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ANALYSIS OF TURBULENT SHEAR FLOWS IN LASER NOZZLES AND CAVITIES

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ANALYSIS OF TURBULENT SHEAR FLOWS IN LASER NOZZLES AND CAVITIES

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An invariant second-order closure program for compressible shear flows has been developed at ARAP. The program has been applied to study a simulation of the mixing region in a HF chemical laser. Considerable insight into the complex processes occurring in laser cavities has been achieved by these studies. The results show that the assumptions used in the eddy viscosity and the turbulent kinetic energy closure methods are not completely valid for nonequilibrium flows such as in the chemical laser system. The results of studies of other shear flows with the same invariant second-order model are in generally good agreement.
ABSTRACT

An invariant second-order closure program for compressible shear flows has been developed at A.R.A.P. The program has been applied to study a simulation of the mixing region in a HF chemical laser. Considerable insight into the complex processes occurring in laser cavities has been achieved by these studies. The results show that the assumptions used in the eddy viscosity and the turbulent kinetic energy closure methods are not completely valid for nonequilibrium flows such as in the chemical laser system.

The results of studies of other shear flows with the same invariant second-order model are in generally good agreement with experimental measurements, but suggest the need for improvement of the pressure diffusion model for high speed compressible flows.

A "typical eddy" box model has been developed for computation of higher-order correlations involving species, temperatures and reaction rate fluctuations for closure of the turbulent, multi-species, reacting flow equations.
# CONTENTS

<table>
<thead>
<tr>
<th>Sections</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>11</td>
</tr>
<tr>
<td>1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>2. PROGRESS REPORT</td>
<td>2</td>
</tr>
<tr>
<td>2.1 Laser Cavity Flow Studies</td>
<td>2</td>
</tr>
<tr>
<td>2.2 Shear Flow Studies</td>
<td>4</td>
</tr>
<tr>
<td>2.3 Reacting Flow Program &quot;Typical Eddy&quot; Box Model</td>
<td>6</td>
</tr>
<tr>
<td>2.4 TENSIR Program</td>
<td>9</td>
</tr>
<tr>
<td>3. CONCLUSIONS</td>
<td>11</td>
</tr>
<tr>
<td>4. REFERENCES</td>
<td>12</td>
</tr>
</tbody>
</table>
1. **INTRODUCTION**

A second-order closure program for the investigation of compressible, chemically reacting, turbulent flow fields is under development at A.R.A.P. For the past several years A.R.A.P. has been in the forefront of the application of second-order modeling techniques to the calculation of turbulent shear flows. These techniques have been successfully applied to the calculation of planetary boundary layers\(^1\), free shear layers\(^2\), axisymmetric wakes\(^3\), flat plate boundary layers\(^4\) and other turbulent flow problems. The new program will extend the methods developed in these studies to compressible flow problems involving highly exothermic chemical reactions (i.e., the turbulent mixing and reaction in a HF chemical laser). The mixing in chemical lasers takes place under conditions of large local heat release. The resulting interaction between the turbulence and the heat release is an important feature of the flow.

During the past year, with support from AFOSR Contract No. F44620-73-C-0027, we have employed the technique of second-order modeling to study various aspects of gas flows in chemical lasers and the effect of Reynolds number and wall roughness on the mixing in the laser cavity. Other problems of particular interest to the Air Force Weapons Laboratory have also been investigated. These studies were summarized in the Interim Report of February 1974\(^5\). In the past four months a number of additional studies on the laser flowfield have been completed and are discussed in this report. The shear flow program has also been used to check some of the third-order models by comparison of program predictions to available experimental data for certain extensively studied
shear flows such as the flat plate boundary layer and the free shear layer. These studies are presented in this progress report.

The development of the reacting flow program is proceeding rapidly. The modeling of the third-order correlations such as $k' c_{\alpha}^2$, $k' c_{\alpha} c_{\beta}$ which appear in the transport equations for the second-order correlations employs a "typical eddy" box model. Extensive testing of the model has been carried out with very good results. The model is described in Section 2.3 of this report. The TENS program takes the basic transport equations in general tensor notation and converts and expands them to the corresponding equations in the desired coordinate system. It was originally written only for Cartesian coordinates. It is being improved and extended to generalized coordinate systems including cylindrical coordinates. A brief description of the program is presented in Section 2.4.

