Vaping could cause lung disease

Original article by James Urquhart. Adapted by Nina Notman.

Researchers predict a long list of harmful compounds produced from heating eliquids

An artificial intelligence-based approach (go.nature.com/3XOvXjg) predicts hundreds of harmful compounds that could form when vape users heat e-cigarette flavour chemicals in vaping devices. The research adds to mounting evidence concerning the safety of vaping, finding that many of the predicted products released by heating flavours are classed as acutely toxic, health hazards or irritants. What's more, their impact on health might take years to emerge.

E-cigarettes heat up e-liquids to produce aerosols, which users inhale. There are tens of thousands of different flavour e-liquids on the market containing ingredients picked from at least 180 commercially available flavour compounds. These flavours were originally developed for the food industry and deemed safe for consumption. However, the long-term health risks of heating and inhaling these chemicals remain unknown.

Flavour chemistry

'The flavours being used in vapes have never been clinically tested for heating to high temperatures with lung inhalation,' says Donal O'Shea, who led this work at the Royal College of Surgeons in Dublin, Ireland. 'It is important to quickly get an understanding of the cocktail of chemicals that vapeusers' lungs are being exposed to.'

Donal's team trained a neural network – a machine-learning model that mimics the human brain – on over 300,000 chemical



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Flavours in vapes are tested as foods, which doesn't consider what happens to their ingredients when vape users heat them to produce aerosols

reactions. It then used this to predict 7307 thermal decomposition products of 180 compounds used as e-liquid flavourings. Further investigation found that 127 of these breakdown products are acutely toxic, 153 are health hazards and 225 are irritants.

Vaping dangers

'From the compounds predicted, chronic obstructive pulmonary disease, cardiovascular disease and cancers could be expected to arise from prolonged exposures,' says Donal. 'The ester flavours are particularly concerning as they produce many reactive carbonyls, alkenes and aromatics and are most popular

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with a younger demographic.' Among the e-liquid flavours that have esters in their ingredients are bubblegum, fruit and citrus-based ones.

'It is crucially important to understand flavourings' health effects, especially given that users essentially inhale these at a high daily frequency, often for years,' comments Hanno Erythropel, an analytical chemist who studies e-liquid flavours at Yale University, US. 'This approach is very interesting and produces results that would never be possible to realise experimentally due to the sheer volume.'

Donal envisages further work to confirm his group's predictions by comparing them with those from other AI training sets, as well as results from the experimental analysis of vape plumes. 'We would also like to expand the chemical reactions to include combustion products and predict the potential for catalysis from the metal components found within vaping devices,' he says.

This story is adapted from the article **AI predicts vape flavours can break down into potentially harmful compounds when heated** in Chemistry World. Read the full article at rsc.li/4eSeMn2.