Appendix: Final form of the algebraic mass flux model

The pertinent facts concerning the computational implementation of the mass flux representation are presented here. The general form of the model, valid for a three-dimensional flow in an inertial system without body forces, is

$$< v_i >= \tau [\nu_0 \delta_{ij} + \nu_1 \tau V_{i,j} + \nu_2 \tau^2 V_{i,k} V_{k,j}] \{v_j v_p\} < \rho >_{,p} < \rho >^{-1}$$

where the viscosity coefficients are functions of the invariants of, $\mathbf{A} = \mathbf{1} + \tau \nabla \mathbf{V}$, and are given by $\nu_0 = (1 - I_A + II_A)/III_A$, $\nu_1 = (2 - I_A)/III_A$, and $\nu_2 = 1/III_A$. The invariants for the tensor are given by

$$
\begin{aligned}
I_A &= \ < A > \\
II_A &= \ 1/2(< A >^2 - < A^2 >) \\
III_A &= \ 1/6(< A >^3 -3 < A >< A^2 > +2 < A^3 >)
\end{aligned}
$$

for which $<>$ indicates the trace of the enclosed matrix. The time scale is defined as $\tau = (M_t k/\varepsilon)/(1 + M_t(\mathcal{P}/\varepsilon - 1))$ The various traces are straightforward to compute using their definition. Their significance can be understood when they are recast in terms of the mean dilatation, rotation and strain:

$$
\begin{aligned}
< A > &= \ 3 + \tau D \\
< A^2 > &= \ 3 + 2\tau D + \tau^2[< S^2 > + < W^2 >] \\
< A^3 > &= \ 3 + 3\tau D + 3\tau^2[< S^2 > + < W^2 >] + \tau^3[< S^3 > +2 < SW^2 > + < W^3 >]
\end{aligned}
$$

$D = S_{jj}$ is the mean dilatation and the strain and rotation tensors are defined: $S_{ij} = 1/2[V_{i,j} + V_{j,i}]$ and $W_{ij} = 1/2[V_{i,j} - V_{j,i}]$. The term τD can be thought of as a ratio of fluctuating to mean dilatation time scales. It is understood to be order one or smaller, $\tau D < 1$.

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turbulence fields in which the production terms play a major role. For flows in which the pressure dilatation covariance plays a major role in transferring energy from its kinetic to potential modes it may be necessary to reevaluate the adequacy of the linear relaxation model.

The form of the mass flux model presented does not include effects associated with rotation or body forces. Both of these effects can be easily incorporated as they do not require any additional modeling; it is simply a matter of retaining the extra terms in the algebraic truncation of the evolution equations. There is an exception; at rapid rotation rates the neglected pressure covariance becomes important and the truncation of the evolution equation used to obtain the model is no longer valid.

The model is realizable for most simple flows though a general proof of its realizability has not been found. These realizability aspects, and the fact that the destabilizing properties associated with isotropic eddy-viscosity models do not appear in this mass flux model, are expected to make it computationally robust.

In the moment evolution equations for a compressible turbulence the mass fluxes appear in several places. In the mean momentum and energy equations the mass flux appears in five different locations, Ristorcelli (1993), and modeling $U_i \simeq V_i$ ignoring the contribution of the mass flux has been shown to be inadequate. In the Reynolds stress equations the mass flux determines the relative importance of the production by the mean flow acceleration, it contributes to the pressure fluxes and the viscous fluxes. It is clear, given the number of times it occurs in the moment evolution equations, that an accurate model for the mass flux is necessary for complex compressible turbulent flows of aerodynamic interest. This is to assess the magnitude of the mass flux in various flows and to include it in a computational model when it is important. There are classes of compressible flows in which the contribution from the mass flux are expected to be small and its inclusion in a computational model is unnecessary.

It is expected that the mass flux will not make much of a contribution to usual unidirectional shear flows such as the flat plate boundary layer and diverse free shear layers, unless there are large density gradients. The mass flux terms are expected to be important in more complex flows: these include flows in which there are mean density gradients due to large Mach number or combustion, separation or reattachment (inflection points), cold wall boundary conditions, mean dilatation, shocks, adverse pressure gradients, or strong streamwise accelerations such as those occurring in ramp type flows.

appearance of the mean velocity gradients in the tensor eddy-viscosity reflects their presence in the production terms in the evolution equation for $< v_i >$. The model predicts countergradient transfer and shows that mean density gradients in one direction can produce a mass flux in a different direction. It form, valid for a general three-dimensional flow, is

$$< \rho v_i >= - < \rho >< v_i >= -\tau [\nu_0 \delta_{ij} + \nu_1 \tau V_{i,j} + \nu_2 \tau^2 V_{i,k} V_{k,j}] \{v_j v_p\} < \rho >_{,p}$$

where $\tau = (M_t k/\varepsilon)/(1 + M_t(\mathcal{P}/\varepsilon - 1))$. The viscosity coefficients, ν_0, ν_1, ν_2, are known functions of the mean velocity gradient, given in terms of the invariants of the tensor $\mathbf{A} = \mathbf{1} + \tau \nabla \mathbf{V}$. They are not adjustable "tuning" coefficients.

The derivation of the expression for $< v_i >$ has involved a minimum number of assumptions regarding the physics of compressible turbulence. It is useful, however, to keep in mind some of the approximations to account for possible discrepancies and to anticipate the classes of flows in which the present form of the model may be inadequate. The assumptions used are:

1) The derivation of an $\mathcal{O}(< \rho\rho >^{1/2} / < \rho >)$ set of evolution equations for the $< v_i >$ showed that the unclosed terms involving correlations with the fluctuating pressure and stress are higher order effects and can therefore be neglected. In the evolution equations there is only one unclosed term, the fluctuating $< v_i v_{k,k} >$ covariance.

2) The form of turbulent diffusion terms appearing in the $< v_i >$ equation, are found to scale with the density intensity, $< \rho\rho >^{1/2} / < \rho >$, for arbitrary inhomogeneity and can therefore be neglected. This is consistent with the truncation of the equation as $(< \rho v_i v_p >< \rho >^{-1})_{,p} = (\{v_i v_p\} - < v_i v_p >)_{,p}$ is an $\mathcal{O}(< \rho\rho >^{1/2} / < \rho >)$ quantity. The difference between $\{v_i v_p\}$ and $< v_i v_p >$ has been seen to be small in the wall bounded flow at $Ma = 4.5$ of Dinavahi and Pruett (1993), as seen in Ristorcelli $et\ al.$ (1993).

