

*Designing the new generation
of plant based foods: from cook
and look to screening solutions
present in nature*

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How do we design products?

Pharmaceutical Industry

- Platform technologies
- AI driven innovation
- 1536 well plates, multipl assays, HT micrscopy
- Petabytes of data



A critical bottleneck limiting the potential of Machine Learning (ML) and Deep Learning (DL) models within the drug discovery and development (DDD) pipeline is the scarcity of high-quality experimental data. **Limited data is not an anomaly but an inherent characteristic of the DDD process.**

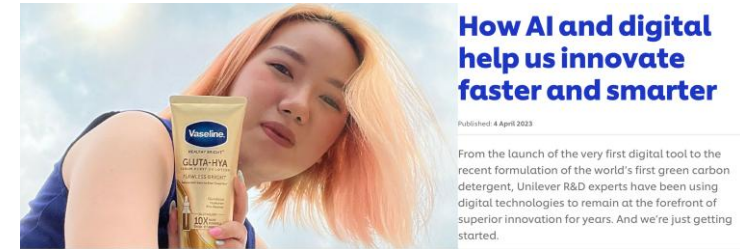
Pallikkavaliyaveetil et al., 2026

Digital Design: Formulated products



L'ORÉAL

Alchemi platform –
predict interactions
of components
before doing
experiments



Optimise formulations (cost reduction)
New products faster on the market

Data generation is now possible

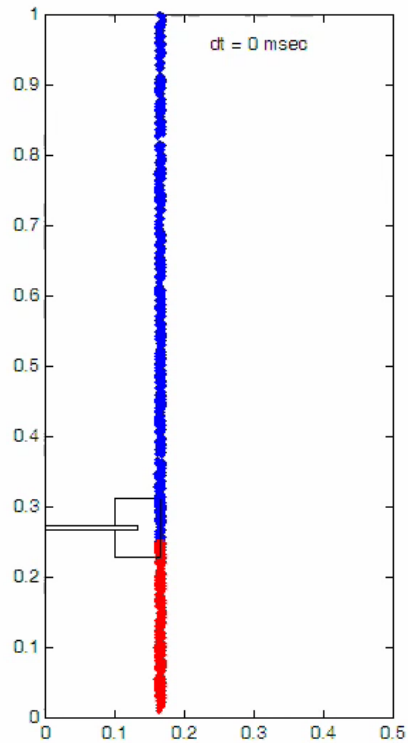
Product Engineering

- FOOD - UoCopenhagen, Chem Eng: UoNottingham (2017-2020), UoBirmingham (2005-2017)
- PhD Food Engineering (*Food Science Rutgers University, USA*), MEng Chemical Engineering (*NTUA, Greece*)
- Track record in the broad area of **formulation engineering**

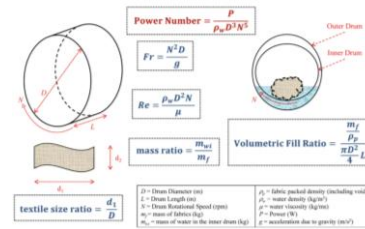
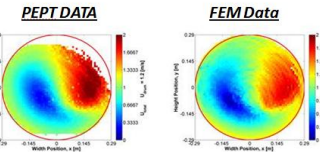
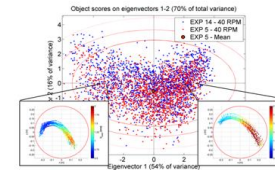


