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Infinitely fast chemistry in two-dimensional Navier-Stokes

Farid Ait Chaalal[†]; Michel Bourqui; Peter Bartello
[†] McGill University, Canada
Leading author: farid.aitchaalal@mail.mcgill.ca

Several previous studies pointed out that unresolved small scales could significantly affect the chemistry in Stratospheric Climate-Chemistry Models. We study the effect of diffusion on a bimolecular chemical reactions in two-dimensional Navier-Stokes flows, an idealized framework for isentropic mixing in the lower stratosphere, in order to understand and quantify these errors of Climate Models. We focus on a chemical reaction between two reactants separated by sharp gradients and limited by mixing: the chemistry is assumed infinitely fast. Particular attention is given to the tracers diffusion, which define an effective resolution. We show that the time derivative of the reactants, hereafter called chemical speed, is proportional to the diffusive flux across the contact line between the reactants. We compute the ensemble means of the contact line length, of the gradient along it and of the reactant time derivative from direct numerical simulations (DNS). We analytically relate these quantities to the Lagrangian straining proprieties of the flow as captured by the finite time Lyapunov exponents (FTLE) and to the box counting dimension D of the contact line. We show that the contact line is initially independent†of the diffusion and grows almost exponentially†at a rate determined by the tails of the FTLE PDF, and then saturates at a value dependant only on the diffusion and D. The gradients are initially proportional to the inverse of the square root of the diffusion and decrease like the mean stretching rate of a Lagrangian parcel in the recent past. In the long time regime, their exponential decay is both determined by D and small values of the FTLE, while the†dependence†to the diffusion can be related to D only. Similar relations can be derived for the diffusive flux along the contact line, and thus for the chemical speed in the infinitely fast case. The chemical speed scales like the diffusion to the power p(t), where p(t) is equal to 1/2 for D=1, and then decreases as time goes to infinity. An initial mainly exponential increase of the chemical speed is determined by the tail of the FTLE PDF, while the long time decay depends on both small values of FTLE and D. All these relations are tested with our DNS, through the direct†computation†of the FTLE and of D.