3) The structural equilibrium assumption, $D/Dt [< v_i >< v_j > /\{v_p v_p\}] = 0$, is used to produce an algebraic expression for the mass flux equation. This allows the material derivative to be expressed in terms the production and dissipation of the turbulence energy. For more rapidly varying flows in which the structural equilibrium is not expected to yield results of adequate accuracy it is possible to carry the full differential equation for the mass flux. Near solid boundaries, were the mass flux is most important, a structural equilibrium is expected to be achieved rapidly and the algebraic form is adequate. It is this fact, coupled with the density intensity truncation of the evolution equation, that enables the mass flux expression to be used all the way to the wall without any $ad\ hoc$ wall function corrections.

4) The algebraic truncation of the evolution equation for $< v_i >$ involves one unclosed term, $< v_i v_{k,k} >$. It has been assumed that it can be represented as a linear relaxation term, $< v_i v_{k,k} >= - < v_i > /\tau_d$ where $\tau_d = M_t k/\varepsilon$. This model for the covariance with the fluctuating dilatation is expected to be adequate for most quasi-equilibrium quasi-homogeneous

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Case 5: Arbitrary two-dimensional mean velocity gradients

For an arbitrarily complex two-dimensional flow, such as the developing wall bounded turbulent boundary layer with separation, $V_{i,j} = [V_{1,1}, V_{1,2}, 0], [V_{2,1}, V_{2,2}, 0]$ is a suitable representation for the velocity gradient field. The viscosity coefficients are given by $\nu_0 = 1$, $\nu_1 = -(1 + \tau D)/III_A$, $\nu_2 = 1/III_A$ where $D = V_{1,1} + V_{2,2}$. The mass fluxes are given by

$$< v_1 > = \frac{\tau}{III_A}[(1 + \tau V_{2,2})\{v_1 v_p\} - \{v_2 v_p\}\tau V_{1,2}] < \rho >_{,p} < \rho >^{-1}$$

$$< v_2 > = \frac{\tau}{III_A}[(1 + \tau V_{1,1})\{v_2 v_p\} - \{v_1 v_p\}\tau V_{2,1}] < \rho >_{,p} < \rho >^{-1}$$

where $III_A = 1 + \tau D + \tau^2(V_{1,1} V_{2,2} - V_{1,2} V_{2,1})$.

Case 6: Arbitrary three-dimensional strain with simple shear

In a general three-dimensional flow the expressions for the invariants are somewhat more complicated. The simplest case, a simple shear with arbitrary three dilatation, is chosen. The velocity gradients are represented by $V_{i,j} = [V_{1,1}, V_{1,2}, 0], [0, V_{2,2}, 0], [0, 0, V_{3,3}]$. The square of the velocity gradient is given by $V_{i,k} V_{k,j} = [(V_{1,1})^2, V_{1,2}(V_{1,1} + V_{2,2}), 0], [0, (V_{2,2})^2, 0][0, 0, (V_{3,3})^2]$. The invariants of $\mathbf{A}$ are $I_A = 3 + \tau D$, $II_A = 3 + 2\tau D + \tau^2(V_{1,1} V_{2,2} + V_{2,2} V_{3,3} + V_{3,3} V_{1,1})$, and $III_A = (1 + \tau V_{1,1})(1 + \tau V_{2,2})(1 + \tau V_{3,3})$. Here, as usual, $D = V_{j,j}$ is the mean dilatation. The viscosity coefficients are a little more complicated - the three-dimensionality of the flow now affects the zeroth-order viscosity coefficient. In the two-dimensional flows $\nu_0 = 1$; here $\nu_0 = (1 + \tau D + \tau^2 d(V_{1,1} V_{2,2} + V_{2,2} V_{3,3} + V_{3,3} V_{1,1}))/III_A$. The higher order viscosity coefficients are given by $\nu_1 = -(1 + \tau D)III_A$, $\nu_2 = 1/III_A$ and the fluxes are written as

$$< v_1 > = \frac{\tau}{III_A}[(1 + \tau(V_{2,2} + V_{3,3}) + \tau^2 V_{2,2} V_{3,3})\{v_1 v_p\}$$
$$-\{v_2 v_p\}\tau V_{1,2}(1 + \tau V_{3,3})] < \rho >_{,p} < \rho >^{-1}$$

$$< v_2 > = \frac{\tau}{III_A}[(1 + \tau(V_{1,1} + V_{3,3}) + \tau^2 V_{1,1} V_{3,3})\{v_2 v_p\}] < \rho >_{,p} < \rho >^{-1}$$

6. Summary and Conclusions

The fluctuating Favre velocity mean, $< v_i >$, is the first-order form of a second-order moment, the mass flux, $< \rho v_i > = - < \rho >< v_i >$. The mass fluxes quantify the difference between Reynolds statistics and the density-weighted Favre statistics, $U_i = V_i + < v_i >$ and $u_i = v_i - < v_i >$, and can be thought of as measuring the effects of compressibility due to variations in density. The effects of the mean density gradients on the anisotropy of the turbulence are fully parameterized by the mass flux.

An algebraic representation for the mass flux has been derived from the transport equation for the Favre fluctuation mean using the structural equilibrium assumption. The mass flux is found to be proportional to the mean density gradients with an anisotropic eddy-viscosity that depends on both the Reynolds stresses *and* the mean velocity gradients. The

isotropic eddy-viscosity model cannot predict; such a model predicts a zero streamwise mass flux.

The predictions of the cross-stream component, $< v_2 >$, are less successful. This is because there are no large production terms in the $< v_2 >$ expression to mask the inaccuracies of the linear relaxation model assumed for the dilatational correlation in a nonequilibrium "newly formed" turbulence. The present temporal DNS is started from a laminar profile and computed through transition. The data shown in the figures represents a flow approximately three eddy-turnovers past the transition, $\varepsilon \delta x / (kU) \simeq 3$. The turbulence field is not fully developed, retaining vestiges of the initial conditions; a linear relaxation model for the correlation with the fluctuating divergence would not be expected to do well in such, a more or less, transitional flow.

