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Use detailed computational fluid dynamics (CFD) models to inform design and operating decisions for state-of-the-art NETL direct air capture (DAC) concept

Reactive Gas-Solid Multiphase Flow Modeling

- Develop a detailed CFD model to predict fluid flow, sorbent kinetics, and gas and solid heat transfer in the reactor
- Provide insights into the dependence of the pressure drop on form factor across the DAC reactor

Absorption Kinetics Model:

$$\frac{dq_t}{dt} = k(q_e - q_t)^2$$

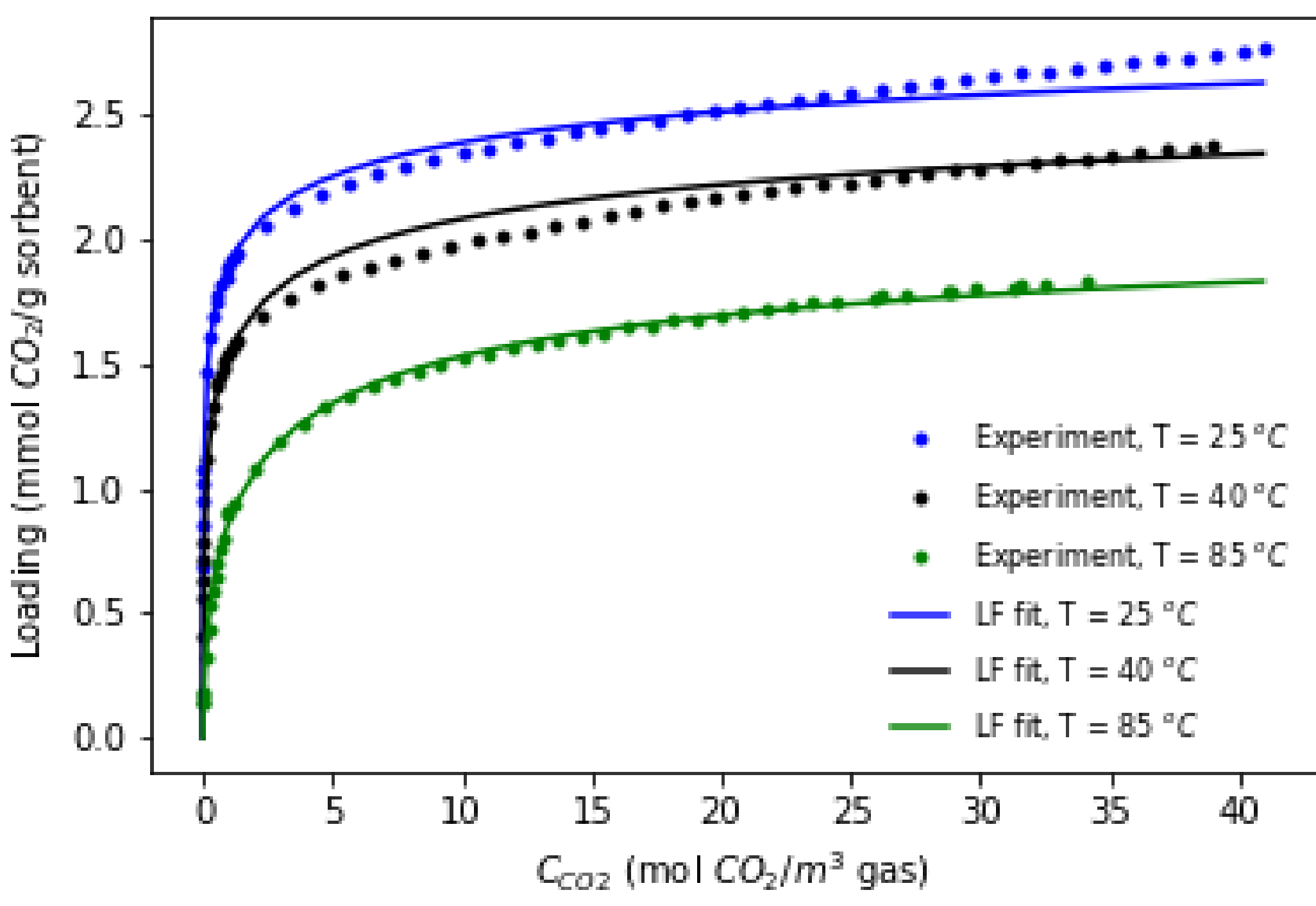
$$q_e = \frac{q_{max} K_{eq} C_{CO_2}^n}{1 + K_{eq} C_{CO_2}^n}$$

