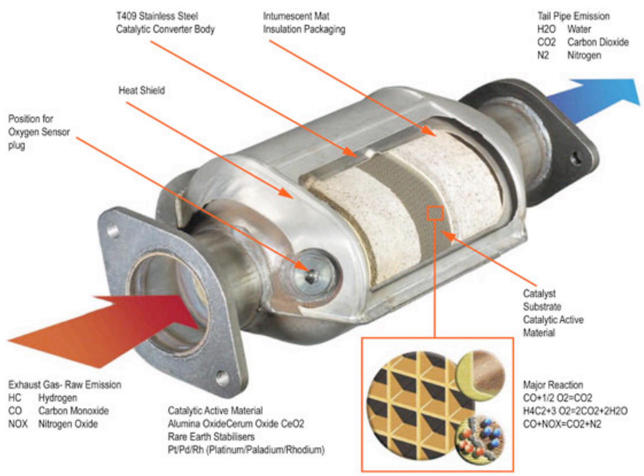
Model Development for a Catalytic Converter

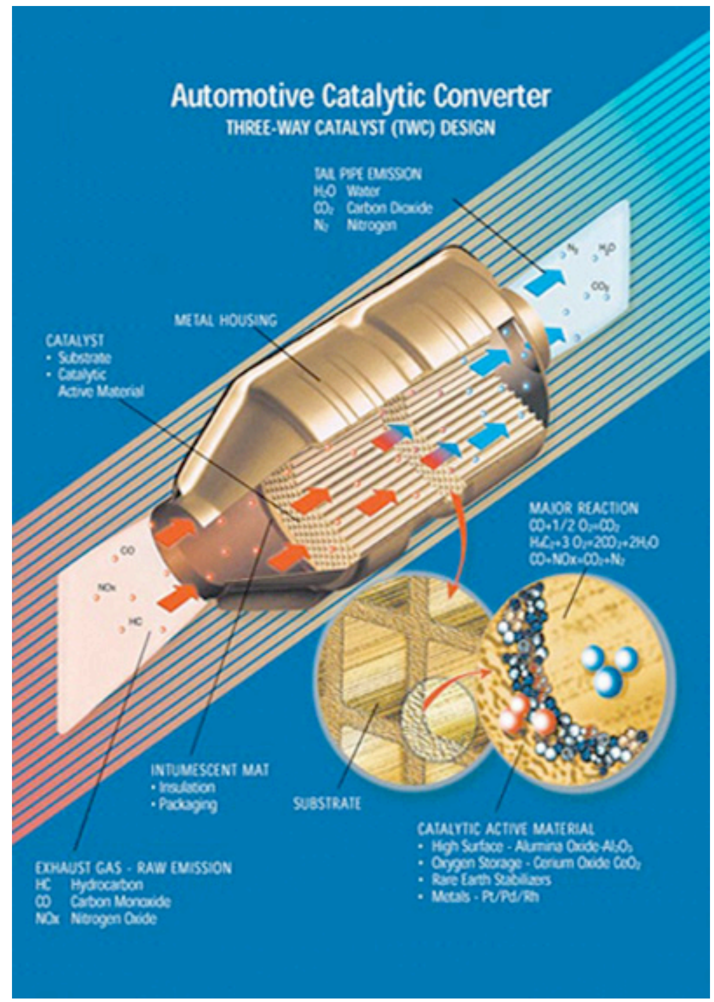
"If there is a regulation that says you have to do something—whether it be putting in seat belts, catalytic converters, clean air for coal plants, clean water—the first tack that the lawyers use, among others things, and that companies use, is that it's going to drive the electricity bill up, drive the cost of cars up, drive everything up. It repeatedly has been demonstrated that once the engineers start thinking about it, it's actually far less than the original estimates. We should remember that when we hear this again, because you will hear it again." Stephen Chu

