Entropy production due to subgrid-scale thermal fluxes with application to breaking gravity waves

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dissipation in nature $\leftrightarrow$ dissipation in modeling

\[
\text{dissipation} = \text{temperature} \times \text{internal entropy production}
\]

resolved scales = reversible energy transformations, forth and back

unresolved scales = resolved kinetic or internal energy are irreversibly converted into internal energy (=dissipation)
work and heat

\[ dU = \delta A + \delta Q \]

macroscopically visible

\[ dU = -pdV + TdS \]

macroscopically invisible

nature, DNS:
\[ \rho \frac{d}{dt} c_v T = -p \nabla \cdot v + \nabla \cdot W + \varepsilon_{vfr} \]

model, RANS:
\[ \rho \frac{d}{dt} c_v T = -p \nabla \cdot v + \nabla \cdot W + \varepsilon_{vfr} \]

\[ \tilde{\rho} \frac{d}{dt} \hat{c}_v \hat{T} = -\tilde{p} \nabla \cdot \hat{v} - \nabla \cdot (\overline{c_v \rho v''T''}) - (p \nabla \cdot v - \tilde{p} \nabla \cdot \hat{v}) + \varepsilon_{tfr} \]

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Consequences of turbulence averaging

\[
\frac{\partial}{\partial t} \bar{\rho} c_v \hat{T} = -\nabla \cdot \left( c_v \bar{\rho} \hat{v} \hat{T} \right) - \bar{p} \nabla \cdot \hat{v} - \nabla \cdot \left( c_v \rho \hat{v}'' T'' \right) - (\bar{p} \nabla \cdot \hat{v} - \bar{p} \nabla \cdot \hat{v}) + \epsilon_{tfr}
\]

\[
\frac{\partial}{\partial t} \bar{\rho} c_v \hat{T} = -c_p \Pi \nabla \cdot (\bar{\rho} \hat{\theta}) - \nabla \cdot \left( c_v \rho \hat{v}'' T'' \right) + \nabla \cdot \left( c_v \rho \hat{v}'' T'' \right) - c_p \Pi \nabla \cdot (\bar{\rho} \hat{\theta}') + \epsilon_{tfr}
\]

Sole approximation: \( \Pi' / \Pi \ll 1 \)
This approximation is common.

\[
\Pi = \left( \frac{p}{p_0} \right)^{R/c_p} \quad T = \Pi \theta
\]
\[ \frac{\partial}{\partial t} \bar{\rho} c_v \hat{T} = -c_p \bar{\rho} \nabla \cdot (\bar{\rho} \mathbf{v} \hat{\theta}) - c_p \bar{\rho} \nabla \cdot (\bar{\rho} \mathbf{v}'') + \varepsilon_{tfr} + \rho \hat{T} \frac{d}{dt} \hat{s} \]

Second law of thermodynamics

\[ \bar{\rho} \frac{d}{dt} \hat{s} = -\nabla \cdot \left( \frac{c_p \rho \mathbf{v}''}{\hat{\theta}} \right) - \frac{c_p \rho \mathbf{v}''}{\hat{\theta}^2} \cdot \nabla \hat{\theta} + \varepsilon_{tfr} / \hat{T} \]

Export / import internal entropy production has to be positive for every single process

Gradient approach:

\[ \rho \mathbf{v}'' = -\rho K^\theta \cdot \nabla \hat{\theta} \]

\[ \sigma_\theta = \frac{c_p \bar{\rho}}{\hat{\theta}^2} K^\theta_{ii} (\partial_i \hat{\theta})^2 \geq 0 \]

Always positive, regardless of stratification

Dissipation by \( \theta \)-diffusion:

\[ \varepsilon_\theta = \hat{T} \sigma_\theta \]
Energy exchange with kinetic energy has not been inspected thoroughly enough!

