

Numerical Methods for Chemical Kinetics

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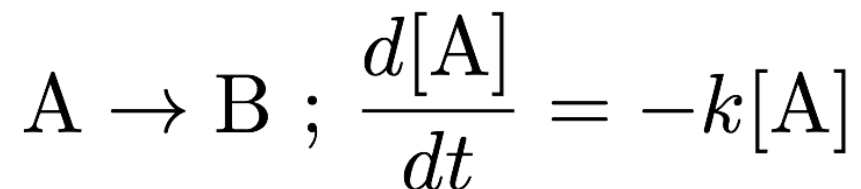
Chemical Kinetics Numerical Methods

- As we have discussed earlier, detailed kinetic behavior is described by a set of rate equations.
- To solve these equations requires that all the rate coefficients and initial concentrations be known.
- Since the thermodynamic state may be changing, one must solve the appropriate conservation equations as well.
- Therefore, depending on the physical system being considered, a large system of differential equations must be solved and support for calculating rate constants and thermodynamic properties provided.



The Stiffness Problem

- Characteristic times for reactions, i.e.



$$[A]_t = [A]_0 e^{-kt} ; \tau = 1/k$$

- For real kinetic mechanisms it is usual for the characteristic reaction times to vary over many orders of magnitude.
- This leads to the so called stiffness problem.

The Stiffness Problem

- If a system of equations is stiff, then the step size needed to solve the system is driven by the dependent variables that are changing the fastest which leads to very slow solutions.
- To overcome this problem, a number of solution methods have been developed, most notably
 - DASPAK¹:
 - Gear method².

1. S. Li and L.R. Petzold, "Software and algorithms for sensitivity analysis of large-scale differential algebraic systems." Journal of Computational and Applied Mathematics, 2000, vol. 125, no. 1/2, pp. 131.

2. Gear, C.W. (1971) Numerical Initial Value Problems in Ordinary Differential Equations. Prentice-Hall, Upper Saddle River.

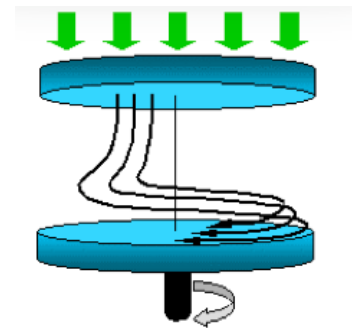
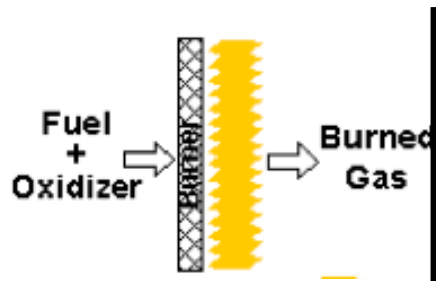
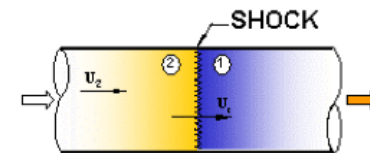
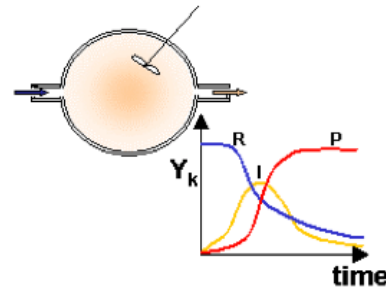
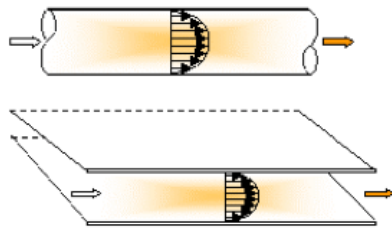
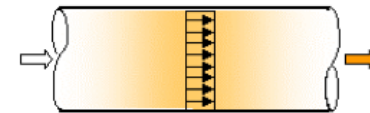
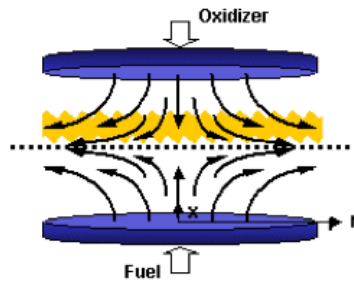
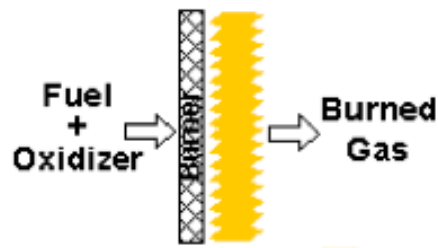


