Turbulence Modeling for Atmospheric Simulations

Geophysical Turbulence Phenomena

NCAR, Boulder, CO, 25 July 2008

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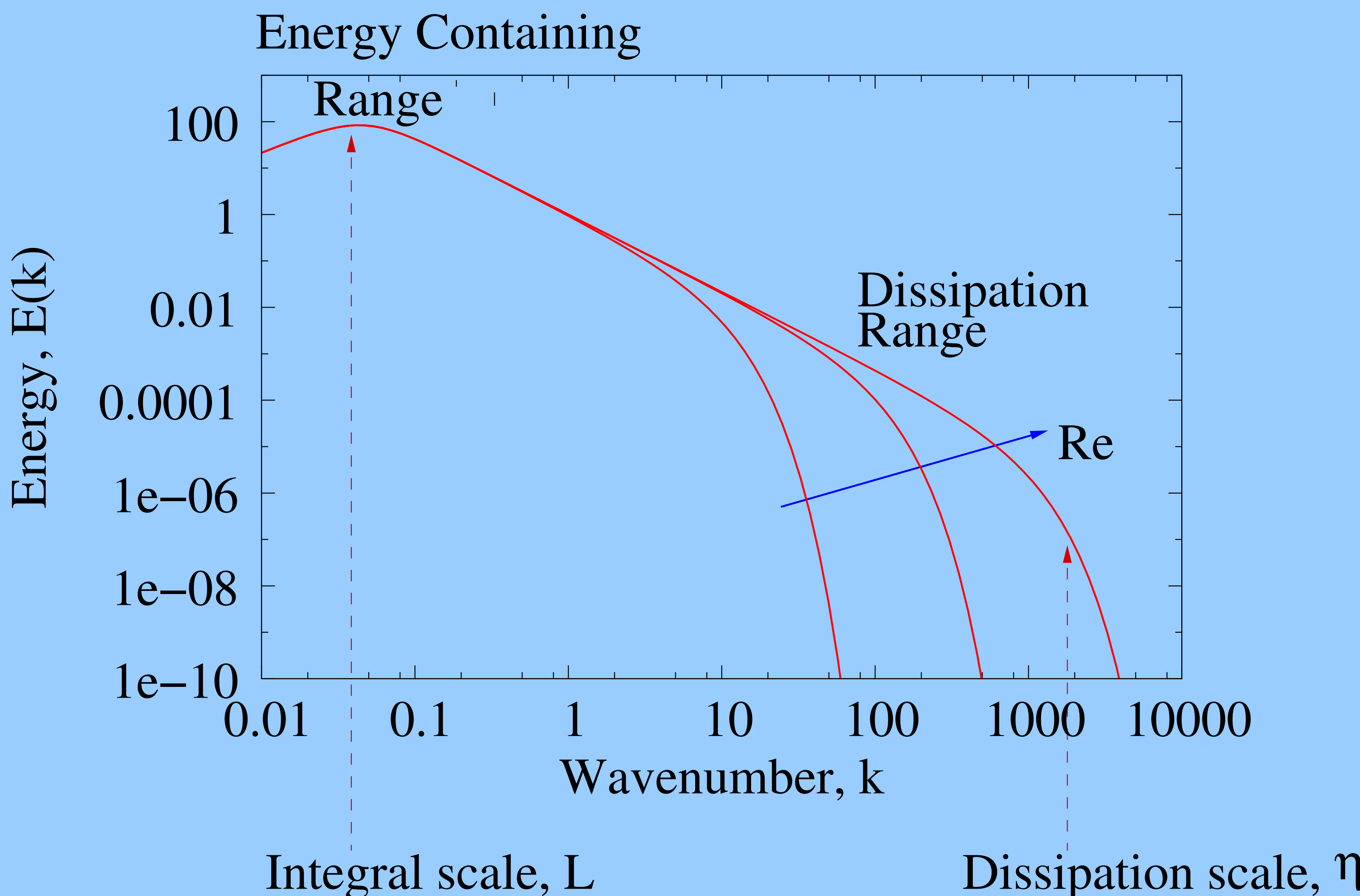
OUTLINE

- Review of the turbulence energy spectrum - enormous range of length scales.
- Reduction of scale range via spatial filtering - Large Eddy Simulation (LES).
- Closure problem - required SubGrid-Scale (SGS) models for flows with significant buoyancy effects.
- Eddy viscosity models.
- Modeling via transport equations.
- Dynamic modeling.
- Failure of LES near the earth's surface - what to do about it.
- Sample simulation results.
- Summary.

TURBULENCE ENERGY SPECTRUM



MESH POINT REQUIREMENTS FOR DNS

- From Turbulence theory, we have the following scaling relation:

$$(L/\eta) \sim Re^{3/4}$$

- Using this information, we can form the following estimate:

Box size $\sim L$
Grid size $\sim \eta$
Number of mesh points in each direction $\sim (L/\eta) \sim Re^{3/4}$
Number of mesh points in 3D $\sim (L/\eta)^3 \sim (Re^{3/4})^3 \sim Re^{9/4}$

- Based on experience

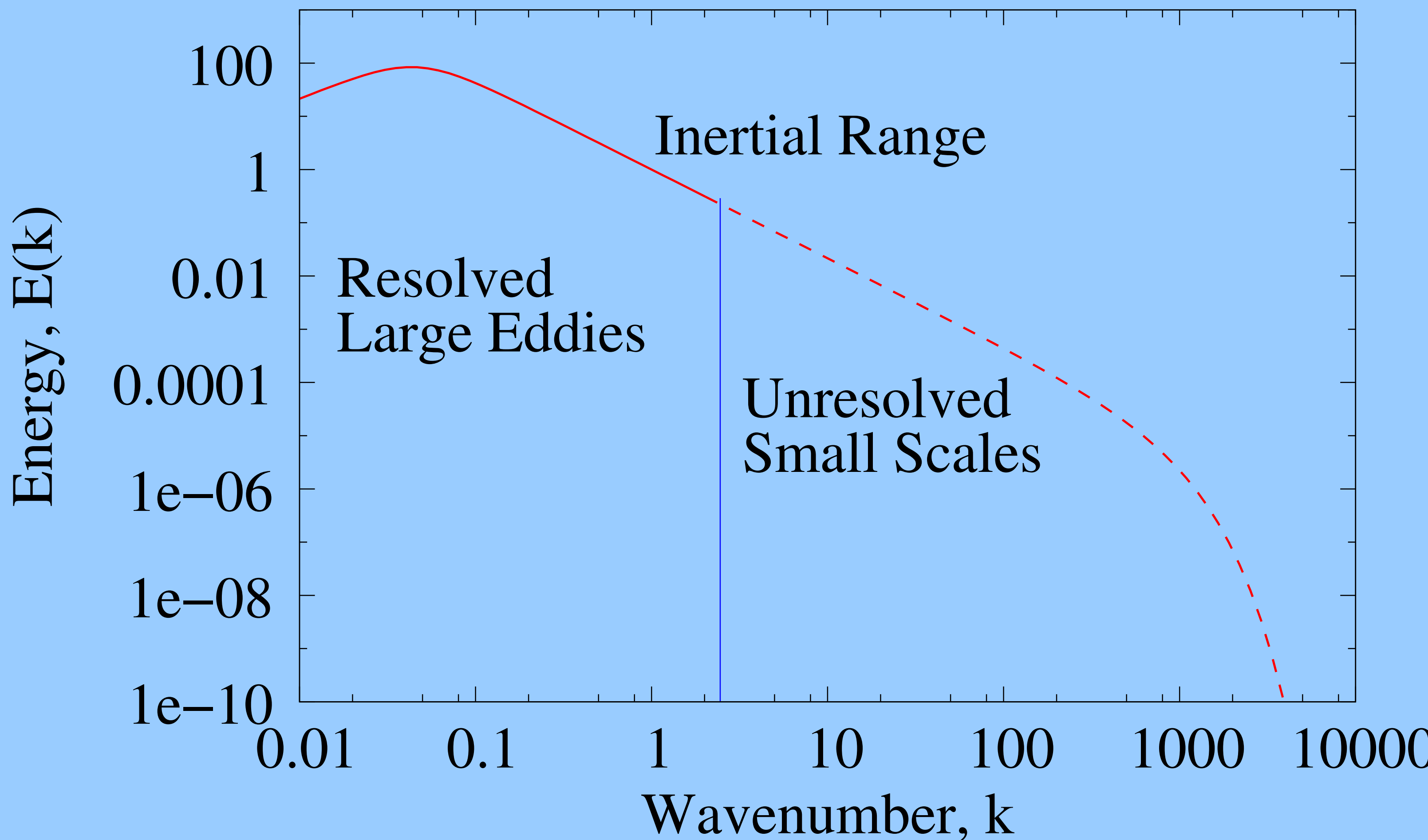
$$N \simeq 6Re^{9/4}$$

- For $Re = 10^6$, this estimate indicates that order 10^{14} mesh points are required!

- *It is simply not possible to simulate all the relevant scales of motion at the high Reynolds numbers found in atmospheric flows.*

LARGE EDDY SIMULATION

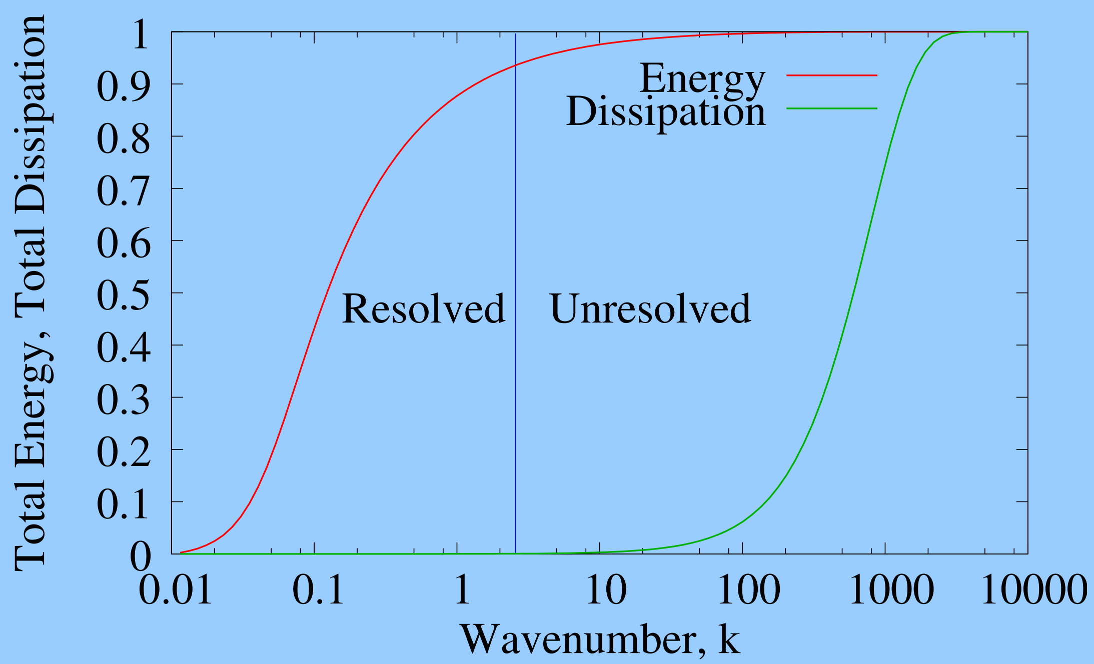
- Our simulations can only resolve the large eddies. We must account for the effects of the unresolved motions via a turbulence model.



