A theoretical study for one-dimensional modeling for VOC in a catalytic converter

Combustion Theory and Modeling
14: 3, 367-379
Chauhan S.
Sharma L.
Srivastave V.K.

The Problem

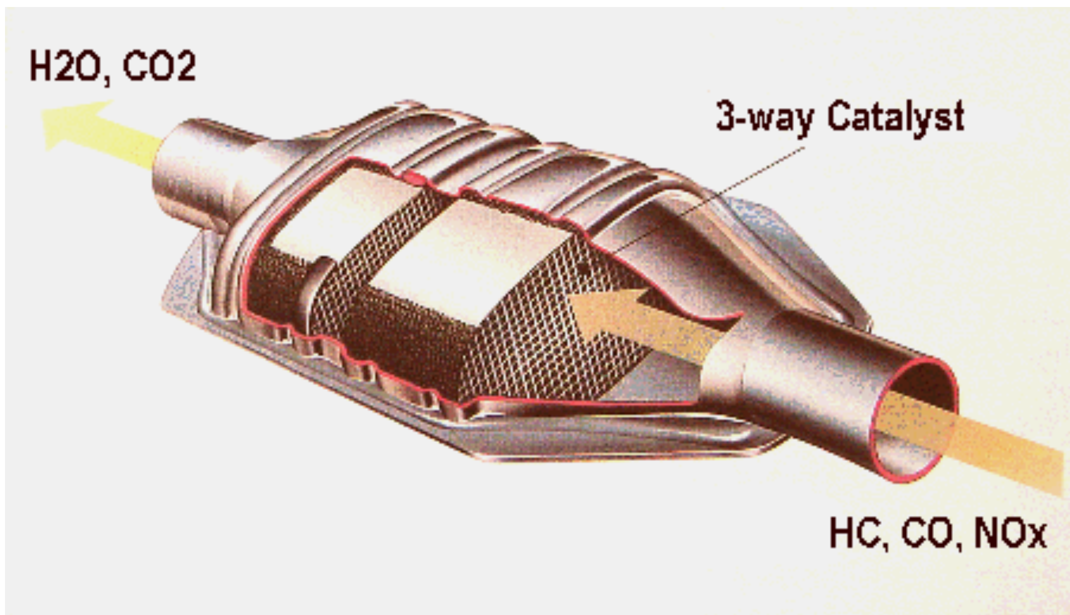
- VOC – (volatile organic compound)
  - –produced from vehicular emissions
  - –exposure–health risks
    - –deteriorate air quality
    - –damage crops
  - –Ex. CO, NO_x, aldehydes
  - –increasing restrictions of the emissions of these compounds

Catalytic Combustion

- Thermal combustion of pollutants requires high temp and produces harmful products
- Catalyst lowers required combustion temp
- Products are H_20 and CO_2
- Combustion occurs on the surface of the catalyst
- Process is highly efficient

Catalytic Converter

- Monolithic Catalysts
  - “honeycomb catalysts”
  - Platinum and Palladium serve as catalyst



Purpose

- Create a mathematical model of a monolithic catalyst in the warm up period
- Model
  - Combustion of acetaldehyde (CH_3CHO)
  - Platinum as catalyst
  - Utilize one dimensional unsteady state model mass and energy balance eqn. for solid and gas phases
  - Solve using the Backward Implicit Method

Assumptions

- Negligible axial diffusion in gas phase.
- Noble metal (catalyst) concentration was kept constant and the catalyst does not deactivate.
- Monolith is cylindrical with circular cross-section channels.
- Gas phase concentration, temperature, velocity and the solid temperature are uniform across the monolith cross-section at any axial position.
- The heat released by the catalytic reactions inside the washcoat was totally transported to the gas phase by convection.
- Heat transfer by radiation within channels and also heat exchange between the substrate and the surroundings at both inlet and an outlet face of the monolith is neglected.
- Non-uniform flow distribution inside the converter is neglected, as one single channel represents the entire monolith.
- Reactor operates in laminar flow region, with fully developed flow in greater part of the reactor and therefore the reacting species are transferred to the wall by molecular diffusion.

Kinetics

- Reaction

  $CH_3CHO + 2.5O_2 \rightarrow 2CO_2 + 2H_2O$

  - Irreversible
- Reaction rate

$$(-r)_{VOC} = k_0 \exp^{(-E/RT_s)} C_i$$

  - Pre-exponential Factor: k_0 = 46.18 m/s
  - Activation Energy: E = 36,374 J/mol

Equations

- Mass balance in gas phase:

$$v\left(\frac{\partial C_g}{\partial x}\right)+k_g S\left(C_g-C_s\right)=\left(\frac{\partial C_g}{\partial t}\right)$$

- Mass balance in solid phase:

$$a(-r)_{VOC}=k_g S(C_g-C_s)$$

- Energy balance in gas phase:

$$-v\rho_g Cp_g\left(\frac{\partial T_g}{\partial x}\right)-hS\left(T_g-T_s\right)=\rho_g Cp_g\left(\frac{\partial T_g}{\partial t}\right)$$

- Energy balance in solid phase:

$$\rho_s Cp_s\left(\frac{\partial T_s}{\partial t}\right)=a\left(-\Delta H\right)(-r)_{VOC}+hS\left(T_g-T_s\right)+\lambda_s\left(\frac{\partial^2 T_s}{\partial x^2}\right)$$

Boundary Conditions

- Entering acetaldehyde concentration through time:

$$C_g(0,t) = C_g^0$$

- Entering gas temp though time:

$$T_g(0,t) = T_g^0$$

- Catalyst temp at t=0:

$$T_s(x,0) = T_s^0$$

- Converter entrance:

$$x = 0, \quad \frac{\partial T_s}{\partial x} = 0$$

- Converter exit:

$$x = L, \quad \frac{\partial T_s}{\partial x} = 0$$

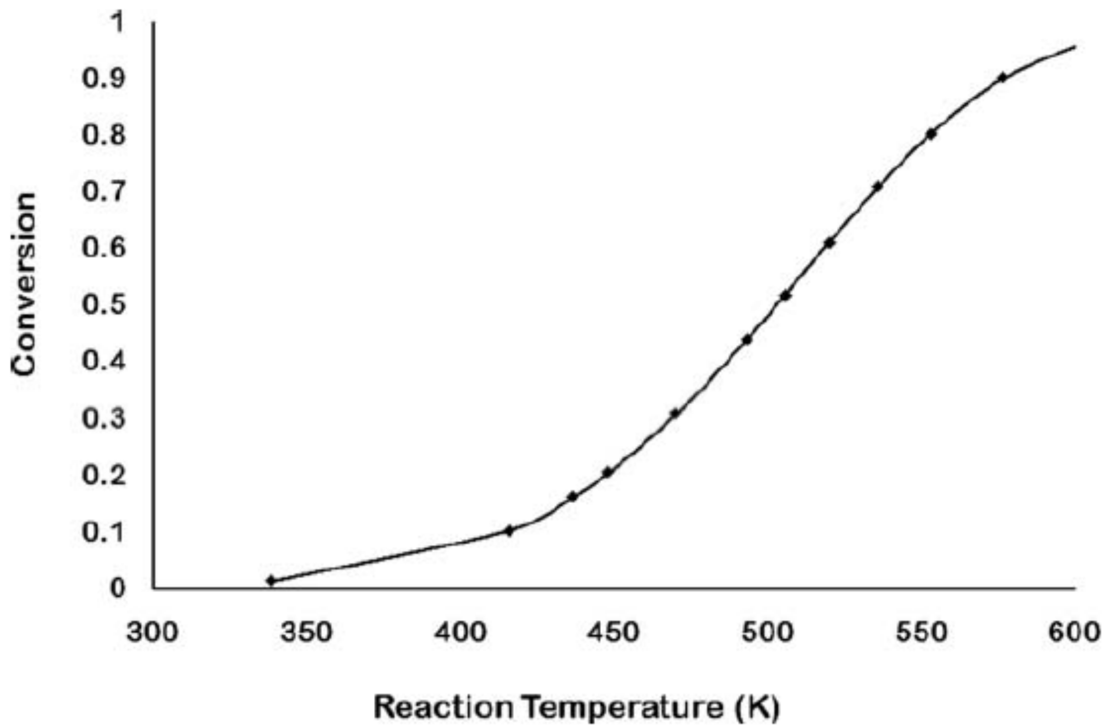
$$x = L, \quad \frac{\partial C_g}{\partial x} = 0$$

$$x = L, \quad \frac{\partial T_g}{\partial x} = 0$$

Results

- Calculated values:
  - Acetaldehyde concentration
  - Gas temperature
  - Solid Catalyst Temperature
- Findings:
  - Temperature of the converter slowly raised
  - Reaction started when converted reached operating temperature
  - Decrease in acetaldehyde due to reaction
    - Decrease to 1.000 to .200 (dimensionless)

Conversion of Acetaldehyde with time



2. Conversion of acetaldehyde (100 ppm) with respect to reaction temperature.

Concentration Variation along length

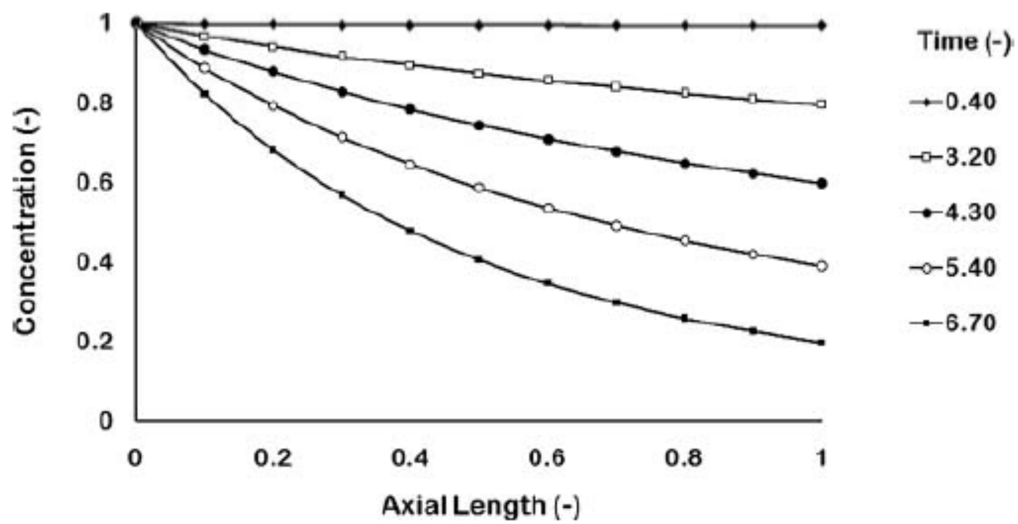


Figure 3. Concentration variation of acetaldehyde (100 ppm) at 723 K along the axial length.

Exit Concentration with respect to time:
with varying inlet temperatures

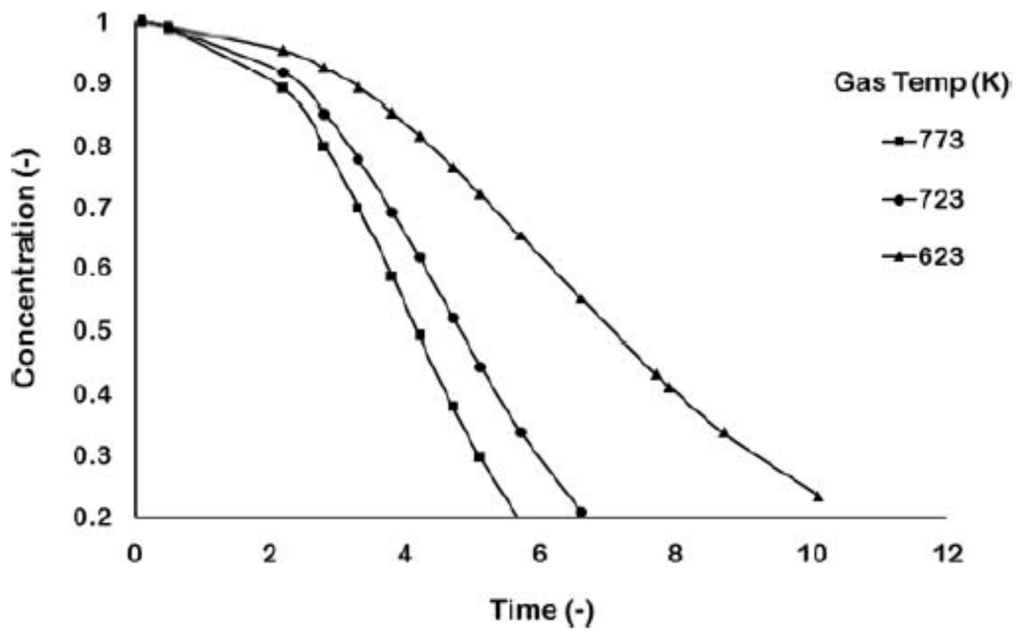


Figure 4. Exit concentration variation of acetaldehyde (100 ppm) with respect to time for different gas inlet temperatures.

Exit Concentration of Acetaldehyde with Aged and New Catalyst

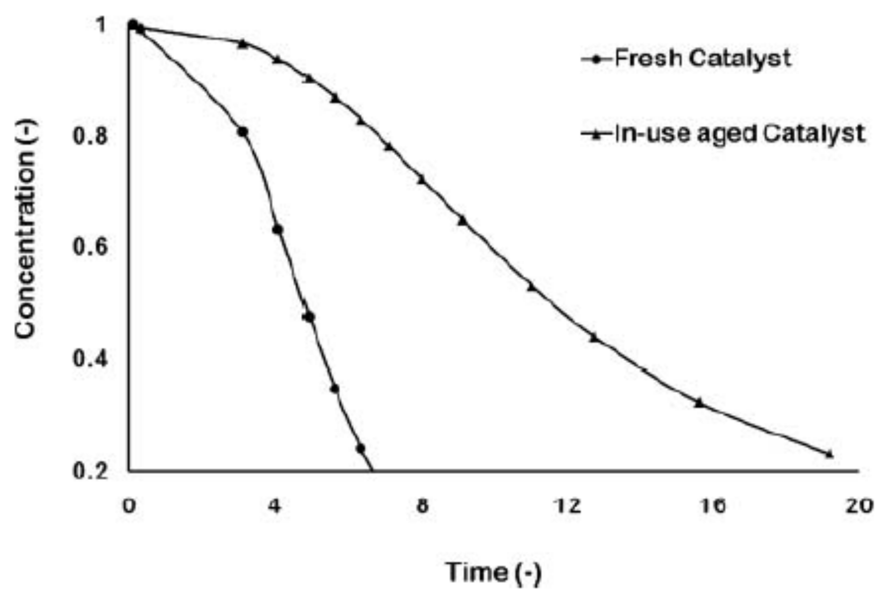


Figure 5. Exit concentration variation for acetaldehyde gas (100 ppm) at 723 K with time for fresh and in use aged catalyst.