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ANALYSIS OF DIFFUSION OF TURBULENT KINETIC ENERGY BY NUMERICAL SIMULATIONS OF NATURAL CONVECTION IN LIQUID METALS

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ABSTRACT

Many turbulence models used in engineering applications solve the transport equation of turbulent kinetic energy k to determine a characteristic velocity scale of turbulence. Meanwhile it is known that for prediction of natural convection flows with second moment closure models the inclusion of diffusive transport of k is essential. However, validation and improvement of closure assumptions for turbulent diffusion is difficult because of lack of accurate experimental information about the correlations $\overline{u_j'p'}$ and $\overline{u_j'u_i'u_i'}/2$, which have to be modelled. In this paper we use the method of direct numerical simulation to provide a database of turbulent Rayleigh-Bénard convection in liquid sodium. The numerical results are used to analyse terms in the transport equation of turbulent kinetic energy, including turbulent diffusion terms. The results reveal that in natural convection the dominant mechanism responsible for diffusive transport is due to pressure fluctuations, not due to triple correlations of velocity fluctuations. This is in contrast to forced flows in which pressure diffusion is of minor importance only. For this reason in standard turbulence models pressure diffusion is usually neglected. Our results indicate that both correlations act in opposite direction. Therefore turbulence models that neglect pressure diffusion cannot correctly predict turbulence in natural convection.

INTRODUCTION

To take advantage of inherent safety features new designs of liquid metal fast breeder reactors aim for example to remove the decay heat completely by natural convection [1]. Results of experiments that are performed in this context in scaled reactor models using water as a model fluid [2] have to be transfered to real reactor conditions. This will mainly be done by computer codes like [3,4]. These codes are based on statistical turbulence models which have to be improved and calibrated to be applicable to heat transfer by natural convection in liquid metals. For this purpose detailed information about turbulence in such flows is needed. However, because of great difficulties in working with liquid metals only few suitable experimental data are available in literature [5].

We use the method of direct numerical simulation to provide data of turbulent convection in liquid metals. However, with present-day computer power the method is limited to the investigation of simple geometries and low turbulence levels only. Nevertheless in this simulations similar physical mechanisms are expected to occur as will be dominant in the real reactor. Thus our numerical results may be helpful to illuminate fundamental statistical features of turbulent convection in liquid metals.

In a previous study [6] we used direct numerical simulation results of turbulent Rayleigh-Bénard convection in liquid sodium to analyse terms in the transport equation of turbulent kinetic energy k. It became evident that in the balance of k diffusive transport is of great importance. This result is in accordance with that from analytical considerations by Lawrence [7]. He found that in case of natural convection without mean flow second moment closure models that do not account for diffusive transport cannot predict turbulent flow. Lawrence concluded that there is a strong need for a physically meaningful diffusion model which is not based on a mean flow. To meet this goal information is required about the correlations which represent turbulent

diffusion. However, measurements of these correlations lack of accuracy or are even lacking completely [8].

The objective of this paper is to perform a detailed analysis of diffusive transport of turbulent kinetic energy in natural convection of liquid sodium by means of direct numerical simulation data. Compared to earlier simulations now an increased turbulence level has been realized so that convective mechanisms are of enhanced importance. Results will be given for turbulent kinetic energy k, for terms in the balance equation of k and especially for the correlations that contribute to diffusive transport of turbulent kinetic energy. The numerical results will be discussed regarding their consequences for adequate modelling of turbulent diffusion of k in natural convection.

1. PHYSICAL AND NUMERICAL MODEL

1.1 Rayleigh-Bénard convection

As a model for investigation of heat transfer phenomena by natural convection we consider the Rayleigh-Bénard convection. The geometry is given by an infinite fluid layer which is confined by two rigid horizontal isothermal walls. The lower one is heated and the upper one is cooled. There are two dimensionless numbers which characterize the problem: The Rayleigh number

$$Ra = \frac{g\beta\Delta T_W \, H^3}{\nu\kappa} \qquad (1)$$

and the Prandtl number

$$Pr = \frac{\nu}{\kappa} \qquad (2)$$

(where g = gravity, β = volume expansion coefficient, ΔT_W = temperature difference of the walls, H = depth of the fluid layer, ν = kinematic viscosity, and κ = thermal diffusivity). From Rayleigh and Prandtl number a further dimensionless number, the Grashof number

$$Gr = \frac{Ra}{Pr}\,, \qquad (3)$$

can be defined.