Consider only vertical fluxes

\[ c_p \bar{\rho} w'' \theta'' \partial_z \Pi = -c_p \bar{\rho} K^\theta \partial_z \left( -\frac{g}{c_p \theta} \right) = \bar{\rho} K^\theta N^2 \]

\[ \bar{\rho} K^\theta N^2 > 0 \]

- gain of internal energy
- entropy production **meaningful**
- loss of resolved kinetic energy
- a force must represent this kinetic energy
- loss in the momentum equation

\[ \bar{\rho} K^\theta N^2 < 0 \]

- loss of internal energy
- entropy production **meaningless**!
- making it meaningful must prevent the gain of resolved kinetic energy
- instead, TKE is generated, but TKE is indistinguishable from internal energy
- the traditional approach (grey box) is safe

Case distinction necessary!
Case distinction: \( N^2 < 0 \)

- omit resolved energy conversion, only applicable to \( N^2 < 0 \)

\[
\frac{\partial}{\partial t} \bar{\rho} c_v \hat{T} = -c_p \bar{\Pi} \nabla \cdot (\bar{\rho} \hat{\nu} \hat{\theta}) - \nabla \cdot \left( c_p \bar{\Pi} \rho v'' \theta'' \right) + \varepsilon_{tfr} \\
\bar{\rho} \frac{\hat{d}}{dt} \hat{s} = -\nabla \cdot \left( \frac{c_p \rho v'' \theta''}{\hat{T}^2} \right) - \frac{c_p \bar{\Pi} \rho v'' \theta''}{\hat{T}^2} \cdot \nabla \hat{T} + \varepsilon_{tfr}/\hat{T}
\]

Gradient approach:

\[
c_p \bar{\Pi} \rho v'' \theta'' = -c_p \bar{\rho} \hat{K}^T \cdot \nabla \hat{T}
\]

\[
\sigma_T = \frac{c_p \bar{\rho}}{\hat{T}^2} \hat{K}^T_{ii} (\partial_i \hat{T})^2 \geq 0
\]

Contradiction to 2nd law, if applied in case of \( N^2 > 0 \)

Formally, this is a temperature diffusion = subscale heat flux.

For unstable stratification \( \partial_z \hat{\theta} \) and \( \partial_z \hat{T} \) are parallel.

Dissipation by T-diffusion: \( \varepsilon_T = \hat{T} \sigma_T \)
Case distinction: $N^2 > 0$

\[
\frac{\partial}{\partial t} \bar{\rho} c_v \hat{T} = -c_p \bar{\Pi} \nabla \cdot (\bar{\rho} \hat{V} \hat{\theta}) - c_p \bar{\Pi} \nabla \cdot (\bar{\rho} v'' \theta'') + \varepsilon_{tfr}
\]

\[
\frac{\partial}{\partial t} \bar{\rho} \left( \frac{\hat{V}^2}{2} + \Phi \right) = -c_p \bar{\rho} \hat{V} \hat{\theta} \cdot \nabla \bar{\Pi} - c_p \bar{\rho} v'' \theta'' \cdot \nabla \bar{\Pi} - \hat{V} \cdot \nabla \bar{\rho} v'' \theta'' - \nabla \left( \bar{\rho} \nabla \left( \frac{\hat{V}^2}{2} + \Phi \right) \right)
\]

Which momentum equation belongs to kinetic energy equation?

Consider only vertical direction.

\[
\frac{\partial}{\partial t} \hat{w} = -g - c_p \hat{\theta} \partial_z \bar{\Pi} - c_p \frac{\rho w'' \theta''}{\bar{\rho} \hat{w}} \partial_z \bar{\Pi}
\]

\[
\frac{\partial}{\partial t} \hat{w} = -g - c_p \hat{\theta} \partial_z \bar{\Pi} - \frac{K^\theta N^2}{\hat{w}}
\]

\[
\frac{\partial}{\partial t} \hat{w} = -g - c_p \hat{\theta} \partial_z \bar{\Pi} - R_w \hat{w}
\]

\[-c_p \hat{\theta} \partial_z \bar{\Pi} = -\frac{1}{\bar{\rho}} \partial_z \bar{\rho} \]

- **new term**
- turbulent pressure gradient term
- similarity to Rayleigh damping

\[R_w = N^2 K^\theta / \hat{w}^2\]

- diffusion coefficient must prevent singularity
- new term leads to downward turbulent $\theta$-flux.
Case distinction: \( N^2 > 0 \)

\[
\frac{\partial}{\partial t} \hat{w} = -g - c_p \hat{\theta} \frac{\partial \Pi}{\partial z} - R_w \hat{w}
\]

\[
R_w = N^2 K^\theta / \hat{w}^2
\]

**Hypothesis:** For shortest resolvable scales, the horizontal wind is damped by vertical diffusion as fast as the vertical wind is damped by Rayleigh damping.

\[
R_w = K^m \frac{\pi^2}{(\Delta z)^2}
\]

\[
K^\theta = K^m \frac{\pi^2 \hat{w}^2}{(\Delta z)^2 N^2}
\]

There is no diffusion for \( \hat{w}^2 = 0 \).

