Turbulence closure in the light of phase transition

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In the present study, new turbulence closure equations are derived in the light of continuous (often termed second-order) phase transition. Closed form Reynolds averaged Navier-Stokes equations due to those closure equations are solved numerically for a plane turbulent free jet. Here, turbulent viscosity is treated as a tensor, unlike eddy viscosity. An overall agreement of the obtained results with the existing literature for the jet flow proves the effectiveness of the new closure equations. Besides, turbulent stresses as a function of normalized mean velocity are found to exhibit their odd and even symmetries, which seem to be the manifestations of the free energy symmetry of continuous phase transition.

Keywords: phase transition, free energy, order parameter, symmetry, closure equation, viscosity tensor.

1. Introduction

Turbulent flow is characterized by a hierarchy of scales of fluctuations ranging from production to dissipation. The dynamics of turbulent flow is governed by the Navier-Stokes equations, whose solution resolving all those scales at high Reynolds number in complex geometries is unlikely to be attainable in the foreseeable future. However, Reynolds averaging and filtering are the two methods that have been used to transform the Navier-Stokes equations so that the small-scale turbulent fluctuations do not have to be directly simulated. Both methods introduce additional terms in the governing equations due to the correlations of fluctuating quantities (i.e., turbulent stresses) that need to be modeled in order to achieve closure. The closure assures a sufficient number of equations for all the unknowns. Turbulence modeling requires that turbulent stresses in the Reynolds averaged Navier-Stokes (RANS) equations be appropriately modeled. Boussinesq hypothesis is the core of all turbulence models that relates the Reynolds stresses to the mean velocity gradients as

\[-u'_i u'_j = \nu_T \left( \frac{\overline{\epsilon}}{c_j} \frac{\partial u}{\partial x_j} + \frac{\overline{\epsilon}}{c_i} \frac{\partial u}{\partial x_i} \right) \] (1)

for incompressible fluid which is analogous to the laminar one with enlarged viscosity called the eddy viscosity. This eddy viscosity requires further modeling as, for example, \( \nu_T = \ell_m^2 \left( \frac{\overline{\epsilon}}{c_j} \frac{\partial u}{\partial x_j} \right) \) after Prandtl, \( \nu_T = C_p \ell_m \sqrt{k} \) after Kolmogorov and Prandtl, \( \nu_T = C_p \ell_m^2 \) after Launder and Spalding, where \( \ell_m \) is the mixing length (closely related to the length scale).

Present endeavor aims at extracting turbulence closure equations by using the features of continuous (also called second-order) phase transition against the order parameter. The concept of order parameter in phase transition has been widely generalized as when an arbitrary system crosses an instability point, only a few variables become relevant and serves as an order parameter, which may be single or coupled variables that distinguishes the ordered from the disordered phase. However, the averaged velocity may be a suitable control parameter for a fluid dynamical system which if adequately tuned, the system can undergo strong qualitative changes in its macroscopic properties and consequently in microscopic properties. Goldenfeld showed that the rise of temperature in metals is similar to the increase in velocity in the fluid flows, the former causes magnetization at critical point and the latter turbulence. This invokes a strong analogy between turbulization and magnetization at critical point. Recently, many researchers have demonstrated both experimentally and numerically by resolving the time and length scales sufficiently close to the critical point that all turbulent flows are closely analogous to the continuous phase transition (CPT). In CPT, Landau-free energy of a system exhibits symmetry against the order parameter. This free energy of the system and the kinetic energy of turbulence are analogous because both near their critical points obey the power-law scaling of the correlation functions.

2. Closure equations due to phase transition

Navier-Stokes equations represent the collective motion of fluid particles. These equations of motion for incompressible fluid are

\[ \frac{\partial \overline{\epsilon}}{\partial t} + u_j \frac{\partial \overline{\epsilon}}{\partial x_j} = -\frac{\partial}{\partial x_j} \left( \frac{P}{\rho} \delta_{ij} + u_j \overline{\alpha} \right) + v \frac{\partial^2 \overline{\epsilon}}{\partial x_j^2}. \] (2)

In collective motion, the most naturally (but not necessarily) chosen order parameter is the predominant velocity. The concept of moving equilibrium states
that the rate of change of each component of Reynolds stress $\overline{u_iu'_j}$ is proportional to the rate of change of turbulence kinetic energy $k$, that is, $\overline{u_iu'_j}$ corresponds to the free energy of phase transition.