WHAT CAN WE RESOLVE?

- The kinetic energy and energy dissipation resolved up to wavenumber k are

$$\text{Energy} = \int_0^k E(k')\,dk' \qquad\qquad \text{Dissipation} = \nu \int_0^k {k'}^2 E(k')\,dk'$$



- *We can resolve nearly all of the kinetic energy (and turbulent transport) but very little of the energy dissipation.*

FILTERING

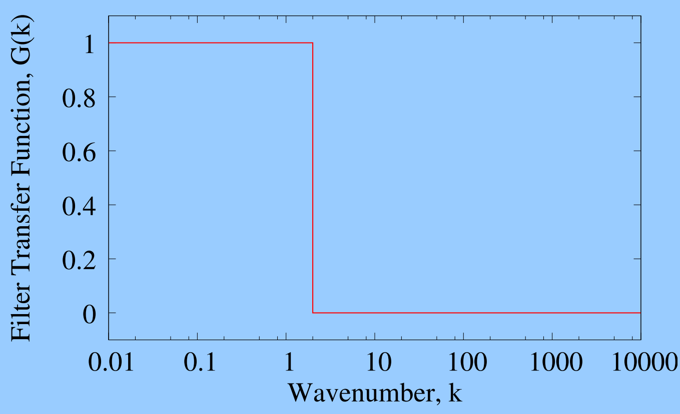
• The separation into large and small scales is accomplished via a spatial filtering operation. In Fourier space this amounts to multiplication by a filter transfer function

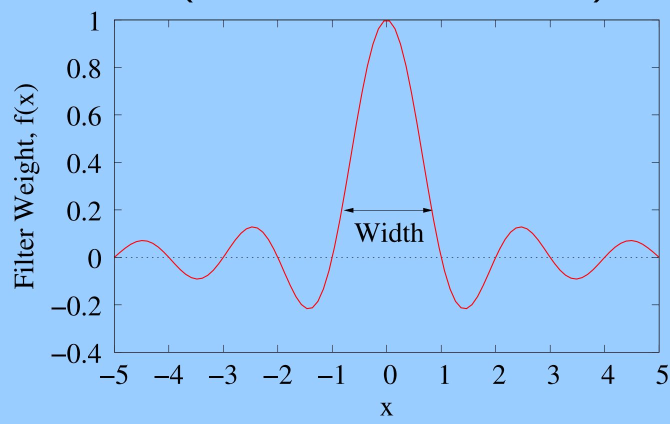
$$\overline{\tilde{u}} = G(k)\tilde{u}(k)$$

Using the convolution theorem, the equivalent operation in physical space is

$$\overline{u} = \int_0^L f(x - x')u(x')\, dx'$$

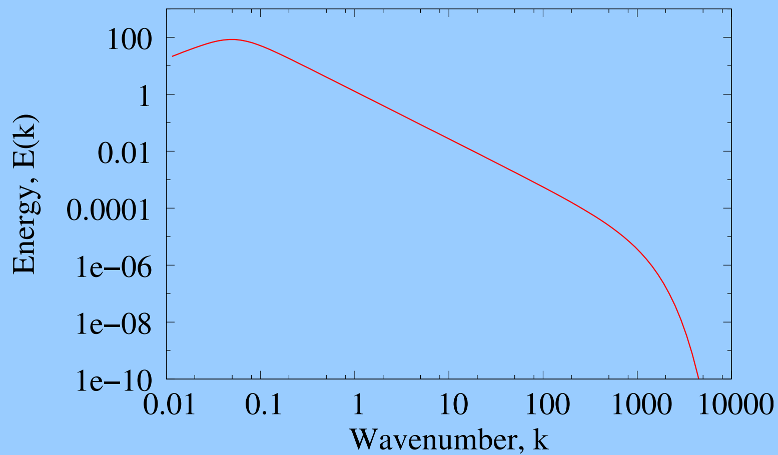
Where $f(x)$ and $G(k)$ are Fourier transform pairs. Spatial filtering amounts to a weighted average of the function over a set region in space (filter length scale).



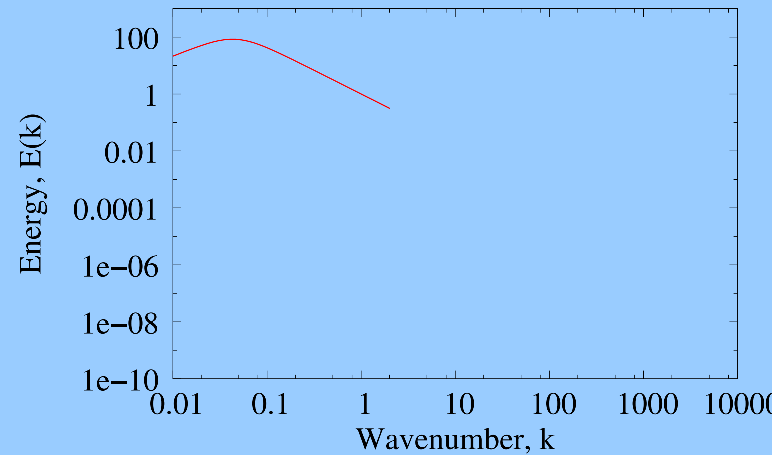


FILTERING EXAMPLE

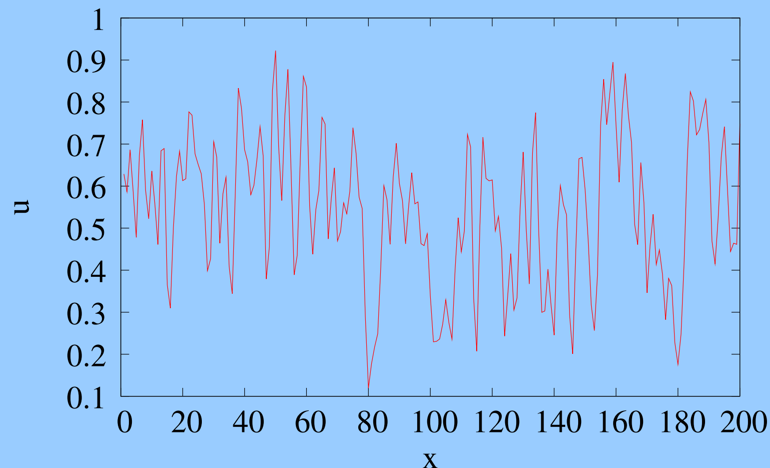
In Fourier space



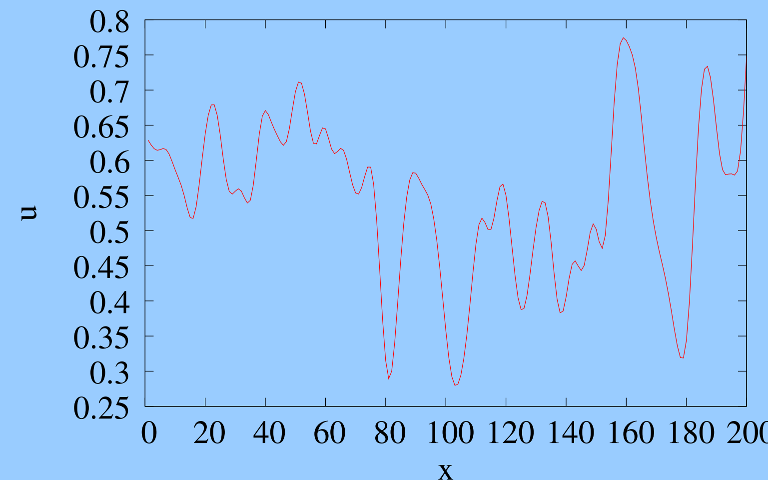
Filter $\longrightarrow$



In physical space



Filter $\longrightarrow$



DERIVATION OF THE LES EQUATIONS

The spatial average (filter) operator is applied to the mass, momentum, and potential temperature equations to give

$$
\begin{aligned}
\frac{\partial \bar{u}_i}{\partial x_i} &= 0 \\
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{u}_i \bar{u}_j\right) &= -\frac{1}{\rho_0}\frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{g}{\theta_0}\bar{\theta}\delta_{i3} + \frac{\partial}{\partial x_j}\left(2\nu \bar{S}_{ij}\right) \\
\frac{\partial \bar{\theta}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\theta}\bar{u}_j\right) &= -\frac{\partial q_j}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial \bar{\theta}}{\partial x_j}\right)
\end{aligned}
$$

Where τ_{ij} and q_i are the unresolved (SubGrid-Scale, SGS) stress and heat flux

$$
\tau_{ij} \equiv \overline{u_i u_j} - \bar{u}_i \bar{u}_j \qquad q_j \equiv \overline{\theta u_j} - \bar{\theta}\bar{u}_j
$$

and where $\bar{S}_{ij}$ is the resolved rate of strain

$$
\bar{S}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)
$$

CLOSURE (TURBULENCE MODEL) REQUIRED

- The SGS stress (τ_{ij}) and SGS heat flux (q_j) appear as unknowns in the filtered momentum and temperature equations.

- Although we can derive exact evolution equations for these quantities, these equations contain additional unknown terms. This is the closure problem.

- We proceed by attempting to relate τ_{ij} and q_j to the resolved flow variables. This process is known as turbulence modeling.

- Unlike turbulence models for the Reynolds averaged equations (classical approach using a long time average), the LES system requires models only for the unresolved transport.

