CHAPTER IV

ENHANCED DECAY PHENOMENON IN CASE OF FIRST ORDER

REACTIONS IN ISOTROPIC TURBULENCE

The contents of this chapter was presented in Xlth CASAMCU Symposium (1984) organised by the Centre of Advanced Study in Applied Mathematics, Calcutta University.
§ 4.1 Introduction:

In Chapter II, we have derived the equation of decay of second order correlations of the gradients of concentration undergoing decay due to diffusivity and chemical reaction at two neighbouring space points as

\[
\left( \frac{\partial}{\partial t} + 2K \right) (\nabla \gamma)^2 R_{ij} - \frac{\partial}{\partial t} \left\{ (\bar{\gamma}^2) \left( \frac{\partial}{\partial t} \nabla \gamma \right)^2 T_{ij} \right\}
= 2D \nabla_i^2 (\nabla \gamma)^2 R_{ij}
\]

...(4.1)

where

\[
(\nabla \gamma)^2 R_{ij} = \frac{\partial \gamma'}{\partial x_i} \frac{\partial \gamma''}{\partial x_j}
\]

\[
(\bar{\gamma}^2) \left( \frac{\partial}{\partial t} \nabla \gamma \right)^2 T_{ij} = \frac{\partial}{\partial x_i} \left( \bar{\gamma} \gamma'' \right) \frac{\partial \gamma''}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \bar{\gamma} \gamma' \right) \frac{\partial \gamma'}{\partial x_i}
\]

where \( \gamma', \gamma'' \) are assumed to be fluctuations of passive reactant concentrations at two neighbouring points \( A(x') \) and \( B(x'') \) respectively, while \( U_i' \), \( U_i'' \) represent the \( i \)-th component of velocity at two points, whereas \( D \) represents the coefficient of diffusivity and \( K \), the chemical reaction
rate constant of the total decay process.

The scalar version of the aforesaid equation (4.1) is obtained in Chapter II in a simplified form

\[
\left( \frac{\partial}{\partial t} + 2 \mathcal{K} \right) \left[ (\nabla \psi)^2 R \right] + 2(\Xi^2) \left( \nabla \psi \right)^2 \left[ \frac{\partial^2 M}{\partial x^2} + \frac{4}{r} \frac{\partial M}{\partial r} \right] = 2 D \left( \nabla \psi \right)^2 \left[ \frac{\partial^2 R}{\partial x^2} + \frac{4}{r} \frac{\partial R}{\partial r} \right]
\]

...(4.2)

\[ \text{cf. equation (2.11) of Chapter II} \]

Further, in Chapter III, we have obtained similar solutions of the above equation (4.2) in terms of the form functions \( \mathcal{R}(\psi) \) and \( \mathcal{M}(\psi) \) where \( \psi = \frac{r}{\lambda \nabla \psi} \). These have been discussed in the context of an apriori assumption that the chemical reaction rate constant is totally negligible. This incidentally leads to the dimensionless equation of the form,

\[
\left[ \frac{d^2}{d\psi^2} \mathcal{R}(\psi) + \frac{4}{\psi} \frac{d}{d\psi} \mathcal{R}(\psi) + 5 \mathcal{R}(\psi) \right] + \frac{1}{4D} \frac{d}{dt} \lambda \nabla \psi \left\{ \psi \frac{d\mathcal{R}}{d\psi} \left( \mathcal{M}(\psi) \right) + 6 \frac{d}{d\psi} \mathcal{M}(\psi) + \frac{4}{\psi} \mathcal{M}(\psi) \right\} = 0
\]

...(4.3)

In the said, chapter, we have seen that in our case also, we come across the well-known power law,
This very much suggests the consistency of our problem. In continuation, we have obtained in our case, the zeroth approximation of the scalar equation (4.2) as,

\[
\frac{\partial}{\partial t} (\nabla \gamma)^2 = - \frac{10 D}{\lambda^2} (\nabla \gamma)^2,
\]

where \(\lambda\) is a well-defined micro-length scale connected with fluctuating \(\gamma\)-field.

In the current chapter, we shall obtain some modifications for the second order correlations \((\nabla \gamma)^2 R_{ij}\) from the case of pure mixing to the case of pure mixing plus chemical reaction of the first order taken into account. This procedure is in the same line as adopted by G.K. Batchelor (1953), T. Tatsumi (1957), Batchelor and Townsend (1948), J. Bass (1954), S. Corrsin (1958), Prem Kumar and S.R. Patel (1975). Thus we shall extend our consideration of self preservation to the region when the chemical reaction rate constant \(K\) is significant.