**Consider isentropes of a breaking gravity wave**

**New procedure**

- wave overturns
- amplitude does not grow

**State of the art**

- wave overturns less
- amplitude grows

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Examplary 2-d modeling with ICON-IAP

ICON-IAP model with hexagonal mesh (QJRMS, 2013)

\[ \Delta z = 250 \text{ m}, \Delta x = 2 \text{ km}, \Delta t = 3 \text{ s}, \]
\[ H = 120 \text{ km}, L = 1200 \text{ km}, T = 32 \text{ h} \]

- \( K^m \) as in Holtslag und Boville (1993)
- initial profile as in Chun and Kim (2008)

- gravity wave generator as in Durran (1999), ceases after 16 hours

Figure 1. The basic-state (a) zonal wind and (b) temperature used for the numerical simulations. These are the July mean values at 35°N from the CIRA climate data.
- isentropes have local minimum at $w = 0$
- gravity wave breaks near the critical level: $m^2 \rightarrow \infty$
- isentropes overturn
- vertical wind shear is large
Downward directed $\theta$ fluxes

$$E_{\text{new}} = \rho K^m w^2 \pi^2 / (\Delta z)^2$$

$$E_{\text{old}} = \rho K^m N^2$$

State of the art

New procedure

wave overturns
amplitude does not grow

$$\hat{w}^2 = 0$$

$$t \quad t + \Delta t$$

Wave overturns less
amplitude grows

$$t \quad t + \Delta t$$

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3 setups

EXP 1: state of the art, inconsistent for $N^2 > 0$

After a long time....

EXP 2: entropically consistent for $N^2 > 0$

Further experiments (not shown):
If
• forcing in $w$-eq. is omitted, but $\theta$-flux is retained in $\theta$-eq,
• typical numerical off-centering in the implicit solver for $w$ is used,
results are very similar to exp 2.

EXP 4: nothing for $N^2 > 0$
Relative static stability $N^2/N^2_{iso}$

EXP 1: state of the are, inconsistent for $N^2>0$

EXP 2: entropically consistent for $N^2>0$

EXP 4: nothing for $N^2>0$

\[ N^2_{iso} = \frac{g^2}{(cpT)} \]

$N^2$ for isothermal stratification
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Temperature profiles

Experiments 1, 2, 4
- sharp maxima, peaks
- sometimes overadiabatic stratification
- no parabolic shape

Lidar-measurements (Liu and Meriwether, 2004)
Horizontal mean and variability of $N^2/N_{iso}^2$
Dissipations rates $\varepsilon_\theta, \varepsilon_T, \varepsilon_{tfr}$

Upper picture:
- $\partial_z \theta \partial_z T$ changes sign at isothermal stratification
- inversion layer ($\partial_z T > 0$) has positive dissipation, but the physical process is wrong
- there should not be any qualitative difference between less and more stable stratification than isothermal stratification, if the stratification is stable

↑ frictional dissipation is 10 times larger than thermal dissipation
← thermal dissipation

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Case distinction for subscale parameterization:

**stable** $N^2 > 0$ and **unstable** $N^2 < 0$

**Energy conversion** between resolved kinetic and internal energy is necessary for $N^2 > 0$.

This requires a new term in the vertical momentum equation.

The friction term converts likewise kinetic energy into internal energy.

But this process is described by tensor fluxes and not by vector fluxes.

---

**New procedure**

\[
\hat{\omega}^2 = 0
\]

wave overturns

amplitude does not grow

---

**State of the art**

\[
\hat{\omega}^2 = 0
\]

wave overturns less

amplitude grows