

Scenario

Cars utilise catalytic convertors to oxidise carbon monoxide in the exhaust gas into carbon dioxide. Current technology relies on alumina nanomaterials loaded with precious group metal nanoparticles. These are wash coated onto cordierite substrates that form the basis of the catalyst support.

This technology suffers from a substantial drawback as the catalytic material only becomes active once it reaches approximately 150°C.

In this problem, you will consider exhaust gas (300°C), containing 1at% carbon monoxide, entering the exhaust pipe (304 stainless steel, 10 cm length, 56mm outer diameter, 1mm wall thickness, initially at 25°C) at a rate of 50 L/s. The upstream face of the pipe is in perfect thermal contact with the exhaust manifold which maintains a constant temperature of 300°C.

The gases pass along the exhaust and through a catalyst (cordierite substrate, 1cm length, initially at 25°C) at the exit of the pipe. The catalyst has elements, each 1 mm thick, arranged in a 10×10 square grid, with 4mm separation between elements. See the provided diagram (page 3) for clarification.

Task

1. Calculate the time taken for the system to reach thermal equilibrium.
2. Prepare a temperature profile of the pipe's external surface along the length over this time period.
3. Prepare a temperature profile across the downstream surface of the catalyst over this time period.
4. Calculate the time taken for exhaust gases exiting the system to contain 0.01at% CO.
5. Prepare a plot of N_{CO} after passing through the exhaust against time over the direction of the time from task 4.
6. Consider the questions at the end.

Assumptions & Quantities

The following quantities may be used. They may be assumed as constant unless specified otherwise.

Gases

Density = 1.15 kg/m³

Thermal conductivity (=0.024 W/K·m)

Dynamic viscosity (=1.7×10⁻⁵ kg/m·s)

Specific heat = 720 J/kg·K

Exhaust gas composition 75% N, 15% O₂, 7% CO₂, 2% H₂O, 1% CO (at%)

Air composition 78% N, 21% O, 1% Ar (at%)

Exhaust gas may be assumed to be incompressible at all temperatures and pressures.

304 stainless steel

Density = 8030 kg/m³

Specific heat capacity = 450+0.28 T J/kg·K (T in °C)

Thermal conductivity = 16.3 W/K·m

Perfectly formed with no welds or breaks in symmetry.

Cordierite

Density = 2300 kg/m³

Specific heat capacity = 900 J/kg·K

Thermal conductivity = 2.5 W/K·m

Fluid flow

The exhaust gases are undergoing purely laminar flow, with no turbulence.

The pressure drop across the length of pipe may be neglected.

The exhaust gases enter the pipe at atmospheric pressure.

The catalyst grid does not induce any pressure drop or turbulence.

Boundary layers may be neglected.

Heat transfer

The thermal contact conductance between cordierite and stainless steel is infinite.

The thermal contact conductance between any solid and any gas is $2 \text{ W/m}^2\cdot\text{K}$.

Air outside the pipe maintains a steady temperature of 25°C .

Reaction Kinetics

The catalyst oxidises CO to CO_2 at the following rate:

$$\frac{\partial^2}{\partial A \partial t} N_{\text{CO}} = -C e^{-E/RT}$$

where T is temperature in Kelvin and R is the ideal gas constant, $E=100000$ and $C = 6.4 \times 10^{14}/\text{m}^2\text{s}$

The enthalpy of the CO oxidation reaction is zero.

You may assume that the surface of the catalyst is perfectly flat and homogeneous. Gases are adsorbed/desorbed instantaneously onto/from this surface with no upper limit on the amount of CO that may be adsorbed on the surface.

You may assume that the diffusion coefficient of CO in the exhaust gas is infinite in the radial direction and zero in the longitudinal direction.

Questions

1. What would happen if the exhaust gases were no longer considered incompressible?
2. How would you simulate the application of thermal insulation to the exterior of the pipe?
3. A new catalyst is developed that becomes operable at 125°C .
 - a. Qualitatively discuss the impact of this change.
 - b. Quantify the impact of this change. How long does it take for the scrubbed exhaust gases to achieve 0.01at% CO? [Use the same rate formula as before, using $E=70000$]
4. Consider the other assumptions given and highlight how the model would have to be altered to adjust for these changes.

