



TCS Digital Skin Twin platform will enable accelerated design and testing of pharmaceutical and cosmetic formulations.

THE CONTEXT



Given the time and cost involved in traditional techniques of designing pharmaceutical and personal care formulations and their in-vitro/in-vivo testing on animals, it has become imperative to supplement or replace some of these elaborate tests with in-silico (digital or computer simulation) tests. Testing of cosmetic formulations on animals and import of cosmetics tested on animals have been banned in various countries across the globe (EU Regulation 1223/2009; Bureau of Indian Standards (BIS), June 2013; California, USA, 2018 etc.). Pharmaceutical and personal care product manufacturers looking for benign and more efficient alternatives to animal testing are therefore seeking innovative solutions based on digital technology.

THE INNOVATION



TCS Research team has developed an in-silico, physics-based skin model based on multi-scale modelling framework and augmented with virtual reality (VR). TCS Digital Skin Twin model represents stratum corneum – the outermost layer of the human skin, which acts as a natural barrier against bacteria and other pathogens.

This model is tested extensively against available experimental data and provides a unique collaborative environment for design of various formulations having nanomaterials leveraging state-of-the-art scientific computing. It helps manufacturers identify non-viable formulations at the early stages of product development, thereby bringing down costs.



KEY CHALLENGE

NON-AVAILABILITY OF EXPERIMENTAL DATA

The human skin permeation of cosmetics & pharmaceutical formulation is proprietary of respective industries and not available in the open domain. Hence, the model is validated against permeation data of simple formulations (having one or two components) available in the open domain. TCS Research team has conducted a Proof of Concept with one personal care major, where the digital model has been used to see the permeation of molecules shared by them. The model was also piloted in real conditions through experiments conducted in collaboration with Harvard University.

CAPTURING COMPLEXITY OF SKIN COMPOSITION

Nature has designed our skin in such a way that even small molecules cannot penetrate the skin barrier. This barrier comes from the outermost layer of skin i.e. stratum corneum, which is made up of dead proteins and almost 300 types (3 classes) of lipids. Modeling all of them will require enormous computational capacity. To overcome this problem, we have selected one representative molecule of each class and built molecular model of lipid layer. This model is further connected to macroscopic skin model utilizing multiscale modelling framework and validated with real skin permeation experiments. Further, we have developed models for other types of lipid molecules which were piloted along with Martin Luther University, Germany.



POTENTIAL IMPACT



The global transdermal/topical drug delivery and cosmetics markets are projected to touch revenues of more than 100 bn (Markets&Markest) and \$350 bn (Marketresearchengine) respectively, by 2023. The regulators, FDA, emphasizing on increment of digital intervention in drug/cosmetics testing paradigm. TCS has completed a PoC with a well-known personal care customer. Patents have been filed in various geographies and can potentially be leveraged into business opportunities.