

On the Modeling of Molecular Mixing in Turbulent Flows

Daniel Werner Meyer-Massetti



Dissertation
ETH No. 17639

In turbulent reactive flows, the contributions of the chemical reactive source terms in the species and energy conservation equations influence not only the distribution of the different chemical compounds but also, through density effects, greatly the flow field. Conventional simulation approaches (RANS or LES) for such flows have the major drawback that these highly non-linear terms appear only in an averaged or filtered and thus unclosed form. Alternatively, a transport equation for the joint probability density function (PDF) of the relevant flow and composition field quantities can be derived and numerically solved. Here, the chemical source terms appear in closed form. Since the PDF contains most often no multi-point statistics, the effect of molecular or thermal diffusion, which would require joint information about the compositions and their gradients, is modeled by a so-called mixing model. Even though research in this field started decades ago and significant progress has been made, there is still room for improvement. The numerous physical properties of molecular diffusion such as linearity or boundedness are difficult to deal with. Furthermore, in both premixed and non-premixed combustion applications, the strong interplay between chemical reaction and molecular diffusion in or near flame fronts is challenging to model. In numerical simulations, these are usually not resolved. In the present work, PDF method issues are addressed. The focus is among other aspects on the development of an accurate and efficient mixing model. The proposed model is based on an idealization of the scalar field in the form of an ensemble of one-dimensional scalar profiles. An assumption about the shape of these profiles is made which leads to a simple parameterization. The dynamics of the unresolved diffusive scalar field lengthscales are modeled by calculating the temporal evolution of the parameterized scalar profiles (PSP). The resulting mixing model is validated and generalized to cope with inhomogeneous multi-scalar mixing scenarios. Finally, it is shown that the PSP model provides a framework to integrate chemical reactions and molecular diffusion into one single model.

DISS. ETH NO. 17639

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MIXING IN TURBULENT FLOWS**

A dissertation submitted to

ETH ZURICH

for the degree of

Doctor of Sciences

presented by

DANIEL WERNER MEYER-MASSETTI

Dipl. Masch. -Ing. ETH/HTL

born on June 27, 1974

citizen of Meggen LU and Aristau AG (Switzerland)

accepted on the recommendation of

Prof. Dr. Patrick Jenny
Prof. Dr. Wolfgang Polifke

2008

Abstract

In turbulent reactive flows, the contributions of the chemical reactive source terms in the species and energy conservation equations influence not only the distribution of the different chemical compounds but also, through density effects, greatly the flow field. Conventional simulation approaches (RANS or LES) for such flows have the major drawback that these highly non-linear terms appear only in an averaged or filtered and thus unclosed form. Alternatively, a transport equation for the joint probability density function (PDF) of the relevant flow and composition field quantities can be derived and numerically solved. Here, the chemical source terms appear in closed form. Since the PDF contains most often no multi-point statistics, the effect of molecular or thermal diffusion, which would require joint information about the compositions and their gradients, is modeled by a so-called mixing model. Even though research in this field started decades ago and significant progress has been made, there is still room for improvement. The numerous physical properties of molecular diffusion such as linearity or boundedness are difficult to deal with. Furthermore, in both premixed and non-premixed combustion applications, the strong interplay between chemical reaction and molecular diffusion in or near flame fronts is challenging to model. In numerical simulations, these are usually not resolved. In the present work, PDF method issues are addressed. The focus is among other aspects on the development of an accurate and efficient mixing model. The proposed model is based on an idealization of the scalar field in the form of an ensemble of one-dimensional scalar profiles. An assumption about the shape of these profiles is made which leads to a simple parameterization. The dynamics of the unresolved diffusive scalar-field lengthscales are modeled by calculating the temporal evolution of the parameterized scalar profiles (PSP). The resulting mixing model is validated and generalized to cope with inhomogeneous multi-scalar mixing scenarios. Finally, it is shown that the PSP model provides a framework to integrate chemical reactions and molecular diffusion into one single model.

Zusammenfassung

Die chemischen Quellterme in den Energie- und Stoffhaltungsgleichungen sind von zentraler Bedeutung bei der Behandlung von turbulenten, reaktiven Strömungen. Einerseits verändern diese die lokalen Stoffkonzentrationen, und andererseits können diese über Dichteänderungen das Strömungsfeld beeinflussen. In konventionellen Lösungsansätzen wie RANS oder LES treten diese stark nichtlinearen Terme in gemittelter oder gefilterter Form auf und sind daher nicht geschlossen. Eine Alternative zu diesen Ansätzen stellen die PDF-Methoden dar. Hier wird eine Transportgleichung für die mehrdimensionale Wahrscheinlichkeitsdichtefunktion oder auf englisch "joint probability density function" (PDF) der relevanten Strömungs- oder Skalarfeldgrößen gelöst. Der chemische Quellterm tritt hier in geschlossener Form auf. Da die PDF allerdings meist nur Einpunktstatistiken repräsentiert, muss der molekulare Mischungsterm, welcher gemeinsame Statistiken von Skalar und Skalargradienten benötigt, mittels eines sogenannten Mischungsmodells geschlossen werden. Obwohl schon seit Jahrzehnten auf diesem Gebiet Forschung betrieben wird und grosse Fortschritte gemacht wurden, gibt es immer noch Verbesserungspotential. Erschwerend sind hier die zahlreichen physikalischen Eigenschaften der molekularen Diffusion wie beispielsweise Gebundenheit oder Linearität. In Anwendungen mit vorgemischter wie auch nicht vorgemischter Verbrennung ist weiter die starke Interaktion zwischen chemischer Reaktion und molekularer Diffusion in der Umgebung der Flammenfront erschwerend. Diese wird üblicherweise in numerischen Simulationen nicht aufgelöst. In der vorliegenden Arbeit werden Problemstellungen in PDF-Methoden betrachtet. Der Schwerpunkt liegt dabei auf der Entwicklung eines genauen und effizienten Mischungsmodells. Das entwickelte Modell basiert auf einer Idealisierung des Skalarfeldes in der Form einer Menge von eindimensionalen Skalarprofilen. Eine Annahme zur Form einzelner Profile führt auf eine einfache Parametrisierung. Durch die Berechnung der zeitlichen Entwicklung der parametrisierten Skalarprofile (PSP) kann die Dynamik der nichtaufgelösten diffusiven Skalarlängenskalen modelliert werden. Das sich ergebende Mischungsmodell wurde validiert und verallgemeinert, um es zur Simulation von inhomogenen Mehrskalarproblemen anwenden zu können. Schliesslich wird gezeigt, dass das PSP-Modell ein Rahmenwerk zur Integration von chemischer Reaktion und molekularer Diffusion innerhalb eines einzigen Modells liefert.