Background

Food Engineering

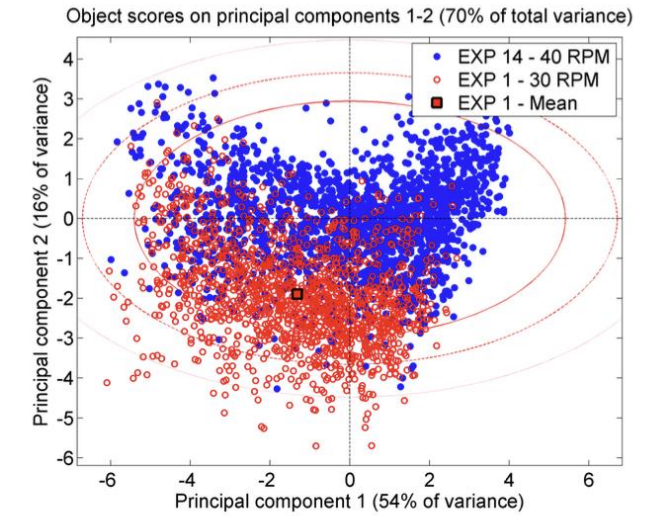
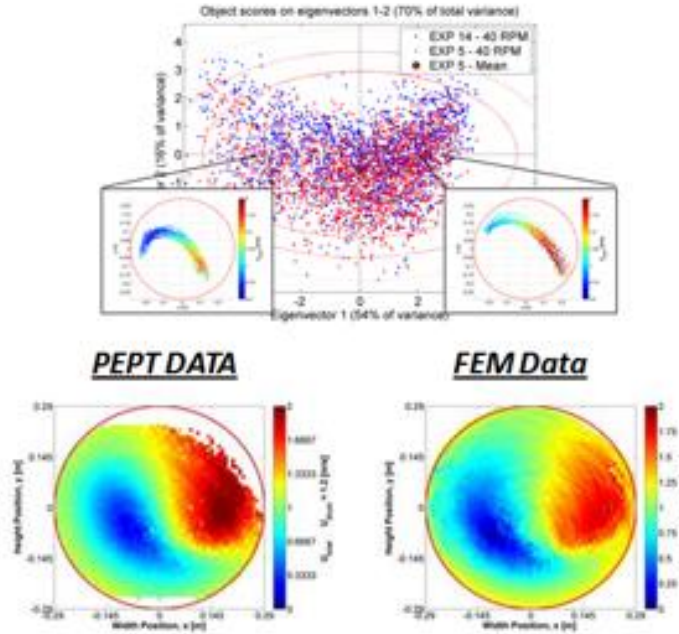
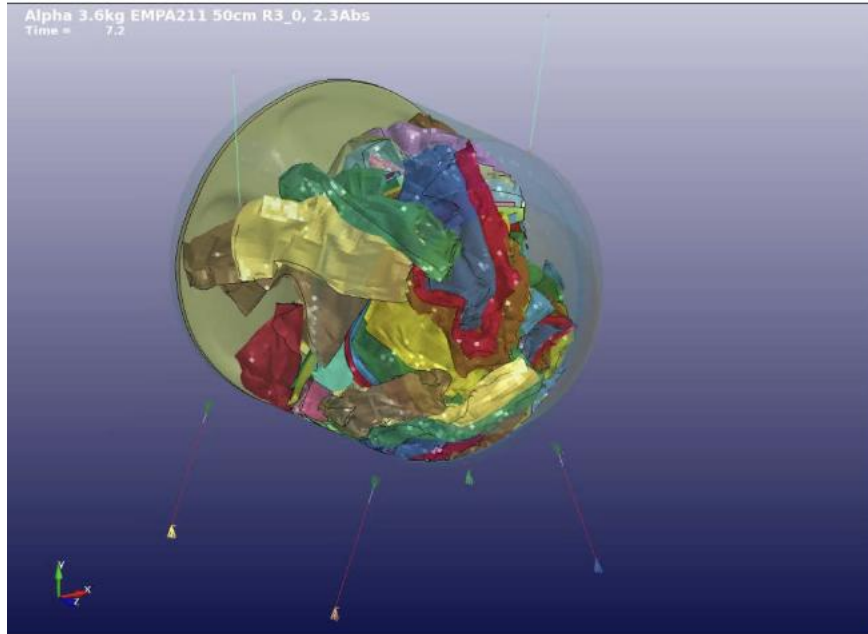


