Application of the Slow Invariant Manifold Correction for Diffusion

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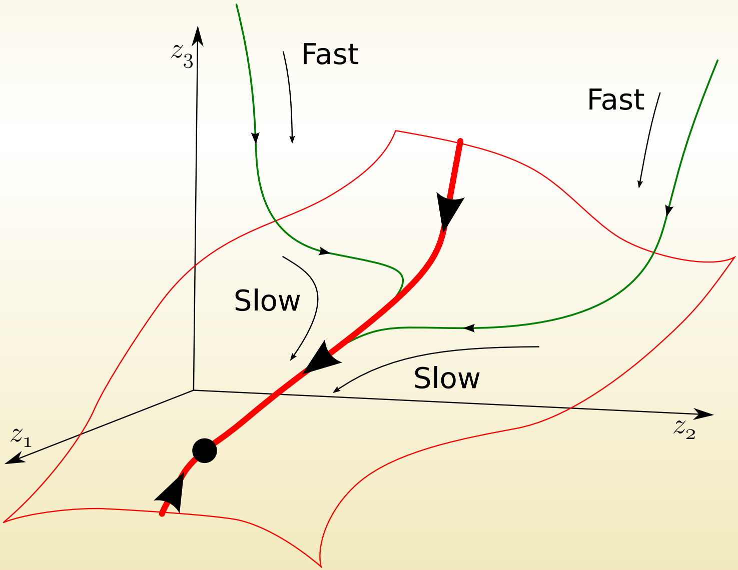
Manifold Methods



Outline

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.
- 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, reaction is fast relative to diffusion, and the short wavelength limit is more appropriate.
- Al-Khateeb, et al. 2009, *Journal of Chemical Physics*, studied an isothermal spatially homogeneous Zel'dovich mechanism and identified a SIM.
- We will employ their model with two key extensions,
  - Adiabatic, spatially homogeneous system, and
  - Isothermal system with diffusion.

Assumptions

Model a system of N species reacting in J reactions with diffusion in one spatial dimension

- Ideal mixture
- Calorically perfect
- Ideal gases
- Constant pressure
- Negligible advection
- Constant specific heat
- Single constant mass diffusivity
- Constant thermal conductivity

Balance Laws

- Evolution of species and energy

$$\begin{aligned} \rho\frac{\partial Y_i}{\partial t} + \frac{\partial j_i^m}{\partial x} &= \mathsf{M}_i\dot{\omega}_i(Y_n, T), \quad \text{for } i, n \in [1, N] \\ \rho\frac{\partial h}{\partial t} + \frac{\partial j^q}{\partial x} &= 0 \end{aligned}$$

- Boundary conditions

$$\begin{aligned} \left.\frac{\partial Y_i}{\partial x}\right|_{x=0} = \left.\frac{\partial Y_i}{\partial x}\right|_{x=\ell} &= 0, \quad \text{for } i \in [1, N] \\ \left.\frac{\partial T}{\partial x}\right|_{x=0} = \left.\frac{\partial T}{\partial x}\right|_{x=\ell} &= 0 \end{aligned}$$

- Initial conditions

$$\begin{aligned} Y_i(x, t=0) &= \tilde{Y}_i(x), \quad \text{for } i \in [1, N] \\ T(x, t=0) &= \tilde{T}(x) \end{aligned}$$

Constitutive Equations

- Simple diffusive flux terms

$$
\begin{aligned}
j_i^m &= -\rho \mathcal{D} \frac{\partial Y_i}{\partial x}, \quad \text{for } i \in [1, N] \\
j^q &= -k \frac{\partial T}{\partial x} + \sum_{i=1}^{N} h_i^f j_i^m
\end{aligned}
$$

- Caloric equation of state

$$
h = \sum_{i=1}^{N} Y_i \left(c_{Pi}(T - T^o) + h_i^f \right)
$$

- Ideal gas equation of state

$$
\rho = \frac{P_o}{\bar{\mathfrak{R}} T} \sum_{i=1}^{N} \frac{\mathsf{M}_i}{Y_i}
$$