Catalytic Converter Properties

Function: Reduce toxicity of engine emissions

- Honeycomb design presently employed to optimize surface area





Two-Way: Performs oxidation tasks; e.g.,

$$2CO + O_2 \rightarrow 2CO_2$$

$$2C_3H_6 + 9O_2 \rightarrow 6CO_2 + 6HO$$

$$2H_2 + O_2 \rightarrow 2H_2O$$

Three-Way: Additionally reduces nitrogen oxides

$$2NO_2 \rightarrow N_2 + 2O_2$$

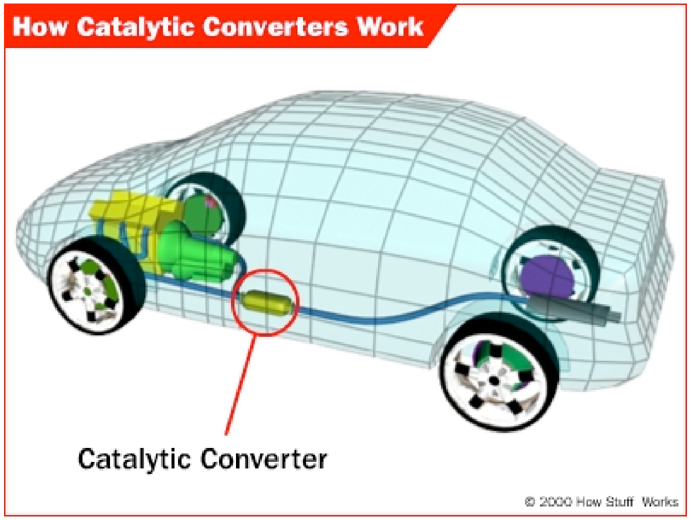
Catalytic Converter Properties

Issues:

- Catalysts: Platinum (Pt), Palladium (Pd) or Rhodium (Rh)
  - All are very expensive, have very limited supply sources, and limited future availability. Price makes them attractive to steal. Recycling is possible.
- Catalysts only work at fairly high temperatures
  - Position near engine but not too close
  - Preheating: Slow with 12 V battery; more effective in hybrids

Control Problem:

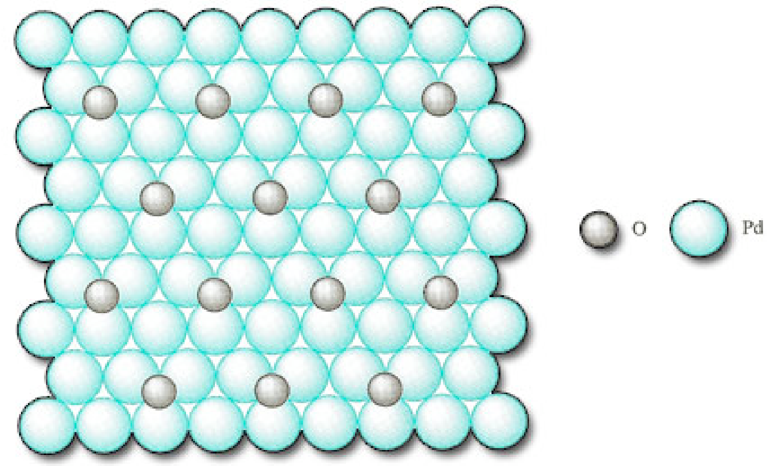
- Design heat source to optimize catalysis without damaging unit.



Oxidation Reactions

Two-Way Oxidation Reactions: Ignore NO reduction

$$
\begin{aligned}
2CO + O_2 &\rightarrow 2CO_2 \\
2C_3H_6 + 9O_2 &\rightarrow 6CO_2 + 6H_2O \\
2H_2 + O_2 &\rightarrow 2H_2O
\end{aligned}
$$



Notation:
$i = 1: \; CO$
$i = 2: \; C_3H_6$
$i = 3: \; H_2$
$i = 4: \; O_2$

Reaction Rates: c_i: Concentration of i^{th} species (mol/cm^3)
c_{NO}: Concentration of NO (non-reacting species) (ppm)

$$R_i = \frac{k_i c_i c_4}{G} \quad \left(\frac{\text{mol } c_i}{\text{cm}^2 \text{Pt} \cdot s} \right) \quad , \; i = 1, 2, 3$$

where

$$G = (1 + K_1 c_1 + K_2 c_2)^2 \left(1 + K_3 c_1^2 c_2^2\right) \left(1 + K_4 c_{NO}^{0.7}\right)$$

Oxidation Reactions

Rate Constants: Based on Arrhenius relation

$$k = Ae^{-E_a/RT}$$

Experimentally Determined Values: see [Oh, Cavendish 1985]

$$k_1 = 6.802 \times 10^{16} \exp(-13,108/T) \quad \left(\frac{\text{cm}^4}{\text{mol}\cdot s}\right)$$

$$k_2 = 1.416 \times 10^{18} \exp(-15,109/T) \quad \left(\frac{\text{cm}^4}{\text{mol}\cdot s}\right)$$

$$k_3 = k_1 \text{ since } \mathrm{H_2} \text{ oxidation inhibited by CO}$$

$$K_1 = 8.099 \times 10^{6} \exp(409/T) \quad \left(\frac{\text{cm}^3}{\text{mol}}\right)$$

$$K_2 = 2.579 \times 10^{8} \exp(-191/T) \quad \left(\frac{\text{cm}^3}{\text{mol}}\right)$$

$$K_3 = 1.13 \times 10^{21} \exp(9,299/T) \quad \left(\frac{\text{cm}^6}{\text{mol}^2}\right)$$

$$K_4 = 3.02 \times 10^{1} \exp(-3,733/T) \quad \left(\frac{\text{cm}^3}{\text{mol}}\right)$$

Note:

$$R_4 = \frac{1}{2}R_1 + \frac{9}{2}R_2 + \frac{1}{2}R_3$$

Device Model

Model Components:

- Conservation of Energy: Heat models
- Conservation of Material: Transport equations

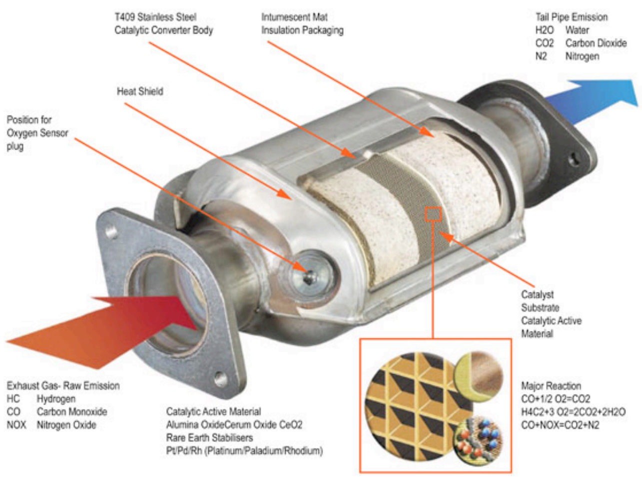
Notation:

T_g: Temperature of gas

T_s: Temperature of solid

c_{gi}: Concentration of species i in bulk gas stream

c_{si}: Concentration of species i in bulk gas stream



Assumptions:

- Ignore channel-to-channel variations
- Assume infinitely long channel

$$0 < x < \infty \, , \; t > 0$$

Heat Models

Heat Conduction in Ceramic:

$$\rho_s C_s \frac{\partial T_s}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial x^2} + Sh(T_g - T_s) + S \sum_{i=1}^{3} R_i(T_s, \vec{c})(-\Delta H)_i + Q\chi_{\text{input}}$$

Parameters:

- ρ_s: Density of the ceramic $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$
- C_s: Specific heat $\left(\frac{\mathrm{J}}{\mathrm{kg \cdot K}}\right)$
- λ_s: Thermal conductivity of solid $\left(\frac{\mathrm{J}}{\mathrm{m \cdot K \cdot s}}\right)$
- h: Heat transfer coefficient $\left(\frac{\mathrm{J}}{\mathrm{m^2 \cdot K \cdot s}}\right)$
- S: Surface to volume ratio of channel $\left(\frac{1}{\mathrm{m}}\right)$
- $-\Delta H$: Heat of i^{th} reaction $\left(\frac{\mathrm{J}}{\mathrm{mol}}\right)$
- Q: Control input

Example:

$$2\mathrm{H_2} + \mathrm{O_2} \rightarrow 2\mathrm{H_2O}$$

$$\Delta H = -285.83\ \mathrm{kJ/mol}$$

Heat Models

Heat Conduction in Ceramic:

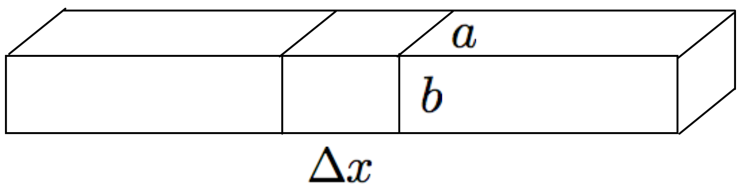
$$\rho_s C_s \frac{\partial T_s}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial x^2} + Sh(T_g - T_s) + S \sum_{i=1}^{3} R_i(T_s, \vec{c})(-\Delta H)_i + Q\chi_{\text{input}}$$

Derivation of 3rd Term: Consider channel with cross-sectional dimensions a and b

$$\frac{\partial(C_s \rho_s ab \Delta x T_s)}{\partial t} = q(t,x) - q(t, x + \Delta x) - 2\Delta x(a+b)h(T_s - T_g)$$

$$\Rightarrow \rho_s C_s \frac{\partial T_s}{\partial t} + \frac{\partial \mu}{\partial x} = Sh(T_g - T_s)$$

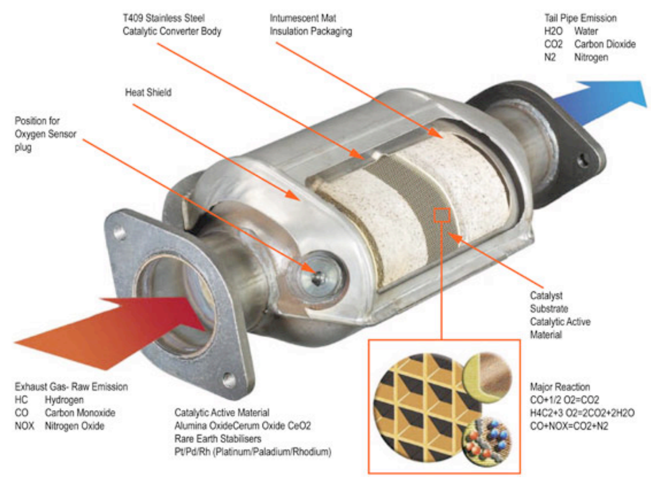
where $S = \dfrac{2(a+b)}{ab}$



Additional Assumption: Diffusion negligible

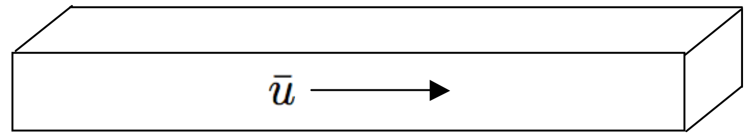
Boundary and Initial Conditions:

- Specify T_s at $x = 0$ for $t > 0$
- Specify T_s at $t = 0$ for all x



Heat Models

Heat Conduction in Exhaust:



- Assumption: Negligible diffusion

$$\rho_g C_g \frac{\partial T_g}{\partial t} + \frac{\partial \mu}{\partial x} = Sh(T_s - T_g)$$

- Constitutive relation: $\mu = \bar{u}\rho_g C_g T_g$

$$\Rightarrow \rho_g C_g \frac{\partial T_g}{\partial t} + \rho_g C_g \bar{u} \frac{\partial T_g}{\partial x} = Sh(T_s - T_g)$$

Steady State Flow:

$$\rho_g C_g \bar{u} \frac{\partial T_g}{\partial x} = Sh(T_s - T_g)$$

Parameters:

ρ_g: Density of the exhaust $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$

C_g: Specific heat $\left(\frac{\mathrm{J}}{\mathrm{kg}\cdot\mathrm{K}}\right)$

$\bar{u}$: Average exhaust velocity $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$

Boundary and Initial Conditions:

- Similar to solid

Reactant Models

Conservation of Reactant Species: Gas

$$\frac{\partial c_{gi}}{\partial t} + \bar{u}\frac{\partial c_{gi}}{\partial x} = k_m S(c_{si} - c_{gi})$$

k_m: Mass transfer coefficient $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$

Conservation of Reactant Species: Solid

$$k_m S(c_{gi} - c_{si}) = SR_i(T_s, \vec{c})$$