**Time-scale structure, spectral properties and model reduction in advection-diffusion and advection-diffusion-reaction systems**


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While nonlinear reaction-diffusion models represent one of the classical prototypes for addressing model reduction, as well as the finite-dimensional representation of infinite-dimensional systems (Partial Differential Equations, PDE), the role of advective terms is often underestimated [1].

In point of fact, the presence of an advecting term $-\mathbf{v} \cdot \nabla \boldsymbol{\phi}$ in the balance equation for a transported family of scalar concentration fields $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_n)$ evolving according to the dimensionless equation

$$\partial_t \boldsymbol{\phi} = -\mathbf{v} \cdot \nabla \boldsymbol{\phi} + \varepsilon \nabla^2 \boldsymbol{\phi} + r(\boldsymbol{\phi}) \tag{1}$$

modifies significantly the time-scale structure of the transport operator. In Eq. (1) $\mathbf{v}$ is a given velocity field, $\mathbf{v} \sim \mathcal{O}(1)$, $\varepsilon = 1/Pe$ is the reciprocal of the Peclet number, and $r(\boldsymbol{\phi})$ is a nonlinear vector-valued function of the concentrations accounting for chemical reactions.

This communication addresses the role of the advective term in transport-reaction model, the interplay between advection and diffusion, and its implications in model reduction of PDEs.

We consider incompressible flows (i.e. $\nabla \cdot \mathbf{v} = 0$), defined in two- and three-dimensional bounded domains, where the velocity field is either autonomous, i.e. $\mathbf{v} = \mathbf{v}(\mathbf{x})$, or time-periodic, i.e. $\mathbf{v}(\mathbf{x}, t+T) = \mathbf{v}(\mathbf{x}, t)$, where $T$ is the period of the flow.

This communication is organized in three main subtopics. First, we analyze the spectral properties of the advection diffusion operator $\mathcal{L}_{\mathbf{v}}$ entering Eq. (1),

$$\mathcal{L}_{\mathbf{v}} = -\mathbf{v}(\mathbf{x}) \cdot \nabla + \varepsilon \nabla^2 \tag{2}$$

in the case of autonomous flows, and of the Poincarè $\mathcal{P}_T$ operator associated with $\mathcal{L}_{\mathbf{v}}$ for time-periodic flows, $\mathcal{P}_T[\phi(\mathbf{x}, t)] = \phi(\mathbf{x}, t+T)$. We consider different classes of boundary conditions, corresponding to closed and open flow domains.

Under mild conditions on the regularity of $\mathbf{v}$, both $\mathrm{e}^{\mathcal{L}_v}$ or $\mathcal{P}_T$ are compact operators, and consequently their spectrum is purely a point spectrum of countably many eigenvalues lying within the unit circle of the complex plane.

The localization of the eigenfunctions of $\mathcal{L}_{\mathbf{v}}$ allows us to derive a universality theory for the spectral properties of the advection-diffusion operators [2,3]. As a consequence of universality, an analytic expression is derived for the scaling exponent $\gamma$ of the real part of the dominant (non-vanishing) eigenvalue $\Lambda$ of $\mathcal{L}_{\mathbf{v}}$ as a function of the Peclet number,

$$\Lambda \sim Pe^{-\gamma}, \qquad Pe \gg 1 \tag{3}$$

where the exponent $\gamma$, $0 \leq \gamma \leq 1$ is universal in the sense that it depends solely on the local properties of the velocity field $\mathbf{v}(\mathbf{x})$ (near a stagnation point for open flows, near a critical point for closed systems). Specifically, the singular scaling $\gamma = 0$, obtained in the case of globally chaotic closed flows, is critically addressed. This communication extends the results obtained in [2,3] to the case of open flows, such as flow in tubes or in static mixers.

In the case of time-periodic velocity fields, no analytical result are available, and the spectrum of $\mathcal{P}_T$ is computed numerically. Specifically, attention is focused on the relation between the spectral properties of $\mathcal{P}_T$, and the flow kinematics associated with $\mathbf{v}(\mathbf{x})$ (expressed by $d\mathbf{x}/dt = \mathbf{v}(\mathbf{x})$), for flows giving rise to partial or globally chaotic kinematics.

The second part of this communication analyzes the dynamic properties of Eq. (1) in the presence of chemical kinetics giving rise to complex (periodic or chaotic) dynamics. The main focus is the stabilizing action of mixing flow fields in the case of small diffusivities (large $Pe$ values).

The third part of this communication focuses on model reduction problems. The results deriving from the spectral analysis of $\mathcal{L}_{\mathbf{v}}$ (or $\mathcal{P}_T$) are useful for addressing the influence of advection in modifying the time-scale structure of the evolution operator, and in interpreting model reduction and finite-dimensional approximation of advecting-diffusion-reacting systems.


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