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Remarks on Turbulent Constitutive Relations

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Remarks on Turbulent Constitutive Relations

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The paper demonstrates that the concept of turbulent constitutive relations introduced by Lumley (1970) can be used to construct general models for various turbulent correlations. Some of Generalized Cayley-Hamilton formulas for relating tensor products of higher extension to tensor products of lower extension are introduced. The combination of dimensional analysis and invariant theory can lead to "turbulent constitutive relations" (or general turbulence models) for, in principle, any turbulent correlations. As examples, the constitutive relations for Reynolds stresses and scalar fluxes are derived. The results are consistent with ones from RNG theory and two-scale DIA method, but with a more general form.

I. Introduction

Lumley[1] discussed some possible constitutive relations for turbulent correlations. One of his conclusions was that turbulent constitutive relations may exist under situations in which the length and time scales of turbulence are smaller than those in the mean flow field so that the effect of initial and boundary conditions on the turbulence is not significant. For example, if an unbounded mean flow evolves slowly in both time and space, there may exist a constitutive relation for turbulent correlations (e.g., Reynolds stresses) which may help to solve the turbulence closure problem in this particular situation. However, in most practical situations, the scales of turbulence are of the same order of magnitude as those of the mean flow field, hence so called turbulent constitutive relations do not exist, and the turbulence closure problem cannot be theoretically solved. The formally derived "turbulent constitutive relations" become at most approximations (turbulence models) to the turbulent correlations whose validity varies from flow to flow. Regardless of the existence of turbulent constitutive relations, the formal procedure of deriving constitutive relations developed in continuum mechanics provides an useful tool for developing general turbulence models.

A constitutive relation developed in continuum mechanics is always of an equilibrium and local form, that is, it is a function of arguments at the present time and the local point. This is, of course, not true for most turbulent flows. For a general turbulent flow, a constitutive relation should contain the time history and spatial information for the arguments in question. However, as a model approximation, we always neglect time and spatial effects and consider the relationship at the present time and the local point as the first order approximation in the time and spatial expansions of the functional form.

The procedure for deriving a constitutive relation usually includes two steps. The first step is to make an assumption about the general relationship between the turbulent correlation and other "known" quantities (which are the arguments of the function) using the information from whatever observations or experience we have. At this stage, dimensional analysis (π theorem) can be used to regroup and reduce the number of independent arguments in question. The second step is to determine the detailed form of the relationship using invariant theory.

In the application of invariant theory, the most important procedure is to determine the number of independent invariants. This determination will become more complicated if the arguments in question have more than two tensors. The number of independent invariants depends on the number of independent tensors which it is possible to form using the arguments in question. In this paper, we shall show a procedure for determining the independent tensors which can be formed by two general tensors using generalized Cayley-Hamilton formulas. Thereafter, as an example, we shall briefly derive a constitutive relation for the turbulent Reynolds stresses. A possible constitutive relation for the scalar flux is also given. This approach can be extended to more complicated turbulent correlations, for example, the high order turbulent correlations appearing in the transport equations of the second order moments.

II. Generalized Cayley-Hamilton formulas

Rivlin[2] showed that there are several generalized Cayley-Hamilton formulas relating matrices (product of several matrices A, B, C ...) of higher extension to matrices of lower extension. Here, we follow Rivlin to derive some relations of this type which will be used latter.

One of Rivlin's basic relations is

$$(ABC + ACB + BCA + BAC + CAB + CBA) - A(trBC - trB\ trC)$$
$$- B(trCA - trC\ trA) - C(trAB - trA\ trB)$$
$$- (BC + CB)trA - (CA + AC)trB - (AB + BA)trC \qquad (1)$$
$$- I(trA\ trB\ trC - trA\ trBC - trB\ trCA$$
$$- trC\ trAB + trABC + trCBA) = 0$$

where I is the unit matrix or identity tensor and tr represents the trace operator.

