AI IN CHEMICAL REGULATION

Current approaches and future potential for integrating Artificial Intelligence (AI) within chemical hazard and risk assessments

Helena Crosland[1#], Hanna Schuster[1], Olha Khomenko[1], Bashir Surfraz[1]
[1]Cambridge Environmental Assessments, Boxworth, UK; [#]Corresponding author: helena.crosland@cea-res.co.uk

CAMBRIDGE ENVIRONMENTAL ASSESSMENTS

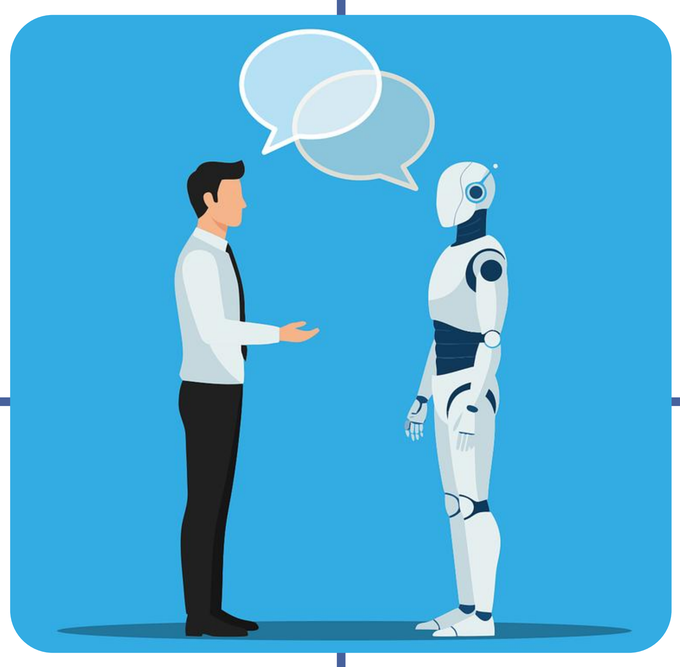
WHAT IS YOUR PERSPECTIVE? DICUSS AI WITH US AT BOOTH #35!

Benefits

- Streamline increasingly complex regulatory processes – automate processes, write summaries, simplify guidance, perform calculations
- Study review/summary
- Study management, inter-lab historical control harmonisation and assessment
- Assist writing code for regulatory purposes e.g. modelling:
  - More accessible/democratic
  - Less time consuming
- Literature searches and other time-consuming activities
- Benefits for resource across all areas: Non-testing 'tools' for investigating hazard and risk

Examples

- Non-Animal Methodologies (NAMs)
  - Many examples of efforts to produce synthetic clinical trial data for pharma (e.g. summarised in Alam et al.)[1]
- Machine learning, extrapolation on techniques such as QSAR (Quantitative Structure-Activity Relationship) to reduce animal testing[2]
- Chemo-informatics[3]
  - Data mining
    - Improve searches
    - Filter data
    - Use Gen AI to 'ask questions' of large data set
    - Help make sense of increasingly complex guidance and RAs



Challenges, Limitations, Concerns

- Moral implications:
  - Environmental impacts
  - Job stability
  - Intellectual property
  - Lack of transparency
  - Misleading?
- Confidentiality
- Domain knowledge remains essential
- Most of the AI tools are black boxes and are hard to QA/QC. GLP?
- Hallucinations: careful peer review of outputs required
- Over-estimation of abilities – use of AI not a replacement for good data!
- Regulators – rate-limiting step to implementation?

On the Horizon

- Could the 'AI bubble' burst?[4]
- Move towards more holistic chemical risk assessments?
  - Weight of Evidence approaches
  - Non-testing methodologies, NAMs
- Increased capacity and flexibility with modelling
- Semi-automation:
  - Code based automation
  - Lower tier assessments
  - Screening processes for low-risk chemicals
  - Importance of (human) QC
- Introduction of harmonized databases/API for PPPs would improve data scraping potential
- Smaller businesses – benefits but may not have capital to implement?
- Regulators - slow to implement/accept?

References:
1 Alam, F., & Alnazzawi, T S M., Mehmood, R., & Al-maghthawi, A. (2025). A Review of the Applications, Benefits, and Challenges of Generative AI for Sustainable Toxicology. Current Research in Toxicology. 8. 100232. 10.1016/j.crtox.2025.100232.
2 Hao, Y., Fan, T., Sun, G., Li, F., Zhang, N., Zhao, L., Zhong, R. Environmental toxicity risk evaluation of nitroaromatic compounds: Machine learning driven binary/multiple classification and design of safe alternatives, Food and Chemical Toxicology, Volume 170, 2022, 113461, ISSN 0278-6915. https://doi.org/10.1016/j.fct.2022.113461.
3 Chetry A B., Ohto K. From molecules to data: the emerging impact of chemoinformatics in chemistry. J Cheminform. 2025 Aug 7;17(1):121. doi: 10.1186/s13321-025-00978-6. PMID: 40775368; PMCID: PMC12333164.
4 Sasha Rogelberg. Benchmark's Bill Gurley: the AI bubble is about to burst—and a reset is coming. Fortune Media. March 17, 2026, 1:23 PM ET. https://fortune.com/2026/03/17/is-ai-bubble-bill-gurley-run-out-of-money/