2. PROGRESS REPORT

2.1 Laser Cavity Flow Studies

The simulation of the mixing processes in a HF chemical laser cavity using our turbulent, compressible, shear flow program showed that at the typical operating conditions ($Re \sim 2000$ for the AFWL HF laser) the turbulence decays rapidly. Under these operating conditions, the performance of the laser would be strongly affected by changes in flow conditions. The turbulence in the region of mixing and chemical reaction is simply the decaying turbulence left over from the wall boundary layers and the recirculation regions at the nozzle exit. These studies also showed that Reynolds numbers of the order of $10^5$ would be necessary to reach significant turbulence levels in
the mixing region which may lead to an improvement in the laser performance.

A comparison of our second-order closure model with the eddy viscosity and the kinetic energy approach has been made for the laser flow problem. Figure 1 shows the results for the computation of an eddy viscosity "constant"

\[
K = \frac{\epsilon_{\text{max}}}{\Delta \hat{u} \times (y_{.75} - y_{.25})} = \frac{-\left( \frac{\hat{u}' \hat{v}'}{\epsilon_{\text{max}}} \right)}{\Delta \hat{u} \times (y_{.75} - y_{.25})}
\]

using the results for the Reynolds stress \(\hat{u}' \hat{v}'\) and the mean axial velocity \(\hat{u}\) obtained from the second-order closure program. We see that \(K\) is neither a constant with the downstream distance \(\Delta x\) nor with the Reynolds number, and the use of a simple eddy viscosity in the mixing region of interest for a chemical laser would be incorrect. The figure also shows the values for \(K\) obtained for a free shear layer for which we see that after a short initial region \(K\) becomes a constant. Therefore, in an equilibrium flow region, the eddy viscosity concept can be used with some degree of success, but for nonequilibrium flows as in a laser cavity a more sophisticated procedure like second-order closure must be used.

An elementary second-order closure procedure is the turbulent kinetic energy closure method as developed, for example, by Harsha. Figures 2a and 2b show the results of our computation of the quantity \(a_1 = \frac{-u'v'}{q'}\) for the laser flow field at \(Re = 2 \times 10^4\) and \(2 \times 10^5\). We see that \(a_1\) can be, to a large extent, treated as a constant across
Figure 1. Variation of the eddy viscosity "constant" in the mixing region of a chemical laser flow simulation.
the flow field. There appears to be some consistent variation in the edge regions of the flow, but there the reliability of the calculations is poor as both $\overline{u'v'}$ and $q^2$ are small in these regions. The results show some effect of the flow Reynolds number with $a_1 = 0.20$ at Re = $2 \times 10^3$ and $a_1 = 0.13-0.16$ at Re = $2 \times 10^5$. Harsha recommends a value of 0.15 from comparisons with different equilibrium shear flows. In general, then, a kinetic energy closure method seems to be considerably more successful than an eddy viscosity model but still falls short of being able to predict the results obtained by a second-order closure procedure.

Our second-order closure program provides detailed information on turbulence components useful for studying the behavior of the cavity flowfield, for example, the study of laser beam degradation due to $\overline{T^2}$ fluctuations presented in an earlier report. A detailed second-order closure program has to be developed in order to correctly incorporate the interaction between the turbulence and the chemistry in a HF laser. We are continuing our development of such a program.

2.2 Shear Flow Studies

An invariant second-order closure model requires the basic assumption that third-order and higher-order correlations that appear in the transport equations for the turbulence stresses can be modeled in terms of the second-order correlations and mean properties in such a way that the model remains invariant with respect to changes in the flow geometry. Models have been developed by us for various third-order correlations. These models are being tested and refined by comparison of model predictions to reliable experimental measurements in various shear flows. A compilation of the models being used in our present programs is presented in reference 2. Some of the
results of our studies on the free shear layer and the flat plate boundary layer are briefly discussed below.

Figure 3 compares the predictions for the effect of the velocity ratio on the spreading parameter $\sigma$ for an incompressible free shear layer against experimental measurements and a generally accepted empirical curve. The results are in excellent agreement. Figures 4 and 5 presents comparisons of our program predictions against Coles' law of the wall profile and correlation of skin friction data for incompressible flat plate boundary layers. The results again are in very good agreement. The model predictions for the detailed turbulent correlations are compared to Klebanoff's measurements in Figure 6. The agreement for $\frac{\sqrt{u'}}{\sqrt{v}}$ is very good. The results for $\sqrt{\frac{u'^2}{v'^2}}$ do not show the sharp peak in the region very near the wall, but the agreement is good for $\sqrt{\frac{u'^2}{v'^2}}$ and $\sqrt{\frac{w'^2}{v'^2}}$ over most of the profile. Our present model predicts virtually the same values for $\sqrt{\frac{v'^2}{w'^2}}$ and $\sqrt{\frac{w'^2}{v'^2}}$ while the measurements show a significant difference.

