A PAT Study of an Industrial Catalytic Hydrogenation of an Active Pharmaceutical Ingredient

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Abstract
Process analytical technologies (PAT) designate the integrated use of industrial process analytical chemistry techniques with classical process systems engineering tools, for the analysis and control of manufacturing processes. In this work we report on the development and integrated use of an at-line monitoring technique with a kinetic model of the process, to establish a basic understanding of an industrial catalytic hydrogenation of an active pharmaceutical ingredient (API). A suitable process spectroscopy technique (NIR) is described to monitor the most relevant reaction constituents, in terms of process performance (product distribution, reagent conversion and catalyst selectivity and stability). A kinetic model is also proposed for the process, which is capable of describing the industrial process under diverse operating conditions. The success of the industrial PAT application described is indicative of this methodology general value for industrial process analysis, control and optimization without production disruption.

Keywords: process analytical technologies (PAT), near-infrared (NIR), multivariate modelling (PLS), pharmaceutical production

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