$$q_{max} = k_1 e^{k_2/T}$$

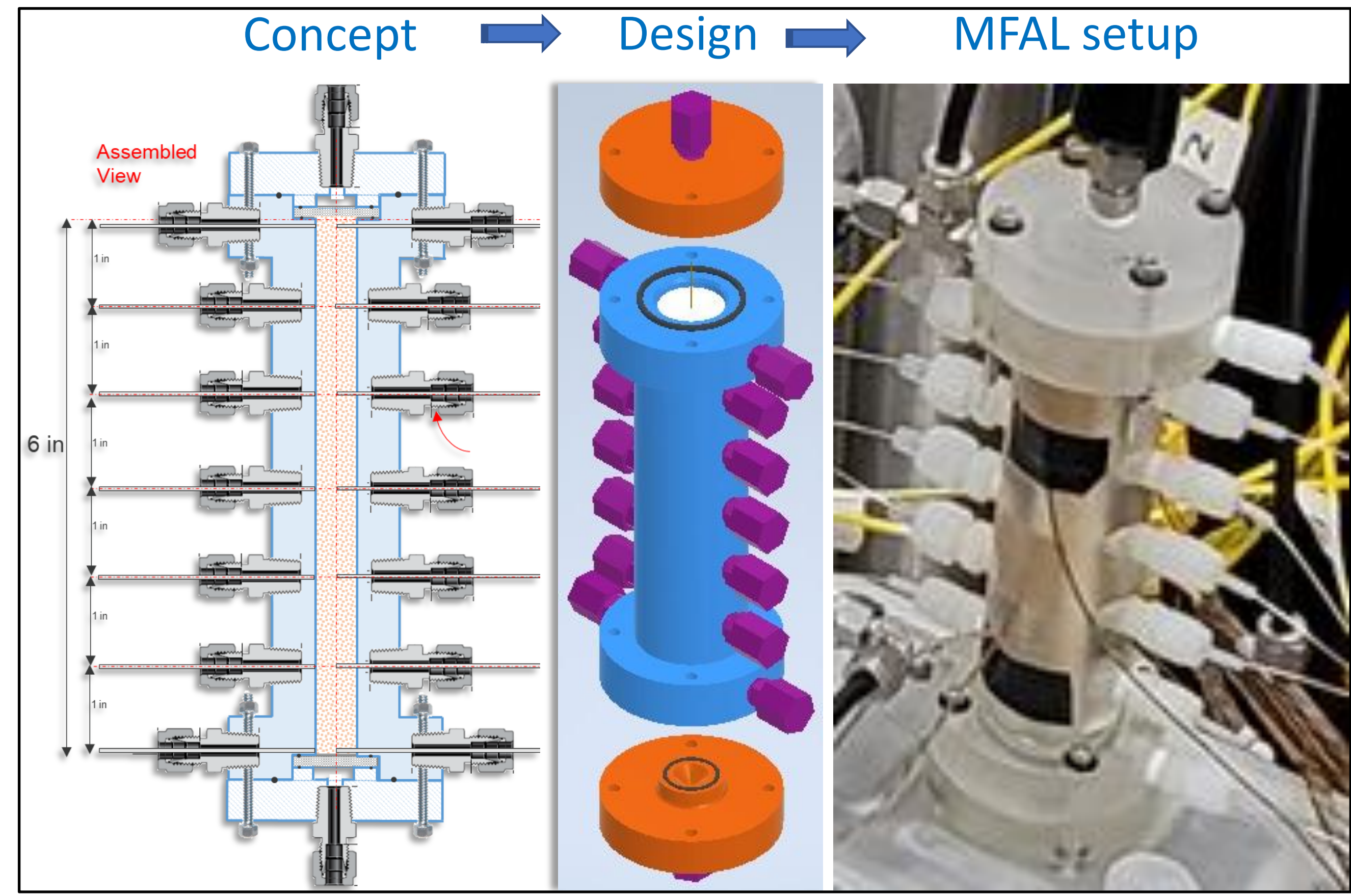
$$n = k_3 e^{k_4/T}$$

$$K_{eq} = k_5 e^{k_6/T}$$

