1D Plug Flow Reactor Model with Surface Chemistry

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Introduction

Cantera:

- An open-source suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and/or transport processes.
- Can be used from Python and Matlab, or in applications written in C/C++ and Fortran 90.
- Applications including combustion, detonations and etc.

Objectives of the project:

- Derive the governing differential algebraic equation (DAE) for a plug flow reactor model with surface chemistry
- Implement the model with proper DAE solver

Problem Solving

$$\frac{d(\rho u A_c)}{dz} = p\sum^{K_g} \dot{s}_k W_k$$

$$\rho u A_c \frac{dY_k}{dz} + Y_k p\sum^{K_g} \dot{s}_k W_k = \dot{\omega}_k W_k A_c + \dot{s}_k W_k p$$

$$\rho u A_c c_p \frac{dT}{dz} + A_c \sum^{K_g} \dot{\omega}_k W_k h_k + p\sum^{K_g} h_k \dot{s}_k W_k = \dot{Q}$$

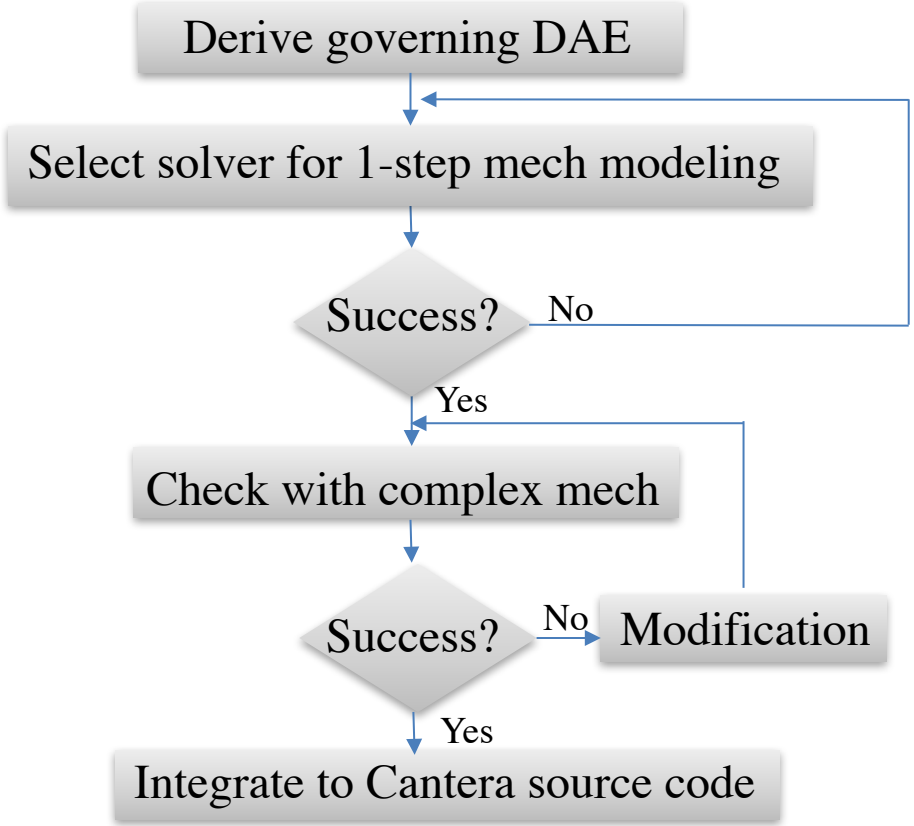
$$\rho u A_c \frac{du}{dz} + u\frac{d(\rho u A_c)}{dz} = -\frac{d(PA_c)}{dz} - \frac{1}{2}\rho u^2 f p$$

$$PW = \rho RT$$

$$\frac{dZ_k}{dt} = \frac{\dot{s}_k \sigma_k}{\Gamma}$$

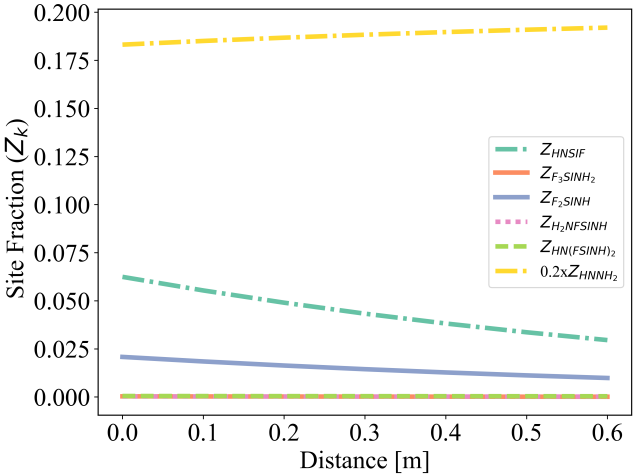
$$\dot{s}_k = 0$$

$$\sum^{K_s} Z_k = 1$$



Results and Applications

Cylindrical, straight-channel, plug-flow reactor



Surface species site fractions vary in the flow direction

Applications of this model:

- Homogeneous and heterogeneous reactions in packed bed
- Deposit thin solid films via chemical vapor deposition