- *SGS models are thus fundamentally different from classical turbulence models. In general, simpler models will suffice for the LES system.*

THE TURBULENT KINETIC ENERGY BUDGET

• An Evolution equation for the resolved turbulent kinetic energy can be formed by taking the dot product of the resolved velocity with the resolved momentum equation

$$\bar{u}_i \frac{\partial \bar{u}_i}{\partial t} = \frac{\partial}{\partial t}\left(\frac{1}{2}\bar{u}_i\bar{u}_i\right) = \frac{\partial}{\partial t}\left(\frac{1}{2}\bar{u}^2\right) =$$

$$\underbrace{-\frac{\partial}{\partial x_j}\left[\left(\frac{1}{2}\bar{u}^2 + \bar{p}\right)\bar{u}_j\right] + \frac{\partial}{\partial x_j}\left[\left(2\nu\bar{S}_{ij} - \tau_{ij}\right)\bar{u}_i\right]}_{\text{Transport}} + \underbrace{\bar{u}_i\bar{u}_j\frac{\partial \bar{u}_i}{\partial x_j}}_{\text{Shear Production}} + \underbrace{\frac{g}{\theta_0}\bar{\theta}\bar{u}_3}_{\text{Buoyancy Product}}$$

$$+ \underbrace{\tau_{ij}\bar{S}_{ij}}_{\text{SGS Dissipation}} \underbrace{- \quad 2\nu\bar{S}_{ij}\bar{S}_{ij}}_{\text{Viscous Dissipation}}$$

BALANCING PRODUCTION AND DISSIPATION

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\bar{u}^2\right) = \ldots \quad \underbrace{\bar{u}_i\bar{u}_j\frac{\partial \bar{u}_i}{\partial x_j}}_{\text{Shear Production}} \quad + \quad \underbrace{\frac{g}{\theta_0}\bar{\theta}\bar{u}_3}_{\text{Buoyancy Production}} \quad + \quad \underbrace{\tau_{ij}\bar{S}_{ij}}_{\text{SGS Dissipation}} \quad \underbrace{- \quad 2\nu\bar{S}_{ij}\bar{S}_{ij}}_{\text{Viscous Dissipation}}$$

- The resolved production is normally positive and is well represented by the resolved-scale motions.

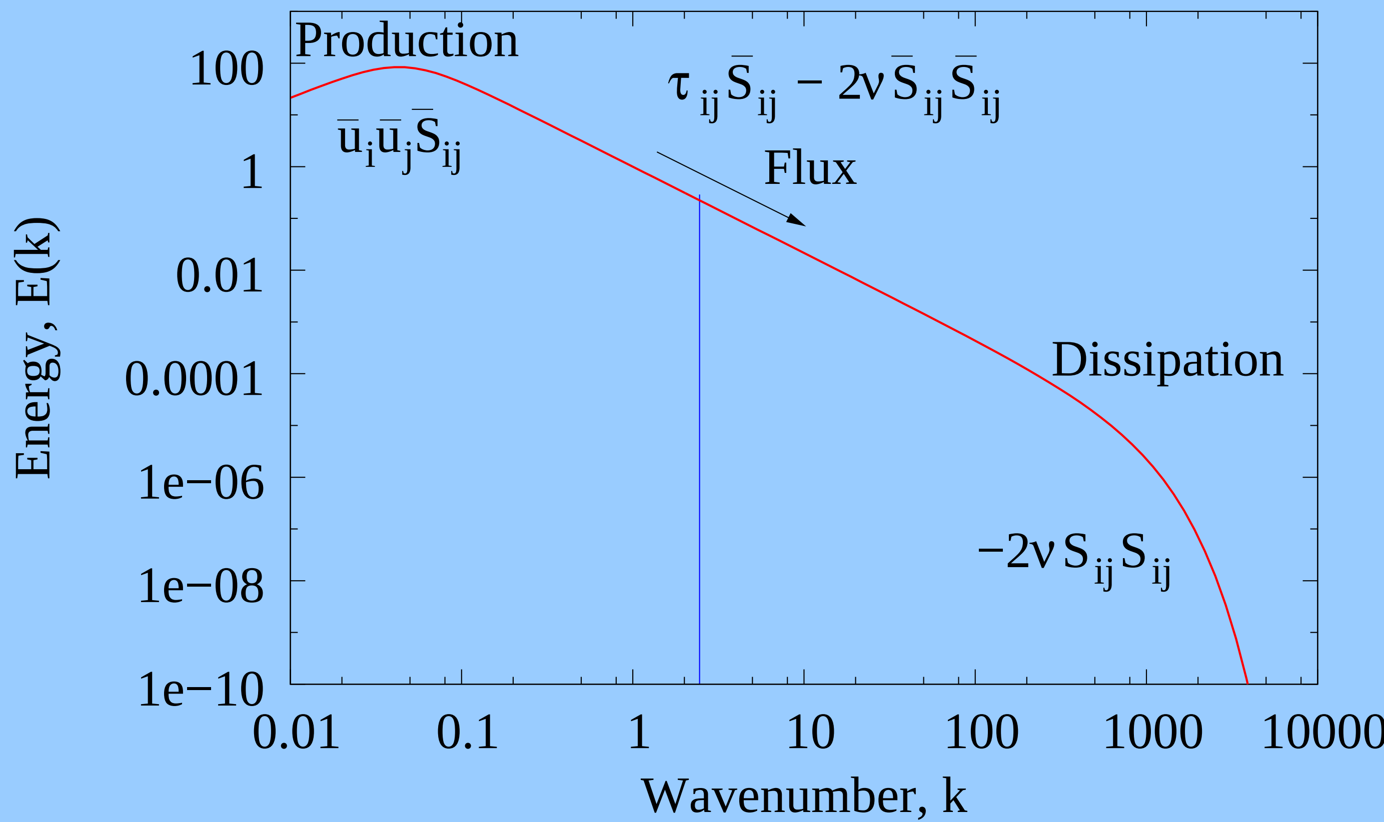
- The resolved viscous dissipation is negative definite.

- Due to the removal of the small scales, however, the resolved dissipation is a small fraction of the total dissipation present in the unfiltered system.

- There is thus a large imbalance between production and dissipation in the filtered system.

- *The primary objective of the SGS model is to provide sufficient dissipation in order to balance the energy budget.*

SPECTRAL VIEW



The energy flux at the filter scale must equal the total dissipation. Thus

$$\tau_{ij}\bar{S}_{ij} - 2\nu\bar{S}_{ij}\bar{S}_{ij} = -2\nu S_{ij}S_{ij}$$

EDDY VISCOSITY MODEL

Eddy viscosity is the simplest way to ensure a proper energy flux

$$\tau_{ij} = -\nu_t \bar{S}_{ij}$$

where ν_t is the *eddy viscosity.* Using this model, the energy balance becomes

$$\begin{aligned} \tau_{ij}\bar{S}_{ij} - 2\nu\bar{S}_{ij}\bar{S}_{ij} &= -2\nu S_{ij}S_{ij} \\ -2\nu_t\bar{S}_{ij}\bar{S}_{ij} - 2\nu\bar{S}_{ij}\bar{S}_{ij} &= -2\nu S_{ij}S_{ij} \\ (\nu + \nu_t)\bar{S}^2 &= \nu S^2 \end{aligned}$$

Thus we can obtain the correct energy flux in order to balance production and dissipation through the correct specification of the eddy viscosity.

SMAGORINSKY MODEL

• Smagorinsky (1961) postulated the following prescription for the SGS eddy viscosity:

$$\nu_t = C_s \underbrace{\Delta}_{\sim l} \underbrace{\Delta|\bar{S}|}_{\sim u}$$

where C_s is a non-dimensional scaling factor, Δ is the mesh spacing, and $|\bar{S}| = \sqrt{2\bar{S}^2}$ is the strain rate magnitude.

• For homogeneous unstratified flows, $C_s \simeq 0.01$. For inhomogeneous and stratified flows, C_s may be required to vary in space and with the relative stability.

HEAT FLUX MODEL

- The simplest heat flux model is the eddy diffusivity model

$$q_j = -\kappa_t \frac{\partial \bar{\theta}}{\partial x_j}$$

where κ_t is the *eddy diffusivity*.

- It is customary to relate κ_t to ν_t via a *turbulent Prandtl number*

$$\mathrm{Pr}_t = \frac{\nu_t}{\kappa_t} \qquad \kappa_t = \frac{\nu_t}{\mathrm{Pr}_t}$$

- For homogeneous, unstratified flows, $\mathrm{Pr}_t \simeq 1$. For inhomogeneous, stratified flows Pr_t may need to vary in space and vary with the relative stability.

MORE COMPLEX EDDY VISCOSITY MODELS

- **TKE model.**
  - Turbulent kinetic energy based eddy viscosity *ala* Deardorff (1980), Moeng (1984).
  - Stability-corrected mixing length scale.
  - Stability-corrected turbulent Prandtl number for heat flux.

- **Dynamic Smagorinsky, dynamic heat flux model.**
  - Parameter-free computation of eddy viscosity and eddy diffusivity.
  - No Prandtl number assumption is necessary.
  - Effect of stability is accounted for automatically.

TKE MODEL

$$\begin{aligned} \tau_{ij} &= -2\nu_t \bar{S}_{ij} \\ q_i &= -k_t \frac{\partial \bar{\theta}}{\partial x_i} \end{aligned}$$

where the eddy viscosity and eddy diffusivity are computed according to

$$\begin{aligned} \nu_t &= C_k l e^{1/2} \\ k_t &= \underbrace{\left(1 + \frac{2l}{\Delta}\right)}_{1/Pr_t} \nu_t \end{aligned}$$

and where l is the mixing length, e is the subgrid-scale kinetic energy, and Δ is the LES filter width. The mixing length is computed via

$$l = \begin{cases} \Delta & \text{convectively unstable} \\ \frac{0.76 e^{1/2}}{\left(\frac{g}{\theta_0}\frac{\partial \theta}{\partial z}\right)^{1/2}} & \text{convectively stable} \end{cases}$$