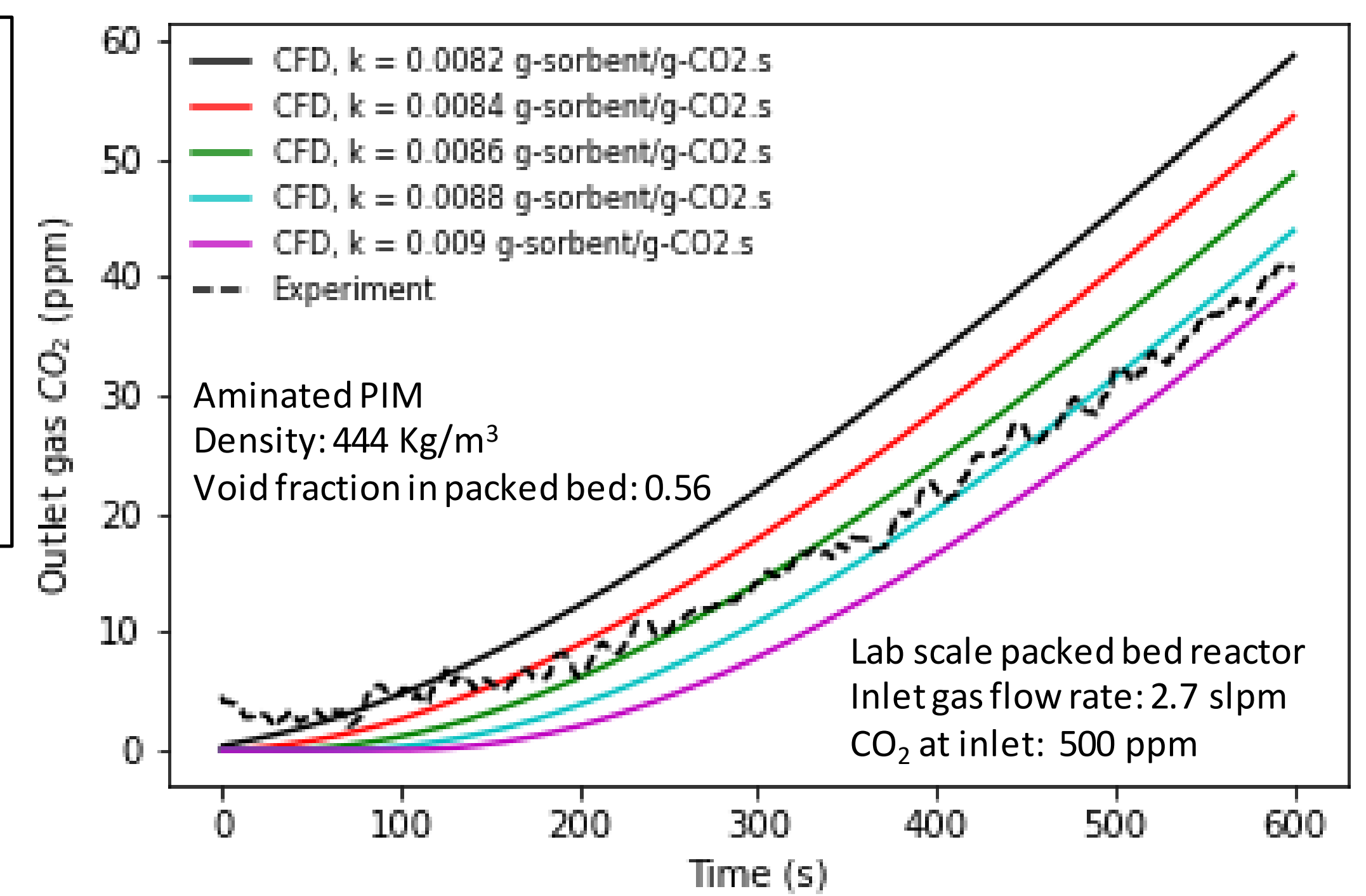
Fit Langmuir-Freundlich isotherm model to experimental data to obtain equilibrium CO₂ loading q_e



