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Combustion Analysis Using Roe's Scheme and the Spalart–Allmaras Model

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The present work describes an efficient computational method for the simulation of turbulent flames. The main three ingredients of the method are Roe's schemes, the Spalart–Allmaras one-equation turbulence model, and a general preconditioning technique. These three ingredients are well known to ensure accuracy, robustness, and generality. The solution of the conservation equations is fully coupled, and the method is implemented in a three-dimensional parallel implicit solver. This potentially allows the use of the same mathematical method for the analysis of turbulent reactive flows at all speeds. The choice of the Spalart–Allmaras model, as opposed to typical two-equation models requires particular attention on the derivation of the micromixing time. Such a derivation is of fundamental importance, for the micromixing time represents the base upon which chemical source terms are built for many combustion models. Deriving a correct model for the micromixing time from the only resolved turbulent quantity kinematic eddy viscosity is challenging. To test the method, two low-Mach-number (0.1–0.2) turbulent reactive flows are simulated using the eddy dissipation model, and the results are compared with both experiments and previous numerical studies. It is established that the proposed method leads to satisfactory results.

Nomenclature

A_{ebu}, B_{ebu} = eddy dissipation model coefficients
C_l, C_μ, A_ε = closure coefficients
C_p = specific heat at constant pressure, $\text{J/kg} \cdot \text{K}$
D = mass diffusion coefficient, m^2/s
D_{kl} = binary mass diffusivity coefficient, m^2/s
$D_{T,k}$ = effective thermal diffusion coefficient, m^2/s
$\mathbf{F}$ = vector of the inviscid flux
$\mathbf{G}$ = vector of the viscous flux
H = total sensible enthalpy of mixture, J/kg
h = sensible enthalpy of mixture, J/kg
h_k = sensible enthalpy of species k, J/kg
h_k^0 = specific enthalpy of formation of species, J/kg
l_t = turbulent integral scale, m
l_ε = characteristic length scale, m
M = Jacobian matrix
M_k = molecular weight of species k, kg/kmol
M_m = modified Jacobian matrix
N = number of chemical species in the system
n_x, n_y, n_z = direction cosines
P = preconditioning matrix
Pr_t = turbulent Prandtl number
p = static pressure, Pa
$\mathbf{Q}$ = vector of conservative variables
$\mathbf{Q}_v$ = vector of viscous primitive variables
q = components of heat flux vector, W/m^2
R_g = universal gas constant, J/mol.K
R_{mix} = mixture specific gas constant, J/kg.K
Re_y = local turbulent Reynolds number
$\mathbf{S}$ = vector of the sources terms
S = mean strain rate, 1/s
S_{ij} = rate of strain tensor, 1/s
Sc_t = turbulent Schmidt number
T = temperature, K
$T_{\text{ref},k}$ = reference temperature for species, k, K
t = time, s
u, v, w = Cartesian component of velocities, m/s
V_n = normal velocity, m/s
V_p = local preconditioning velocity, m/s
x, y, z = Cartesian coordinates
Y = mass fraction
y^+ = normalized wall distance
δ_{ij} = Kronecker's delta function
ε = dissipation rate of turbulent kinetic energy, m^2/s^3
κ = turbulent kinetic energy, m^2/s^2
λ = thermal conductivity or matrix eigenvalue, $\text{W/m} \cdot \text{K}$
λ_ε = damping function
μ = dynamic viscosity, kg/m.s
ν = kinematic viscosity, m^2/s
$\tilde{\nu}$ = Spalart–Allmaras transported variable, m^2/s
ν_t = kinematic eddy viscosity, m^2/s
$\nu'_{i,r}$ = stoichiometric coefficient for the ith reactant in reaction r

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