Your Submission

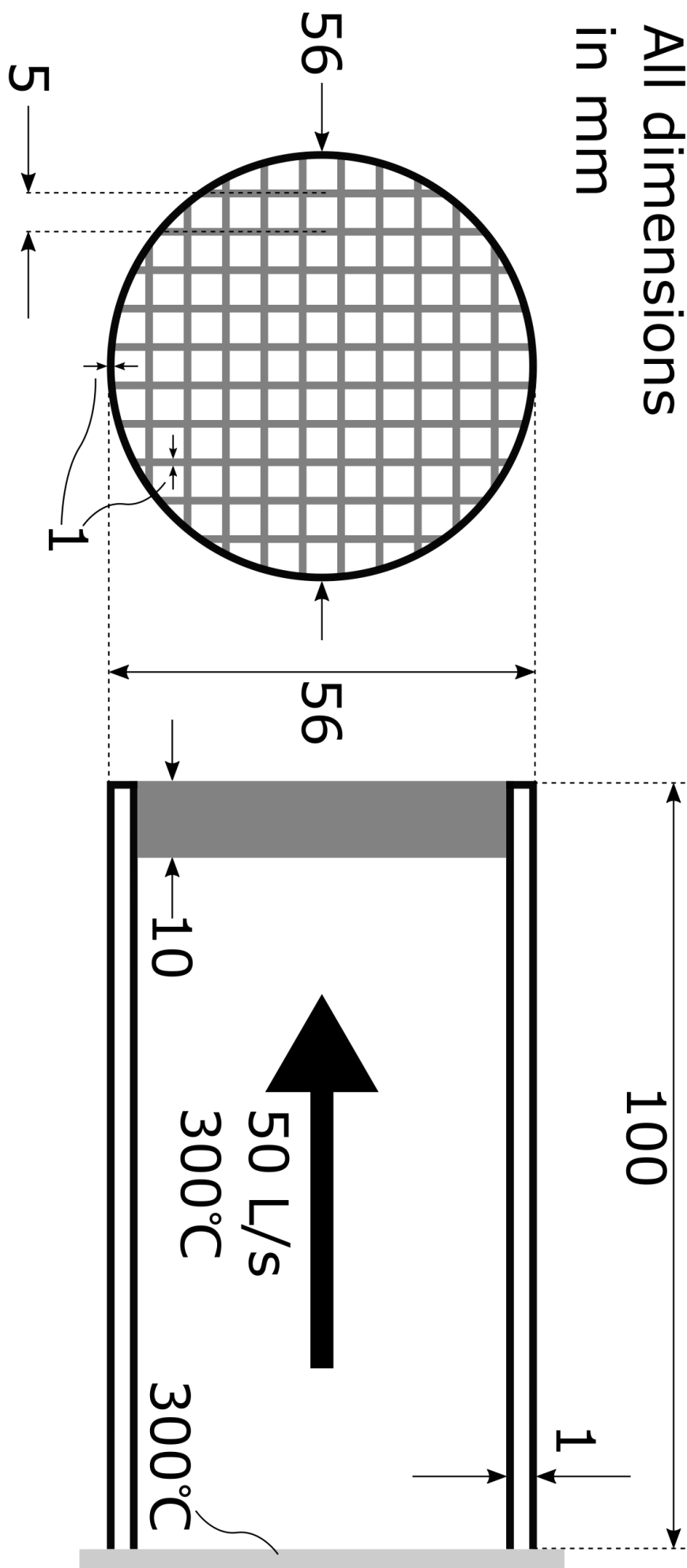
You must provide hand written and scanned, or computer typed notes of the relevant calculations from the notes required to complete the calculations. (30% of the rubric)

You may work cooperatively as a class using any programming language or any commercial or freeware package to solve the problem. However each student must make an individual submission prepared without collaboration that indicates how the code/programme/package was used, either through an explanation of the code or through a description of the necessary input and output files. (30% of the rubric).

You must include the responses to the tasks requested. (10% for the final figures and plots).

You must answer all the questions asked. (30% of the rubric).

Deadline: 0900 27th February 2020



Change Log

v1.1

- Add assumption about neglecting enthalpy of reaction.
- Rephrase Q3b.
- Provide new reaction rate formula for Q3b.
- Rephrased Heat Transfer assumptions (thermal contact *conductance* not *resistance*)
- Included deadline.
- Adjusted exhaust gas composition and added composition of air.
- Clarified diagram and scenario wording about the pipe boundary conditions.

v1.2

- Changed title of 'Reaction Rate' section to 'Reaction Kinetics'.
- Rephrased surface adsorption statement.
- Added statement about CO diffusivity in exhaust gas.

v1.2.1

- Changed 'equilibrium' to 'thermal equilibrium' in the tasks.
- Changed [CO] to N_{CO} in the tasks.