KINETIC ENERGY TRANSPORT EQUATION

$$\left(\frac{\partial}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j}\right) e = P + B - \epsilon + D$$

where

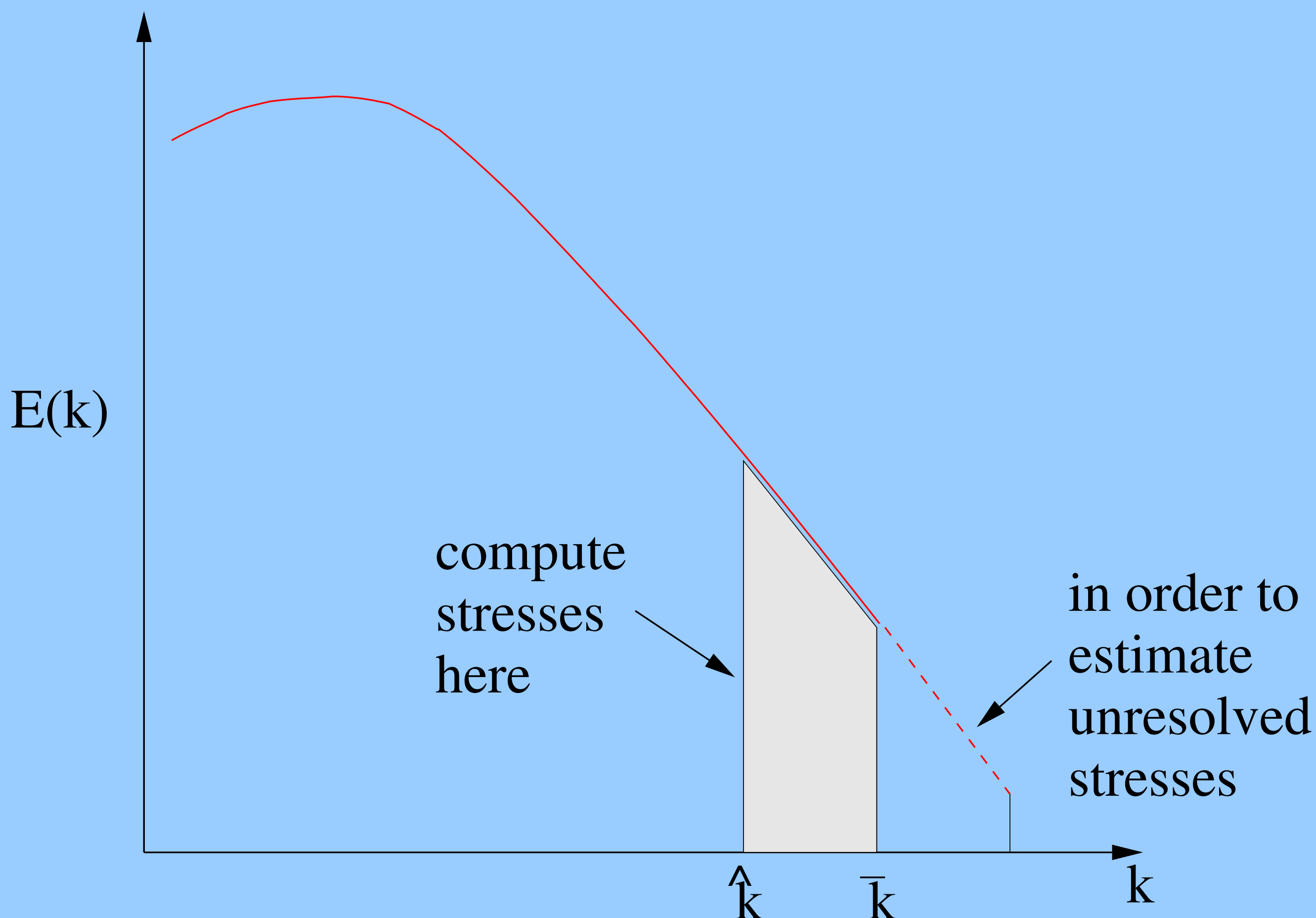
$$\begin{aligned} P &= -\tau_{ij}\bar{S}_{ij} \\ B &= \frac{g}{\theta_0} q_3 \\ \epsilon &= C_\epsilon \frac{e^{3/2}}{l} \\ D &= \frac{\partial}{\partial x_i}\left(2\nu_t \frac{\partial e}{\partial x_i}\right) \end{aligned}$$

The constants are set as follows:

$$C_k = 0.1 \qquad C_\epsilon = 0.93$$

DYNAMIC MODEL

The dynamic model makes use of scale-similarity ideas in order to estimate SGS stresses from the stresses produced by the smallest resolved length scales.



SOLUTION FOR C_s

Grid level: $\overline{u}_i$; $\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \simeq -2(C_s \overline{\Delta})^2 |\overline{S}| \overline{S}_{ij}$

Test level: $\widehat{u}_i$; $T_{ij} = \widehat{\overline{u_i u_j}} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j \simeq -2(C_s \widehat{\Delta})^2 |\widehat{S}| \widehat{S}_{ij}$

Germano's identity:

$$T_{ij} - \widehat{\tau}_{ij} \equiv L_{ij} = \underbrace{\widehat{\overline{u}_i \overline{u}_j} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j}_{\text{computable}}$$

Postulate Smagorinsky models at both the test and grid scales, substitute into Germano's identity

$$-2(C_s \overline{\Delta})^2 \underbrace{\left(\frac{\widehat{\Delta}^2}{\overline{\Delta}^2} |\widehat{S}| \widehat{S}_i j - \widehat{|\overline{S}| \overline{S}_{ij}} \right)}_{M_{ij}} = L_{ij} - \frac{1}{3} L_{kk}$$

Least squares solution for C_s

$$(C_s \overline{\Delta})^2 = -\frac{1}{2} \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}$$

SOLUTION FOR C_h

Grid level: $\overline{\theta}$; $\quad q_i = \overline{u_i\theta} - \overline{u}_i\overline{\theta} \quad \simeq \quad -(C_h\overline{\Delta})^2|\overline{S}|\frac{\partial\overline{\theta}}{\partial x_i}$

Test level: $\widehat{\theta}$; $\quad Q_i = \widehat{\overline{u_i\theta}} - \widehat{\overline{u}}_i\widehat{\overline{\theta}} \quad \simeq \quad -(C_h\widehat{\Delta})^2|\widehat{S}|\frac{\partial\widehat{\theta}}{\partial x_i}$

Germano's identity for scalar flux:

$$Q_i - \widehat{q}_i \equiv H_i = \underbrace{\widehat{\overline{u}_i\overline{\theta}} - \widehat{\overline{u}}_i\widehat{\overline{\theta}}}_{\text{computable}}$$

Postulate gradient diffusion models at both the test and grid scales, substitute into Germano's identity

$$-(C_h\overline{\Delta})^2 \underbrace{\left(\frac{\widehat{\Delta}^2}{\overline{\Delta}^2}|\widehat{S}|\frac{\partial\widehat{\theta}}{\partial x_i} - \widehat{|\overline{S}|\frac{\partial\overline{\theta}}{\partial x_i}} \right)}_{N_i} = H_i$$

Least squares solution for C_h

$$(C_h\overline{\Delta})^2 = -\frac{\langle H_i N_i \rangle}{\langle N_i N_i \rangle}$$

ADVANTAGES OF THE DYNAMIC PROCEDURE

- The model constants C_s and C_h are computed as a function of space and time as the simulation evolves.

- Stability and the necessary damping near the surface are accounted for automatically.

- No external inputs are required.

But ...

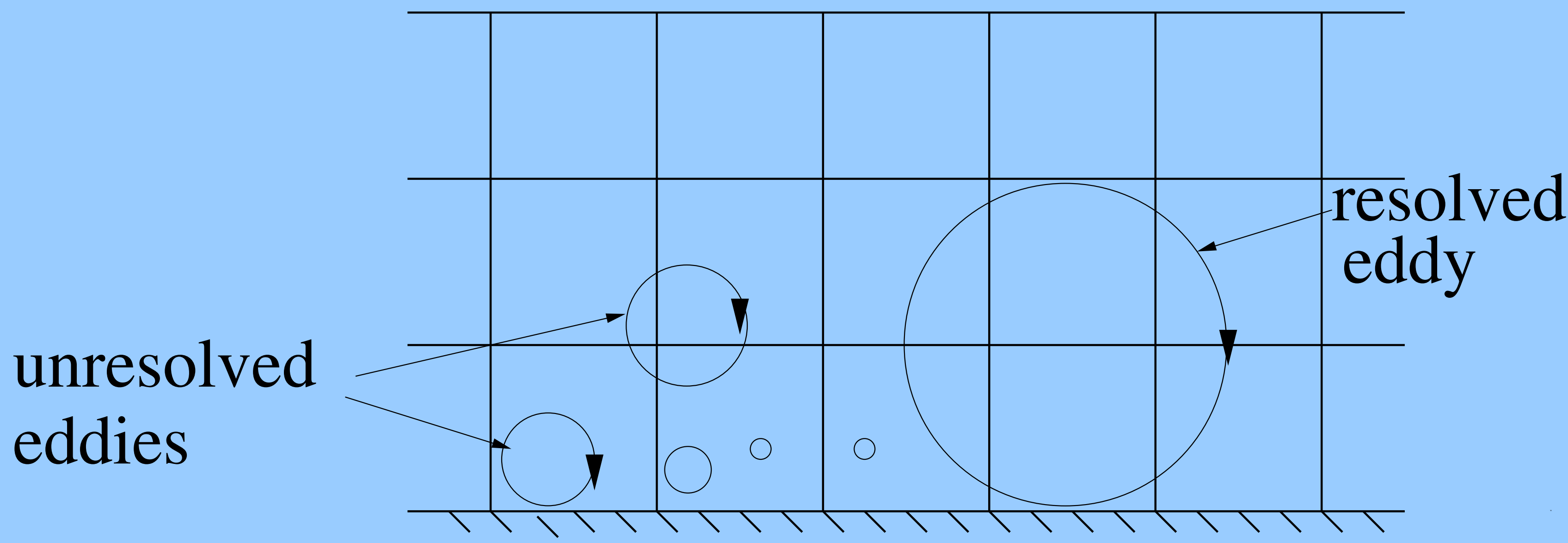
- The filter scale must be in the inertial range.

- This requirement is almost never met near the surface for the atmospheric boundary layer or at coarse resolution away from the surface.

NEAR-SURFACE ISSUES

Following Sullivan *et al.* (1994) we reason as follows:

- In the absence of strong buoyant forcing, the size of the dominant eddies in the near-surface region scales with the distance from the surface.



NEAR-SURFACE ISSUES

Following Sullivan *et al.* (1994) we reason as follows:

- In the absence of strong buoyant forcing, the size of the dominant eddies in the near-surface region scales with the distance from the surface.

- We can not possibly resolve these eddies with conventional LES methods.

- The representation of the flow in the near-surface region is thus more like a Reynolds Averaged Navier Stokes (RANS) computation.

- It is therefore sensible to make use of RANS modeling ideas for the near-surface layer.

TWO-PART EDDY VISCOSITY MODEL

Sullivan's ideas can be realized via a two-part eddy viscosity model

$$\tau_{ij} = -\underbrace{2\gamma(z)\nu_t S_{ij}}_{\text{LES part}} - \underbrace{2V_T\langle S_{ij}\rangle}_{\text{RANS part}}$$

$$V_T = 2C_R\Delta^2|\langle S\rangle|$$

- The RANS part is active mainly in the near-surface region; $\langle S\rangle$ is maximum at the surface and falls off like $1/z$ with height.

- In the case of the tke model, the LES part is multiplied by $\gamma(z)$, an isotropy (damping) function that reduces its influence near the surface. The dynamic model does this automatically and thus no isotropy function is used in this case.