Chemkin and Cantera

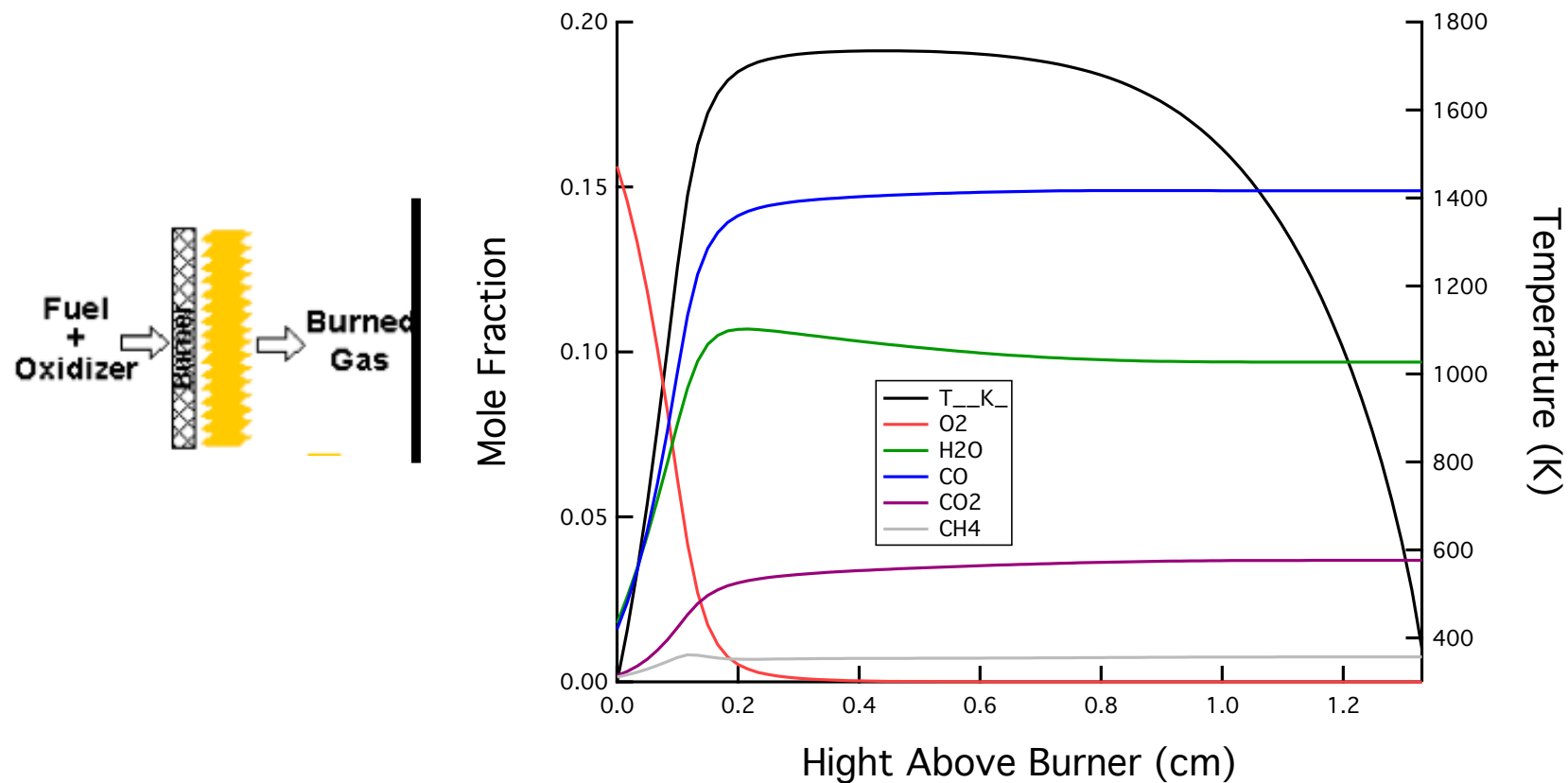
- Chemkin and Cantera are codes designed for solving model problems chemical kinetic problems.
- Chemkin, originally developed by Sandia National Laboratories, is a commercial code now distributed by ANSYS. \$\$\$\$\$\$
- Cantera is an open source code, written in C++ and run via Python or Matlab.



Types of Model Problems



Stagnation Flame Example



Complex Problems

- To solve complex problems, full CFD with reactions is required.
- i.e. Wind tunnel fire:

