysis of the governing processes that play a role in determining such high efficiencies has not yet been carried out.

In the current work, we present a multi-scale dynamic model as a means of understanding and optimizing the precursor utilization during ALD on nanoparticles and nanoporous micron-sized particles in FBRs. We use as a case study the deposition of alumina through trimethylaluminum and water on both titania nanoparticles and nanoporous micron-sized alumina particles at reduced (~1 mbar) and atmospheric pressure. In doing so, we assess the effect of precursor transport, from the inlet of the reactor till the particles active surface, on the precursor utilization efficiency. In particular, we elucidate the effect of pressure, reactor height, average bubble size and internal structure of both nanoparticle agglomerates and nanoporous micron-sized particles. Finally, We show that fluidized-bed ALD on high-surface-area powders is a forgiving process that can be carried out with virtually no precursor waste.

Keywords: Atomic layer deposition; Nanostructured materials; Fluidized bed reactors; process efficiency; Modeling