Replacing C with A in Eq.(1), we obtain

$$ABA = -A^2B - BA^2 + A(trAB - trA\ trB)$$
$$+ \frac{1}{2}B(trA^2 - trA\ trA) + (AB + BA)trA + A^2trB \qquad (2)$$
$$+ I[trA^2B - trA\ trAB + \frac{1}{2}trB(trA\ trA - trA^2)]$$

Replacing C with B in Eq.(1), we obtain

$$BAB = -B^2A - AB^2 + B(trBA - trB\ trA)$$
$$+ \frac{1}{2}A(trB^2 - trB\ trB) + (BA + AB)trB + B^2trA \qquad (3)$$
$$+ I[trB^2A - trB\ trBA + \frac{1}{2}trA(trB\ trB - trB^2)]$$

Eqs.(2) and (3) indicate that the matrices ABA and BAB of extension 3 can be expressed by polynomials of matrices of extension 2 or less.

Multiplying Eq.(2) by A both on the left and on the right, and then adding the results, we obtain

$$ABA^2 + A^2BA = ABA\ trA + A^2\ trAB + A(trA^2B - trA\ trAB)$$
$$- B\ detA + I\ detA\ trB \qquad (4)$$

where det is the determinant operator. Multiplying Eq.(3) by B on the left and on the right, and then adding the results, we obtain

$$BAB^2 + B^2AB = BAB\ trB + B^2\ trBA + B(trB^2A - trB\ trBA)$$
$$- A\ detB + I\ detB\ trA \qquad (5)$$

It follows from Eqs.(2) and (3) that the right hand side of Eqs.(4) and (5) is a polynomial of matrices of extension 2 or less.

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Replacing B with B^2 in Eq.(4), we obtain

$$AB^2A^2 + A^2B^2A = AB^2A \ trA \ + \ A^2 \ trAB^2 + A(trA^2B^2 \ - \ trA \ trAB^2)$$
$$- B^2 \ detA \ + \ I \ detA \ trB^2 \tag{6}$$

Replacing A with A^2 in Eq.(5), we obtain

$$BA^2B^2 + B^2A^2B = BA^2B \ trB \ + \ B^2 \ trBA^2 + B(trB^2A^2 \ - \ trB \ trBA^2)$$
$$- A^2 \ detB \ + \ I \ detB \ trA^2 \tag{7}$$

Replacing B with B^2 in Eq.(2), we obtain

$$AB^2A = -A^2B^2 \ - \ B^2A^2 \ + \ A(trAB^2 \ - \ trA \ trB^2)$$
$$+ \frac{1}{2} \ B^2(trA^2 \ - \ trA \ trA) \ + \ (AB^2 + B^2A)trA \ + \ A^2trB^2 \tag{8}$$
$$+ I[trA^2B^2 \ - \ trA \ trAB^2 + \frac{1}{2}trB^2(trA \ trA - \ trA^2)]$$

Replacing A with A^2 in Eq.(3), we obtain

$$BA^2B = -B^2A^2 \ - \ A^2B^2 \ + \ B(trBA^2 \ - \ trB \ trA^2)$$
$$+ \frac{1}{2} \ A^2(trB^2 \ - \ trB \ trB) \ + \ (BA^2 + A^2B)trB \ + \ B^2trA^2 \tag{9}$$
$$+ I[trB^2A^2 \ - \ trB \ trBA^2 + \frac{1}{2}trA^2(trB \ trB - \ trB^2)]$$

Eqs.(8) and (9) indicate that the matrices AB^2A and BA^2B of extension 3 can be expressed by polynomials of matrices of extension 2 or less. As a result, the right hand sides of Eqs.(6) and (7) are also polynomials of matrices of extension 2 or less.

III. Number of independent tensors formed by two general tensors

Now let us show that the number of independent tensors formed by two general tensors A and B is 18.