Constitutive Equations

- Molar production rate

$$
\begin{aligned}
\dot{\omega}_i &= \sum_{j=1}^{J} \nu_{ij} r_j, \quad \text{for } i \in [1, N] \\
r_j &= k_j \left(\prod_{i=1}^{N} \left(\frac{\rho Y_i}{\mathsf{M}_i} \right)^{\nu'_{ij}} - \frac{1}{K_j^c} \prod_{i=1}^{N} \left(\frac{\rho Y_i}{\mathsf{M}_i} \right)^{\nu''_{ij}} \right), \quad \text{for } j \in [1, J] \\
k_j &= a_j T^{\beta_j} \exp\left(\frac{-\bar{E}_j}{\bar{\mathfrak{R}} T} \right), \quad \text{for } j \in [1, J] \\
K_j^c &= \exp\left(\frac{-\sum_{i=1}^{N} \bar{g}_i^o \nu_{ij}}{\bar{\mathfrak{R}} T} \right), \quad \text{for } j \in [1, J]
\end{aligned}
$$

Generalized Shvab-Zel'dovich

- Certain linear combinations of molar production rate sum to zero,

$$\frac{\partial}{\partial t}\left(\sum_{i=1}^{N}\varphi_{li}\frac{Y_i}{\mathsf{M}_i}\right)=\mathcal{D}\frac{\partial^2}{\partial x^2}\left(\sum_{i=1}^{N}\varphi_{li}\frac{Y_i}{\mathsf{M}_i}\right),\quad \text{for } l\in[1,L]$$

- In adiabatic systems, when the Lewis number is unity

$$\frac{\partial}{\partial t}\underbrace{\left(c_P(T-T^o)+\sum_{i=1}^{N}h_i^f Y_i\right)}_{h}=\mathcal{D}\frac{\partial^2}{\partial x^2}\underbrace{\left(c_P(T-T^o)+\sum_{i=1}^{N}h_i^f Y_i\right)}_{h}$$

- If initially spatially homogeneous, these PDEs can be integrated

$$\sum_{i=1}^{N}\varphi_{li}\frac{Y_i}{\mathsf{M}_i} = \sum_{i=1}^{N}\varphi_{li}\frac{\tilde{Y}_i}{\mathsf{M}_i},\quad \text{for } l\in[1,L]$$

$$c_P(T-T^o)+\sum_{i=1}^{N}h_i^f Y_i = c_P(\tilde{T}-T^o)+\sum_{i=1}^{N}h_i^f \tilde{Y}_i$$

Reduced Variables

- The L species algebraic constraints can be used to reduce N PDEs to $N - L$ PDEs
- Transform to specific mole concentrations

$$z_i = \frac{Y_i}{\mathsf{M}_i}, \quad \text{for } i \in [1, N-L]$$

- Evolution of remaining L species and temperature are coupled to these reduced variables by the algebraic constraints

$$\begin{aligned} \frac{\partial z_i}{\partial t} &= \frac{\dot{\omega}(z_n, T)}{\rho} + \mathcal{D}\frac{\partial^2 z_i}{\partial x^2}, \quad \text{for } i, n \in [1, N-L] \\ T &= \begin{cases} \tilde{T}, & \text{if isothermal} \\ \dfrac{h - \sum_{i=1}^{N} \hat{z}_i(z_n)\bar{h}_i^f}{\sum_{i=1}^{N} \hat{z}_i(z_n)\bar{c}_{Pi}} + T^o, & \text{if adiabatic} \end{cases} \end{aligned}$$

Galerkin Reduction to ODEs

- Assume a spectral decomposition

$$z_i(x,t) = \sum_{m=0}^{\infty} z_{i,m}(t)\phi_m(x), \quad \text{for } i \in [1, N-L]$$

- Orthogonal basis functions, $\phi_m(x)$, are eigenfunctions of diffusive operator that match boundary conditions

$$\phi_m(x) = \cos\left(\frac{m\pi x}{\ell}\right), \quad \text{for } m \in [0,\infty)$$

- Finite system of ODEs for amplitude evolution are recovered by taking the inner product with ϕ_n, and truncated at M

$$\frac{dz_{i,m}}{dt} = \underbrace{\frac{\langle \phi_m, \dot{\omega}_i \left(\sum_{m=0}^{\infty} z_{i,n}\phi_n\right)\rangle}{\langle \phi_m, \phi_m \rangle}}_{\dot{\omega}_{i,m}} - \underbrace{\frac{m^2\pi^2\mathcal{D}}{\ell^2}}_{\frac{m^2}{\tau_\mathcal{D}}} z_{i,m}, \qquad \begin{array}{c}\text{for } i \in [1, N-L], \\ \text{and } m \in [0, M]\end{array}$$

- Diffusion time scale defined as $\tau_\mathcal{D} \equiv \dfrac{\ell^2}{\pi^2\mathcal{D}}$

Example Problem

Zel'dovich reaction mechanism

$$N + NO \leftrightharpoons N_2 + O$$
$$N + O_2 \leftrightharpoons NO + O$$

- $N = 5$ species
- $J = 2$ reactions
- $L = 3$ constraints
- $N - L = 2$ reduced variables

  $z_1 = z_{NO},\ z_2 = z_N$

- Isobaric, $P = 1.6629\ bar$

We examine two limits:

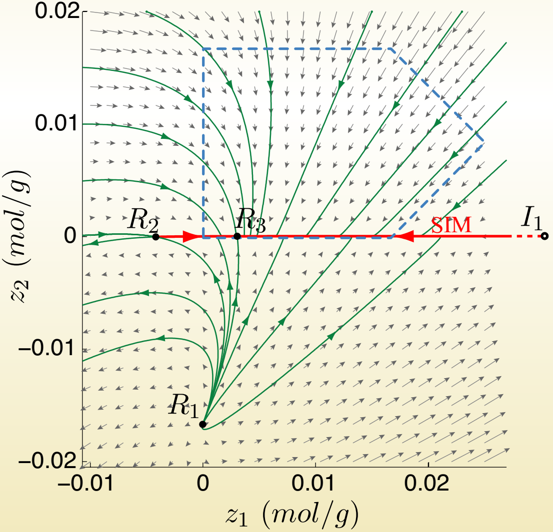
- Isothermal
  - $T = 4000\ K$
  - Bimolecular, isochoric
- Adiabatic
  - $h = 9.0376 \times 10^{10}\ erg/g$
  - Enthalpy chosen such that physical equilibrium is at $T = 4000\ K$

Spatially Homogeneous Isothermal Phase Space

- Identify equilibria
- Characterize equilibria by eigenvalues of their Jacobian matrix

$$\mathsf{J}_{ij} = \frac{\partial \dot{\omega}_i}{\partial z_j}$$

- Classify time scales, reciprocal of eigenvalues, as fast and slow
- SIM is a heteroclinic orbit from saddle to sink



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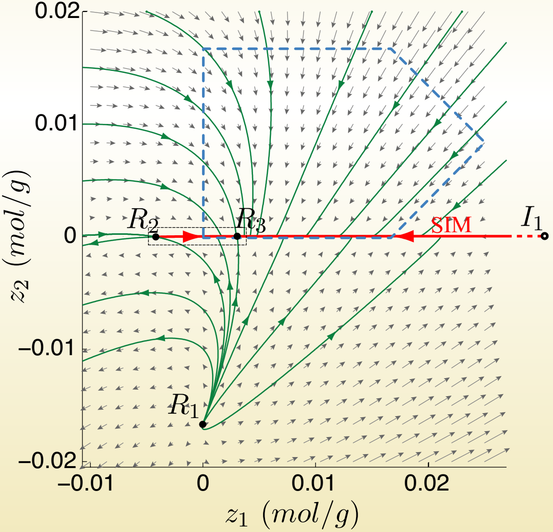

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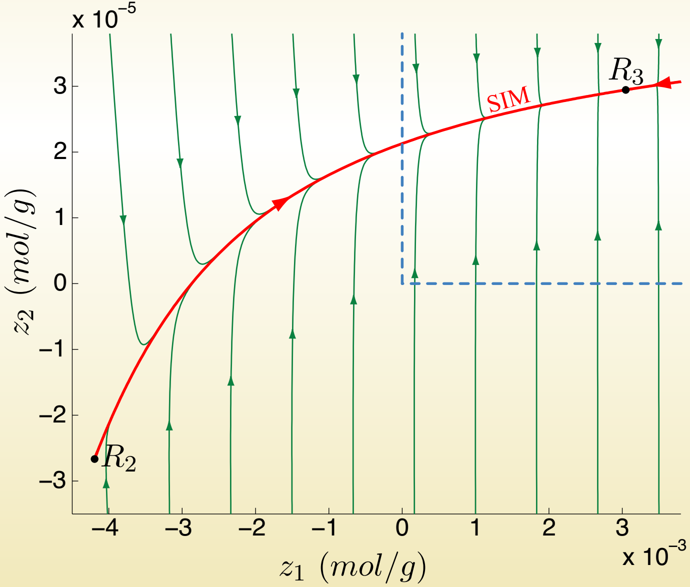

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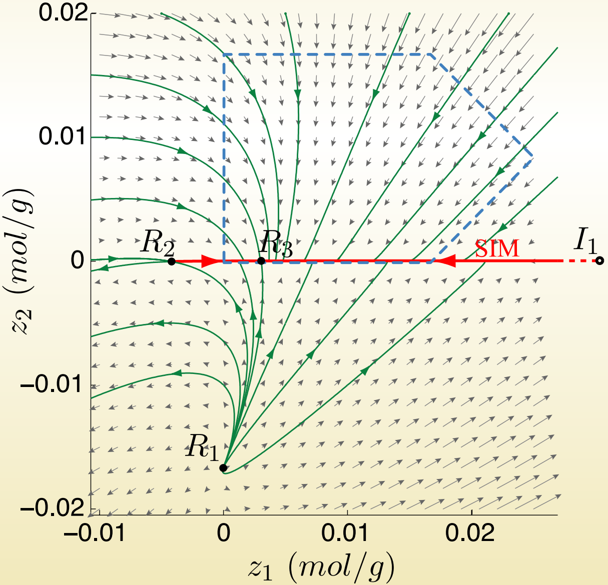

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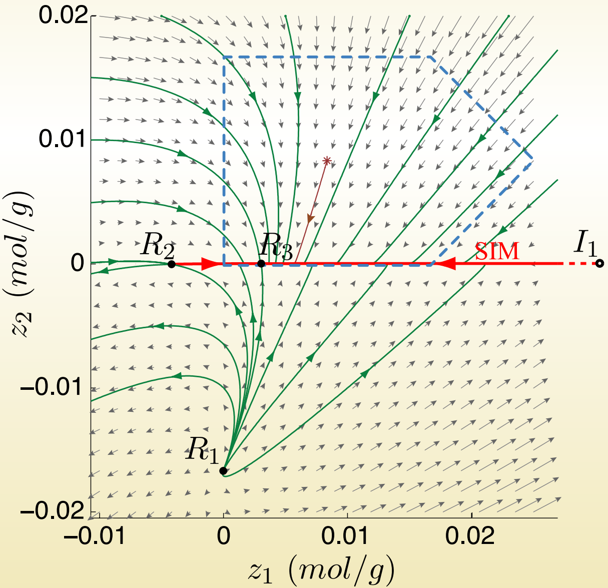
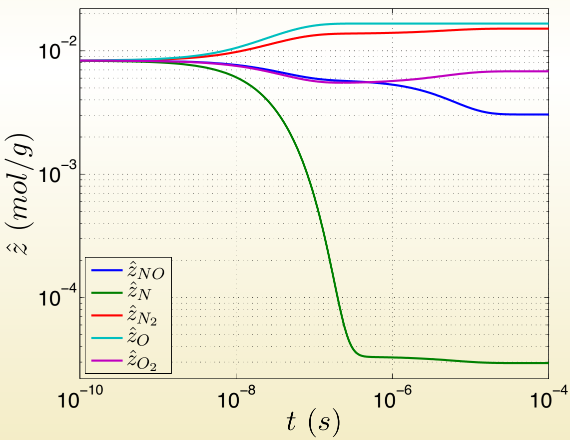
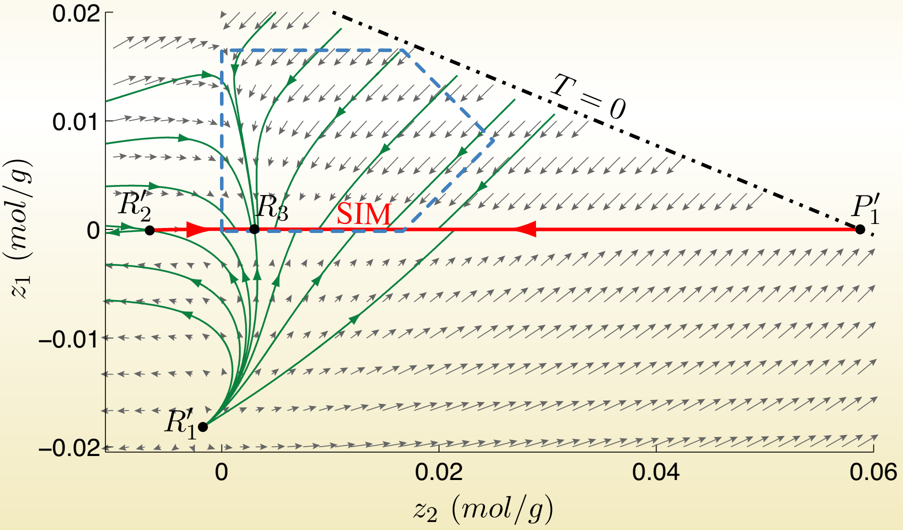


Spatially Homogeneous Isothermal Evolution

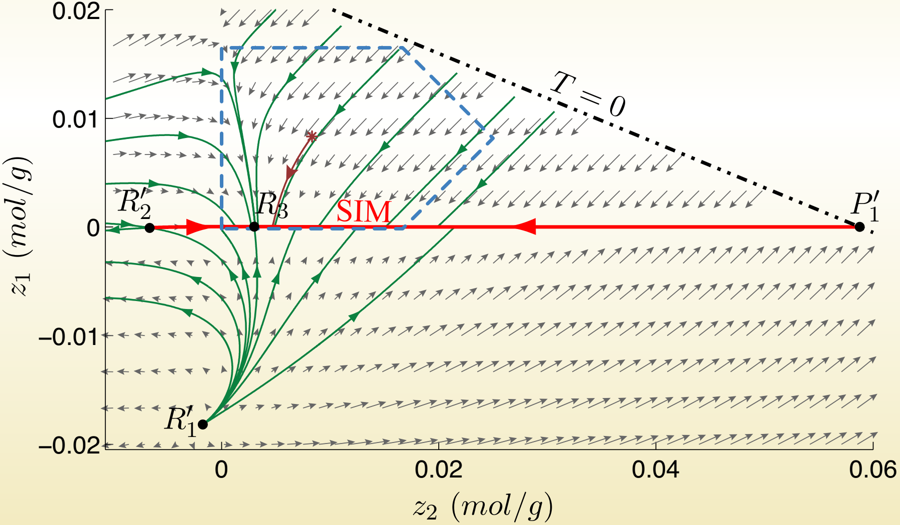
- Fast and slow time scales apparent
- Observed time scales correspond to reciprocal of equilibrium eigenvalues
- Fast – evolution toward SIM
- Slow – evolution along SIM toward equilibrium



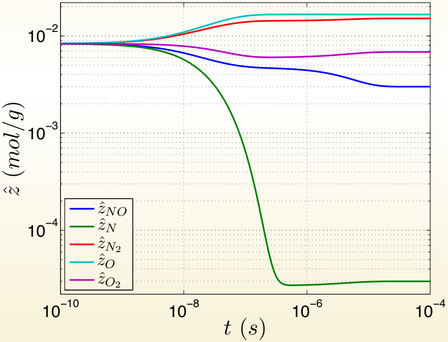
Spatially Homogeneous Adiabatic Phase Space