In this paper we discuss results of simulations performed for the Prandtl number of liquid sodium (Pr = 0.006) and Rayleigh numbers of Ra = 3,000, 6,000, 12,000 and 24,000. The Grashof number is up to $Gr = 4 \cdot 10^6$ and therefore the velocity field is clearly turbulent whereas the temperature field is in the transition range between laminar and turbulent flow.

1.2 Simulation method

The method of direct numerical simulation of turbulence does not involve any empirical model assumptions of turbulence. In accordance with the features of turbulence the full conservation equations of mass, momentum, and thermal energy have to be solved in three dimensions and in time, using grids which resolve the largest and smallest scales of turbulence.

The computer code TURBIT is based on a finite volume method and allows for direct and large eddy simulation of turbulent flow in simple channel geometries [9]. The basic equations are solved in dimensionless form. For normalization the channel height H, velocity $u_0 = (g\beta\Delta T_w H)^{1/2}$, time H/u_0, pressure ρu_0^2, and temperature difference between walls ΔT_w are used. The Boussinesq approximation is assumed to be valid. If the Einstein summation rule is applied to all terms bearing the same subscript twice, the governing equations can be written as

$$\frac{\partial u_i}{\partial x_i} = 0 \qquad (4)$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = - \frac{\partial p}{\partial x_i} - \left(T_{ref} - T \right) \delta_{i3} + \frac{1}{\sqrt{Gr}} \frac{\partial^2 u_i}{\partial x_j^2} \qquad (5)$$

$$\frac{\partial T}{\partial t} + \frac{\partial (T u_j)}{\partial x_j} = \frac{1}{Pr\sqrt{Gr}} \frac{\partial^2 T}{\partial x_j^2} \,. \qquad (6)$$

Here Cartesian co-ordinates are used with x_1 and x_2 horizontal and x_3 directed upwards. Spatial discretization is done by second order central finite differences, defined on a staggered grid. For time integration of the momentum equation the explicit Euler-Leapfrog scheme is used in conjunction with the projection method of Chorin. Time integration of the thermal energy equation is done by the semi-implicit Leapfrog-Crank-Nicholson scheme which improves considerably the efficiency with simulations of liquid metal convection [10]. For Rayleigh-Bénard convection periodic boundary conditions are used in the horizontal directions whereas at the lower and upper wall no slip condition and constant wall temperatures are specified.

Grids used in direct numerical simulation have to meet several requirements to ensure physical relevance of the results. The grid widths Δx_i have to be fine enough to resolve the smallest scales of turbulence and the thin boundary layers. The horizontal extensions $X_{1,2}$ have to be large enough to allow for development of large scale structures. For turbulent convection in liquid metals there is only little experimental information and numerical experience available to specify adequate grids. Therefore we first performed comprehensive numerical studies [6] to ensure that the requirements mentioned above are met by our grids. The parameters of the simulations are given in Table 1. The numbers of mesh cells N_i follow directly from the values chosen for X_i and Δx_i, except for the vertical direction in which nonequidistant grid-spacing is used. The simulations with $3{,}000 \leq Ra \leq 12{,}000$ are started from fluid at rest and linear mean temperature profile on which random fluctuations are superimposed. For the simulation with Ra = 24,000 the final data of the simulation with Ra = 12,000 are used as initial data.

2. SIMULATION RESULTS

2.1 Verification

For purpose of verification of the code we performed a numerical simulation of Rayleigh-Bénard convection in air (Pr = 0.71). The Rayleigh-number Ra = 630,000 corresponds to that of an experiment by Deardorff & Willis [11]. Our numerical results agree well with the experimental ones, see [12]. For Rayleigh-Bénard convection in liquid sodium no other experimental data are available for verification than those given by Kek [13]. In this experiment, where two different channel heights (H = 15.5 mm and H = 46.5 mm) were used, Rayleigh numbers up to Ra = 250,000 were realized. In Fig. 1 measured values of the Nusselt number are given for Rayleigh numbers Ra ≤ 30,000 only. In the numerical simulation the Nusselt number does not approach a constant value but varries in time. In Fig. 1 the corresponding range of Nusselt numbers