It must be pointed out that other measurements of $\sqrt{\frac{w'^2}{v'^2}}$ indicate considerable uncertainties in the values for this term but, nevertheless, our incompressible model needs some modifications for this aspect of the experimental data.

The present compressible model neglects pressure diffusion effects and a recent study\textsuperscript{7} seems to indicate that it might become important even at moderate Mach numbers. Some of the disagreement between the model predictions and the experimental data for compressible flows presented below could be due to the pressure diffusion term. We are presently modifying the program to incorporate our pressure diffusion model and to determine the effects of this term.
Present study ($\sigma_0 = 11$)

Experimental data compiled by Birch & Eggers

$\frac{\sigma_0}{\sigma} = \frac{\bar{u}_1 - \bar{u}_2}{\bar{u}_1 + \bar{u}_2}$

Figure 3. Variation of spreading rate with velocity ratio for a free shear layer.
Figure 4. Mean velocity profiles in the incompressible flat plate boundary layer.

Model parameters

\[ a = 3.25 \]
\[ b = 0.125 \]
\[ \beta = 0 \]
\[ \alpha = 0.65 \]
\[ \Lambda_{\text{MAX}} = 0.17 \delta_{99} \]
Figure 5. Skin friction coefficient as a function of Reynolds number.
Figure 6. Comparison of experimental results and model predictions in an incompressible flat plate boundary layer.
Figure 7 shows the effect of Mach number on the spreading rate for a free shear layer. The predicted Mach number effect is smaller than suggested by the experimental measurements. This is believed to be partly due to the difference in the velocity ratios (numerical problems in the computer program do not allow shear layer runs for \( u_2/u_1 < 0.1 \)) and partly due to the neglect of pressure diffusion effects. The results of Oh support this conclusion.

Figure 8 compares the prediction for \( \sqrt{u'^2} \) for a compressible boundary layer against very recent measurements by Johnson. This result also suggests that further model improvements are necessary for compressible flows to predict details of the flow. The present model does an excellent job of predicting the effect of Mach number on the skin friction as shown in Figure 9, where model results are compared with previous experimental and analytical studies.

2.3 Reacting Flow Program
"Typical Eddy" Box Model

The set of second-order closure equations governing the mixing and reaction of a compressible, turbulent, multicomponent flow system contain a number of new and difficult third-order correlations, such as \( k'c'_\alpha c'_\beta \), \( k'c'_\alpha \), \( k'c'_\alpha c'_\alpha \), etc. These terms being correlations of scalar quantities are somewhat more difficult to model than correlations involving vector terms. During the past year, with additional support from NASA, we have developed a "typical eddy" box model that is very promising for the modeling of these terms and the closure of the reacting flow equations.

The model can be looked at in two ways. First, one might consider the model to be a straightforward way of expressing the higher-order correlations of scalar fluctuations that occur in the
$u_2/u_1 = .2, .6 \circ \text{Present results}$

$u_2/u_1 = 0 \{\quad \Box \quad \square \quad \square \quad \Delta \quad \text{Data compiled by Oh}$

$\nabla \quad \text{Data compiled by Birch & Eggers}$

Figure 7. Effect of Mach number on free shear layer spreading rate.
Figure 8. Distribution of the normalized velocity fluctuations across the boundary layer

\[ \frac{\sqrt{u'v'}}{u_T} \]

Present study

\( M_e = 2.9 \)

\( y/\delta \)
Figure 9. Comparison of experimental results and model predictions for the variation of skin friction coefficient with Mach number.
equations for the second-order correlations of fluctuating scalars
in terms of the second-order correlations and the means of the
scalars. Second, it can be looked at as a way of generating the
most important features of any distribution function for the
turbulence quantities that affect the chemical behavior of the
system.

The model we have selected is the following:

We define the most typical eddy that will pass a point in the re-
acting flow at any time. For the purpose of computing scalar
correlations, the extent of this eddy in time is unimportant and
is taken equal to one. Consider a chemical reaction in which two
species, say, $\alpha$ and $\beta$, react to form a third species $\gamma$.
The typical eddy of extent unity in time has the following
structure. For a time $\varepsilon_1$ out of the total unit time, the eddy
contains only the species $\alpha$. For a time equal to $\varepsilon_2$, the
eddy contains only the species $\beta$. For a time equal to $\varepsilon_3$,
the eddy contains only the species $\gamma$. For times equal $\varepsilon_4$,
$\varepsilon_5$, and $\varepsilon_6$, the eddy contains $1/2 \alpha$ and $1/2 \beta$,
$1/2 \alpha$ and $1/2 \gamma$, and $1/2 \beta$ and $1/2 \gamma$ by mass, respectively, in a state of
molecular mixedness. In addition, for a time equal to