The poor agreement in the expression for the cross-stream mass flux cannot be explained by the fact that the data comes from a temporal DNS. The expression for the mass flux model is from its evolution equation which is independent of the mean flow equation calculation. Thus, the problem often seen in comparing Reynolds stress model calculations to temporal DNS simulations, in which there is a forcing term in the equations to compensate for the boundary layer growth, do not appear here.

Case 4: Plane strain with mean dilatation

For a plane strain with arbitrary non-zero dilatation, $V_{i,j} = V_{1,1}\,\delta_{i1}\delta_{j1} + V_{2,2}\,\delta_{i2}\delta_{j2}$, and the viscosity coefficients take on the following simple values $\nu_0 = 1$, $\nu_1 = -(1 + \tau(V_{1,1} + V_{2,2}))/III_A$, $\nu_2 = 1/III_A$ where $III_A = (1 + \tau V_{1,1})(1 + \tau V_{2,2})$. The fluxes are given by the simple expressions

$$< v_1 >= \frac{\tau}{(1+\tau V_{1,1})} \{v_1 v_p\} < \rho >_{,p} < \rho >^{-1}$$
$$< v_2 >= \frac{\tau}{(1+\tau V_{2,2})} \{v_2 v_p\} < \rho >_{,p} < \rho >^{-1} .$$

Clearly the model is fully realizable and the destabilization of more rudimentary models, noted by Zeman and Coleman (1991), for a flow with large normal strain is not an issue. Note that in very high strains, say the normal passage through a shock, the dependence on the phenomenological parameter τ_d, absorbed in τ is lost. Here, again, $\tau = (M_t k/\varepsilon)/(1 + M_t(\mathcal{P}/\varepsilon - 1))$.

In mean mean field with a large dilatational component, it is more useful to consider a mean velocity gradient described of the form $V_{i,j} = V_{1,1}\,((1+D)\delta_{i1}\delta_{j1} - \delta_{i2}\delta_{j2})$. The viscosity coefficients take on the following values $\nu_0 = 1$, $\nu_1 = -1(1 + D\tau V_{1,1})/III_A$, $\nu_2 = 1/III_A$. The streamwise and cross-stream components of the Favre fluctuation mean, in a flow with arbitrary density gradient, become

$$< v_1 >= \frac{\tau}{1+(1+D)\tau V_{1,1}} \{v_1 v_p\} < \rho >_{,p} < \rho >^{-1}$$

$$< v_2 >= \frac{\tau}{1-\tau V_{1,1}} \{v_2 v_p\} < \rho >_{,p} < \rho >^{-1}$$

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in which the eigenvalue of the Reynolds stress vanishes will also vanish. It is interesting to compare the expression for the mass flux to Zeman's (1993). In an equilibrium turbulence, for which $\mathcal{P} = \varepsilon$, and in the limit of small velocity gradients the present model simplifies, to within a constant of proportionality, to Zeman's model. Comparisons of this model with the DNS data in a wall bounded compressible flow shows that it does not successfully capture the results known from DNS. The neglected terms involving the velocity gradients are essential. After all the terms with the mean velocity gradients represent the production terms, which are typically not negligible, in the mass flux equation. Computations with the neglected velocity gradient capture the near wall behavior very nicely, as will be seen in the next case.

Case 3: Simple shear, $\mathbf{V}_{i,j} = \mathbf{V}_{1,2}\,\delta_{i1}\delta_{j2}$

In problems of engineering interest the turbulence will be anisotropic and there will be nonnegligible gradients in the mean velocity field and the production terms for the mass flux need to be included in the algebraic expression. For the simple shear, $V_{i,j} = V_{1,2}\,\delta_{i1}\delta_{j2}$, a surprisingly simple expression for the mass flux is possible. The computation is easily carried out by hand using $< v_p > (\delta_{ip} + \tau V_{i,p}) = \tau\{v_i v_p\} < \rho >_{,p} < \rho >^{-1}$. Using the inversion formula the invariants of $\mathbf{A}$ are $I_A = 3$, $II_A = 3$, $III_A = 1$ and the viscosity coefficients take on the simple values $\nu_0 = 1, \nu_1 = -1, \nu_2 = 1$ and, as the square of the mean velocity gradient is zero, the expression for the mass flux becomes

$$< v_i >= \tau[\delta_{ij} - \tau V_{1,2}\,\delta_{i1}\delta_{j2}]\{v_j v_p\} < \rho >_{,p} < \rho >^{-1}$$

The streamwise and cross-stream components of the Favre fluctuation mean, in a flow with only a cross-stream density gradient, become

$$< v_1 >= \tau[\{v_1 v_2\} - \tau V_{1,2}\{v_2 v_2\}] < \rho >_{,2} < \rho >^{-1}$$
$$< v_2 >= \tau\{v_2 v_2\} < \rho >_{,2} < \rho >^{-1}.$$

Note that the effects of the production of $< v_i >$ by the mean shear, proportional to $V_{1,2}$, are included in the expressions for the streamwise mass flux. This is similar to the normal Reynolds stresses in a unidirectional shear: the production mechanism is in the equations of the streamwise component of the energy and therefore it is larger than the spanwise and cross-stream components of the turbulence energy. Computations, shown in Figure 3, with this model are very successful for the streamwise component $< v_1 >$. The peak in $< v_1 >$ is captured surprisingly well in size and location. This behavior can not be captured without the inclusion of the $V_{1,2}\{v_2 v_2\}$ term. The small velocity gradient limit expression, case 2 above, which is essentially the algebraic form both Zeman and Cole (1991) and Rubesin (1990) substantially underpredicts the near-wall peak of the mass flux. Note that a streamwise mass flux is engendered by a cross-stream density gradient. This is a behavior that an

Case 1: Isotropic turbulence with small velocity gradients, $\tau \nabla \mathbf{V} << 1$

In this case $\tau \nabla \mathbf{V} << 1$, $\mathcal{P} = 0$ and the time scale $\tau = (M_t k/\varepsilon)/(1 + M_t(\mathcal{P}/\varepsilon - 1))$. The eddy-viscosity tensor assumes the form $\tau \{v_j v_p\} \sim M_t(k/\varepsilon)2k\delta_{jp}/(1 - M_t)$ and the model is

$$< v_i > \sim \frac{M_t}{1-M_t}(k/\varepsilon)2k < \rho >_{,i} < \rho >^{-1} .$$

