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A modeling-optimization framework for assessment of CO₂ absorption capacity by novel amine solutions: IDMA2P, 1DEA2P, DEEA, and DEAB

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Highlights:

- A modeling-optimization framework was developed to assess the CO₂ absorption capacity for novel amine solutions.
- Different thermodynamic models such as Kent-Eisenberg modified Kent-Eisenberg, and Deshmukh–Mather were applied.
- A Back-propagation neural network model and an orthogonal array design (OAD) method were developed.
- The Deshmukh–Mather model predicted the CO₂ loading data of four amine solutions with an AARD% of 2.63.
- The satisfactory error for a modeling-optimization framework calculated to be less than 4%.

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