$$
1 + \left(1 + \frac{\alpha'\beta'}{\bar{\alpha} \beta'}\right) \times \left(1 + \frac{\alpha'\gamma'}{\bar{\alpha} \gamma'}\right) \times \left(1 + \frac{\beta'\gamma'}{\bar{\beta} \gamma'}\right)
$$

the eddy will contain $\alpha$, $\beta$, and $\gamma$ uniformly mixed on the
molecular level according to the mean mass fractions $\bar{\alpha}$, $\bar{\beta}$,
and $\bar{\gamma}$.

A typical eddy may then be drawn as in Figure 10a insofar
as the partitioning of time in the eddy into various species is
concerned. Note, since the total time of the eddy is unity, that
\[ \bar{a}, \bar{\beta}, \alpha'\beta', \alpha'\gamma', \beta'\gamma' \]
\[ \epsilon_7 = 1 + \left( 1 + \frac{\alpha'\beta'}{\alpha \beta} \right) \left( 1 + \frac{\alpha'\gamma'}{\alpha \gamma} \right) \left( 1 + \frac{\beta'\gamma'}{\beta \gamma} \right) \]

Figure 10a

\[ \bar{T}, \bar{T}'^2, \alpha'\bar{T}', \beta'\bar{T}' \]
\[ \bar{C}_{\rho_4} T_4 = \alpha_4 C_{\rho_4} T_a + \beta_4 C_{\rho_4} T_\beta \]
\[ \bar{C}_{\rho_5} T_5 = \alpha_5 C_{\rho_5} T_a + \gamma_5 C_{\rho_5} T_\gamma \]
\[ \bar{C}_{\rho_6} T_6 = \beta_6 C_{\rho_6} T_\beta + \gamma_6 C_{\rho_6} T_\gamma \]
\[ \bar{C}_{\rho_7} T_7 = \bar{\alpha} C_{\rho_7} T_a + \bar{\beta} C_{\rho_7} T_\beta + \gamma C_{\rho_7} T_\gamma \]

Figure 10b

\[ k_i = AT_i^n \exp \left( - \frac{E_A}{RT_i} \right) \]

note \( \bar{k} \neq k(\bar{T}) \)

Figure 10c

Figure 10. Nine parameter "Typical Eddy" Model for Three Species Flow System.
the sum of the times \( \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \) and \( \epsilon_6 \) is

\[
\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4 + \epsilon_5 + \epsilon_6 = - \left( 1 + \frac{\alpha' \beta'}{\alpha \beta} \right) \left( 1 + \frac{\alpha' \gamma'}{\alpha \gamma} \right) \left( 1 + \frac{\beta' \gamma'}{\beta \gamma} \right)
\]

Thus, there are only five unknowns necessary to define the eddy. Five equations are available to determine these unknowns. Independent equations are available for \( \alpha, \beta, \alpha' \beta', \alpha' \gamma', \) and \( \beta' \gamma' \), and, therefore, we are able at all times to define an eddy in terms of only the mean and second-order correlations that are being calculated. This model allows calculation of any higher-order correlations of mass fractions in terms of \( \bar{\alpha}, \bar{\beta}, \alpha' \beta', \alpha' \gamma', \) and \( \beta' \gamma' \).

To proceed with the calculation of other higher-order correlations involving the scalar \( T \) (temperature), we make the following additional assumptions. For the time \( \epsilon_1 \) when the eddy contains only \( \alpha \), the base temperature of the eddy is \( T_\alpha \); for the time \( \epsilon_2 \) when the eddy contains all \( \beta \), the base temperature is \( T_\beta \); for the time \( \epsilon_3 \) when the eddy is all \( \gamma \), the base temperature is \( T_\gamma \). For the times \( \epsilon_4 \) when the eddy consists of \( \frac{1}{2} \alpha \) and \( \frac{1}{2} \beta \) by mass, the base temperature is taken to be the appropriately weighted mean of \( T_\alpha \) and \( T_\beta \). We do likewise for cells containing \( \frac{1}{2} \alpha \) and \( \frac{1}{2} \gamma \) and for those containing \( \frac{1}{2} \beta \) and \( \frac{1}{2} \gamma \) by mass. We also do likewise for the cell containing \( \bar{\alpha}, \bar{\beta}, \) and \( \bar{\gamma} \). Since the model must admit temperature fluctuations whose distribution functions are almost Gaussian when only one species is present, we will assume that each cell spends one-half its time at a temperature \( \Delta T \) above its base temperature. This temperature model may be drawn as shown in Figure 10b. We see that there are four unknowns in this temperature model: \( T_\alpha, T_\beta, T_\gamma, \) and \( \Delta T \). There are four equations to solve these quantities, for the eddy must have the average.
temperature $\tilde{T}$, and the correlations $\tilde{T}^2$, $\tilde{\alpha}' \tilde{T}'$, and $\tilde{\beta}' \tilde{T}'$ that are available from the equations that are carried along to define the flow.