This can be compared to the usual eddy-viscosity model: $< v_i >= (\mu_T/ < \rho >^2 \text{Pr}_t \rho) < \rho >_{,j}$ in which $\mu_T = C_\mu f_\mu < \rho > k^2/\epsilon$ and thus

$$< v_i > \sim (k/\varepsilon)k < \rho >_{,i} < \rho >^{-1} .$$

The usual eddy-viscosity form misses the dependence on M_t which is necessary if the $< v_i >$ are to vanish in the absence of compressibility effects. Thus, apart from the M_t scaling, a scalar viscosity assumption will work, in the limit of an isotropic turbulence with negligible mean velocity gradients. Note that this form in a boundary layer flow with cross-stream density gradient cannot predict a streamwise mass flux. It can only predict a mass flux down the density gradient. In problems of engineering interest there will be countergradient transport, as has been seen in the $Ma = 4.5$ data of Dinavahi *et al.* (1993), and an eddy-viscosity gradient transport hypothesis is inappropriate. These inadequacies have also been noted by Taulbee and VanOsdol (1991).

The major shortcoming of the eddy-viscosity assumption is realizability and its impact on computability in compressible closures. In the Reynolds stress equations for arbitrary mean flow accelerations, a gradient transport assumption for $< v_i >$ can cause the acceleration production mechanism to destabilize the computations. For example if $\{v_\alpha v_\alpha\}$, in the Reynolds stress equations above, vanishes, $< v_\alpha >$ must also vanish in order to keep that eigenvalue of the Reynolds stress from going negative, as a finite $< v_i >$ in $< v_i >< \rho > D/Dt \ V_j$ will cause negative energies for arbitrary mean acceleration. This cannot be accomplished with the eddy-viscosity form of the model. Gatski (1993) has used a scalar eddy-viscosity representation and found it to be computationally destabilizing. Zeman and Coleman (1991) have also pointed out that inadequate representations of the mass flux can destabilize computations in flows when the acceleration terms is important. This occurs, for example, in the passage through a shock or in flows in which the mean strain or mean dilatation are important.

Case 2: Anisotropic turbulence with small mean velocity gradients, $\tau \nabla \mathbf{V} << 1$

In the case $\tau \nabla \mathbf{V} << 1$ and when the turbulence is anisotropic the expression for the mass flux becomes

$$< v_i >= \tau \{v_i v_p\} < \rho >_{,p} < \rho >^{-1}$$

where $\tau = (M_t k/\varepsilon)/(1 + M_t(\mathcal{P}/\varepsilon - 1))$. Note that this expression for the mass flux allows for countergradient transfer and is realizable: the mass flux in the direction of the principal axis

significant features: 1) the mass flux in one direction, as might be expected from continuity considerations, is influenced by the mass flux in another direction and 2) the contraction of the density gradient on the Reynolds stress allows countergradient transfer. In simple cases this set of equations is easily solved by hand. Performing the general inversion the model can be written in symbolic form as

$$< v_i > = \tau \mathcal{T}_{ij} \{v_j v_p\} < \rho >_{,p} < \rho >^{-1}$$

where $\mathcal{T}_{ij} = (\delta_{ij} + \tau V_{i,j})^{-1}$. This is an anisotropic eddy-viscosity model in which the eddy-viscosity tensor $\nu_{jp} = \mathcal{T}_{ji} \{v_i v_p\}$ is a function of the Reynolds stresses and the mean flow gradients. Though this form suggests the structure of the model it is not in a form most suitable for computation. Recourse to the Cayley-Hamilton theorem allows $\mathcal{T}_{ij}$ to be written in terms of the invariants and the first and second powers of the matrix:

$$III_A \mathbf{A}^{-1} = \mathbf{A}^2 - I_A \mathbf{A} + II_A \mathbf{1}$$

Substituting $\mathbf{A} = \mathbf{1} + \tau \nabla \mathbf{V}$ produces an expression for the inverse

$$III_A (\mathbf{1} + \tau \nabla \mathbf{V})^{-1} = (1 - I_A + II_A)\mathbf{1} + (2 - I_A)\tau \nabla \mathbf{V} + \tau^2 (\nabla \mathbf{V})^2$$

and the final model can be written, in ascending powers of ratios of time scales, as

$$< v_i > = \tau [\nu_0 \delta_{ij} + \nu_1 \tau V_{i,j} + \nu_2 \tau^2 V_{i,k} V_{k,j}] \{v_j v_p\} < \rho >_{,p} < \rho >^{-1} .$$

The nondimensional "viscosity" coefficients, ν_0, ν_1, ν_2 are known in terms of the mean deformation; they are not phenomenological parameters that require calibration to experiments which then limit the application of the model to flows not too different from that for which the model has been calibrated. Only one phenomenological assumption - to obtain the relaxation model for the correlation with the fluctuating dilatation - has been made. The invariants and the viscosity coefficients are given in the Appendix that summarizes the final form of the model.

5. Discussion and implementation of the mass flux model in simple flows

Formidable as the algebraic expression for the mass flux may appears there are some simple expressions for the $< v_i >$ possible. Though the representation is valid for arbitrary three-dimensional flows several cases with two-dimensional mean fields are investigated in order to understand the effects of different mean deformations. One three dimensional field is considered in order to anticipate the effects the three-dimensionality of the flow might have on the mass flux expressions.

form of the evolution equation for Favre fluctuation mean is now:

$$< v_i > (\mathcal{P} - \varepsilon)/k = - < v_p > V_{i,p} + \{v_i v_p\} < \rho >_{,p} < \rho >^{-1} + < v_i v_{p,p} > .$$

The body force terms and the Coriolis terms have not been carried, however the analysis can be carried quite easily with them as they do not constitute unknown terms that require closure.

It remains to close the last term on the right hand side. It is possible, in situations with large density and velocity gradients, to neglect the correlation with the fluctuating divergence. This is equivalent to the assumption that the mean flow gradients of density and velocity are large and set the balance to lowest order. It can, however, be shown that the correlation with the fluctuating divergence scales with mean flow gradients and is therefore not negligible in a general flow. Moreover there are times when the difference between the mean production terms is small which means that the contribution from $< v_i v_{p,p} >$ will be important.

