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Do parameterizations obey the second law of thermodynamics?

Almut Gaßmann (1) and Hans-Joachim Herzog (2)
(1) IAP, Kühlungsborn, Germany (gassmann@iap-kborn.de), (2) Nansenstr. 20, Potsdam, Germany (hans.herzog@online.de)

Numerical models of the atmosphere should fulfill fundamental physical laws. They imitate reversible and irreversible processes. Modern dynamical cores describe exclusively reversible processes. Hence, the parameterizations have exclusively to decribe irreversible processes. The associated second law of thermodynamics requires positive local internal entropy production and dissipation of available energy. In order to guarantee this positivity in numerical simulations, subgrid-scale turbulent fluxes of heat, water vapor, and momentum are required to depend on numerically resolved gradients in a unique way. The task of parameterization remains to deliver phenomenological coefficients.

Inspecting commonly used parameterizations for subgrid-fluxes, we find that some of them obey the second law of thermodynamics, and some do not. The conforming approaches are the Smagorinsky momentum diffusion, phase changes, and sedimentation fluxes for hydrometeors. Conventional turbulent heat flux parameterizations conform if interpreted together with mechanical turbulence, but this approach is problematic with respect to the energetics. A new water vapor flux formulation is derived from the requirement of locally positive entropy production. The conventional and the new water vapor fluxes are compared using high-resolution radiosonde data. Conventional water vapor fluxes are wrong by up to 10% and exhibit a negative bias.

Two numerical tests with the ICON-IAP model are performed to compare conventional and entropy-consistent parameterizations. The dry-atmosphere Boulder windstorm test case delivers negative dissipation rates for a conventional turbulent heat flux parameterization. An idealized tropical cyclone test case shows high dissipation rates associated with friction and diffusive sedimentation fluxes.