DETERMINATION OF C_R

Determine C_R such that the mean speed derivative matches with similarity theory at the first grid point.

Postulate a constant stress layer near the surface. Then the computed total stress at the first grid point should satisfy

$$\left[\langle\tau_{13}\rangle_1^2 + \langle\tau_{23}\rangle_1^2\right]^{1/2} + \left[\langle u'w'\rangle_1^2 + \langle v'w'\rangle_1^2\right]^{1/2} = u_*$$

Mean SGS stress, neglecting the fluctuating strain at the first grid point;

$$\begin{aligned}
\langle\tau_{13}\rangle_1 &\simeq -2\left(\langle\gamma\nu_t\rangle_1 + V_{T1}\right)\langle\frac{\partial u}{\partial z}\rangle_1 \\
\langle\tau_{23}\rangle_1 &\simeq -2\left(\langle\gamma\nu_t\rangle_1 + V_{T1}\right)\langle\frac{\partial v}{\partial z}\rangle_1
\end{aligned}$$

The surface stress condition then becomes

$$2\left(\langle\gamma\nu_t\rangle_1 + V_{T1}\right)\left[\left(\frac{\partial\langle u\rangle_1}{\partial z}\right)^2 + \left(\frac{\partial\langle v\rangle_1}{\partial z}\right)^2\right]^{1/2} + \left[\langle u'w'\rangle_1^2 + \langle v'w'\rangle_1^2\right]^{1/2} = u_*$$

Neglect the turning of the mean wind speed at the first grid point:

$$\left[\left(\frac{\partial\langle u\rangle_1}{\partial z}\right)^2 + \left(\frac{\partial\langle v\rangle_1}{\partial z}\right)^2\right]^{1/2} \simeq \frac{\partial U_{s1}}{\partial z} = \frac{u_*\phi_m(z_1)}{kz_1}$$

solve for V_{T1}

$$V_{T1} = \frac{u_* k z_1}{\phi_m(z_1)} - \langle\gamma\nu_t\rangle_1 - \frac{kz_1}{u_*\phi_m(z_1)}\left[\langle u'w'\rangle_1^2 + \langle v'w'\rangle_1^2\right]^{1/2}$$

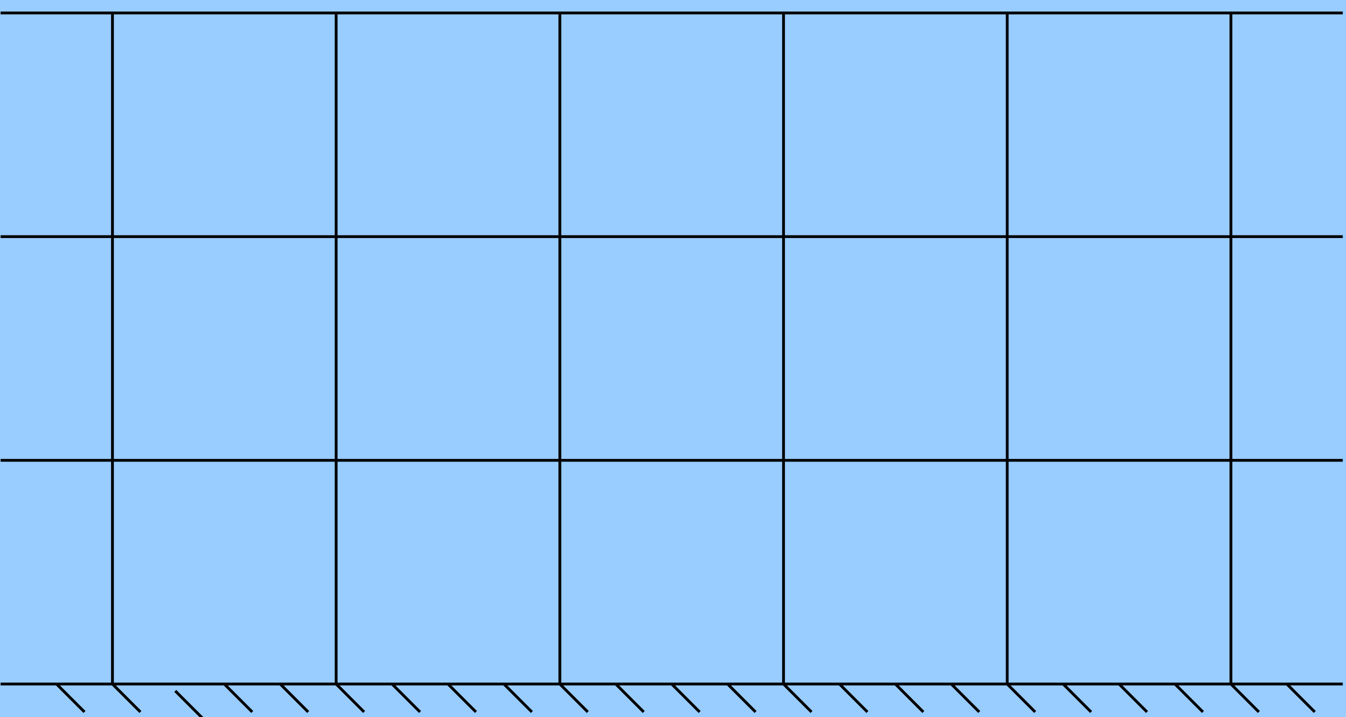
At any other height

$$V_T = V_{T1}\frac{|\langle S\rangle|}{|\langle S\rangle|_1}$$

BOUNDARY CONDITIONS

$$\frac{du}{dz}, \frac{dv}{dz} = 0 \qquad \frac{dw}{dz} = -\left[\frac{du}{dx} + \frac{dv}{dy} \right]$$

P specified ala Klemp & Durran 1983



u, v, w=0 $\quad \theta = \theta(t)$

τ_{13}, τ_{23}, q_3 specified

SURFACE BOUNDARY CONDITIONS

$$\tau_{13}(x,y,z_1) = -u_*^2 \left[\frac{\langle U_s \rangle u'(x,y) + U_s(x,y)\langle u \rangle}{\langle U_s \rangle \sqrt{\langle u \rangle^2 + \langle v \rangle^2}} \right]_1$$

$$\tau_{23}(x,y,z_1) = -u_*^2 \left[\frac{\langle U_s \rangle v'(x,y) + U_s(x,y)\langle v \rangle}{\langle U_s \rangle \sqrt{\langle u \rangle^2 + \langle v \rangle^2}} \right]_1$$

$$q_3(x,y,z_1) = -Q_* \left[\frac{\langle U_s \rangle \theta'(x,y) + U_s(x,y)\langle \theta - \theta_0 \rangle}{\langle U_s \rangle (\langle \theta \rangle - \theta_0)} \right]_1$$

where

$$u'(x,y,z) = u(x,y,z) - \langle u \rangle, \quad \text{etc.} \qquad U_s(x,y,z) = \sqrt{u(x,y,z)^2 + v(x,y,z)^2}$$

These forms obey the constraints

$$\sqrt{\langle \tau_{13}(x,y,z_1) \rangle^2 + \langle \tau_{23}(x,y,z_1) \rangle^2} = u_*^2$$

$$\langle q_3(x,y,z_1) \rangle = Q_*$$

ESTIMATION OF SURFACE FLUXES

Use surface similarity theory:

$$\langle U_s \rangle_1 = \frac{u_*}{k}\left[\log\left(\frac{z_1}{z_0}\right) + \beta_m\left(\frac{z_1}{L}\right)\right]$$

$$\langle \theta \rangle_1 - \theta_0 = \frac{Q_*}{u_* k}\left[\log\left(\frac{z_1}{z_0}\right) + \beta_h\left(\frac{z_1}{L}\right)\right]$$

Solve for u_* and Q_*:

$$u_* = \frac{\langle U_s \rangle_1 k}{\log\left(\frac{z_1}{z_0}\right) + \beta_m\left(\frac{z_1}{L}\right)}$$

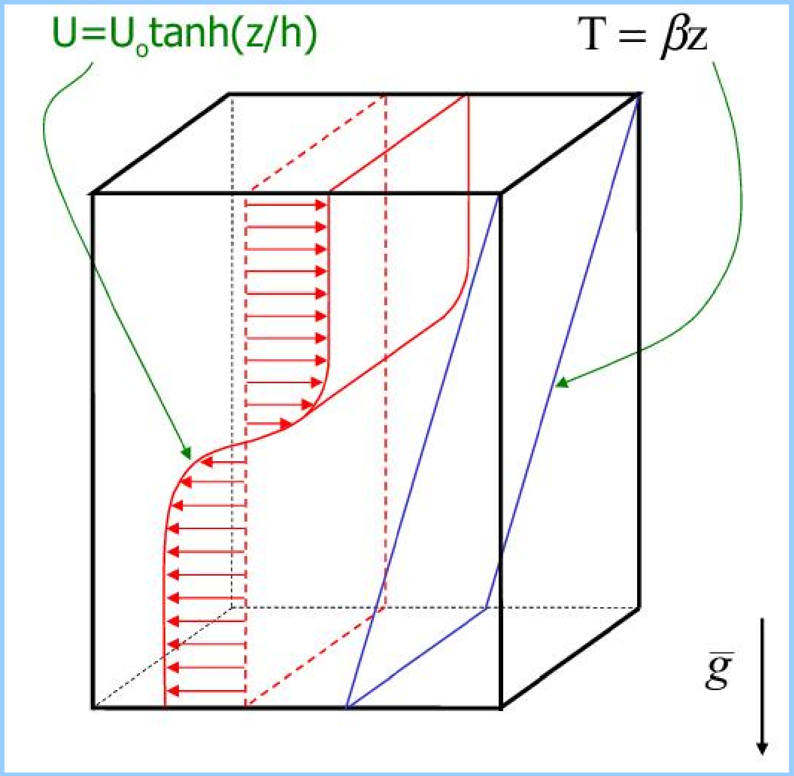
$$Q_* = \frac{(\langle \theta \rangle_1 - \theta_0) u_* k}{\log\left(\frac{z_1}{z_0}\right) + \beta_h\left(\frac{z_1}{L}\right)}$$

The constants are set as follows:

