Analysis and modelling of the effective reaction rate in a developing mixing layer using OpenFOAM libraries

K. Wędolowski*† (kjwed@okwf.fuw.edu.pl)¹,², K. Bajer¹,², and K. Kwiatkowski¹,²

¹Institute of Geophysics, Faculty of Physics, University of Warsaw, Poland
²Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Poland

March 25, 2011

Chemically reacting flows are ubiquitous in both environmental and industrial systems [4]. Vortical structures occurring in a turbulent flow enhance mixing, which is of great importance in the case of non-premixed reaction [6, 3]. The enhancement of diffusion and of the reaction rate was subject of many studies in two- and three-dimensional flows [1, 7]. Equations governing the concentrations of the chemically reacting species are nonlinear. Consequently, they cannot be simply averaged without producing additional terms that need to be modelled and parametrised. Moreover we should not assume that the solution of such equation is linearly dependent on the coefficients describing a particular reaction, e.g. the Damköhler number (Da). The main goal of this work is to analyse in detail this dependence in a developing mixing layer. Numerical simulations of the chemically reacting shear layer were performed, for example by Riley et. al (1985). Experimental work on this issue was conducted by Bilger et. al. (1991).

We simulate an unbounded domain filled with two initially non-premixed, chemically reacting species. In this paper we consider just a simple passive reaction of the second order. The temporally developing, incompressible mixing layer (Fig.1) evolves subject to the periodic boundary conditions in the streamwise direction. Flow instabilities develop in a quite different manner in two- and three-dimensional models. For this reason both cases are analysed separately. So far two dimensional simulations have been done and three-dimensional computations are in progress. In both cases we solve Navier-Stokes equation formulated in terms of the vorticity and the velocity vector potential.

New solvers have been created with OpenFOAM libraries in order to solve the transport equation for the vorticity and the Poisson equation for the vector potential. In the two-dimensional case we simplify calculations assuming that the vector potential has only one component. This formulation of the Navier-Stokes equation proved to be very efficient when compared to solvers

†Corresponding Author: K. Wędolowski
using the PISO algorithm. We have achieved approximately 20-25% shorter time of computations in both two- and three-dimensional cases.

The results are compared to the case of the steady, laminar shear flow (Fig. 2). It is found that slow and fast reactions respond in different ways to the fluctuations of the reactant concentration. Faster reactions appeared to have smaller effective reaction rate increase than the slower one and more quickly achieve its stabilisation.

References