

Technical University of Denmark



Substrates adoption methodology (SAM) to achieve “Fast, Flexible, Future (F3)” pharmaceutical production processes

Singh, Ravendra; Rozada-Sanchez, Raquel; Wrate, Tim; Muller, Frans; Gernaey, Krist V.; Gani, Rafiqul; Woodley, John

Publication date:
2011

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):

Singh, R., Rozada-Sanchez, R., Wrate, T., Muller, F., Gernaey, K., Gani, R., & Woodley, J. (2011). Substrates adoption methodology (SAM) to achieve “Fast, Flexible, Future (F3)” pharmaceutical production processes. Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.

DTU Library

Technical Information Center of Denmark

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Substrates adoption methodology (SAM) to achieve “Fast, Flexible, Future (F³)” pharmaceutical production processes

Ravendra Singh¹, Raquel Rozada-Sanchez², Tim Wrate², Frans Muller², Krist V. Gernaey¹, Rafiqul Gani¹, John M. Woodley¹

¹Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

²AstraZeneca Limited, Charter Way, Silk Road Business Park, Macclesfield, Cheshire SK10 2NA, UK

There is a significant cost associated with process development of a portfolio of pharmaceutical products, few of which will reach the market. Continuous processing will increase the “chemical space” which can increase development efficiency. For example one, particularly attractive option is to develop manufacturing processes based on modular continuous systems; a flexible generic continuous modular plant which can be adapted for different substrates. In the work reported here, a substrates adoption methodology (SAM) has been developed. The proposed SAM identifies the necessary changes to a *template* recipe & flowsheet in order to adapt it for a given substrate. The changes can be related to reagents (e.g. reducing agent, solvent, catalyst), process conditions (e.g. operating temperature, flow rates), as well as in the physical arrangement (configuration) of the modular process equipment within the template. In this way the substrates adoption methodology helps to achieve “fast, flexible, future (F³)” pharmaceutical production processes by adapting a recently designed generic modular process-plant. The supporting tools for the substrate adoption are: (1) an ontological knowledge-base consisting of the properties of substances, reaction characteristics and characteristics of unit operations; and (2) a model library consisting of the mathematical models. The objective of this presentation is two-fold: First to highlight the substrates adoption framework and the associated models, methods and tools, and second to demonstrate its applications using a pharmaceutical manufacturing case study involving the nitro reduction of 2-Nitro-4'-chlorodiphenylamine.

¹ F3 Factory project, European Community's 7th Framework Program under grant agreement n° 228867
<http://www.f3factory.com/scripts/pages/en/home.php>