The correlation with the divergence will be represented by a linear relaxation model. This linear relaxation model is chosen on the grounds that $< v_i v_{p,p} >$ and $< v_i >$ have the same tensorial properties. Both belong to the same symmetry groups, satisfying the same reflectional and rotational properties, vanishing in isotropic turbulence and in an equilibrium homogeneous turbulence. From a computational point of view, a linear relaxation form is desirable as it avoids the possibility of a singularity in the inversion of the velocity gradient during a computation and is consistent with realizability. A linear relaxation with time scale τ_d

$$< v_i v_{p,p} >= - < v_i > /\tau_d$$

is chosen. Zeman and Coleman (1991) have also used a linear relaxation with acoustic time scale for this correlation. The time scale, τ_d, in the model for $< v_i v_{p,p} >= - < v_i > /\tau_d$ may be thought of as a dilatational time scale. The time scale, τ_d, is the *only* phenomenological parameter assumed to obtained the present model for the mass flux. Computations using the acoustic time scale, $\tau_d = M_t k/\varepsilon$, to represent the dilatational time scale have been successful. The present model will use this approximation for the dilatational time scale. There are other possibilities though at this time, given the success of the present model, there is little motivation for further investigation.

Substituting for the unknown correlation with the fluctuating divergence in the algebraic truncation of the evolution equation for $< v_i >$ produces

$$< v_p > (\delta_{ip} + \tau V_{i,p}) = \tau \{v_i v_p\} < \rho >_{,p} < \rho >^{-1} .$$

where $\tau = (M_t k/\varepsilon)/(1 + M_t(\mathcal{P}/\varepsilon - 1))$ The model is now a set of three coupled linear algebraic equations of the form $A_{ip} < v_p >= b_i$. Inspection of the equations reveals two

an evolution equation *independent* of complicating correlations with the pressure and viscous surface forces. Note that the fact that $\{v_i v_j\} - < v_i v_j > = < \rho v_i v_j > < \rho >^{-1}$ and that $< \rho^* v_i v_p > = < \rho > \{v_i v_p\}$ has been used. The inhomogeneous diffusion term $[\{v_i v_j\} - < v_i v_j >]$ is an $\mathcal{O}\left(\sqrt{\sigma}\right)$ term, as can be seen by the data presented in Dinavahi *et al.* (1993), and can in general be neglected. In a homogeneous turbulence it is zero, of course.

This very simple equation for $< v_i >$ results from the fact that, in the Favre setting, surface forces are carried using the Reynolds decomposition while volume forces appear naturally in the Favre variables. The first-moment of the fluctuating surface forces (pressure, viscosity) appearing in the equation for $< v_i >$ are zero and no complicating models for these terms are required. This combined with the peculiarity of the fluctuating Favre mean allows $< \rho v_i > = - < \rho > < v_i >$ and leads one to work with the first-moment form $< v_i >$ of the second-moment $< \rho v_i >$. Thus a simple evolution equation for the mass flux that highlights the zeroeth order effects associated with the volumetric compressibility while relegating the higher order effects of the surface forces to a higher order equation in the expansion is obtained.

4. An algebraic expression for the Favre-velocity perturbation

To obtain the mass flux, $< \rho v_i > = - < \rho > < v_i >$, an equation for the Favre fluctuation mean, $< v_i >$, with *only one* unknown term, the correlation with the fluctuating divergence $< v_i v_{p,p} >$, has been derived. The evolution equation obtained for the Favre fluctuation mean is simple enough to carry in turbulence simulations. However it is still simpler and less expensive to carry an algebraic expression. This is now derived.

A direct algebraic truncation of the evolution equation will describe the fixed points of the $< v_i >$. An algebraic truncation following the procedure used in algebraic stress models will give the fixed points of $< v_i > / \{v_p v_p\}^{1/2}$. This is done by assuming a structural equilibrium of the form $D/Dt \left[< v_i > / \{v_p v_p\}^{1/2} \right] = 0$ allowing the convective derivatives, $D/Dt < v_i >$ to be expressed in terms of the right hand side of the evolution equation for the turbulence energy:

$$\frac{D}{Dt} < v_i > = \frac{< v_i >}{\{v_p v_p\}} \frac{D}{Dt} \{v_q v_q\} = < v_i > (\mathcal{P} - \varepsilon)/k$$

which allows the evolution of the $< v_i >$ to reflect the changes in the energy of the local turbulence field. Here $\mathcal{P}$, ε, are the production and the dissipation in the turbulent kinetic energy equation where $k = 1/2\{v_p v_p\}$ is the specific kinetic energy.

In the near wall region, where the mass flux is expected to be the most important, the flow will attain a structural equilibrium rapidly and such an approximation will be adequate. Note that the equality $\mathcal{P} = \varepsilon$ corresponds to the fixed point $D/Dt < v_i > = 0$. The algebraic

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neglecting $< v_i >$ as $U_i = V_i + < v_i >$. It is clear that this approximation is only valid when $< v_i >$ and its gradients are negligible. The data of Dinavahi *et al.* (1993b) indicates that this approximation is a poor one in the wall bounded flow. In fact, in some portions of the turbulent boundary layer, the mass fluxes' contribution to the viscous terms is as high as 25%. Figure 2, taken from Ristorcelli *et al.* (1993), shows the second cross-stream derivatives of the U_i, V_i and $< v_i >$. The mass flux terms also contribute to the pressure and viscous work terms in the mean energy equation.

It is clear, given the number of times it occurs in the moment evolution equations, that an expression for the mass flux for general compressible turbulent flows of aerodynamic interest. is necessary. An evolution equation and a model for $< v_i >$ are important: 1) to be able to estimate the importance of $< v_i >$ in different flows, 2) to know what to do about it when it is important, and 3) to be able to relate experimental values to computational results.