In view of relating the features of phase transition to the dynamics of turbulence, an implicit function $f(u_i, u'_j) = 0$ for RANS equation (2) is written as

$$f(u_i, u'_j) = \frac{d\overline{u_i}}{dt} + \frac{\partial}{\partial x_j} \left( \frac{\rho}{\nu^2} \delta_{ij} + \overline{u'_i u'_j} \right) - \nu \frac{\partial^2 \overline{u_i}}{\partial x_j^2}.$$ (3)

The differential form of the implicit function is

$$\left( \frac{\partial f}{\partial \overline{u_i}} \right) d\overline{u_i} + \left( \frac{\partial f}{\partial u'_j} \right) \overline{u'_j} = 0.$$ At the point of phase transition, the fluctuation correlations $\overline{u'_i u'_j}$ become maximum, that is, $d\overline{u'_i u'_j}$ become zero leading to $\partial f / \partial \overline{u_i} = 0$ because $d\overline{u_i}(x) = 0$ is unrealistic.

Equation $\partial f / \partial \overline{u_i} = 0$ is the first derivative of the free energy (RANS equation) with respect to the order parameter $\overline{u_i}$ that expresses the state of turbulence in terms of free energy equilibrium and thus combines the dynamics of turbulence with that of CPT as

$$\frac{\partial}{\partial \overline{u_i}} \frac{\partial}{\partial x_j} \left( \frac{\rho}{\nu^2} \delta_{ij} + \overline{u'_i u'_j} \right) = 0.$$ (4)

This equation can be written by using an entity $f_j(\overline{u_i}, \overline{u'_j}) / \partial x_j = 0$ due to the continuity equation as

$$\frac{\partial}{\partial \overline{u_i}} \frac{\partial}{\partial x_j} \left( \frac{\rho}{\nu^2} \delta_{ij} + \overline{u'_i u'_j} \right) = f_j(\overline{u_i}) \frac{\partial \overline{u_i}}{\partial x_j}$$ (5)

which, upon integration yields

$$\overline{u_i u'_j} = -\frac{\rho}{\nu^2} \delta_{ij} + \int f_j(\overline{u_i}) d\overline{u_i} d\overline{u'_j}.$$ (6)

Let the free energy of turbulence be defined as

$$F_{ij} = \overline{u_i u'_j} - b_n \overline{u_i u'_j} \overline{u/u_c}^{ij}$$ (7)

where the first term on the right-hand side is the energy that enters into the turbulence by the interaction of fluctuations and mean field shear, and the second term is the energy that leaves the turbulence due to the coupling between turbulent fluctuations and order parameter, and all these energies finally dissipate as heat. The indices $(i)$ and $(j)$ in the parentheses indicate that they are not summed over. Here $\overline{u}$ -velocity is the order parameter being the predominant one and normalized by centerline velocity $u_c$, and $b_n$ is a constant to accommodate the effect of normalization of the order parameter. Landau-free energy is a thermodynamic potential of a system despite being expressed as a function of the order parameter and its conjugate external field. Turbulence-free energy in Eq. (7) is a close analog to the thermodynamic potential form of Landau-free energy.

On replacing $\overline{u_i u'_j}$ by $\overline{u_i u'_j} - B_i(\overline{u}/u_c) \delta_{ij}$, Eq. (6) becomes

$$\overline{u_i u'_j} = \left( B_i u^{-3}/u_c - \frac{\rho}{\nu^2} \right) \delta_{ij} + \int f_j(\overline{u_i}) d\overline{u_i} d\overline{u'_j}$$ (8)

where $B_i$ is a constant tensor and $\overline{u_i u'_j}$ is replaced by $\overline{u^2}$ using order of magnitude reasoning. Equation (8) may be written further as

$$\overline{u_i u'_j} = C_{ij}(\overline{u}^3 + u_c^{-1} - \frac{\rho}{\nu^2}) \delta_{ij} + \int f_j(\overline{u_i}) d\overline{u_i} d\overline{u'_j}$$ (9)

where $C_{ij}$ are the scaling constants for a balance between the turbulent and the mean quantities of the equation, and the function $f_j(\overline{u_i})$ is ascertained later.