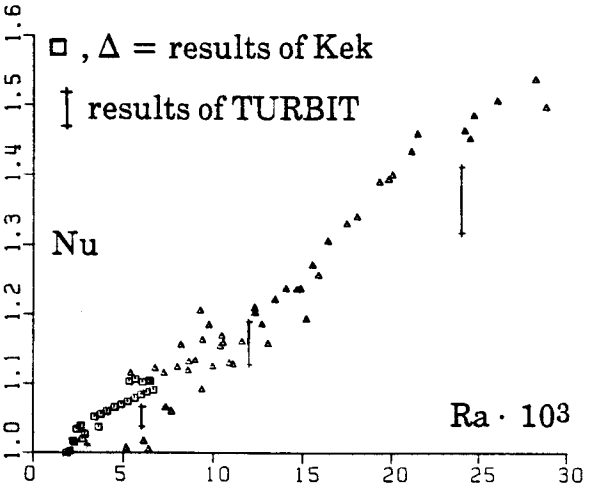

Fig. 1: Nusselt number as function of the Rayleigh number.

Tab.1: Flow parameter and grid data of the simulations.

Ra	Pr	Gr	$X_{1,2}$	$\Delta x_{1,2}$	Δx_{3w}	$N_{1,2}$	N_3
3,000	0.006	$5 \cdot 10^5$	8.0	0.0625	0.01	128	31
6,000	0.006	10^6	8.0	0.040	0.01	200	31
12,000	0.006	$2 \cdot 10^6$	8.0	0.032	0.005	250	39
24,000	0.006	$4 \cdot 10^6$	8.0	0.032	0.005	250	39
630,000	0.71	$8.9 \cdot 10^5$	7.92	0.0396	0.005	200	39

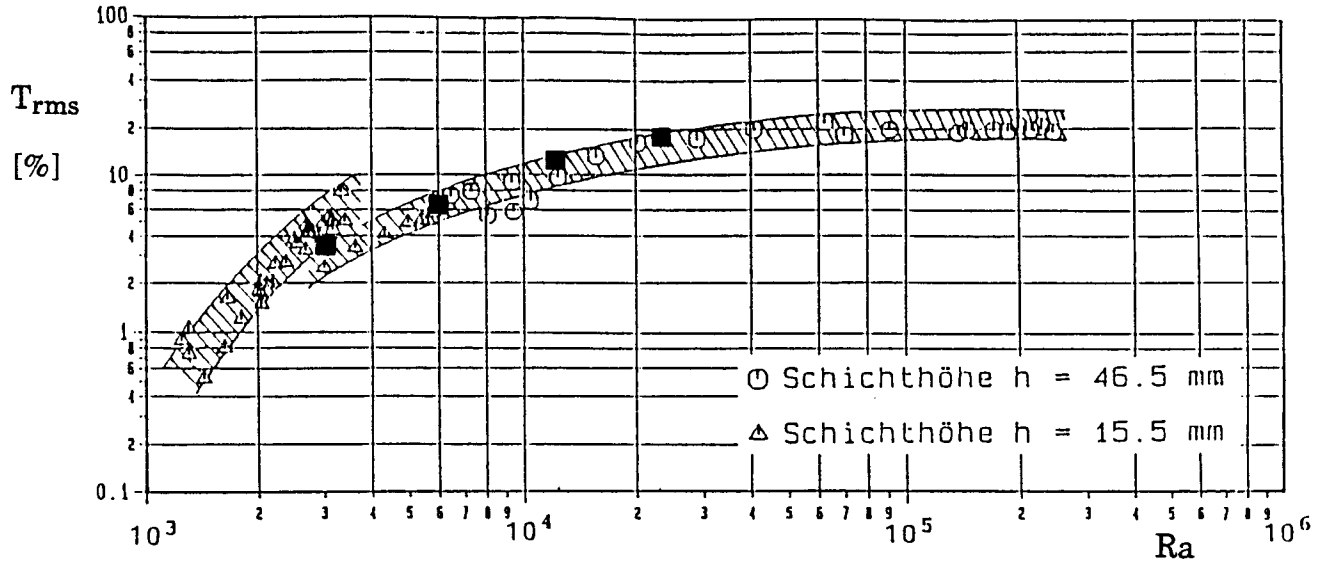

Fig. 2: RMS-values of temperature fluctuations in liquid sodium in the centre of the layer as function of the Rayleigh number, taken from Kek [13]: ○ , Δ = results of Kek, ■ results of TURBIT

observed in the simulations are indicated by vertical bars. In general the numerical results for the Nusselt number are somewhat lower than the experimental ones. However, new unpublished data of measurements in the same channel give Nusselt numbers which are also somewhat lower than the previous ones and thus do better agree with the simulation results.

