Systematic multi-scale model development strategy for fragrance spraying process and transport

Heitzig, Martina; Gregson, Chistopher; Sin, Gürkan; Gani, Rafiqul

Publication date:
2011

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

Citation (APA):
Heitzig, M., Gregson, C., Sin, G., & Gani, R. (2011). Systematic multi-scale model development strategy for fragrance spraying process and transport. Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.

Systematic Multi-Scale Model Development Strategy for Fragrance Spraying Process and Transport

Martina Heitzig, Technical University of Denmark, Lyngby, Denmark; Chistopher Gregson, [b]Firmenich Inc., Plainsboro, NJ USA; Gürkan Sin, Technical University of Denmark, Lyngby, Denmark; Rafiqul Gani, Technical University of Denmark, Lyngby, Denmark

Model-based computer aided product-process engineering has attained increased importance in a number of industries, including pharmaceuticals, petrochemicals, fine chemicals, polymers, biotechnology, food, energy and water. This trend is set to continue due to the substantial benefits computer-aided methods provide. The key prerequisite of computer-aided product-process engineering is however the availability of models of different types, forms and application modes. The problems to be solved in product-process design are often complex and on multiple scales and therefore model development is a non trivial time-consuming task involving numerous steps, expert skills and different modelling tools.

This has motivated the development of systematic methodologies to efficiently develop, analyse, identify, validate and apply the models for the complex systems under investigation in product-process design, as well as the implementation of these methods into a computer-aided modelling framework. The main benefit of this work is to increase the efficiency of the modelling process (saving time and resources).

Computer-aided modelling framework

The developed modelling framework is structured based on the work-flow and data-flow the modeller needs to follow to fulfil the desired modelling task. The framework consists of two main parts (work-flows) for model development. The first part is dedicated to single-scale model development while the second part supports the modeller during multi-scale scenario development and comparison. The second part of the modelling framework manages different multi-scale scenarios, supports in the systematic derivation of a new scenario

and links the models for the different scales according to the linking scheme of the multi-scale scenario. The single-scale model development part supports the modeller in model documentation, construction and analysis. Different models for properties, phenomena, unit operations and processes can be developed and analysed here or are retrieved from model libraries. The model equations are introduced in a simple text format and are translated by reverse polish notation (RPN). A model object is generated which can be applied in a stand-alone-mode, stored in libraries and/or linked to other models. Once the models have been constructed and analysed the modelling framework incorporates work-flows for model identification and validation as well as for model application for simulation or optimization.

Case study

In this contribution, the emphasis is on the application of the developed modelling framework in an industrial case study which is related to a multi-scale modelling problem of an aerosol system. The spraying process of a fragrance product is modelled. Initially, a mixture of the fragrance product and a propellant is contained inside a pressurized can. The pressure drop caused by releasing the fragrance product to the atmosphere results in heavy evaporation of the propellant and the formation of droplets by the remaining liquid. The required models for the system can be subdivided into two parts.

Part I: Modelling of the release process from the pressurized can and prediction of the initial droplet size distribution, composition and temperature of the droplets.

Part II: Modelling of the transport of the formed aerosol.

The developed model is to be applied to predict and evaluate the product qualities and performance.