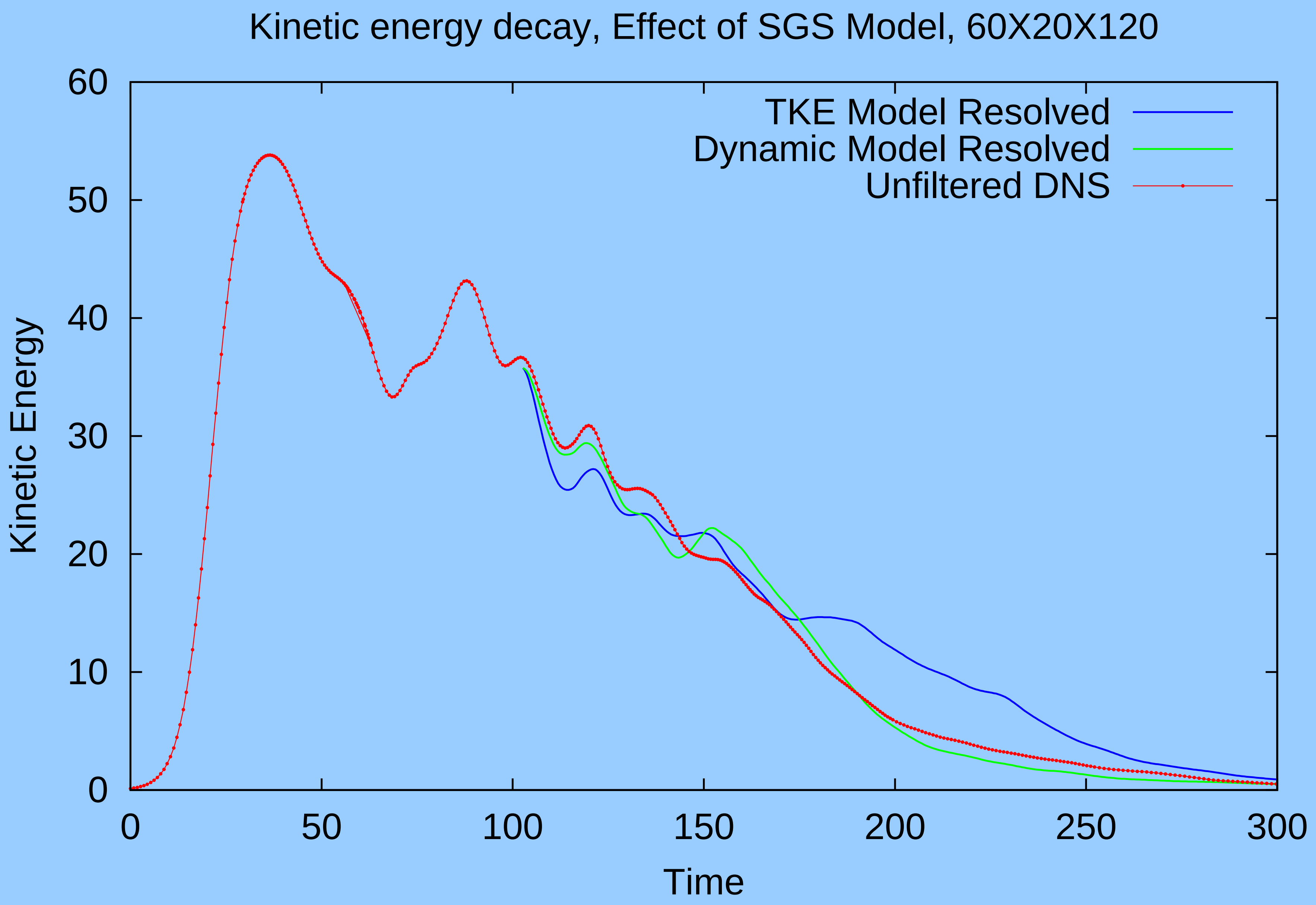
$$\beta_m = 5.0 \qquad \beta_h = 5.0 \qquad k = 0.4$$

KELVIN-HELMHOLTZ TEST PROBLEM

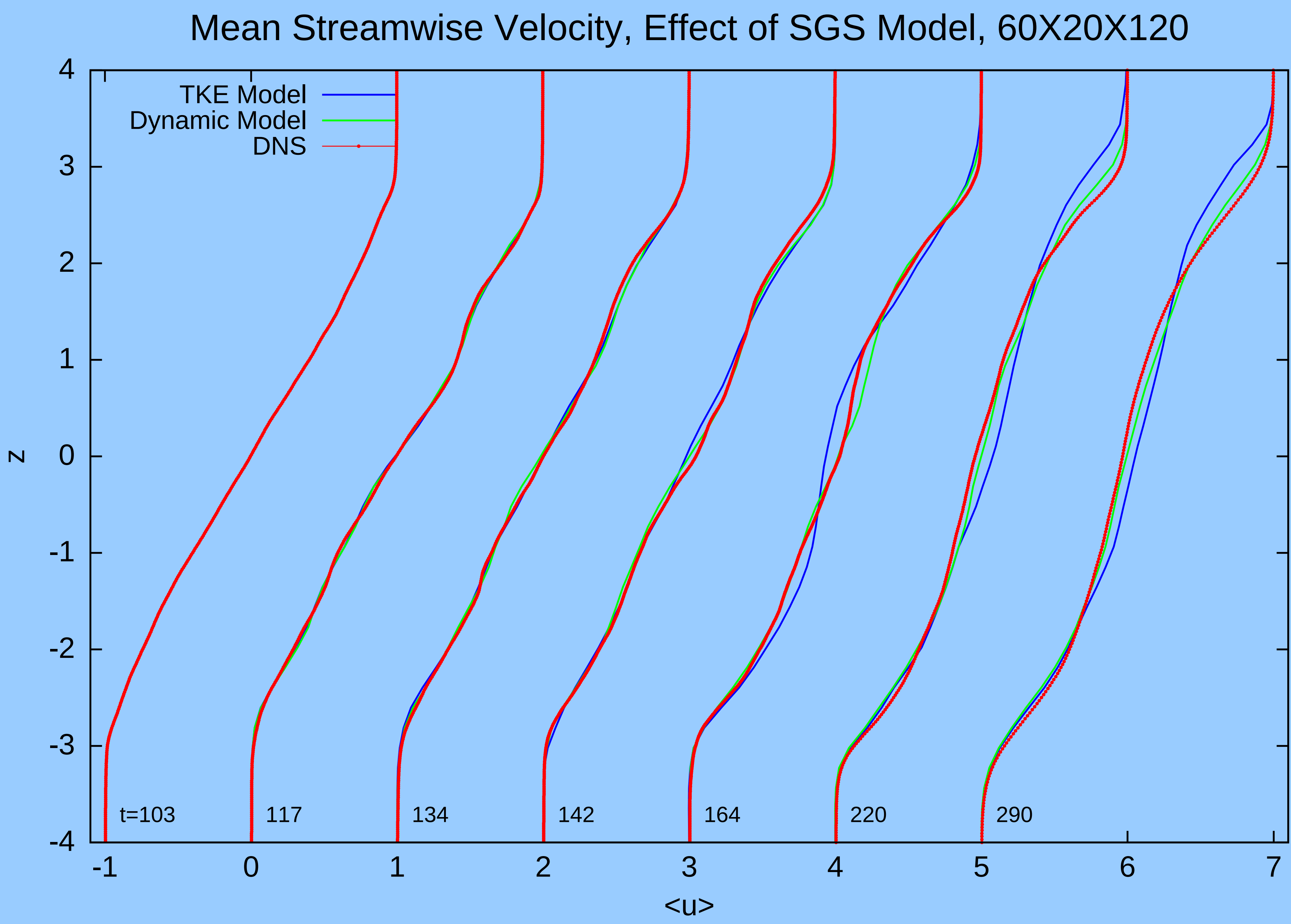
- Simulate a wind shear event in a stable atmosphere $Re = 2000$, $Ri = 0.05$.
- Compare the LES results with DNS computed on a much finer (factor of 12 in each direction) mesh.
- Compare the TKE with the dynamic Smagorinsky model.



