

Fully funded PhD studentship at University of Surrey, in collaboration with Unilever, on

“Multi-scale modelling of dermal absorption, disposition, systemic circulation and liver metabolism of xenobiotics”

Project description

Computational modelling of transdermal permeation and cellular metabolism of topically administered chemicals is an important non-animal approach to safety assurance and product development in the consumer goods, agrochemical and pharmaceutical sectors. Promising developments have been made in recent years in dermatokinetic modelling of dermal bioavailability, physiologically-based pharmacokinetic modelling (PBPK) of chemical transport and distribution in whole body, as well as systems biology modelling of metabolic networks. In particular, models for dermatokinetics are being progressed from simplistic compartment-based approach to including microscopic heterogeneous skin physiology, notably the brick-and-mortar structure of the stratum corneum and shunt pathways (hair follicles, sweat ducts, etc.). In addition, state-of-the-art systems biology models can describe thousands of metabolites and reactions.

At University of Surrey, we have been closely collaborating with Unilever in developing advanced computational models for skin absorption (see *Chen T, Lian G, Kattou P (2016). In silico modelling of transdermal and systemic kinetics of topically applied solutes: Model development and initial validation for transdermal nicotine, Pharmaceutical Research, in press; doi: 10.1007/s11095-016-1900-x*). This project aims to further this research to systematically study the role of metabolism and ionisation in skin absorption. We will explore the integration of systems biology metabolic network model into our existing biophysical permeation model. Furthermore, existing QSPR (quantitative structure-property relationships) models will be extended to consider the impact of ionisation on transport properties in skin, which will in turn improve the accuracy of the multi-scale model. By the end of the project, the student will be an expert in computational modelling, skin biophysics and biochemistry, and systems biology, which are highly sought-after skills by the industries of pharmaceuticals, personal care, cosmetics, agrochemical and other chemical sectors. The student will have close interaction with scientists at Unilever, the industrial sponsor, through secondment and visit, thus developing an understanding and valuable experience in industrial research and development.

Residence eligibility

This studentship is funded by the BBSRC Industrial CASE scheme with Unilever being the industrial sponsor. As such the candidates must meet the following eligibility criteria set by the BBSRC:

- Settled status in the UK, meaning they have no restrictions on how long they can stay; and
- Been 'ordinarily resident' in the UK for 3 years prior to the start of the studentship. This means they must have been normally residing in the UK (apart from temporary or occasional absences); and
- Not been residing in the UK wholly or mainly for the purpose of full-time education. (This does not apply to UK or EU nationals).

The studentship will last for four years. It will cover the tuition fee at UK/EU level, and provide a PhD stipend (c. £18,000 per annum), as well as generous budget for training activities (workshops, conferences, etc.).

Ideally the candidate should be ready to start on **1st October 2016**, or soon afterwards.

Academic requirement:

- A relevant degree (first or upper second) in engineering, physics or chemistry.
- Experience in computer programming and/or mathematical modelling.
- A Master's degree is not a pre-requisite but would be looked upon favourably.
- Non-native speakers of English who did not study in an English speaking country will be required to have IELTS 6.5 or above.

The application shall include:

- 1) Cover letter (max 1 page) explaining your interest and suitability for the project.
- 2) CV (max 2 pages).
- 3) Published work such as journals and conference articles.
- 4) Copy of your academic transcripts.
- 5) Copy of your MSc dissertation (if appropriate).
- 6) Names and contact information of at least two referees.
- 7) If applicable, a copy of a valid IELTS certificate from the past two years.

Applications and any enquiries should be emailed to Dr Tao Chen (t.chen@surrey.ac.uk), Department of Chemical and Process Engineering, University of Surrey. Applications will be reviewed when received, and shortlisted candidates will be interviewed. The position will remain open until a suitable candidate is found.