Fig. 2 shows results of Kek for the variance of temperature fluctuations in channel midwidth as function of the Rayleigh number. Additionally, numerical results of TURBIT are given for four Rayleigh numbers. The calculated values of T_{rms} are well within the band of experimental data.

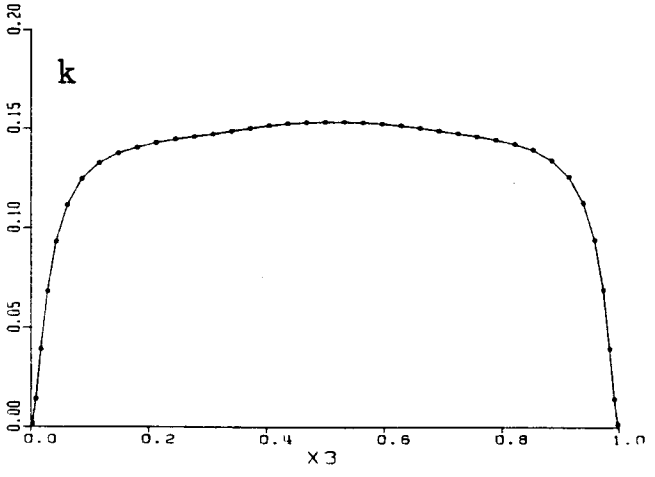

Fig. 3: Vertical profile of turbulent kinetic energy k for liquid sodium, Ra = 24,000.

2.2 Balance of turbulent kinetic energy

Before we analyse terms in the transport equation of turbulent kinetic energy we first present results for $k = 1/2\ u_i'u_i'$ itself. The vertical profile ($x_3 = 0$: lower wall, $x_3 = 1$: upper wall) of k for the simulation with Pr = 0.006 and Ra = 24,000 is given in Fig. 3. We identify a strong increase of k in the viscous boundary layer whereas only a small increase is observed between the edge of the boundary layer and the middle of the channel, where k reaches its maximum.

In turbulent Rayleigh-Bénard convection long time averaged mean velocities are zero. Therefore in the transport equation of turbulent kinetic energy [14] no convective transport and no production of k by interaction of shear stresses and mean velocity gradients is present. In fully developed flow the balance equation of turbulent kinetic energy in dimensionless form reduces to

$$0 = D + G - \varepsilon, \qquad (7)$$

where

$$D = \frac{\partial}{\partial x_3}\left[-\overline{u_3' k} - \overline{u_3' p'} + \frac{1}{\sqrt{Gr}} \frac{\partial k}{\partial x_3} \right],$$

$$G = \overline{u_3' T'} ,$$

$$\varepsilon = \frac{1}{\sqrt{Gr}} \overline{\frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j}} .$$

Here D denotes the diffusion of k, consisting of a turbulent part (first two terms) and a molecular part (third term). The production term G is the vertical turbulent heat flux and ε is the dissipation of turbulent kinetic energy.

In order to obtain reasonable statistical data from the numerical results at a position x_3 = const., averages $\bar{y}$ for a calculated variable y are formed over horizontal planes. These results are averaged over typically 10 to 20 time steps which are equidistantly distributed at the end of the simulated problem time. In Fig. 4 we give vertical profiles of D, G and ε. The dissipation ε is about constant in the centre of the channel and increases near the walls. The production term G vanishes in the thermal and viscous boundary layers near the walls, where heat is mainly transported by conduction, and increases away from the walls. The diffusive term D is responsible for vertical redistribution of k. It transports turbulent kinetic energy produced by G from the centre of the channel to the walls where it balances the dissipation ε. We find that in natural convection there is no local equilibrium between production and dissipation of k.