The concentration model and the temperature model just described allow one to compute any higher-order correlation of scalar fluctuations involving concentrations or temperatures. The second-and higher-order correlations involving the fluctuations of reaction rate constant $k'$ can also be calculated from the model just given. This is so because for each half cell shown in Figure 10, it is possible to calculate the instantaneous reaction rate $k$ so that the reaction rate distribution may be plotted as in Figure 10c. From this figure it is possible to calculate $k' \alpha'$, $k' \beta'$, $k' \gamma'$, or any other higher-order correlation of $k'$ with fluctuations in concentration or temperature.

The above simple model has been constructed after studying a number of other models and comparing the results of the model predictions to exact solutions of the reaction equations. Details of these studies are available in reference 9. The final model selected is believed to be capable of providing the proper closure of the equations and to make second-order closure computation of exothermic reacting flows possible for the first time.

2.4 TENSIR Program

In 1970 when A.R.A.P. first approached the task of numerically solving the modeled equations for compressible turbulent flow, it was decided that portions of the process of producing the required program should be automated. In this way, much tedious algebra and detailed coding could be handled automatically and a major source of errors eliminated.
Two program systems were developed to accomplish this task. The first program, TENSR, accepted differential equations in tensor notation as input. The program expanded the terms according to the summation convention \((A^m B_m \rightarrow A^1 B_1 + A^2 B_2 + A^3 B_3)\), and reproduced separate versions of the equations for each specified value of the free index or indices \((C_1 = D_1 \rightarrow C_2 = D_2, C_3 = D_3)\). In addition, TENSR did extensive checking of the validity of the inputs, allowed the substitution of symbols \((U, 0 \rightarrow U, 1 + U, 2 + U, 3 = 0 \rightarrow U, 1 + V, 2 + W, 3 = 0)\), and evaluated individual components of the Kronecker delta and the metric tensor. The output of TENSR was edited by hand to remove terms not applicable to the problem at hand, i.e., terms that were negligible under the boundary-layer assumptions.

The resulting equations were inputs to the second program system, DIFFR, which constructed FORTRAN statements for computing the coefficients of the finite-difference equations corresponding to the input differential equations.

These programs were very successful. However, there was a major restriction. Covariant differentiation was taken to be the same as partial differentiation. In other words, the Christoffel symbols were taken to be zero. The results were valid only for systems for which all the elements of the metric tensor are constants. Thus, the only applications were for Cartesian coordinates.

For the present effort it became necessary to solve even more complicated equations in cylindrical coordinates. Therefore, the TENSR system has been revised so that it automatically produces the Christoffel symbols associated with covariant differentiation. Orthogonality was not assumed, so that it is possible for example, to introduce streamline coordinates by defining the metric appropriately.
In making the revisions, other changes are being made in TENSER as experience with it has shown these changes to be desirable. These include changing the verification section to make the verification routine more efficient. Another change will make it possible to automatically accomplish at least some of the editing to remove negligible terms (mentioned above), if TENSER is so instructed.

No major changes have been made in DIFFR, nor are any contemplated. However, a successor program has been written which produces more efficient FORTRAN coding from that produced by DIFFR.

3. CONCLUSIONS

Considerable insight into the complex processes occurring in laser cavities has been achieved through the use of an invariant second-order closure model of the turbulent flow equations. The assumptions used in the eddy viscosity method and the kinetic energy method are not completely valid for nonequilibrium flows such as in the chemical laser system.

Studies of different incompressible shear flows with the same basic second-order model demonstrates that the general features of such flows are described very well by an invariant model. It is believed that with a little more modeling effort for compressible flows (especially for the pressure diffusion terms) all the important details of compressible flows can also be adequately calculated by our second-order closure scheme without abandoning the notion of invariance.

Significant progress has been made towards a reacting flow program with the development of the "typical eddy" box model for computation of correlations involving species, temperature and reaction rate fluctuations.
4. REFERENCES


