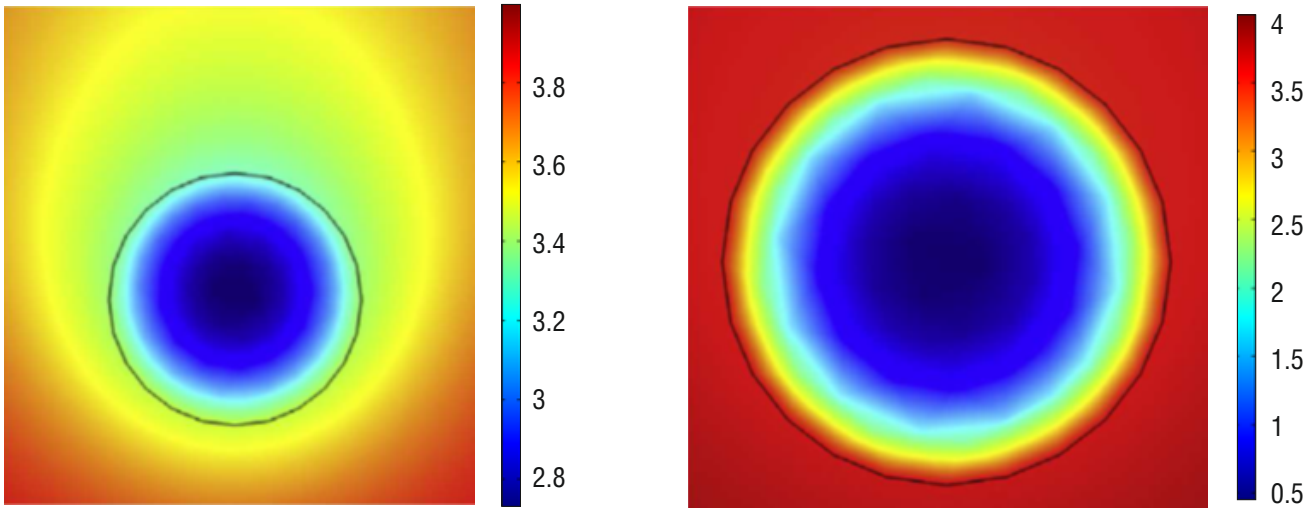
Diffusion and decomposition of SO_3 in non-isothermal catalyst particles



Concentration profiles (in mol/m^3) of SO_3 in catalyst pellet (right) and catalyst foam (left)

*Endothermicity of SO_3 decomposition reaction leads to high thermal gradients and lower reaction rates within the catalyst particles. Catalyst parameters, which can be tuned to minimize the gradients (concentration and temperature), are identified in this study.**

Hydrogen is considered as a clean energy carrier in the future energy system. Sulphur-based water splitting processes (Iodine-Sulphur and Hybrid-Sulphur) are efficient andgreen technologies for hydrogen production. Decomposition of sulphuric acid is the high temperature and energy intensive step in these processes.

A recent report, (S. Sujeesh et al., 2021, 'Kinetic study and modeling of sulphuric acid decomposition using Cr-Fe2O3 catalyst for sulphur based water splitting processes' Int J Hydrogen Energy , 46: 27282-27292) shows that the chromium doped iron oxide catalyst ($Cr\text{-}Fe_2O_3$) particles; less porous 'pellet' and porous 'foam' are non-isothermal particles for decomposition of SO_3. This is due to high endothermicity of SO_3 decomposition reaction. Multiphysics numerical simulations of diffusion and decomposition of reactant, So_3 in these non-isothermal particles are carried out by solving multi-physics reactive species transport, fluid flow and energy transport in porous media.

Kinetic parameters (activation energy and frequency factor) and effectiveness factor of $Cr\text{-}Fe_2O_3$ catalysts (pellet and foam) obtained from experimental studies are also reported in this work. Experimental study shows strong pore diffusion resistance (small internal effectiveness factor) in these catalyst types. Effectiveness factor (η) of these non-isothermal catalyst particles can be maximised by tuning various catalyst parameters such as particle size, porosity and effective thermal conductivity for which numerical simulations are immensely useful.