3. An evolution equation for the Favre velocity perturbation

Consider the evolution equations for the total velocity and density fields:

$$\rho^*,_t + (\rho^* u_p^*),_p = 0$$

$$(\rho^* u_i^*),_t + (\rho^* u_p^* u_i^*),_p + 2\epsilon_{ikp}\Omega_k \rho^* u_p^* = -p_i^* + \rho^* f_i^* + \sigma_{ij,j}^*$$

where $\sigma_{ij}^* = \mu^*[u_i^*,_j + u_j^*,_i - 2/3 u_q^*,_q \delta_{ij}]$. To a very good approximation the viscosity is independent of density: it will be taken to be equal to its local mean value and correlations between the viscosity and velocity will be considered as higher order effects and neglected. The evolution equation for the fluctuations around the Favre-mean momentum are obtained by subtracting the evolution equation for the mean momentum $< \rho > V_i$ from the equation for $\rho^* u_i^*$ to obtain an equation for $\rho^* v_i$. As $< \rho^* v_i >= 0$, a straightforward time-average of this equation does not produce any results. The equation is rewritten in its nonconservative instantaneous form:

$$\rho^* v_i,_t + \rho^* (V_p + v_p) v_i,_p + (\rho^* v_p V_i),_p - < \rho^* v_i v_p >,_p + 2\epsilon_{ikp}\Omega_k \rho^* v_p =$$
$$-p_i + \rho^* f_i + \sigma_{ij,j}^u - \rho L_{vf} V_i + V_i (\rho^* v_p),_p$$

where $\sigma_{ij}^u = < \mu > [u_i,_j + u_j,_i - 2/3 u_q,_q \delta_{ij}]$ and $L_{vf} V_i = V_i,_t + V_p V_i,_p + 2\epsilon_{ikp}\Omega_k V_p - F_i$. The term $\rho L_{vf} V_i$ reflects the coupling between the fluctuating density and the mean flow. Dividing by the total density, ρ^*, expanding using the binomial theorem, and averaging produces an evolution equation for $< v_i >$ in which successive terms scale as $\sqrt{\sigma}$, where $\sigma =< \rho^2 > / < \rho >^2$ is the normalized density variance.

Keeping only lowest order terms produces

$$< v_i >,_t + V_p < v_i >,_p + 2\epsilon_{ikp}\Omega_k < v_p >= - < v_p > V_i,_p + \{v_i v_p\} < \rho >,_p < \rho >^{-1} + < v_i v_p,_p >$$
$$+ [\{v_p v_i\} - < v_p v_i >],_p - < f_i > + \mathcal{O}\left(\sqrt{\sigma}\right)$$

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The second moment equations for a compressible flow are written, without approximation and after some manipulation, as

$$
\begin{aligned}
D/Dt \left(<\rho> \{v_i v_j\} \right) = & \; - <\rho> \{v_i v_p\} V_{j,p} - <\rho> \{v_j v_p\} V_{i,p} + \Pi_{ij} + 2/3 <pv_{k,k}> \delta_{ij} \\
& -[<pv_i> \delta_{pj} + <pv_j> \delta_{ip} + <\rho> \{v_i v_j v_p\} - <v_j \sigma_{ip}^u> - <v_i \sigma_{jp}^u>]_{,p} \\
& + <v_j> [-P_{,i} + \Sigma_{ik,k} + <\sigma_{ik}>_{,k}] + <v_i> [-P_{,j} + \Sigma_{jk,k} + <\sigma_{jk}>_{,k}] \\
& - <u_{j,p} \sigma_{ip}^u> - <u_{i,p} \sigma_{jp}^u>
\end{aligned}
$$

where the mean momentum equations have been used and $\sigma_{ij} = <\mu> [v_{i,j} + v_{j,i} - 2/3 v_{q,q} \delta_{ij}]$, $\Sigma_{ij} = <\mu> [V_{i,j} + V_{j,i} - 2/3 V_{q,q} \delta_{ij}]$ and $\sigma_{ij}^u = <\mu> [u_{i,j} + u_{j,i} - 2/3 u_{q,q} \delta_{ij}]$. The form of the equations above reflects the following manipulations: 1) The deviatoric part of the pressure-strain correlation is defined as $\Pi_{ij} = <p(v_{i,j} + v_{j,i})> - 2/3 <pv_{k,k}> \delta_{ij}$ and 2) the identity $v_i = u_i + <v_i>$ has been used to rewrite the transport terms in v_i variables while keeping the dissipation terms in u_i variables. In the equations for the Favre-averaged Reynolds stress the terms arising from surface forces appear naturally in (U_i, u_i) variables while the problem is posed in (V_i, v_i) variables. In recasting the Reynolds variables terms in Favre variables the mass flux, $<v_i>$, makes several different contributions to the Reynolds stress equations and, of course, to the $k = 1/2 \{v_j v_j\}$ equation. It multiplies the mean flow acceleration which is a new turbulence production mechanism important in flows with strong mean pressure gradients, shocks and expansion fans, and in any flows that have strong streamwise accelerations. The mass flux also contributes to the viscous diffusion of the Reynolds stresses a term that is important in the near wall region which is also where the mass flux terms are important. Note that $\sigma_{ij}^u = \sigma_{ij} - <\sigma_{ij}>$ allows the viscous transport terms to be recast in the Favre variables and that mass flux terms and their derivatives will appear. The mass flux also contributes to the Reynolds stress equations through the pressure flux to which it is coupled by the equation of state: for an ideal gas $<pv_j> = P[<\rho v_j> <\rho>^{-1} + \{\theta v_j\} T^{-1}]$. In the adiabatic case the pressure flux can be written, to first order, as $<pv_j> = P\gamma <\rho v_j> <\rho>^{-1} = c^2 <\rho v_j>$. Results from some numerical simulations have shown that the pressure and density fluctuations of the turbulence passing through a weak shock can be related through such a rule, Lee (1992). This is not found to be true for the wall bounded flow of Dinavahi and Pruett (1993) as shown in Dinavahi *et al.* (1993). Lee has also found that the pressure flux (as well as the pressure-dilatation) is primarily responsible for the rapid evolution of turbulent kinetic energy downstream of a weak shock.

In the mean momentum and mean energy equations the viscous terms appear in Reynolds variables, $\Sigma_{ij}(U) = <\mu> [U_{i,j} + U_{j,i} - 2/3 U_{q,q} \delta_{ij}]$. When the problem is recast in Favre variables, the viscous terms become functions of the Favre mean velocity and the Favre fluctuation mean. It is typical to approximate $U_i \simeq V_i$ to close the equation. This involves

on the turbulence. An anisotropy tensor based on the Reynolds variables is defined as $b_{ij}^r = < u_i u_j > / < u_p u_p > - 1/3\delta_{ij}$. A similar anisotropy tensor using the Favre variables can also be defined: $b_{ij}^f = < v_i v_j > / < v_p v_p > - 1/3\delta_{ij}$. An energy weighted deviation of the anisotropy tensor from its density-weighted equivalent is given solely in terms of the Favre fluctuation mean:

$$< v_p v_p > b_{ij}^f - < u_p u_p > b_{ij}^r = < v_i >< v_j > -1/3 < v_q >< v_q > \delta_{ij}.$$

Note that there are only three independent quantities $< v_i >$. ¿From a heuristic point of view this is pleasantly consistent: the effect of mean flow gradients, $V_{i,j}$, is parameterized by the six components of the anisotropy tensor while the effect of the mean density gradients, the vector $< \rho >_{,i}$, is parameterized by the three components of the mass flux.