Product Engineering

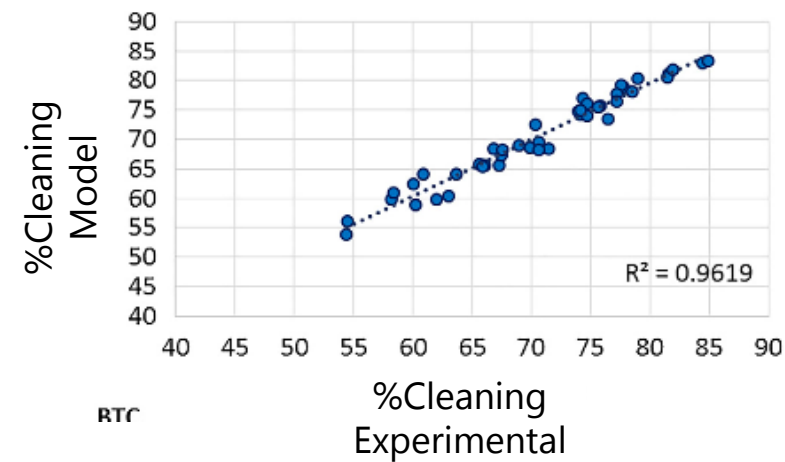
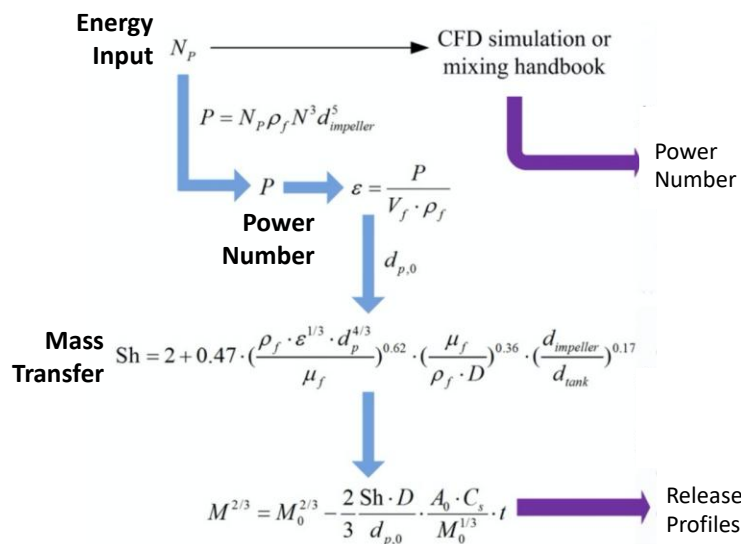
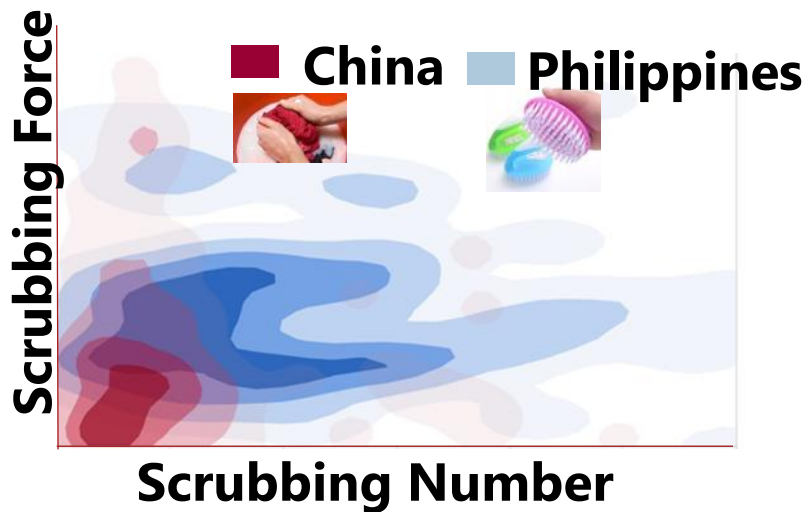
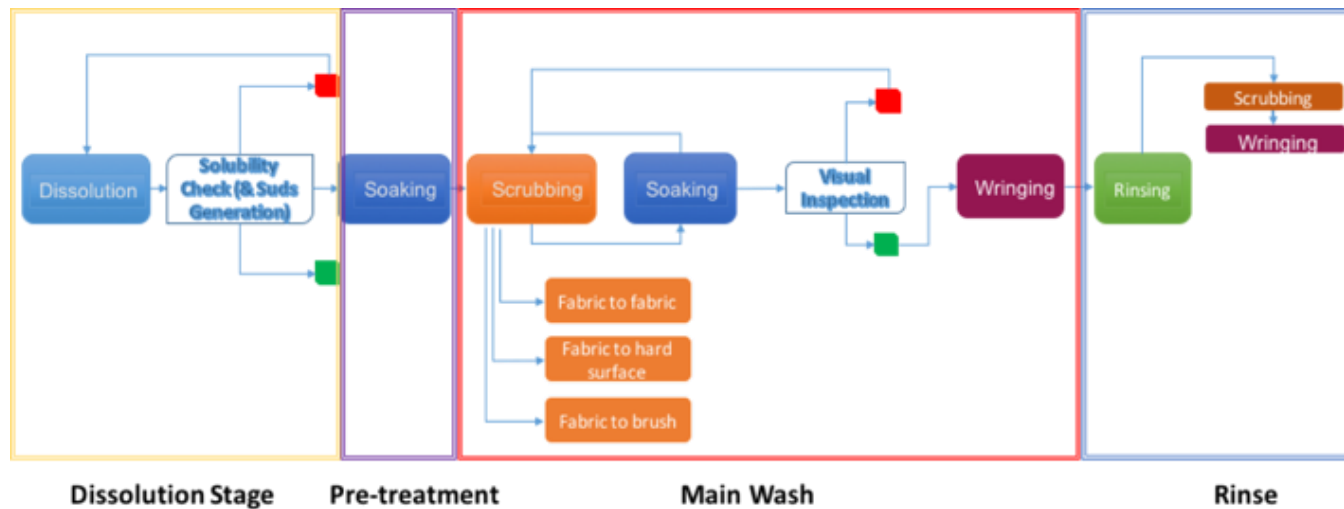


