Diffusion Effects on Slow Invariant Manifolds

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Motivation and background

- Detailed kinetics are essential for accurate modeling of reactive systems.

- Reactive systems induce a wide range of spatial and temporal scales, and subsequently severe stiffness occurs.

- The spatial and temporal scales are coupled by the underlying physics of the problem, $\ell_D = \sqrt{D\tau_R}$.

- Computational cost for reactive flow simulations increases with the range of scales present, the number of reactions and species, and the size of the spatial domain.

- Manifold methods provide a potential for computational savings.
Motivation and background

- Manifold methods are typically spatially homogeneous, yet most engineering applications require spatial variation.

- Diffusion is often modeled with a correction to the spatially homogeneous methods in the long wavelength limit.

- However, for thin regions of flames, diffusion is fast relative to reaction and the short wavelength limit is more appropriate.

- This analysis considers the short wavelength limit by the use of a Galerkin projection.
Mathematical model

- Spatially homogeneous system,
  \[ \frac{dz}{dt} = f(z). \]

- Simple mass diffusion,
  \[ \frac{\partial z}{\partial t} = f(z) + D \frac{\partial^2 z}{\partial x^2}. \]

- Boundary conditions,
  \[ \frac{\partial z}{\partial x} \bigg|_{x=0} = \frac{\partial z}{\partial x} \bigg|_{x=L} = 0. \]
Galerkin projection

- Assume infinite series solution,
  \[
  z = z_i = \sum_{m=0}^{\infty} z_{i,m}(t)\phi_m(x), \quad i = 1, \ldots, R.
  \]

- Complete set of basis functions, with eigenvalues \( \mu_n = -(n \pi / L)^2 \),
  \[
  \phi_n = \cos \left( \frac{n\pi}{L} x \right), \quad n = 0, \ldots, N, \ldots, \infty.
  \]

- Inner product of governing PDE with basis functions,
  \[
  \frac{dz_{i,n}}{dt} = \frac{\langle \phi_n, f_i(\sum_{m=0}^{\infty} z_{i,m}\phi_m) \rangle}{\langle \phi_n, \phi_n \rangle} + \mu_n D z_{i,n}.
  \]

- Truncate series at sufficiently large \( N \).
**Example problem**

**Zel’dovich mechanism**

\[
\begin{align*}
N + NO & \rightleftharpoons N_2 + O \\
N + O_2 & \rightleftharpoons NO + O
\end{align*}
\]

- Isothermal and isochoric, 
  \(T = 3500 \text{ } K\).
- Bimolecular, isobaric, 
  \(P = 1.455 \text{ } \text{bar}\).
- 5 species, 3 constraints,
- Reduces to 2 free variables, 
  \(z_1 = z_{NO}, \ z_2 = z_{N}\).
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Spatially homogeneous \((\mathcal{N} = 0)\)

Results similar to Al-Khateeb et al., J. Chem. Phys., 2009.
Jacobian and time scales

- Jacobian matrix,
  \[ \mathbf{J} = \frac{\partial \mathbf{f}}{\partial \mathbf{z}}. \]
- Eigenvalues of Jacobian at equilibrium, \( \lambda \).
- Classification of equilibria:
  - \( e_0 \) – Sink (Physical),
  - \( e_1 \) – Saddle (+, −).
- Timescales,
  \[ \tau = \frac{1}{\lambda}. \]

Spatially homogeneous \((\mathcal{N} = 0)\)
Short wavelength limit

- Short, finite length scale, $\mathcal{N} = 1$,

\[
\frac{dz_{i,0}}{dt} = f_i(z_{j,0}),
\]

\[
\frac{dz_{i,1}}{dt} = f_{i,1}(z_{j,0}, z_{j,1}) - \frac{\pi^2 D}{L^2} z_{i,1}.
\]

- Analysis for longer lengths with larger $\mathcal{N}$ is consistent with $\mathcal{N} = 1$.

- Spatially homogeneous phase space is $z_{i,0}$ subspace.

- The Jacobian of spatially homogenous equilibria retain original eigenvalues and gain additional diffusion-modified eigenvalues.
- Eigenvalues of $\mathcal{N} = 1$ system,

  $\lambda_{i,0} = \lambda_i,$

  $\lambda_{i,1} = \lambda_i - \frac{\pi^2 D}{L^2}.$

- Character of $e_0$ remains a sink.

- Character of $e_1$ saddle changes $(+, -, -, -) / (+, +, -, -).$

- This change is indicative of a bifurcation in the system.
When $L$ is increased, $e_1$ changes from 1 to 2 positive eigenvalues.

Where this change occurs, 2 additional equilibria converge from the complex domain through $e_1$ and emerge in real space.

These 2 additional equilibria have heteroclinic orbits that connect to $e_0$ and are $(+, -, -, -)$.

For this system with the given parameters this occurs at $L = 0.2745 \text{ mm}$. 
Time scales as a function of length

At equilibrium $e_0$

\[ L = 10 \, \mu m \quad L = 0.2745 \, mm \]

\[ L (m) \quad \tau (s) \]

- $\lambda_{1,0}$
- $\lambda_{1,1}$
- $\lambda_{2,0}$
- $\lambda_{2,1}$

$J. \ Mengers \ (Notre \ Dame)$

Diffusion Effects on SIMs
Evolution at $L = 10 \, \mu m$
Evolution at $L = 0.2745 \ mm$

![Graph showing the evolution of concentration $z$ over time $t$ for different conditions.]

![3D graph showing the concentration $z_1$ over distance $x$ and time $t$.]
Phase space diagrams

$L = 10 \, \mu m$
Phase space diagrams

$L = 0.2745 \; \text{mm}$
Phase space diagrams

$L = 10 \, \mu m$

![Phase space diagram with axes labeled](image-url)
Phase space diagrams

$L = 0.2745 \text{ mm}$
Conclusions

- For long wavelengths, reaction governs the time scales.

- For short wavelengths, diffusion dictates the fast time scales; however, slower reaction time scales are still present.

- The boundary between short and long wavelengths is identified by this method.

- This method isolates the slowest dynamics making it ideal for reduction technique.

- It is easily extended to larger $N$ to evaluate systems with longer domain lengths.

- This technique provides a framework for further evaluation of the coupling of spatial and temporal scales.
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