## 599e Use of Computational Fluid Dynamics for Catalyst Deactivation at Commercial Plants

Sue Degaleesan, Janine A. Toner, and Jonathan H. Worstell

The Shell Higher Olefins Process (SHOP) isomerizes alpha olefins to internal olefins using a proprietary catalyst. This catalyst must be deactivated at the end of its process life. Deactivation of this catalyst includes and a hydrocarbon wash step followed by flooding the reactor with water, which generates significant heat. Thus, flow distribution through the reactor is important. Computational fluid dynamic (CFD) models were developed to study the flow distribution through a SHOP isomerization reactor for both the water flooding step and the hydrocarbon washing step. Results show that there are flow distribution issues associated with both process steps. Flow maldistribution in the bottom conical section of the reactor leads to "dead zones". Flow maldistribution results in relatively more active catalyst in these "dead zones" of the reactor which potentially leads to more active localized deactivation, with rapid by-product formation and heat generation, causing disintegration of the catalyst to form fines. Utilization of this information has led to significant changes in reactor operation in the SHOP plants.