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The figure shows a comparison of the pentakis(dimethylamido) tantalum (PDMAT) mass carryover for pulsed delivery from two relatively simple flow over vessel designs. (A "flow over vessel" refers to a vessel through which carrier gas flows but which has no dip tube: the gas inlet and outlet ports open directly into the vessel head space.) The involves CFD comparison simulations for two vessels that each have a 1.5 L volume but different heights and diameters. The 1:1 vessel has an internal



diameter and internal height of 12.7 cm and 12.4 cm, respectively. The 2:1 vessel has an internal diameter and internal height of 15.5 cm and 8.0 cm, respectively. Also shown are mass carryover values for the 1:1 vessel measured with a non-dispersive infrared gas analyzer. Conditions for these comparisons are 2 s PDMAT injection followed by a 16 s purge with a 1.0 SLM argon flow rate, 4.09 kPa pressure, 75 °C vessel temperature, and 200 g PDMAT fill. The results indicate that, after the first injection, an increase in mass carryover and improved reproducibility likely can be obtained by increasing the cross sectional area occupied by the precursor. These trends are attributed to an increase in PDMAT diffusing into the head space during the idle. Hence, any process parameter change that tends to reduce the binary diffusion coefficient, e.g., higher pressure or lower temperature, will counteract the improvement observed with the 2:1 vessel compared to the 1:1 vessel. This illustrates the need to understand the origin of any improvements and to identify the process parameter range under which the improvements may be observed.