3. Application to a plane jet flow

The derived closure equations are applied to unclosed RANS equations for a plane jet as a test case.
Plane jets are free shear flows where fluids coming out from a two-dimensional (2D) orifice mix with the ambient fluid and develop through three successive distinct regions, namely initial, intermediate, and developed regions (Fig. 1). Initial region (at $x/h\leq5$) is characterized by the presence of a potential core of uniform axial velocity that is in laminar state, intermediate region by the transition state and developed region by the turbulent state. Literature shows a large scatter of the downstream distance at which the jet becomes fully developed, ranging from $5h$ to $25h$, depending on its initial conditions (e.g., Reynolds number at exit and nozzle geometry). This jet grows non-linearly in the developing (initial and intermediate) region and linearly in the developed (self-similar) region. The governing equations and their initial and boundary conditions, determination of the constants $C_{ij}$ and function $f_j(u_i)$, the closure equations in $(x,y,z)$ coordinates, and description of the plotting of turbulent stresses are presented in this section.

### 3.1 Governing equations

Continuity and RANS equations describing a steady plane turbulent jet flow for incompressible fluid are

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (10)$$

$$-\frac{\partial \bar{u}_j}{\partial x_j} = \frac{1}{\rho} \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \bar{u}_i}{\partial x_j} - \bar{u}_i \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (11)$$

where $-\bar{u}_j \frac{\partial \bar{u}_j}{\partial x_j} = \nu_{\tau_{ij}}/c_{ij} \left( \bar{u}_i/\bar{c} \right)$ is the turbulent stress and strain rate relation and $\nu_{\tau_{ij}}$ the turbulent viscosity tensor. Equations (9)-(11) are in closed form and need to be solved to extract mean and turbulence quantities of the flow.

### 3.2 Initial and boundary conditions

In free jet flow, the initial conditions are

$$\bar{u}(0,y\leq0.5h) = u_0, \quad \bar{u}(0,y>0.5h) = 0 \quad \text{and} \quad \bar{v}(0,y) = 0$$

where $h$ is the orifice height and $u_0$ the uniform jet exit velocity. The boundary conditions are: $\phi$ (general flow variable) attains ambient conditions at the jet outer edge, $\bar{\phi}/\bar{c} = 0$ at the outflow, and $\bar{\phi}/\bar{v} = 0$ at the symmetry axis except $\bar{v} = 0$ and $\bar{u}/\bar{v} = 0$.

### 3.3 Determination of $C_{ij}$

The concept of moving equilibrium may be read in explicit form as

$$\bar{u}_i \bar{u}_j = a_{ij}(\delta_{ij} \pm \epsilon_{ijk} \dot{k}) \quad (12)$$

where $a_{ij}$ are the proportionality constants. From Eqs. (9) and (12), one can write

$$\bar{u}_i \bar{u}_j = \left( B_i \bar{u}_i^3 / u_c - \frac{p}{\rho} \right) \delta_{ij} + \int f_j(u_i) \bar{u}_i \bar{u}_j \sim (\delta_{ij} \pm \epsilon_{ijk} \dot{k}). \quad (13)$$

This equation indicates that $C_{ij}$ of Eq. (9) and $a_{ij}$ of Eq. (12) are structurally similar, and hence $a_{ij} = C_{ij}$ for $C_{ij}$ is a constant. Using $\bar{u}/\bar{v} / \sqrt{\bar{u}} \approx 0.46 \times 0.35$ for turbulent flows and $\bar{u}/\bar{v} \approx 1.4 \bar{v}$ for plane jet flow in free jet flow, along with Eq. (12), the constants are evaluated to be $a_{ij} = 0.87$, $a_{ij} = 0.62$ and $a_{ij} = 0.35$. The values of $C_{ij}$ are calculated later by knowing the value of $C_{ij}$.