In order to introduce the chemical reaction rate constant \(K\) in the above analysis. We need recast \(R(\psi)\) and \(\mathcal{M}(\psi)\) as to be denoted by \(R^m(\psi)\) and \(\mathcal{M}^m(\psi)\) where

\[
(\nabla \gamma)^2 R^m(\psi^m) = (\nabla \gamma)^2 R^0(\psi) e^{2Kt}
\]
and
\[(\bar{\psi}^2)^{1/2} (\text{grad} \, \gamma^m)^2 \mathcal{M}^m (\psi^m) = (\bar{\psi}^2)^{1/2} (\text{grad} \, \gamma)^2 \mathcal{M}^0 (\gamma) e^{2\kappa t}\]
where \(\mathcal{R}^0(\gamma), \mathcal{M}^0(\psi)\) are the solutions corresponding to \(\kappa = 0\), these being discussed with respective notations as \(\mathcal{R}(\psi)\) and \(\mathcal{M}(\psi)\) in Chapter III.

\textit{§ 4.2 Derivation of the solutions of the proposed modified equation:}

Multiplying both sides of the equation (4.2) by \(e^{2\kappa t}\), we obtain,
\[
\frac{\partial}{\partial t} \left\{ e^{2\kappa t} (\text{grad} \, \gamma)^2 R \right\} + 2 (\bar{\psi}^2)^{1/2} (\text{grad} \, \gamma)^2 \left\{ \frac{\partial^2}{\partial r^2} (Me^{2\kappa t}) \right\} \\
+ \frac{4}{\bar{r}} \frac{\partial}{\partial r} \left( Me^{2\kappa t} \right) \\
= 2D \left( \text{grad} \, \gamma \right)^2 \left\{ \frac{\partial^2}{\partial r^2} (Re^{2\kappa t}) \right\} \\
+ \frac{4}{\bar{r}} \frac{\partial}{\partial r} (Re^{2\kappa t})
\]
\[(4.5)\]

This gives the whole length of the equation (4.2) when the chemical reaction rate constant \(\kappa\) is not negligible. Proceeding in a similar manner as in the last chapter and considering series expansion at \(r = 0\), we get the diffusion equation in this case as
\[
\frac{d}{dt} \left\{ (\nabla \gamma^m)^2 \right\} = - \frac{10 D}{\lambda^m \nabla \gamma} (\nabla \gamma^m)^2
\]

...(4.6)

where the above equation (4.6) is the modified version of (4.4) under the modification,

\[
(\nabla \gamma^m)^2 = e^{2Kt} (\nabla \gamma)^2
\]

...(4.7)

The diffusion equation given by (4.6) in this modified case, i.e. when the chemical reaction rate $K$ is taken into account, is of the same type as the case when $K=0$ given by the relation (4.4). If we now compare these two equations, we can easily obtain

\[
-\frac{10 D e^{2Kt}}{\lambda^m \nabla \gamma} (\nabla \gamma)^2 = e^{2Kt} \frac{d}{dt} (\nabla \gamma)^2 + 2 K e^{2Kt} (\nabla \gamma)^2
\]

or,

\[
-\frac{10 D e^{2Kt}}{\lambda^m \nabla \gamma} (\nabla \gamma)^2 = e^{2Kt} \frac{(-10 D)(\nabla \gamma)^2}{\lambda^2 \nabla \gamma} + 2 K e^{2Kt} (\nabla \gamma)^2
\]

or,

\[
\frac{1}{\lambda^2 \nabla \gamma} - \frac{1}{\lambda^m \nabla \gamma} = \frac{K}{5D}
\]

...(4.8)

