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A modulated gradient model for passive scalar transport in large-eddy simulations of neutral atmospheric boundary layer

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As a simple approach alternative to eddy-viscosity model, a nonlinear subgrid-scale (SGS) flux model is introduced and implemented in simulations of neutral atmospheric boundary layers with a constant surface flux of a passive scalar. This approach is based on the Taylor expansion of the SGS flux, and uses local equilibrium hypothesis to evaluate the SGS velocity scale and the SGS scalar concentration scale. To resolve the instability issue of the original gradient model and ensure numerical stability, a clipping procedure is adopted to avoid local negative SGS production for the scalar variance. The model formulation using constant coefficients is assessed through a systematic comparison with well-established empirical results and theoretical predictions of a variety of flow statistics. Results show good agreement with reference results and a significant improvement compared to simulations using traditional eddy-viscosity models. For instance, the model is capable to reproduce the expected similarity scalar profile and power-law power spectra. Simulations also yield reasonable flow structures and scalar statistics.