### 3.4 $f_j(u_i)$ and closure equations in $(x,y,z)$

The free energy of turbulence $\bar{u}_i \bar{u}_j$ may be expressed by a fourth degree polynomial of normalized velocity $\bar{u}/u_c$ with a view to capture the free energy symmetry of continuous phase transition. Analysis of turbulent shear stress data of plane and circular jets show that the coefficient of the fourth-order term is insignificant compared to other coefficients of that polynomial in the initial region of the jet while the same is more significant than or comparable to other coefficients in the intermediate and self-similar regions. Furthermore, the coefficients of the second-order term of the polynomials are found small, which is inconsistent with the order of magnitude estimate of $\bar{u}/\bar{v}$ by dimensional analysis. It seems now that $\bar{u}/\bar{v}$ is best expressed by a third degree polynomial of $\bar{u}/u_c$ in the initial region of the jet and by a fourth degree polynomial beyond the initial region. Such a polynomial may be assumed as

$$-\bar{u}/\bar{v}/u_c^2 = c_1 \left( U - U^2 + U^3 - U^4 \right)$$

for the turbulent shear stress. This shear stress is generally symmetric with respect to the origin (called odd symmetric) while the normal stresses are symmetric with respect to the axis (called even symmetric). Hence, turbulent normal stress function may be obtained by integrating the above polynomial as
\[ \overline{u'u^\prime} = C_n \left( U_1 - \frac{L}{2} U + \frac{L}{4} U^2 - \frac{L}{5} U^3 + \frac{L}{5} U^4 + \text{rest} \right) \]

which further can be approximated as
\[ u'u^\prime = C_n U \exp(-\alpha U) \] where \( U = \overline{u}/u_c \), and \( C_n, C_n, \) and \( \alpha \) are constants. This is because an odd symmetric function, either by differentiation once or by integration, becomes even symmetric and vice-versa.

The function \( f_s(\overline{u}) \) for the Reynolds stresses is obtained from Eq. (5), discarding the pressure term by using their functional form for the normal stress and by using the highest order term of the polynomial for the shear stress. The derived function \( f_s(\overline{u}) \) for the axial normal stress \( \overline{u'u^\prime} \) is
\[ f_s(\overline{u}) = C_n \alpha u_c, \beta (-2 + \beta u) \exp(-\beta U) \] (14a)
where \( \beta = \alpha u_c, \) for the transverse normal stress \( v^\prime v^\prime \) is
\[ f_s(\overline{u}) = C_n (\alpha \overline{u}/u_c) (2 \beta u^\prime) \exp(-\beta U) \] (14b)
and for the shear stress \( u^\prime v^\prime \) is
\[ f_s(\overline{u}) = C_n (\beta \overline{u}/u_c) \exp(-\beta U) \] (14c)
That is \( f_s(\overline{u}) = C_n \overline{u}/u_c \) for the initial region of the jet and \( f_s(\overline{u}) = C_n \overline{u}/u_c^2 \) beyond the initial region. The highest order term is used instead of the entire polynomial for the shear stress as this requires known values of the coefficients that might cause ascertaining \( f_s(\overline{u}) \) unlikely. Further, the function \( f_s(\overline{u}) \) is the second derivative of the highest order term of the polynomial, as a result, retains the same characteristics of \( f_s(\overline{u}) \) if derived by using the entire polynomial. Above reasons justify the use of the highest order term instead of the entire polynomial to determine \( f_s(\overline{u}) \).

Using the functions \( f_s(\overline{u}), f_s(v^\prime v^\prime) \) and \( f_s(u^\prime v^\prime) \), closure equation (9) in \((x,y,z)\) coordinates becomes

\[ \overline{u'u^\prime} = C_{11} \left( B_1 \overline{u}/u_c - \frac{\overline{u}}{\rho} + \int f_s(\overline{u}) d\overline{u}d\overline{u} \right) \] (15a)
\[ \overline{v'v'} = C_{22} \left( B_2 \overline{u}/u_c - \frac{\overline{u}}{\rho} + \int f_s(\overline{u}) d\overline{u}d\overline{u} \right) \] (15b)
\[ \overline{u'v'} = C_{12} \int f_s(\overline{u}) d\overline{u}d\overline{v} \] (15c)