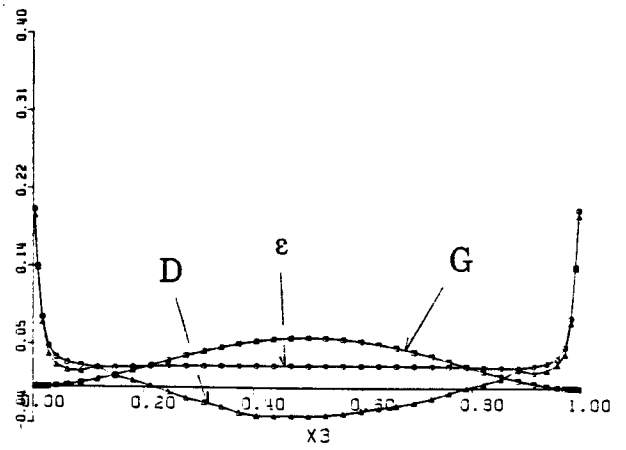

Fig. 4: Vertical profiles of balance terms of the k-equation for liquid sodium, Ra = 24,000: □ G, Δ D, o ε.

2.3 Analysis of diffusive transport of turbulent kinetic energy

In turbulent flows the molecular diffusion of k is only of importance near the walls, whereas outside the thin viscous boundary layers turbulent diffusion is dominant. The turbulent diffusion consists of two parts: a triple correlation of velocity fluctuations and a pressure-velocity correlation (see diffusion term D in Equation (7)). As these correlations are unknown the turbulent diffusion has to be modelled to close the kinetic energy equation. Usually, the pressure diffusion is either neglected or only indirectly taken into account as it is modelled in common with the triple correlation of velocity fluctuations [15]. The diffusion model commonly used in standard second moment closures is in accordance to the gradient diffusion assumption and in analogy with the eddy diffusivity hypothesis:

$$- \overline{u_3' \frac{u_i' u_i'}{2}} = \frac{\nu_t}{\sigma_k} \frac{\partial k}{\partial x_3} . \qquad (8)$$

Here σ_k is a turbulent Prandtl number for k, usually taken to be $\sigma_k \approx 1$ [15].

Lumley [16] proposed to account for the pressure flux term via

$$\overline{u_3' p'} = - \frac{1}{5} \overline{u_3' u_i' u_i'} . \qquad (9)$$

However, this relation has not been verified experimentally because of lack of data of pressure-velocity correlations [8]. Shabbir & Taulbee [17] used experimental data for mean velocity, mean temperature and kinetic energy of the buoyant axisymmetric plume to obtain Reynolds stresses and heat fluxes from closure formulations and compared the results with the measured values of Reynolds stresses and turbulent heat fluxes. To determine the unknown dissipation they balanced the turbulent energy equation and used proposal (9) to evaluate the pressure transport. The authors emphasize that the pressure diffusion is significant for this type of flow and has to be taken into account rather than simply neglecting it.

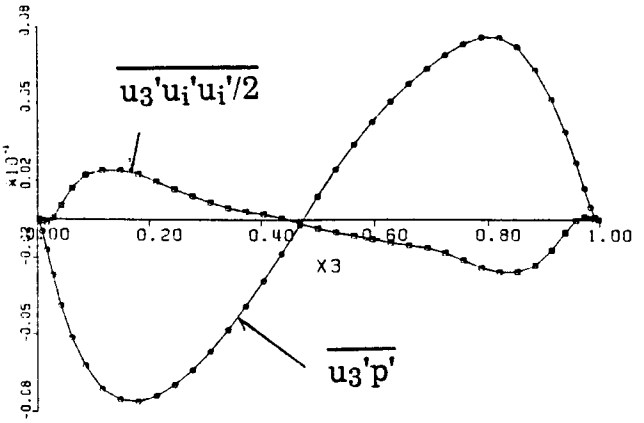

Fig. 5: Vertical profiles of correlations in the diffusion term of the k-equation (Pr = 0.006, Ra = 24,000).