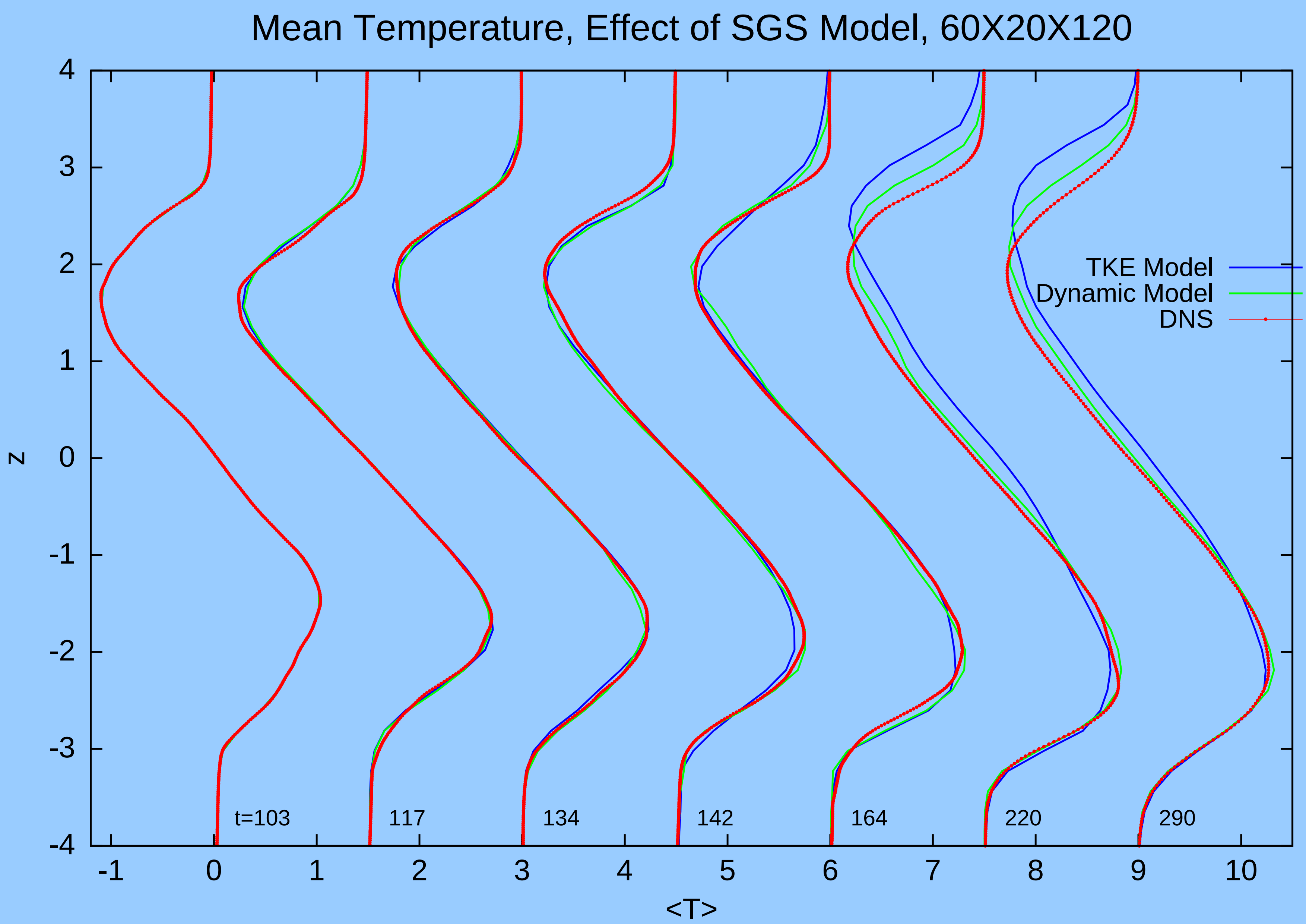
RESULTS - KE DECAY



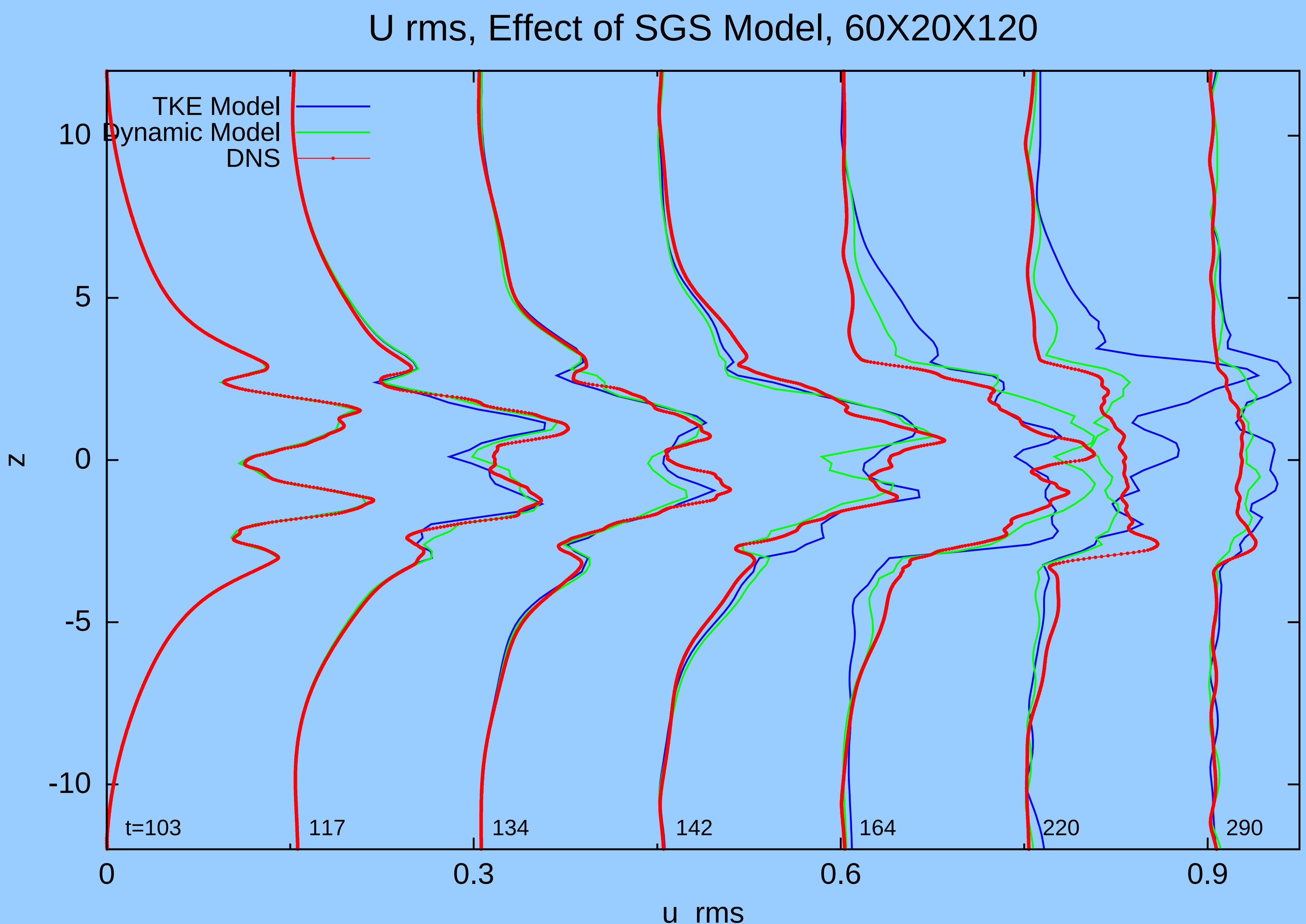
RESULTS - MEAN STREAMWISE VELOCITY



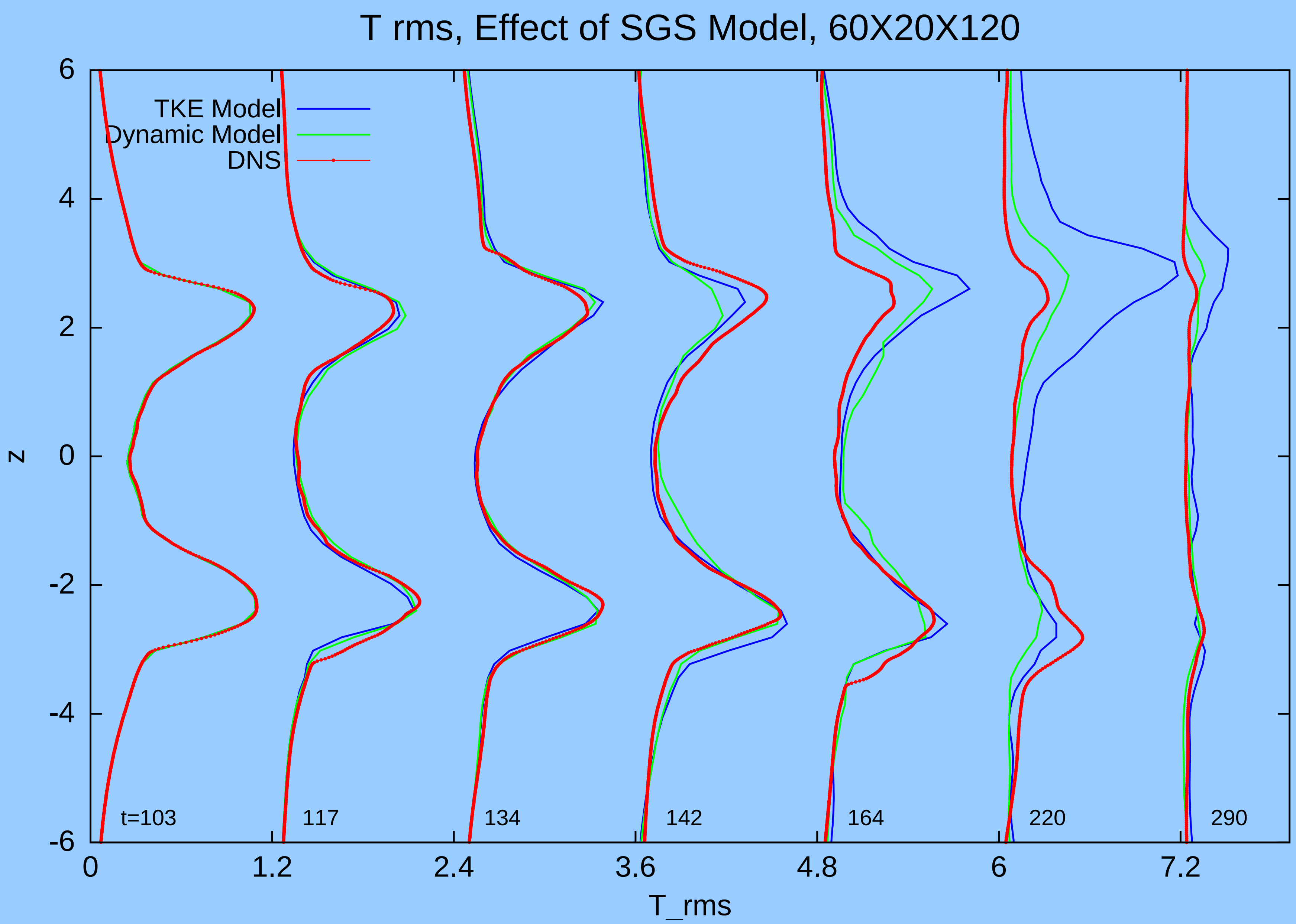
RESULTS - MEAN POTENTIAL TEMPERATURE



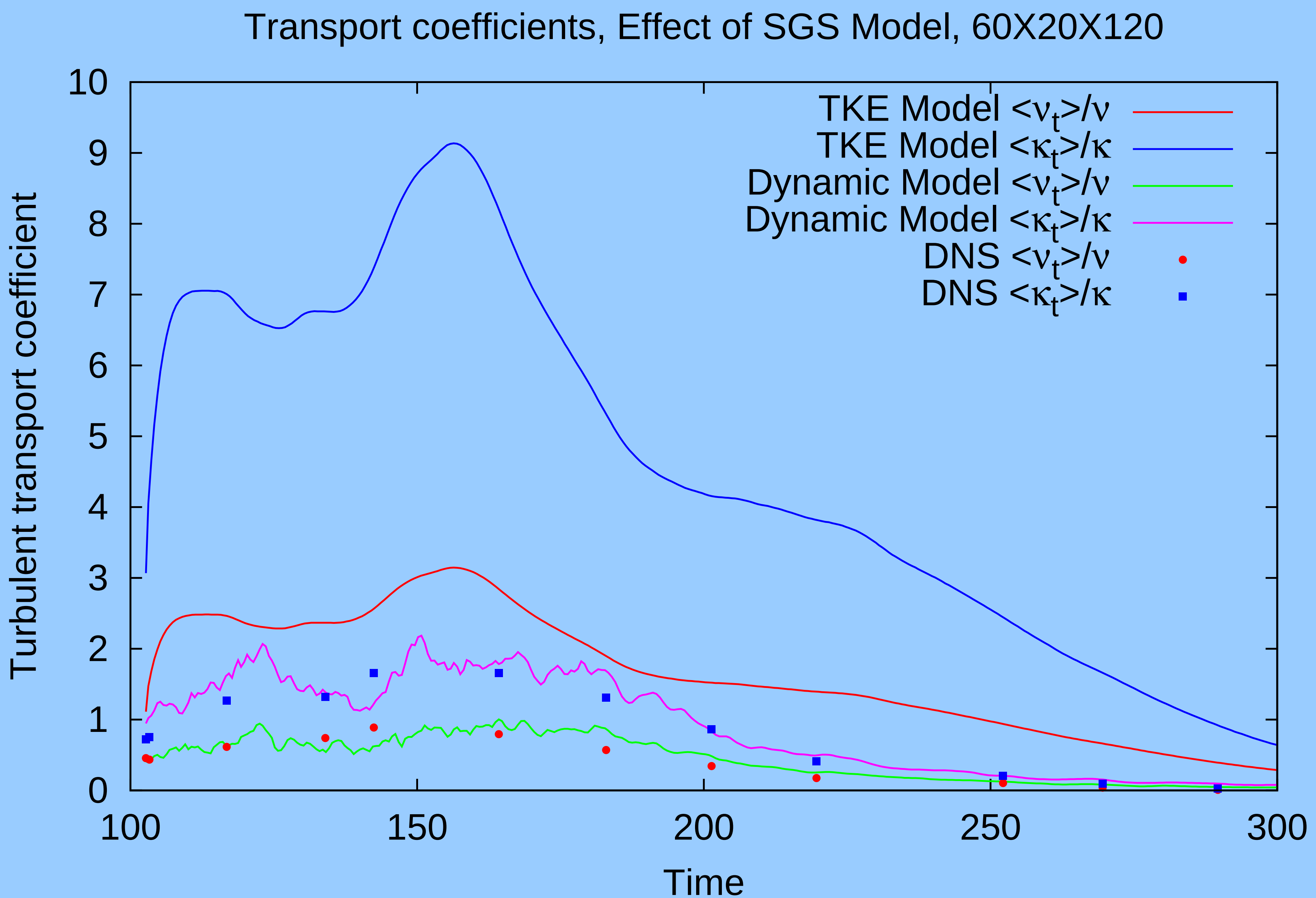
RESULTS - STREAMWISE VELOCITY FLUCTUATION



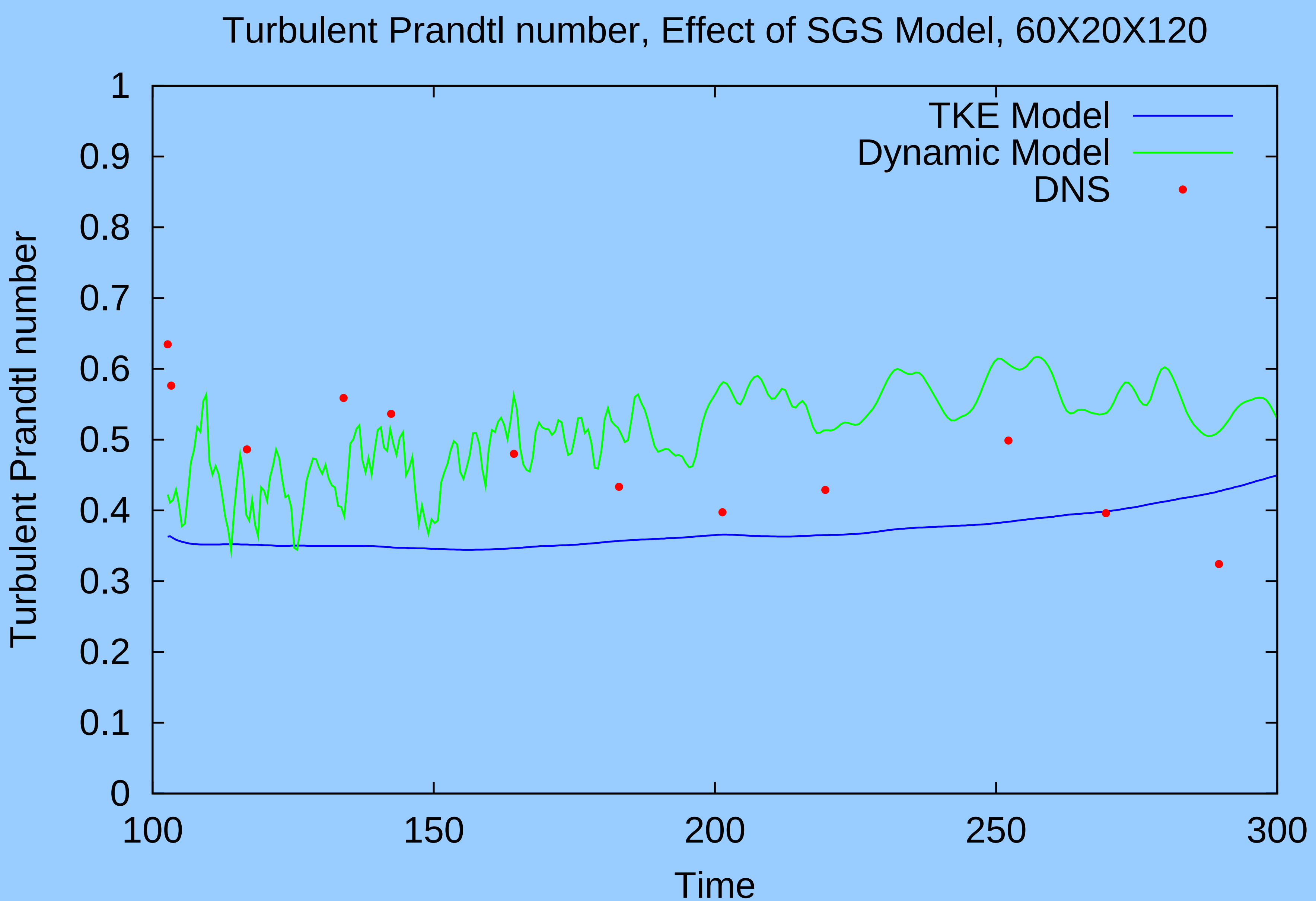
RESULTS - POTENTIAL TEMPERATURE FLUCTUATION



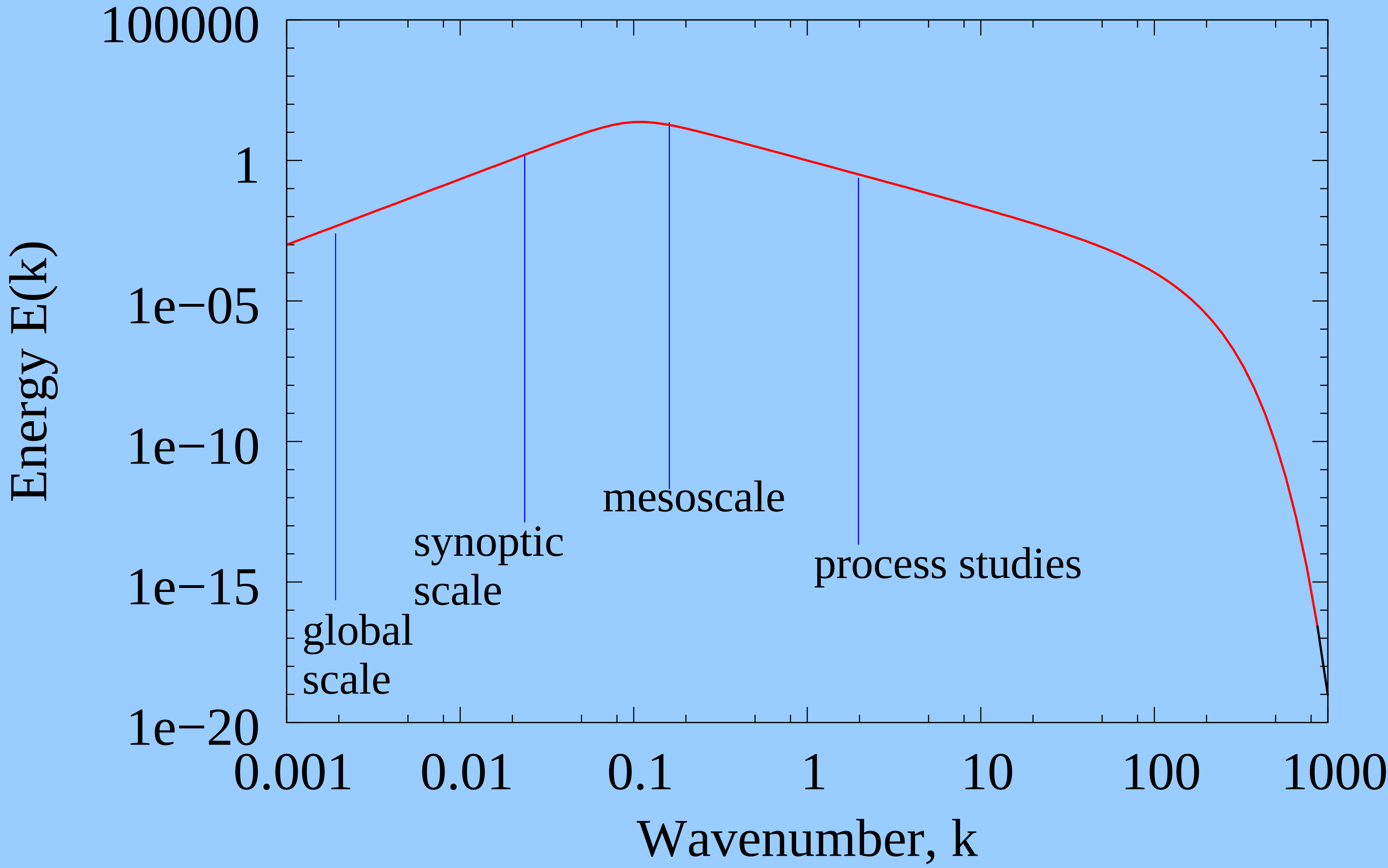
RESULTS - EDDY VISCOSITY AND DIFFUSIVITY



RESULTS - TURBULENT PRANDTL NUMBER



HOW WELL RESOLVED ARE ATMOSPHERIC SIMULATIONS?



IS IT REALLY LES?

- Detailed process studies are LES (by construction).

- Mesoscale simulation may barely satisfy the requirements of LES.

- Synoptic scale and larger simulations typically do not resolve the integral scale and thus violate the underlying ideas of LES (i.e. bulk of the turbulent transport is *not resolved*).

- Turbulence modeling for large-scale simulations proceed along the same lines but with lots of ad hoc modifications.

SUMMARY

- It is impossible to resolve all relevant length scales in turbulent atmospheric flows.

- We apply a spatial filter to eliminate small scales and then account for their effects through a turbulence model.

- The turbulence model must supply the correct energy flux at the filter cutoff in order to balance production and dissipation.

- Simple eddy viscosity models can achieve such a balance.

- Many different approaches exist for scaling the eddy viscosity.

- Dynamic modeling is self-calibrating but requires the filter cutoff to be in the inertial range.

- The LES approach is successful if the resolution is adequate and the model is well calibrated.