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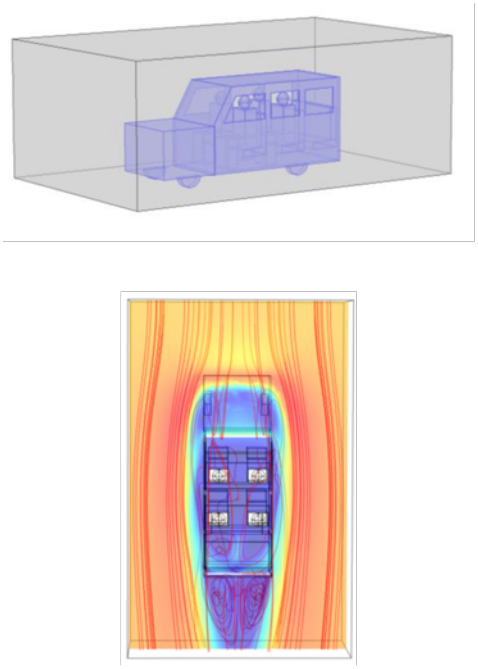
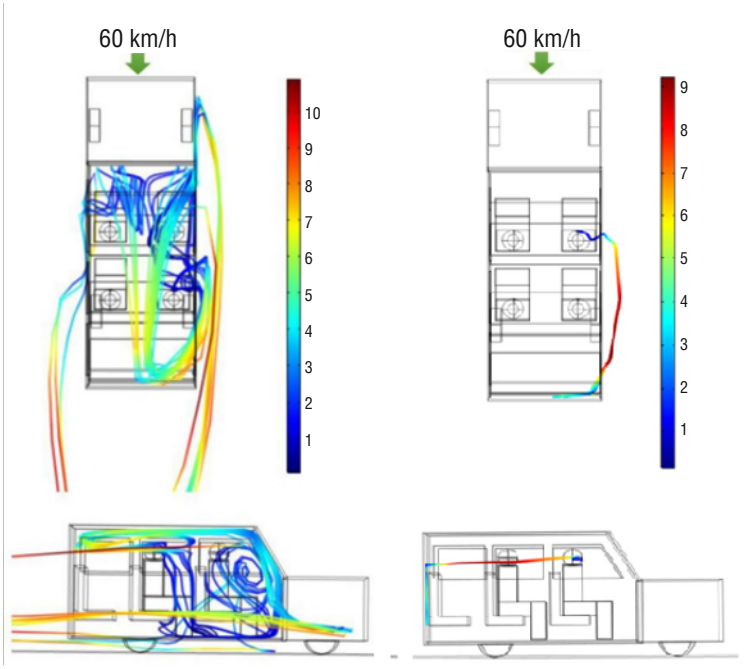
Dispersion of aerosols inside SUV



Computational domain (top) and streams lines showing formation of wakes behind the SUV (bottom)



Trajectories of the ejected aerosols when a person sitting in 2nd row speaks (left) and when a person sitting in driver's seat speaks (right). The colour scales show the velocity (in m/s)

Risk assesment for each passenger travelling in a SUV for four different scenarios. Significant recirculation of aerosols is possible even if all windows are completely open.*

COVID-19rages on. Now that we need to live with the virus the onus is on us to prevent ourselves from contracting it. As life limps back to normalcy travelling of more than one person in a car/taxi becomes common. In Indian context we often travel in a non- air-conditioned car with windows open. In a recent study, (Sen & Singh, 2021, Physics of Fluids, 33(9): pp.095117) we have reported how aerosols (produced as one of the passengers speaks without mask on) can spread across the vehicle and affect other three co-passengers in a SUV (6 seater). Air exchange with the surroundings through open windows strongly affect the state of dispersion. An Euler-Lagrangian 3D CFD model implemented in COMSOL Multiphysics is used for the study.