$$\begin{cases} \frac{dC_1}{dt} = \frac{Q_1}{V_1} (C_2 - C_1) \\ \frac{dC_2}{dt} = \frac{Q_2}{V_2} (C_1 - C_2) + \frac{Q_3}{V_2} (C_3 - C_2) \\ \frac{dC_{3,z}}{dt} = \frac{Q_3}{V_3} (C_2 - C_3) + k_0 \cdot \frac{4}{d_f} \cdot \frac{(1 - \varepsilon(t))}{\varepsilon(t)} \cdot (C_{4,z} - C_{3,z}) \\ \frac{dC_{4,z}}{dt} = +k_0 \cdot \frac{4}{d_f} \cdot \frac{(1 - \varepsilon(t))}{\varepsilon(t)} \cdot (C_{3,z} - C_{4,z}) + \text{Intrinsic Removal Rate} \\ \frac{dC_{5,z}}{dt} = - \text{Intrinsic Removal Rate} \end{cases}$$

Finite Element model – Comparison with the experiments

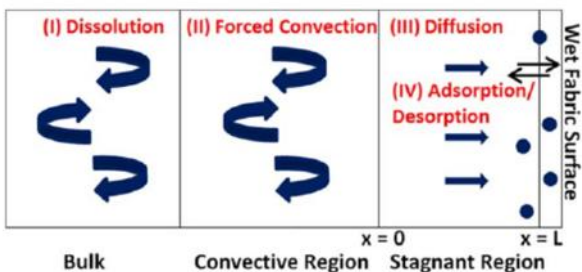


Understand Consumers: A Product Engineer's Approach



The work (1 paper- out of 3): Coarse grain

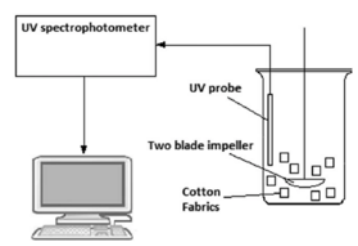
Conceptual Framework



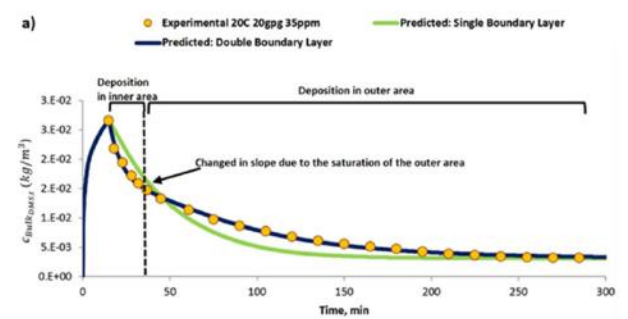
2 pages of equations (ODEs)