With this we obtain a relation connecting the two length scales i.e. one length scale for $K=0$ and the other for $K \neq 0$
We now proceed to obtain the self-preserving solutions of the modified equation (4.5). If we introduce the scalars $R^m$ and $M^m$, which are modified versions of the scalars $R$ and $M$, the equation (4.5) may be rewritten as

$$\frac{\partial}{\partial t} \left\{ (\nabla m)^2 R^m \right\} + 2(u^2)^{1/2} (\nabla m)^2 \left\{ \frac{\partial^2 R^m}{\partial x^2} + \frac{4}{r} \frac{\partial R^m}{\partial r} \right\} = \kappa D (\nabla m)^2 \left\{ \frac{\partial^2 R^m}{\partial x^2} + \frac{4}{r} \frac{\partial R^m}{\partial r} \right\}$$

where

$$(\nabla m)^2 R^m = (\nabla m)^2 e^{2\kappa t} R$$

and

$$(u^2)^{1/2} (\nabla m)^2 M^m = (u^2)^{1/2} (\nabla m)^2 e^{2\kappa t} M$$

We now substitute $R^m (r,t) = R^m (\psi m)$ and

$$M^m (r,t) = r M^m (\psi m) = \psi \nabla m \nabla \psi m \psi m$$

where,

$$\psi m = \frac{r}{\lambda m \nabla m}$$

With usual procedure, we obtain the self-preserving solution as
The equation (4.11) is similar to the equation (3.24) of Chapter III in case of pure mixing, with \( \mathcal{R}(\psi) \), \( \mathcal{M}(\psi) \) only replaced by \( \mathcal{R}^m(\psi) \) and \( \mathcal{M}^m(\psi) \) respectively and \( \lambda \text{ grade } \gamma \) is replaced by \( \lambda \text{ mgrad } \gamma \), where

\[
\frac{1}{\lambda^2 \text{ grad } \gamma} - \frac{1}{\lambda^2 \text{ mgrad } \gamma} = \frac{\mathcal{K}}{5D}
\]

and \( \psi_m = \frac{r}{\lambda \text{ mgrad } \gamma} \) along with \( \psi = \frac{\psi}{\lambda \text{ grad } \gamma} \) leads to the transformation of the independent variable \( \psi \) given by the relation

\[
\psi_m = \frac{\lambda \text{ grad } \gamma}{\lambda \text{ mgrad } \gamma} \cdot \psi
\]

...(4.12)

In this case, the conditions for self-preservation gives
\[
\frac{1}{4D} \frac{d}{dt} \lambda^m \nabla \gamma = \text{constant} = C_1 \text{ (say)}
\]
and
\[
(\bar{u}^2)^{1/2} \frac{\lambda^m \nabla \gamma}{D} = \text{constant} = C_2 \text{ (say)}
\]
Assuming a power law of decay of \((\nabla \gamma^m)^2\) as
\[
(\nabla \gamma^m)^2 \sim t^{-m}, m > 0,
\] ...

the diffusion equation (4.6) gives
\[
\lambda^m \nabla \gamma = \frac{10D}{m} t
\] ...

From the second self-preserving condition, applying (4.14)
we find
\[
\bar{u}^2 \sim t^{-1}
\] ...

which is the universal decay law for the velocity field also obtained in Chapter III. \(\text{cf.} \ (3.29) \) Chapter III.

In the present case, from (4.13) and (4.14)
\[
(\nabla \gamma)^2 = e^{-2\lambda t} (\nabla \gamma^m)^2
\]
\[
\sim e^{-2\lambda t} t^{-m}, m > 0
\] ...

comparing this relation (4.16) with a similar relation (3.27) of Chapter III, we get,
This means that when we know the law of decay determined by $n$ we need modify $n$ to be supplemented by $-\frac{2Kt}{\log t}$ to give us revised power law of decay in case $K$ is no more negligible.

§ 4.3 Conclusion:

Thus what we have obtained as similar solutions in regard to $\psi = \frac{r}{\lambda \text{grad} \gamma}$ in absence of chemical reactions will turn out to be true for chemical processes reconsidered when we replace $\psi$ by $\psi_m$ given by (4.12). This transformation (4.12) is easily calculated with the help of the relation (4.8) and $\lambda \text{grad} \gamma$ obtained in the previous chapter in case of pure mixing. We also observe that the power law of decay of $(\text{grad} \gamma)^2$ in Chapter III, when $K=0$ has the form given by (3.27) and in this case when $K \neq 0$, $(\text{grad} \gamma)^2$ decays at a faster rate, as is seen from (4.15). This decay law being a similar power law multiplied by the factor $e^{-2Kt}$, $K$ being the chemical reaction rate constant.
Hence, if it is required to eliminate a scalar contaminant from a pollution, it is to be mixed with some type of reactant with chemical reaction rate constant $\mathcal{K}$ as high as possible. The decay of $\nabla y$ and as such of $\gamma$ becomes much more rapid with time due to the presence of the factor $e^{-2\mathcal{K}t}$. 