Four sets of scenarios of practical interest have been considered. The first set shows the effect of vehicle speed on aerosol transport, the second set describes what happens when some of the windows are closed while the third describes how aerosol transport is affected by position of the passenger speaking. The fourth set of simulations describe how a gush of cross-wind affects aerosol transport. Simulation results reveal that when all windows are open aerosols can go out of one window and then return back to the vehicle interior through another window. Results also reveal that when passenger sitting in the second row speaks the aerosols generated may sweep the entire volume of the vehicle interior before going out through the open windows.

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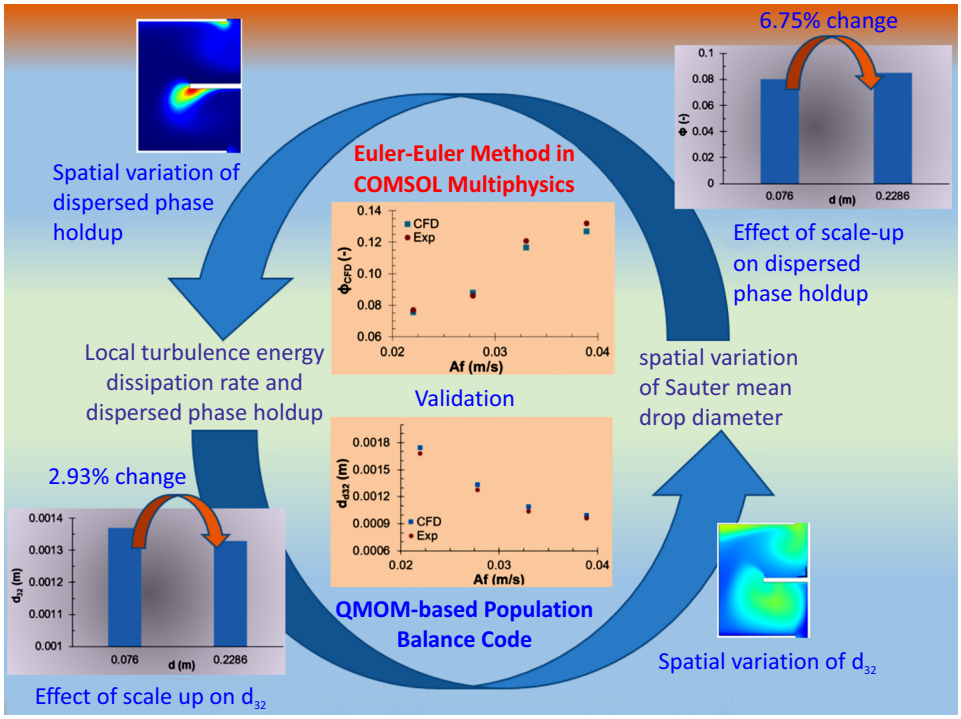
CFD–PB modelling of pulsed disc and doughnut column



Coupled CFD-PB modelling is used to estimate dispersed phase holdup and Sauter mean drop diameter for liquid-liquid two-phase flow in a pulsed disc and doughnut column.*

PULSED DISC and DOUGHNUT COLUMN (PDDC) is a modified design of PULSED SIEVE PLATE COLUMN (PSPC). In a PDDC, sieve plates are replaced by disc and doughnut shaped plates. Unlike a PSPC which has sieve plates containing small holes, internals of PDDC allow it to handle feed containing solids without tendency of chocking. For identical geometry and operating conditions, a PDDC has higher dispersed phase holdup than a PSPC resulting in lower HETP in PDDC compared to PSPC.In a recent article (Sarkar et al., 2020, 'CFD-PB Modelling of Liquid-liquid Two-phase Flow in Pulsed Disc and Doughnut Column', Solvent Extraction and Ion Exchange, 38:536) CFD-Population Balance (CFD-PB) modelling to estimate dispersed phase holdup and Sauter mean drop diameter in a PPDC is reported. Prediction of these hydrodynamic variables is important to estimate specific interfacial area available for mass transfer. An in-house Quadrature Method of Moment (QMOM) code is coupled with a CFD solver using the methodology pictorially shown above. The CFD-PB model is validated with experimentally measured dispersed phase holdup and drop diameter. Further, the CFD-PB model is used to check the validity of the scale-up scheme proposed in literature.

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