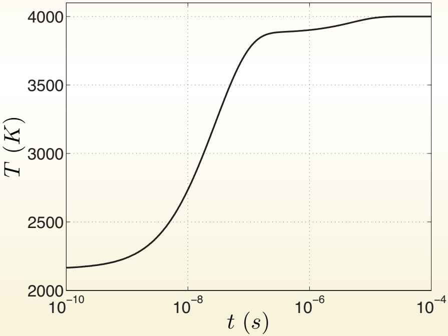


Spatially Homogeneous Adiabatic Phase Space



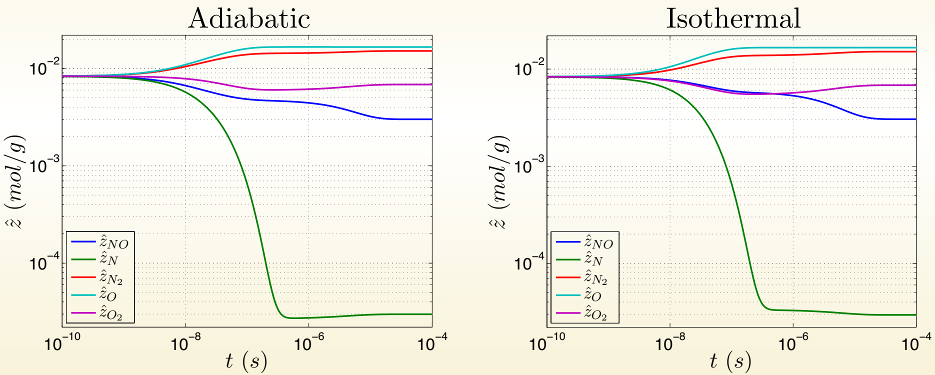
Spatially Homogeneous Adiabatic Evolution





- Again, the fast and slow time scales are consistent with equilibrium eigenvalues
- Now, they are apparent in temperature as well as species evolution

Spatially Homogeneous Adiabatic Evolution



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Isothermal Diffusion Correction – Galerkin Projection

- We now examine the spatially inhomogeneous isothermal case
- In the Galerkin projection we find an infinite spectrum of diffusion modified eigenvalues

$$\lambda_{i,m} = \lambda_i - \frac{m^2}{\tau_{\mathcal{D}}}, \quad \text{for } i \in [1, N-L], \text{ and } m \in [0, \infty)$$

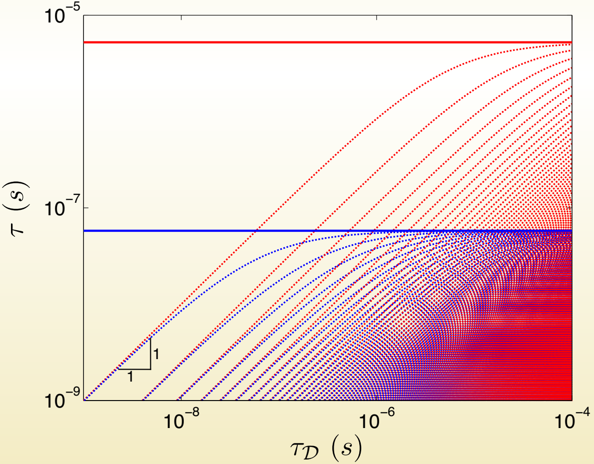
- Recall that the diffusion time scale is related to the length scale

$$\tau_{\mathcal{D}} = \frac{\ell^2}{\pi^2 \mathcal{D}}$$

- For any given $\tau_{\mathcal{D}}$, truncation at a sufficiently large M is necessary to fully resolve the spatial and temporal scale coupling

Galerkin Projection – Time Scales

- Infinite spectrum of diffusion modified eigenvalues
- For fast diffusion time scales truncate at $M = 1$ is adequate



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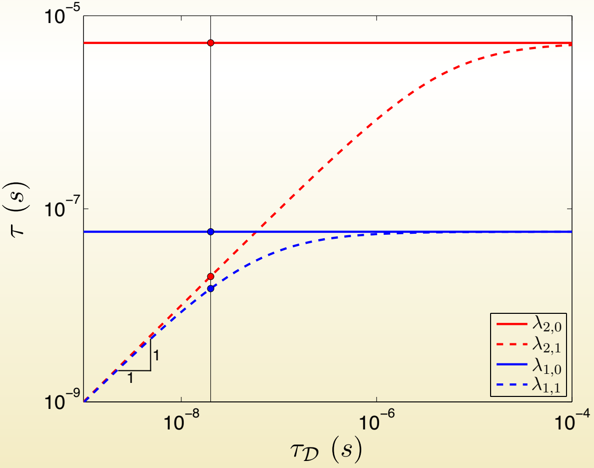
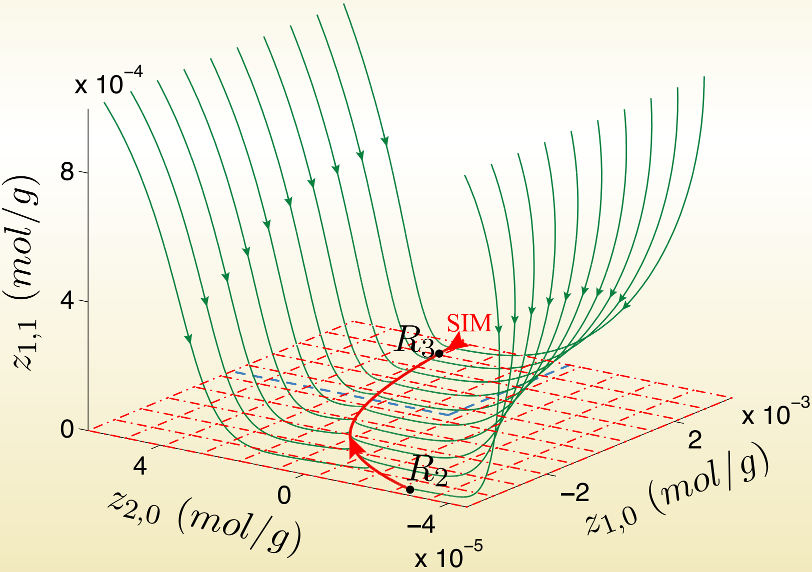
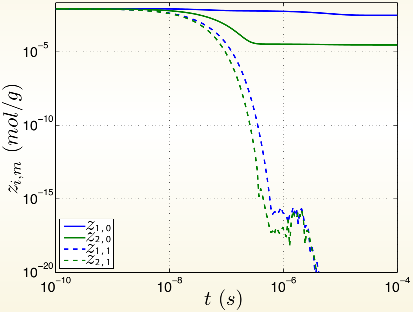
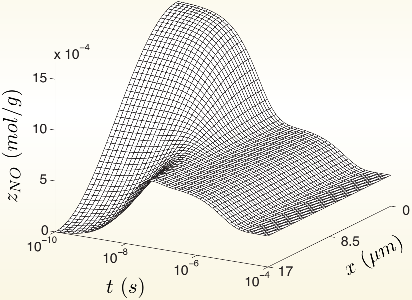


Diffusion Correction Isothermal Phase Space



Diffusion Correction Isothermal Evolution





- Two additional fast time scales from diffusion
- Spatially inhomogeneous amplitudes decay earlier than either reaction time scale
- Our $\tau_{\mathcal{D}}$ choice with $\mathcal{D} = 14\ cm^2/s$ yields length scale $\ell = 17\ \mu m$.

Conclusions

- The SIM isolates the slowest dynamics making it ideal for a reduction technique.
- The SIM is found for a spatially homogeneous adiabatic system, providing a framework for finding SIMs on other non-isothermal systems.
- For sufficiently short length scales, diffusion time scales are faster than reaction time scales, and the system dynamics are dominated by reaction.
- When lengths are near or above a critical length where the diffusion time scale is on the same order as reaction time scales, diffusion will play a more important role.
- In the limit of large length scales, a truncation at $M = 1$ is insufficient, and more terms are required to fully resolve the dynamics.

Acknowledgments

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