$$\begin{aligned}
 (u \cdot D) &= u \cdot \nabla u + \nu \nabla^2 u \\
 &= \sqrt{(p-a)^2 - b^2} \sqrt{(p-a)} \left(p = \frac{a+b+c}{2} \right) \quad b = \frac{ad}{c} \quad r \\
 \ln \lg a + \lg b - \frac{1}{2} [\lg(a+b) + \lg(a-b)] &= \epsilon \\
 \beta_a &= \frac{2}{b+c} \sqrt{bc(p-a)} \quad S = ah = abs \sin \alpha \\
 b^2 + \dots + (n-1)ab^{n-1} + b^n &= x^2 = px + q \quad (x) a^{n-1} \\
 \frac{A-B}{2} \cos \frac{C}{2} &= a = \frac{bc}{d} \quad \sin A + \sin B = 2 \cos \\
 a:b:c &= d:e:f \quad c = \frac{ad}{b} \quad m_a = \frac{1}{2} \sqrt{2b^2 + 2c^2 - a^2} \\
 n &= m \log_a \frac{c}{b} \quad m_a = \frac{1}{2} \sqrt{2b^2 + 2c^2 - a^2} \\
 r^2 + i \sin 30^\circ &= \frac{\sqrt{3}}{2} + \frac{1}{2} i \quad b = \frac{ad}{c} \quad Z_1 = \cos 30^\circ \\
 \lg b &= S = \frac{d \cdot h}{b} = a \sin \alpha \quad \lg \frac{a}{b} = \lg a - t \\
 &= \sin \alpha \cos \beta + \cos \alpha \sin \beta \quad S = ph \quad \sin(\alpha + \beta) \\
 &= \sin \alpha \cos \beta + \cos \alpha \sin \beta \quad \sin(\alpha + \beta) \approx \sin \alpha \cos \beta
 \end{aligned}$$

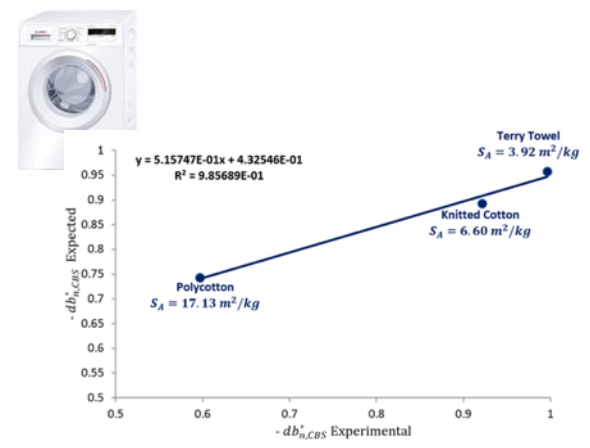
Experimental Set-up (Higher Throuput)



Prediction for deposition to fabrics: Use experimental data for models



Correlates with phenomena in real world



$$\begin{aligned}
 (u \cdot D) &= u \cdot \nabla u + \nu \nabla^2 u \\
 &= \sqrt{(p-a)^2 - b^2} \sqrt{(p-a)} \left(p = \frac{a+b+c}{2} \right) \quad b = \frac{ad}{c} \quad r \\
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 \end{aligned}$$



Molecular Understanding (ab initio models)



Hybrid Models



"Big" Data approaches

Digital: Expore possibilities for digital technology on inovation

How will our labs look in the future?

Pasteur's lab



Food Science lab (now)



According to ChatGP
This is a typical lab
now

How will labs look in 20 years??



ChatGPT