There are some interesting properties of the mass flux that can be surmised from the above relationships. The most striking, and this is a rigorous result, is that in 1) an isotropic turbulence and or in 2) a statistically stationary homogeneous turbulence with mean velocity gradients and with no mean density gradients, $< v_i > \equiv 0$ and the Reynolds and Favre variables are equivalent:

$$
\begin{aligned}
U_i &= V_i \\
u_i &= v_i \\
< v_i v_j > &= < u_i u_j > \\
b_{ij}^f &= b_{ij}^r.
\end{aligned}
$$

Similar results hold for relationships between the various moments of u_i and v_i as can be easily derived. These results come from the following two facts: 1) in an isotropic field all vector statistics are zero; 2) in a statistically stationary homogeneous field, whose directional characteristics are solely determined by the mean velocity gradients, which are invariant to coordinate reflection, all quantities not invariant to coordinate reflection are zero. This has been recognized, in the context of compressible turbulence, by Blaisdell (1991). In short, in isotropic or homogeneous turbulence without mean density gradients, there is no difference between the problem posed in Reynolds or Favre variables. This is an important and serious issue affecting the validity of conclusions about the performance of compressible turbulence models which have been developed and tested in homogeneous or isotropic flows. On the other hand it suggests the appropriateness of the incompressible turbulence modeling framework in building models for the compressible flow as they are consistent in the isotropic and homogeneous limit, for arbitrary turbulent Mach number.

decompositions of the velocity field. They are related by

$$U_i = V_i + <v_i>$$
$$u_i = v_i - <v_i>.$$

The fluctuating Favre mean quantifies the difference between the Favre-mean and the Reynolds-mean velocities, V_i and U_i, as well as the difference between the instantaneous fluctuating portions of these two fields. Note that because of the definition of the Favre-average of the Favre-deviation, $<\rho^* v_i> \equiv <\rho> \{v_i\} = 0$,

$$- <\rho><v_i> = <\rho v_i>,$$

the time average of the fluctuating Favre velocity and the mass flux are equivalent quantities (apart from a scaling by the local mean density). Because of the peculiarities of the density-weighted averaging operation, a second-order statistic, $<\rho v_i>$, can be expressed as the product of two first-order statistics, $- <\rho><v_i>$. The two phrases mass flux and Favre fluctuation mean will be used interchangeably. The primes on the fluctuating density have been dropped.

As $U_i = V_i + <v_i>$, the $<v_i>$ quantify the difference between the unweighted or Reynolds mean, U_i, and the density-weighted mean, V_i, and represent the effects of compressibility through variations in density. Data from $Ma = 4.5$ DNS computations of Dinavahi and Pruett (1993) in unidirectional developing wall bounded flow indicate that the approximation of $U_i \simeq V_i$ in the wall region is inadequate. In this flow, in which $M_t \simeq 0.3$ and there is a four-fold variation of the mean density over the boundary layer. In data taken from that simulation, shown in Figure 1, it was unexpectedly found that $<v_2>$ is larger than either U_2 and V_2. It is large enough to cause U_2 and V_2 to have different signs. This is an indication that the net fluid particle transport and the net momentum transport are in opposite directions. The point is that this is a nominally simple flow, in comparison to those of practical interest, no inflection points, no change of geometry, no substantial heat transfer, no cold wall boundary conditions with the concomitant change in sign of the mean density gradient, in which the approximation $U_2 \simeq V_2$ was expected to be adequate and they are not even of the same sign.

In comparing experimental data and computational results the mass flux plays a role in relating the Reynolds stresses in Favre, v_i, variables and Reynolds, u_i, variables:

$$<v_i v_j> = <u_i u_j> + <v_i><v_j>.$$

The moments involving u_i are experimentally measured while those involving v_i come from the calculations. As it is a vector it describes the anisotropic effects compressibility has

no unknown correlations with viscous and pressure terms appear. The evolution equation is simple enough to carry as an additional differential equation in turbulence simulations, as Zeman and Cole (1991) have proposed. Nonetheless an algebraic truncation of the equation is derived as a further simplification of the problem applicable to most compressible flows of engineering interest. The algebraic truncation, similar to that used in algebraic stress models, assumes a structural equilibrium which relates the material derivative in the fluctuating Favre mean equation to the production and dissipation in the kinetic energy equation. The truncation produces a set of three coupled algebraic equations, of the form $A_{ij} < v_j > = b_i$. Application of the Cayley-Hamilton theorem produces an explicit closed form expression for the $< v_i >$. The $< v_i >$ are found to be proportional to the density gradients with an eddy-viscosity tensor dependent on the Reynolds stress and the mean deformation. The fluctuating Favre mean is then related back to mass flux using the well known relation between the two quantities.

This article is organized in the following manner. After motivating the investigation in section two, section three describes the derivation of an evolution equation for the mass flux. In the following section an algebraic model for the mass flux is obtained. The general expression for the $< v_i >$ is then specialized to several simple mean flows in order to highlight the physics. It is found that, in the limit of isotropic turbulence with negligible mean velocity gradients, the derived expression reduces to the usual scalar eddy-viscosity form derived using a gradient transfer assumption. The model is tested in the $Ma = 4.5$ wall bounded DNS of Dinavahi and Pruett (1992).