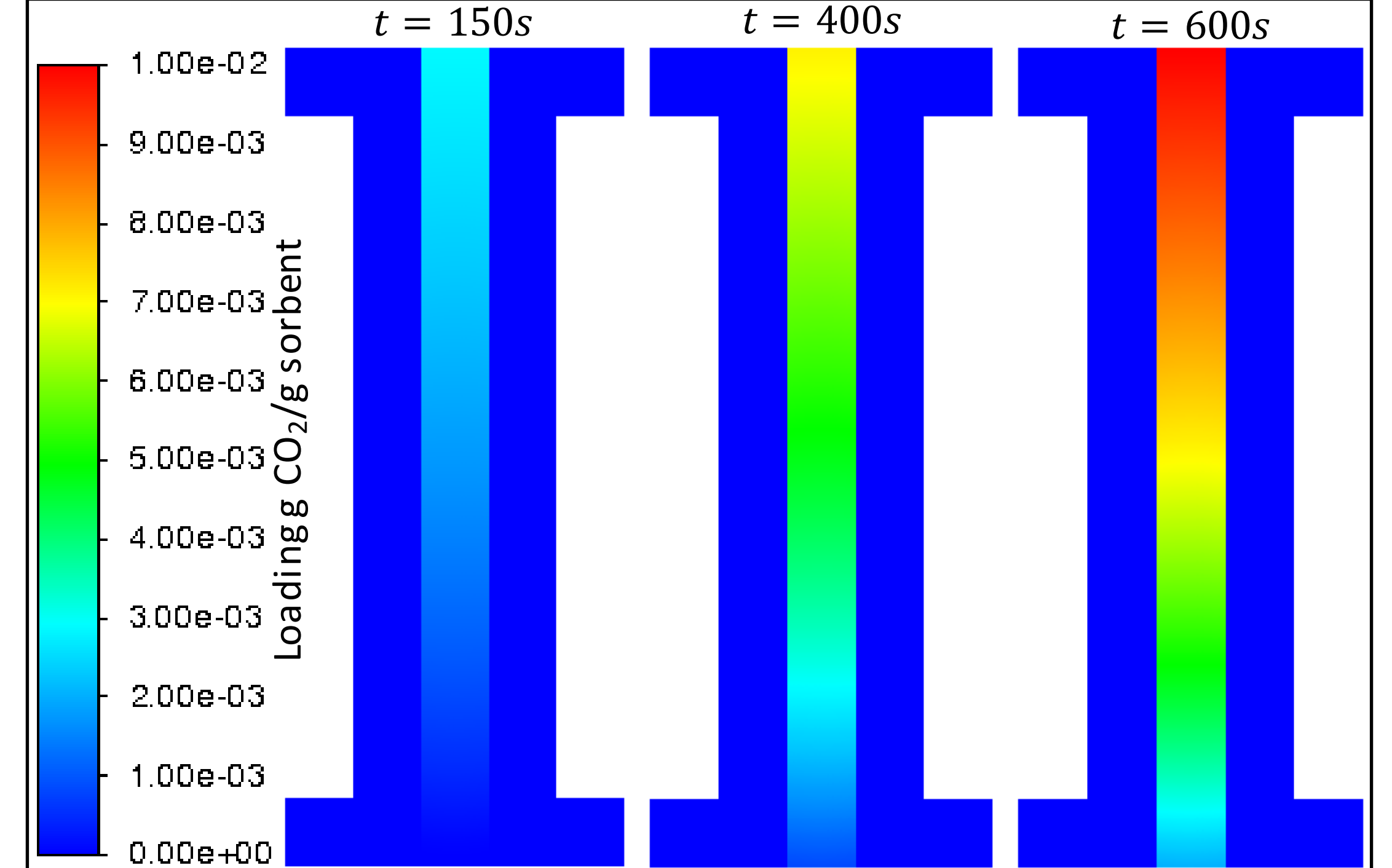
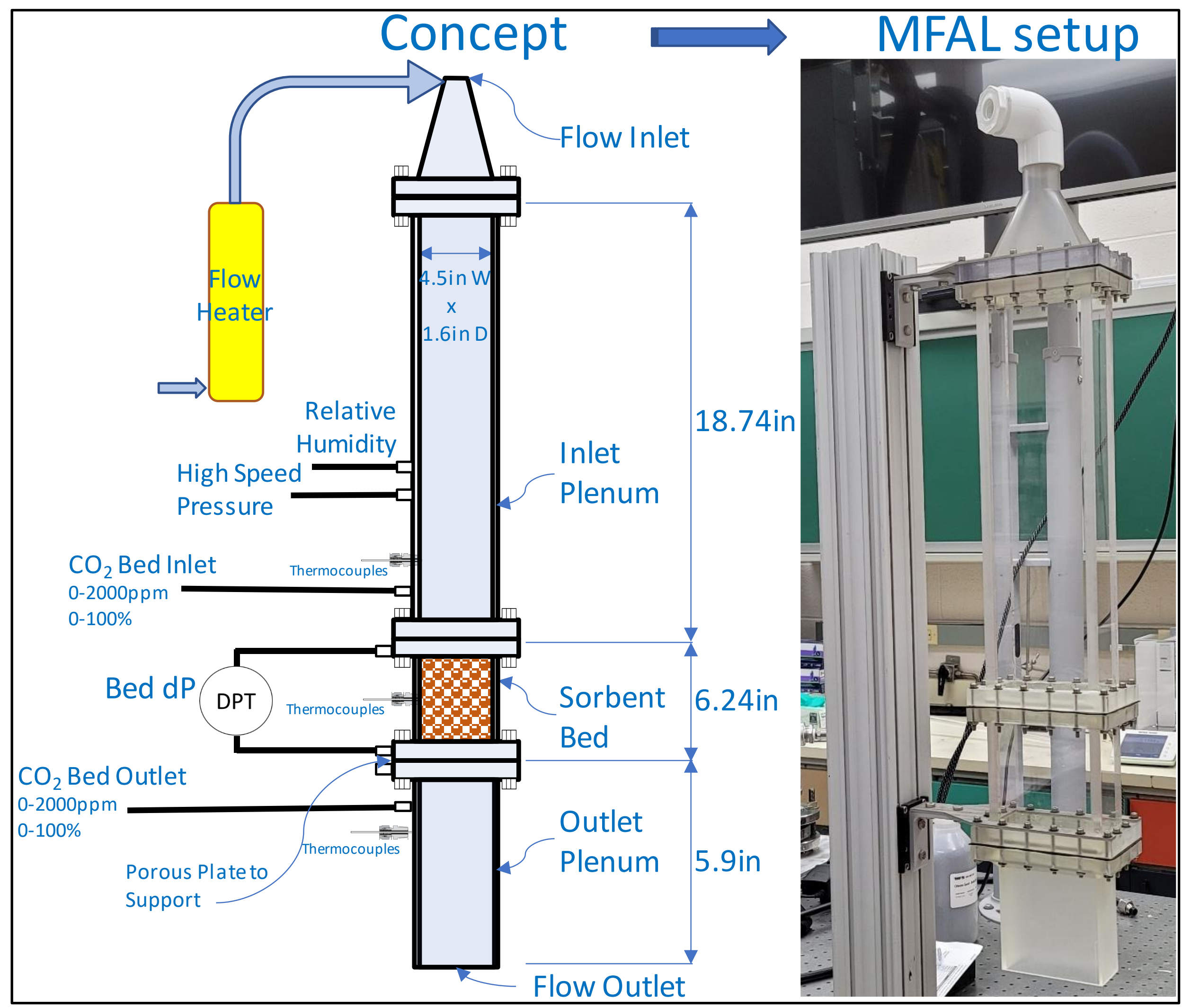
Lab-scale and bench-scale packed bed experiments are performed to calibrate the reaction rate and pressure drop across the bed



The rate constant k calibration: CFD vs. experimental breakthrough curves. CFD simulations were performed using porous media model. Predicted $k = 0.0088 \text{ g CO}_2/\text{g sorbent.s}$



Future Work: Develop kinetic model to incorporate the effects on humidity on the CO₂ adsorption. Develop CFD model to determine the effect of pressure drop on the sorbent arrangement in the DAC reactor and investigate the hydrodynamics in the bench-scale DAC bed.



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