### 3.5 Plotting of Reynolds stresses

Equation (15a) is in the velocity domain and, by simplifying, may be reduced to
\[ \overline{u'u^\prime} = \int f_s(\overline{u}) d\overline{u}d\overline{u} \] (16)
which may also be written in the space domain as
\[ \overline{u'u^\prime} = \int f_s(\overline{u}) \left( \frac{\partial \overline{u}}{\partial y} \right)^2 dydy \] (17)
It can be shown that \( \overline{u'u^\prime} = \beta \overline{u'u^\prime} \) for \( \beta \) is a constant greater than unity. The graphs of \( \overline{u'u^\prime} \) and \( \overline{u'u^\prime} \) against \( y \)-axis are not equal in area because of the difference in integration limits across the stream between the outer edge and centerline of the jet. In the former case, the limits cover the entire velocity domain and in the latter case, they cover half of the space domain. Now, \( \int \overline{u'u^\prime} dy' = \int \overline{u'u^\prime} dy \) where \( y' = \lambda y \) for \( \lambda \) is a constant, and this relation leads to \( \beta = \lambda \).
Hence, Reynolds stresses due to Eqs. (15) must be plotted as \( \beta \overline{u'u^\prime} \) against \( \lambda y \).

### 4. Numerical strategies

A CFD (Computational Fluid Dynamics) code is developed for solving 2D steady flow based on finite volume method and rectangular structured grid\(^{22}\). SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm of Patankar and Spalding\(^{23}\) is employed to solve the equations (9)-(11) governing the plane turbulent free jet. Discretization of the governing equations, computational grids, and grid convergence test are described in this section.

#### 4.1 Discretization and computational grids

The convective and diffusive terms of the transport equations for \( \phi \) are discretized using the second-order upwind difference scheme and the second-order central difference scheme in the staggered grid, respectively, with cell centers for \( \overline{u} \) at \((i, j)\), for \( \overline{v} \) at \((i, j)\), for \( \overline{p} \), \( \overline{u'u^\prime} \) and \( \overline{v'v'} \) at \((i, j)\), and for \( \overline{u'v'} \) at \((i, j)\). The discretized equations are solved iteratively using the line-by-line tridiagonal matrix algorithm\(^{24}\) (TDMA). The momentum and pressure correction equations are provided with a suitable number of sweeps. All variables \((\overline{u, v, p})\) are weighted with very low under-relaxation factors (order of 0-1) for the stability of the numerical scheme. The flow variables are further expressed by a weighted average of their neighbors in
each iteration after obtaining them using TDMA. This procedure ensures the stability of the numerical scheme by reducing the oscillations of strain rates in turbulent viscosity calculation from the stress and strain rate relation.

![Fig. 2 Computational grids for a plane turbulent jet.](image)

The flow domain is constructed over $40h \times 20h$ in $x,y$-directions with grids as in Fig. 2. Grids are uniform inside the orifice and varying outside it in $y$-direction, and uniform in $x$-direction as in the figure. The solutions are duly converged with the normalized residuals of $1.2 \times 10^{-4}$, $6.0 \times 10^{-6}$ and $6.4 \times 10^{-5}$ for $u$, $v$ and mass, respectively.

![Fig. 3 Axial mean velocity profiles at $x/h=5$.](image)

4.2 Grid convergence test

The present simulation is performed for a plane turbulent free jet with Reynolds number $Re=3.2 \times 10^4$, orifice height $h=0.04m$, and velocity at exit $u_e=12$ m/s. A grid convergence test is carried out with the three grid sizes termed coarse, medium and fine which are $170 \times 146$, $232 \times 166$ and $282 \times 184$ in $x,y$-directions having a grid refinement factor of 1.45 between the coarse and fine grids. Figure 3 depicts the mean axial velocity profiles at $x/h=5$ for the three grid sets. Grid refinement shows successful convergence for those three grid resolutions. The results presented here are obtained by using the fine mesh.

5. Results and discussion

Closed form RANS equations (9)-(11), governing the turbulent flow, are solved numerically for a plane jet. The used numerical scheme is found to produce stable solutions for $B_1=2.4$ and $B_2=1.8$, and for $C_{f1}=0.048$, $C_{f2}=0.034$ and $C_{f3}=0.019$ that are obtained by using the relation $C_{fij}=a_{ij}/C_o$ for a minimum value of $C_o=18.2$. Values of other constants appearing in the functions $f_1(u)$ for turbulent shear and normal stresses from the stable numerical scheme are $C_1=320$, $C_2=5.8$ and $C_3=3$ in the initial region of the jet and $C_4=240$, $C_5=7.4$ and $C_6=2$ beyond the initial region. This section presents axial velocity, transverse velocity, and turbulent stresses that are extracted in the present simulation and their comparison with the existing theoretical, experimental (Exp), and numerical data on planar turbulent jets. Klein et al. performed direct numerical simulation (DNS) of a turbulent plane jet with $Re=4 \times 10^5$ and compared their results (e.g., mean velocity and Reynolds stresses) with the results of several authors and found them in good agreement. Hesch et al. made RANS simulation of a plane jet with $Re=3 \times 10^5$ using the standard $k-\varepsilon$ turbulence model and compared their results with the existing data. Ramaprian and Chandrasekhar with $Re=1.6 \times 10^5$ have experimentally investigated the plane jets and presented the profiles of mean velocity and turbulent stresses.

![Fig. 4 Axial mean velocity profiles.](image)
Mean axial velocity $\bar{u}/u_c$ is presented in Fig. 4 against the transverse distance $y/h$ at axial locations $x/h=2, 5, 8$ and $12$. This figure illustrates that the jet grows with the axial distance due to the entrainment of ambient fluid, and its maximum velocity decreases due to the loss of momentum caused by the interaction with the ambient fluid. Figure 5 presents normalized mean velocity $\bar{u}/u_c$ against $y/y_{1/2}$ at axial location $x/h=12$ along with Gaussian curve $18$ of the form $\bar{u}/u_c = \exp(-0.693\eta^2)$ and DNS results$19$ where $\eta=y/y_{1/2}$, and $y_{1/2}$ is the jet’s half-width. The figure shows that results from the present simulation and DNS compare well with the Gaussian curve. Transverse velocity $\bar{v}/u_c$ is depicted in Fig. 6 against $y/y_{1/2}$ at axial locations $x/h=8$ and $12$, and found to have achieved free-stream value at some larger distance $y/y_{1/2}>3.5$ (not shown). DNS$19$ and experimental$25$ data for $\bar{v}$-velocity provided in the figure are in satisfactory agreement with the present simulation.

Reynolds normal stresses $\bar{u}'u_c^2$ and $\bar{v}'v_c^2$, and shear stress $\bar{u}'v_c$ are calculated from Eq. (15) and plotted in Figs. 7-9 against $y/y_{1/2}$ at $x/h=8$ and $12$ for $\lambda=1.5$ (a constant appeared in Sec. 3.5). Calculated stresses from DNS$19$, RANS simulation$20$ and measurements$25$ are added to compare in those figures. All turbulent stresses, $\bar{u}'u_c$, $\bar{v}'v_c$ and $\bar{u}'v_c$ from the present simulation, are observed in close agreement with the stresses from measurement and simulations.

### 6. Conclusions

The new closure equations derived by considering turbulence as CPT are utilized here to get the closed form RANS equations. The numerical solution of those equations for a plane jet flow provides the mean axial and transverse velocities, and turbulent stresses. Extracted results from the simulation are found to be in overall agreement with the existing data, showing the effectiveness of the closure equations. Turbulent stresses of the jet as functions of normalized mean axial velocity confirm their odd and even symmetries, and
owning of the additional term like the one in Landau-free energy expansion, and thus demonstrate the phenomenological relations with phase transition and restate that laminar-turbulent transition undergoes a continuous phase transition.

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Comments: a) Revision of implicit function and turbulence-free energy in Sec. 2 cause minor changes in the results. b) Revision of Eq. (14c) in Sec. 3.4 does not affect the results. c) Revision in Sec. 3.5 provides more clarity.