Rivlin[2] showed that any matrix product in two 3×3 matrices may be expressed as a polynomial of these matrices of extension 4 or less. For example, suppose we have a matrix product Π of extension 5:

$$\Pi = ABA^2B^2A \tag{10}$$

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This can be written as

$$\Pi = ACA \tag{11}$$

where $C = BA^2B^2$. From Eq.(2), Π may be viewed as a polynomial of matrices in A and C of extension 2 or less. Note that C itself is a matrix in A and B of extension 3, therefore, Π may be expressed by a polynomial in A, B of extension 4 or less. Therefore, we only need to consider the possible matrices (or tensors) of extension 4 or less formed by A and B.

We now show that there are only two independent tensors of extension 4. The possible tensors of extension 4 are the following 8 tensors:

$$ABA^2B^2, \ BAB^2A^2, \ A^2BAB^2, \ B^2ABA^2,$$
$$AB^2A^2B, \ BA^2B^2A, \ A^2B^2AB, \ B^2A^2BA. \tag{12}$$

With Eqs.(4) and (2), A^2BAB^2 can be expressed by ABA^2B^2 plus a polynomial in A and B of extension 3 or less. Similarly, with Eqs.(5) and (3), $B^2ABA^2 = -BAB^2A^2 +$ polynomial in A and B of extension 3 or less, with Eqs.(7) and (9), $AB^2A^2B = -ABA^2B^2 +$ polynomial in A and B of extension 3 or less, with Eqs.(6) and (8), $BA^2B^2A = -BAB^2A^2 +$ polynomial in A and B of extension 3 or less. From Eqs.(4) and (5), we may show that $A^2B^2AB = ABA^2B^2 +$ polynomial in A and B of extension 3 or less, and that $B^2A^2BA = BAB^2A^2 +$ polynomial in A and B of extension 3 or less. Therefore, only two tensors of extension 4 in Eq.(12) are independent, we select them as

$$ABA^2B^2, \quad BAB^2A^2 \tag{13}$$

Now we show that there are only four independent tensors of extension 3. The possible tensors of extension 3 are the following 8 tensors:

$$ABA^2, A^2BA, BAB^2, B^2AB, AB^2A^2, A^2B^2A, BA^2B^2, B^2A^2B \tag{14}$$

Using Eqs.(4), (5), (6) and (7), we find that only four of them in Eq.(14) are independent. Let us select them as

$$ABA^2, BAB^2, AB^2A^2, BA^2B^2 \tag{15}$$

There are eight possible tensors of extension 2 which are all independent:

$$AB, \ BA, \ AB^2, \ B^2A,$$
$$A^2B, \ BA^2, \ A^2B^2, \ B^2A^2. \tag{16}$$

There are four possible tensors of extension 1 which are also independent:

$$A, \ A^2, \ B, \ B^2. \tag{17}$$

Therefore, we have proved that only 18 tensors can be formed independently by two general tensors.

IV. Constitutive relation for Reynolds stresses $\overline{u_i u_j}$

We assume

$$\overline{u_i u_j} = F_{ij}(U_{i,j}, \ k, \ \varepsilon)$$

which indicates that the turbulent stresses depend on the mean velocity gradient $U_{i,j}$ and the scales of turbulence characterized by the turbulent kinetic energy k and its dissipation rate ε. Applying the π theorem, the arguments can be regrouped as

$$A_{ij} = \frac{k}{\varepsilon} U_{i,j}$$

Accordingly, we may write

$$\frac{\overline{u_i u_j}}{2k} = F_{ij}(A_{ij})$$

Noting that A_{ij} is a general tensor, if we define its transpose as

$$B_{ij} = A_{ij}^T = \frac{k}{\varepsilon} U_{j,i} \tag{18}$$

then, $B \neq A$. In order to obtain a general relationship, we first look for a general tensorial form of $F_{ij}(A_{ij}, B_{ij})$, then replace B_{ij} by A_{ij}^T. We have proven that the independent tensors formed by A and B are the following 18 tensors:

$$
\begin{aligned}
&A, A^2, B, B^2, \\
&AB, BA, AB^2, A^2B, BA^2, B^2A, A^2B^2, B^2A^2, \\
&ABA^2, BAB^2, AB^2A^2, BA^2B^2, \\
&ABA^2B^2, BAB^2A^2.
\end{aligned} \tag{19}
$$

Following Lumley[3] and applying invariant theory, we may obtain

$$
\begin{aligned}
\frac{\overline{u_i u_j}}{2k} = {} & a_1 \delta_{ij} + a_2 A + a_3 B + a_4 A^2 + a_5 B^2 \\
& + a_6 AB + a_7 BA + a_8 AB^2 + a_9 A^2 B \\
& + a_{10} BA^2 + a_{11} B^2 A + a_{12} A^2 B^2 + a_{13} B^2 A^2 \\
& + a_{14} ABA^2 + a_{15} BAB^2 + a_{16} AB^2 A^2 + a_{17} BA^2 B^2 \\
& + a_{18} ABA^2 B^2 + a_{19} BAB^2 A^2
\end{aligned} \tag{20}
$$

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where $a_1 - a_{19}$ are scalar functions of the invariants of the tensors in question.

Using the conditions: $\overline{u_i u_j} = \overline{u_j u_i}$, $\overline{u_i u_i} = 2k$ and $B_{ij} = A_{ij}^T = A_{ji}$, we obtain

$$a_2 = a_3, \quad a_4 = a_5, \quad a_8 = a_9, \quad a_{10} = a_{11},$$
$$a_{14} = a_{15} = a_{16} = a_{17} = a_{18} = a_{19} = 0 \tag{21}$$

and

$$a_1 = \frac{1}{3}\big[1 - 2a_2 A_{ii} - 2a_4 A_{ij} B_{ij} - (a_6 + a_7)A_{ij}B_{ji}$$
$$- 2(a_8 + a_{10})A_{ij}B_{ji}^2 - (a_{12} + a_{13})A_{ij}^2 B_{ji}^2\big] \tag{22}$$

Therefore, we obtain

$$\overline{u_i u_j} = \frac{2}{3}k\delta_{ij} + 2a_2\frac{K^2}{\varepsilon}(U_{i,j} + U_{j,i} - \frac{2}{3}U_{i,i}\delta_{i,j})$$
$$+ 2a_4\frac{K^3}{\varepsilon^2}(U_{i,k}U_{k,j} + U_{j,k}U_{k,i} - \frac{2}{3}\mathrm{II}\delta_{ij})$$
$$+ 2a_6\frac{K^3}{\varepsilon^2}(U_{i,k}U_{j,k} - \frac{1}{3}\tilde{\mathrm{II}}\delta_{ij})$$
$$+ 2a_7\frac{K^3}{\varepsilon^2}(U_{k,i}U_{k,j} - \frac{1}{3}\tilde{\mathrm{II}}\delta_{ij})$$
$$+ 2a_8\frac{K^4}{\varepsilon^3}(U_{i,k}U_{j,k}^2 + U_{i,k}^2 U_{j,k} - \frac{2}{3}\tilde{\bar{\mathrm{II}}}\delta_{ij}) \tag{23}$$
$$+ 2a_{10}\frac{K^4}{\varepsilon^3}(U_{k,i}U_{k,j}^2 + U_{k,j}U_{k,i}^2 - \frac{2}{3}\tilde{\bar{\mathrm{II}}}\delta_{ij})$$
$$+ 2a_{12}\frac{K^4}{\varepsilon^3}(U_{i,k}^2 U_{j,k}^2 - \frac{1}{3}\bar{\bar{\mathrm{II}}}\delta_{ij})$$
$$+ 2a_{13}\frac{K^4}{\varepsilon^3}(U_{k,i}^2 U_{k,j}^2 - \frac{1}{3}\bar{\bar{\mathrm{II}}}\delta_{ij})$$

where

$$\mathrm{II} = U_{i,j}U_{j,i}, \qquad \tilde{\mathrm{II}} = U_{i,j}U_{i,j}, \qquad \tilde{\bar{\mathrm{II}}} = U_{i,j}U_{i,j}^2, \qquad \bar{\bar{\mathrm{II}}} = U_{i,j}^2 U_{i,j}^2 \tag{24}$$

It is noticed that the first two terms on the right hand side of Eq.(23) represent the standard k-ε eddy viscosity model, and that the first five terms of Eq.(23) are of the same form as the models derived from both the two-scale DIA approach (Yoshizawa[4]) and the RNG method (Rubinstein and Barton[5]).

Eq.(23) is a general model for $\overline{u_i u_j}$. It contains 8 undetermined coefficients which are, in general, scalar functions of various invariants of the tensors in question, for example, $S_{ij}S_{ij}$ and $\Omega_{ij}\Omega_{ij}$ which are $(\tilde{\mathrm{II}} + \mathrm{II})/2$ and $(\tilde{\mathrm{II}} - \mathrm{II})/2$ respectively. The detailed forms of these

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scalar functions must be determined by other model constraints, for example, realizability, and by experimental data. Eq.(23) contains 9 terms; however, its quadratic tensorial form may be sufficient for practical applications, expecially when $|U_{i,j}|k/\varepsilon$ is less than one.

V. Constitutive relation for Scalar Flux $\overline{\theta u_i}$

We assume

$$\overline{\theta u_i} = F_i(U_{i,j}, T_{,i}, k, \varepsilon, \overline{\theta^2}, \varepsilon_\theta) \tag{25}$$

where $\overline{\theta^2}$ is the variance of a fluctuating scalar and ε_θ is its dissipation rate. Eq.(25) indicates that the scalar flux depends on not only the mean scalar gradient $T_{,i}$, but also the mean velocity gradient $U_{i,j}$ and the scales of both velocity and scalar fluctuations characterized by k, ε, θ^2, ε_θ.

Applying the π theorem, we have:

$$A_{ij} = \frac{k}{\varepsilon}U_{i,j}, \qquad \Theta_{,i} = \frac{k}{(\varepsilon\varepsilon_\theta)^{1/2}}T_{,i}, \qquad r = \frac{k}{\varepsilon}\bigg/\frac{\overline{\theta^2}}{\varepsilon_\theta}$$

Accordingly, we may write

$$\frac{\overline{\theta u_i}}{(\overline{\theta^2}k)^{1/2}} = F_i(A_{ij}, \Theta_{,i}, r) \tag{26}$$

Using arguments similar to the ones made above for Reynolds stresses, we obtain

$$
\begin{aligned}
\overline{\theta u_i} ={}& a_1 k\Big(\frac{k}{\varepsilon}\frac{\overline{\theta^2}}{\varepsilon_\theta}\Big)^{1/2}T_{,i} + \frac{k^2}{\varepsilon}\Big(\frac{k}{\varepsilon}\frac{\overline{\theta^2}}{\varepsilon_\theta}\Big)^{1/2}(a_2 U_{i,j} + a_3 U_{j,i})T_{,j} \\
&+ \frac{k^3}{\varepsilon^2}\Big(\frac{k}{\varepsilon}\frac{\overline{\theta^2}}{\varepsilon_\theta}\Big)^{1/2}(a_4 U_{i,k}U_{k,j} + a_5 U_{j,k}U_{k,i} + a_6 U_{i,k}U_{j,k} + a_7 U_{k,i}U_{k,j})\,T_{,j} \\
&+ \frac{k^4}{\varepsilon^3}\Big(\frac{k}{\varepsilon}\frac{\overline{\theta^2}}{\varepsilon_\theta}\Big)^{1/2}(a_8 U_{i,k}U_{j,k}^2 + a_9 U_{i,k}^2 U_{j,k} + a_{10}U_{k,i}U_{k,j}^2 + a_{11}U_{k,i}^2 U_{k,j})\,T_{,j} \\
&+ \frac{k^5}{\varepsilon^4}\Big(\frac{k}{\varepsilon}\frac{\overline{\theta^2}}{\varepsilon_\theta}\Big)^{1/2}(a_{12}U_{i,k}^2 U_{j,k}^2 + a_{13}U_{k,i}^2 U_{k,j}^2 \\
&\qquad\qquad + a_{14}U_{i,k}U_{\ell,k}U_{\ell,j}^2 + a_{15}U_{k,i}U_{k,\ell}U_{j,\ell}^2)\,T_{,j} \\
&+ \frac{k^6}{\varepsilon^5}\Big(\frac{k}{\varepsilon}\frac{\overline{\theta^2}}{\varepsilon_\theta}\Big)^{1/2}(a_{16}U_{i,k}U_{\ell,k}^2 U_{\ell,j}^2 + a_{17}U_{k,i}U_{k,\ell}^2 U_{j,\ell}^2 \\
&\qquad\qquad + a_{18}U_{i,k}U_{\ell,k}U_{\ell,m}^2 U_{j,m}^2 + a_{19}U_{k,i}U_{k,\ell}U_{m,\ell}^2 U_{m,j}^2)\,T_{,j}
\end{aligned}
\tag{27}
$$

