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Large eddy computational fluid dynamic symulations of drug dissolution in a USP II apparatus

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The popularity of the oral route as the most common route for drug administration is due to its convenience, low cost, and high patient compliance. In the development of new products, it is essential to ensure that the tablet dissolves at a certain time and place. It is a time- consuming and resource-intensive process to develop pills conventionally.

This study is part of a larger research plan to develop a user-friendly drug dissolution prediction methodology using an *in-silico* approach. At this stage of the research, a numerical model is developed that uses the fundamentals of computational fluid dynamics and drug release/disintegration kinetics to estimate drug dissolution time in a laboratory-controlled system. In addition, it is assumed that the tablet consists only of a single active pharmaceutical ingredient.

The Finite Volume solver based on the OpenFOAM toolkit was used to determine the dissolution of paracetamol tablets and the diffusive/convective transport in the USP II dissolution apparatus. The design of the apparatus determines the formation of the velocity field, the turbulent and convective transfer, and the rate of heat and mass transfer, which directly affect the mixing efficiency. The water flow was described by incompressible Navier-Stokes equations and turbulence was modeled with the Large Eddy Simulation turbulence model. In comparison, the analysis of published studies shows that the simplest RANS-type models are generally used to simulate the dissolution processes in USP apparatuses. The interaction between the non-rotational and rotational domains of the FV mesh was provided by the built-in GGI facilities of OpenFOAM. Validation with laboratory experiments shows that the main tendencies of the drug solution process are captured by the Computational Fluid Dynamics model.

Biography

Normunds Jekabsons received his PhD at Lulea University of Technology (Sweden) in 2002. He is a lecturer and the leading researcher at the University of Latvia. He has extensive experience in numerical methods and their application to solve various types of engineering problems. He has coordinated several national and international research projects, including EEA/Norway Grants and the ESA projects. He has international collaboration experience (e.g., the Lule University of Technology (Sweden), the University of Tartu (Estonia), the Arctic University of Norway, and the Paul Scherrer Institute (Switzerland)). He is the author of more than 30 Scopus-referenced papers.

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