2. Preliminary exposition

In general, upper case letters will be used to denote mean quantities except in the case of the mean density, $< \rho >$, since ρ which has no convenient upper case form. The averaging operation is indicated using the angle brackets for time means, $< v_i v_j >$, and the curly brackets for the density-weighted or Favre mean, $\{v_i v_j\}$, where $< \rho > \{v_i v_j\} = < \rho^* v_i v_j >$ and the asterisk denotes the full field, $\rho^* = < \rho > + \rho'$. The dependent variables are decomposed according to

$$
\begin{aligned}
u_i^* &= U_i + u_i & &\text{where } < u_i > = 0 \\
u_i^* &= V_i + v_i & &\text{where } \{v_i\} = 0 \\
\rho^* &= < \rho > + \rho' & &\text{where } < \rho' > = 0 \\
p^* &= P + p & &\text{where } < p > = 0 \\
T^* &= T + \theta & &\text{where } \{\theta\} = 0
\end{aligned}
$$

As both the Reynolds and the Favre velocities appear naturally in the evolution equations for a compressible turbulence it is necessary to carry both the Favre and the Reynolds

Others have recognized the importance of the mass flux and several models have been proposed. Taulbee and VanOsdol (1991) have derived a modeled equation for the mass flux. In their equation they keep the correlations with the surface forces which are modeled assuming a homogeneous turbulence and the validity of Morkovin's hypothesis. In the present asymptotic derivation these terms scale with the density intensity and are found to be of higher order; the present asymptotic derivation of the transport equation for the mass flux keeps only the zeroeth terms to keep the model simple and to avoid the loss of accuracy associated with the individual approximations made in many models. They also use a gradient transfer assumption for the turbulent diffusion. Due to the different manipulation to obtain an equation for the the Favre fluctuation equation, the turbulent diffusion is found to be proportional to the difference between the Favre and Reynolds averaged Reynolds stresses; as this is a higher order term, scaling as the density intensity, there is no need to model it. The Taulbee and VanOsdol model requires the solution of two modeled differential equations, one for the mass flux and one for the density variance which appears as a source term in their modeled mass flux equation. In the present derivation of the evolution equation for the mass flux only one unknown, the covariance with the fluctuating dilatation, requires modeling. There is no need for a separate equation for the density variance.

Zeman and Coleman (1991) have also proposed a mass flux model. Their modeled equation, which has been tested in the turbulence through a shock simulations of Lee (1992) is very similar to the one derived in this article. They also propose an algebraic expression for the mass flux to which the present model simplifies to, in the limit of negligible mean deformation. Our work has shown that the inclusion of the mean velocity gradients is essential to capturing the near wall maxima of the mass flux. After all, the mean velocity gradients are a major portion of the production terms of the mass flux in its transport equation.

Rubesin (1990) has also proposed a mass flux model. It assumes that 1) the fluctuations obey a polytropic gas law 2) the specific heats are constant allowing the fluctuating density to be written in terms of the fluctuating enthalpy and that 3) the fluctuating enthalpy can be related to the mean enthalpy using a gradient transfer hypothesis. The Rubesin model requires the polytropic index as an input. Dinavahi *et al.* (1993) and Ristorcelli *et al.* (1993) in a temporal DNS have shown that the polytropic index varies substantially over the width of the turbulent boundary layer. The Rubesin model also predicts a mass flux only when there is a heat flux, while the present model derived from the exact evolution equation, predicts a mass flux whenever there are mean density gradients.

The present model for the mass flux starts with the exact evolution equation for the mass flux. An equation for the fluctuating Favre mean is then developed in a power series in the fluctuating density intensity. To zeroeth order there is only one unknown correlation and

1. Introduction

This article presents a derivation of a representation for the *non-zero first-moment* of the fluctuating velocity field, the time average of the fluctuating component of the Favre velocity, $<v_i>$. Mathematically $<v_i>$ represents the difference between unweighted and density weighted averages of the velocity field and is therefore a measure of the effects of compressibility through variations in density. It plays an important role in parameterizing the anisotropic effects of compressibility associated with the mean dilatation and gradients in the mean velocity and density. Experimentally it is an important quantity that allows Favre-averaged numerical results to be related to time-averaged experimental results. The need to consider this quantity is motivated by its frequent contributions to the first and second-order moment equations in two-equation $k-\varepsilon$ type turbulence closures as well as in Reynolds stress closures. In the mean momentum equations the mass flux makes a contribution to the viscous terms. In the mean energy equations the mass flux makes a contribution to the viscous, the pressure work, and the pressure flux terms. In the Reynolds stress equations the viscous terms appear naturally in Reynolds variables while the problem is posed in Favre variables. In the process of splitting the viscous terms into the viscous transport terms, carried in Favre variables, and the dissipation terms, carried in Reynolds variables, important contributions from the mass flux appear. The accurate accounting of these terms is important for any consistent near wall modeling and the retention of the mass flux terms is important in complex compressible turbulent flows. These contributions have been investigated in detail in Ristorcelli (1993). The mass flux also determines the importance of two production mechanisms one due to the acceleration of the mean flow and the other due to viscous effects associated with the Favre fluctuation mean.

Many of these contributions are neglected in turbulence closure models. This is a result of assuming that the Favre mean velocities are suitable approximations to the Reynolds mean velocities. This approximation is not appropriate in complex flows of practical interest. The retention of the mass flux terms will be necessary in complex compressible turbulent flows: these include flows in which there are mean density gradients due to large Mach number, combustion, separation or reattachment (inflection points), cold wall boundary conditions, mean dilatation, shocks, adverse pressure gradients, or strong streamwise accelerations. Even in this nominally simple compressible flow, such as a supersonic wall bounded boundary layer which has a four-fold variation of the mean density over the width of the boundary layer, the mass flux is not negligible. Dinavahi *et al.* (1993b), in a Mach 4.5 wall bounded DNS, has found that the cross-stream Favre mean and Reynolds mean velocities have different signs attesting to the fact that the mass flux is not small with respect to the mean velocities.

A REPRESENTATION FOR THE TURBULENT MASS FLUX CONTRIBUTION TO REYNOLDS-STRESS AND TWO-EQUATION CLOSURES FOR COMPRESSIBLE TURBULENCE

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ABSTRACT

The turbulent mass flux, or equivalently the fluctuating Favre velocity mean, appears in the first and second moment equations of compressible $k - \varepsilon$ and Reynolds stress closures. Mathematically it is the difference between the unweighted and density-weighted averages of the velocity field and is therefore a measure of the effects of compressibility through variations in density. It appears to be fundamental to an inhomogeneous compressible turbulence, in which it characterizes the effects of the mean density gradients, in the same way the anisotropy tensor characterizes the effects of the mean velocity gradients. An evolution equation for the turbulent mass flux is derived. A truncation of this equation produces an algebraic expression for the mass flux. The mass flux is found to be proportional to the mean density gradients with a tensor eddy-viscosity that depends on both the mean deformation and the Reynolds stresses. The model is tested in a wall bounded DNS at Mach 4.5 with notable results.