The coefficients $a_1 - a_{19}$ are, in general, functions of the time scale ratio r and the other invariants of tensors in question.

If we assume the time scale ratio $r \approx$ constant, for example, $\overline{\theta^2}/\varepsilon_\theta \approx k/\varepsilon$, then Eq.(27) becomes

$$
\begin{aligned}
\overline{\theta u_i} = {} & a_1 \frac{k^2}{\varepsilon} T_{,i} + \frac{k^3}{\varepsilon^2}(a_2 U_{i,j} + a_3 U_{j,i}) T_{,j} \\
& + \frac{k^4}{\varepsilon^3}(a_4 U_{i,k} U_{k,j} + a_5 U_{j,k} U_{k,i} + a_6 U_{i,k} U_{j,k} + a_7 U_{k,i} U_{k,j}) \, T_{,j} \\
& + \frac{k^5}{\varepsilon^4}(a_8 U_{i,k} U_{j,k}^2 + a_9 U_{i,k}^2 U_{j,k} + a_{10} U_{k,i} U_{k,j}^2 + a_{11} U_{k,i}^2 U_{k,j}) \, T_{,j} \\
& + \frac{k^6}{\varepsilon^5}(a_{12} U_{i,k}^2 U_{j,k}^2 + a_{13} U_{k,i}^2 U_{k,j}^2 \\
& \qquad + a_{14} U_{i,k} U_{\ell,k} U_{\ell,j}^2 + a_{15} U_{k,i} U_{k,\ell} U_{j,\ell}^2) \, T_{,j} \\
& + \frac{k^7}{\varepsilon^6}(a_{16} U_{i,k} U_{\ell,k}^2 U_{\ell,j}^2 + a_{17} U_{k,i} U_{k,\ell}^2 U_{j,\ell}^2 \\
& \qquad + a_{18} U_{i,k} U_{\ell,k} U_{\ell,m}^2 U_{j,m}^2 + a_{19} U_{k,i} U_{k,\ell} U_{m,\ell}^2 U_{m,j}^2) \, T_{,j}
\end{aligned}
\tag{28}
$$

It is interesting to note that the conventional eddy viscosity model for the scalar flux is just the first term on the right hand side of Eq.(27) or (28), and that the models derived from two-scale DIA (Yoshizawa[6]) and RNG method (Rubinstein and Barton[7]) are the first two terms of Eq.(28).

VI. Conclusion

We have demonstrated that the combination of dimensional analysis and invariant theory is a powerful tool for developing "turbulent constitutive relations" (or general turbulence models) for various turbulence correlations. The way of forming generalized Cayley-Hamilton formulas for determining independent tensors is also shown. As examples, the general turbulence models for Reynolds stresses and scalar fluxes are derived. The results from RNG theory and the two-scale DIA method are the first few terms of the constitutive relations derived in this paper. This technique can be extended to other turbulence correlations including higher order correlations appearing in second order closures.

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