In Fig. 5 we give vertical profiles of the correlations $\overline{u_3'u_i'u_i'}/2$ and $\overline{u_3'p'}$ calculated from results of our numerical simulation. The proposal of Lumley to model both correlations with reverse sign seems to be correct with the exception of the near wall regions. However, Fig. 5 shows that for this type of flow diffusive transport is mainly caused by pressure fluctuations not by triple correlations of velocity fluctuations. To clarify, whether the dominance of pressure diffusion is a special feature of liquid metal convection or not, analysis of $\overline{u_3'p'}$ and $\overline{u_3'u_i'u_i'}/2$ was also performed for the simulation of Rayleigh-Bénard convection in air used in the verification process. The results are given in Fig. 6. The pressure correlation shows very similar behaviour as compared to the results of the simulation with sodium, whereas the profiles of the triple correlations are clearly different. Nevertheless, it becomes evident that in natural convection without mean flow the relevant physical mechanism responsible for diffusive transport is due to pressure fluctuations. This finding is in contrast to forced flows where triple correlations are dominant and pressure diffusion is only of minor importance.

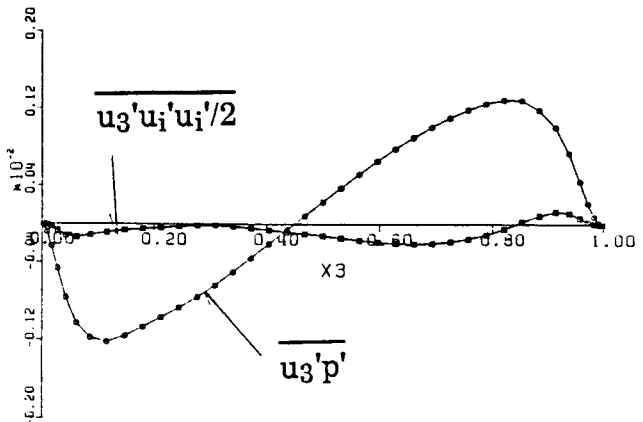

Fig. 6: Vertical profiles of correlations in the diffusion term of the k-equation for air, Ra = 630,000.

CONCLUSION

The method of direct numerical simulation was used to provide a data base of turbulent Rayleigh-Bénard convection in liquid sodium. The results were used to analyse analytical terms of the transport equation of turbulent kinetic energy.

The production of turbulent kinetic energy in purely buoyant flows is due to the vertical turbulent heat flux. In the simulation considered here, this term is zero at the walls and maximum at channel midwidth. The dissipation is about constant in the centre of the channel and increases in the viscous boundary layers near the walls. The diffusion is responsible for redistribution of turbulent kinetic energy from the centre of the channel to the near wall regions. Thus, in turbulence modelling of natural convection it is essential to account for diffusive transport.

Both correlations representing turbulent diffusive transport are analysed from the numerical results. It became evident that in natural convection turbulent diffusion of k is mainly caused by the interaction of pressure- and velocity-fluctuations, not by triple correlations of velocity fluctuations. As the latter correlation is dominant in forced flows in many turbulence models pressure diffusion is neglected and only the triple correlation is modelled. However, with the exception of the near wall regions both correlations are found to act in opposite direction. Thus, turbulence models that take into consideration only triple correlations of velocity fluctuations cannot correctly predict the diffusive transport in natural convection. We conclude that adequate modelling of pressure diffusion is of essential relevance for prediction of natural convection by models using second moment closure.

NOMENCLATURE

D	diffusion term in the k-equation
G	production term in the k-equation
Gr	Grashof number
g	gravitational acceleration
H	depth of the fluid layer
k	turbulent kinetic energy
N_i	Number of mesh cells
Nu	Nusselt-number
Pr	Prandtl-number
p	pressure
Ra	Rayleigh-number
T	temperature
T_{ref}	reference temperature (volume average in the entire channel)
ΔT_w	temperature difference between walls
t	time
u_i	components of velocity-vector
u_o	velocity used for normalization
$X_{1,2}$	horizontal extensions of the channel in terms of H
x_i	Cartesian co-ordinates
Δx_i	grid width
β	volumetric expansion coefficient
δ_{ij}	Kronecker delta
ε	dissipation of k
κ	molecular thermal diffusivity
ν	kinematic viscosity
ν_t	turbulent viscosity
ρ	fluid density
σ_k	coefficient in turbulence models
y'	fluctuating part of variable y
$\overline{y}$	mean value of variable y

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