

Section 1: Supplementary calculations and reasoning

1.1 Fourier's Second law

To calculate the heat flux into a given differential volume, Fourier's second law may be used:

$$\begin{aligned}\frac{\delta T}{\delta t} &= \frac{k}{\rho c} \nabla^2 T(x, y, z, t) \\ \frac{1}{\delta t} &= \frac{Vk}{mc\delta T} \nabla^2 T(x, y, z, t) \\ \frac{mc\delta T}{\delta t} &= Vk \nabla^2 T(x, y, z, t) \\ dQ &= k \nabla^2 T(x, y, z, t) dV\end{aligned}$$

Where k is the thermal conductivity of the material,
 $T(x, y, z, t)$ is the scalar temperature field
and dQ is the total heat into an infinitesimal volume dV per second

Taking a second derivative from first principles is shown as follows:

$$\begin{aligned}\frac{\delta T}{\delta x} &= \lim_{h \rightarrow 0} \frac{T(x + \Delta h, y, z, t) - T(x, y, z, t)}{\Delta h} \\ \frac{\delta^2 T}{\delta x^2} &= \lim_{h \rightarrow 0} \left[\frac{T(x + \Delta h, y, z, t) - T(x, y, z, t)}{\Delta h} - \frac{T(x, y, z, t) - T(x - \Delta h, y, z, t)}{\Delta h} \right]\end{aligned}$$

As the pipe has been discretised into cubic nodes, each interior pipe node (nodes not on the surface) is surrounded by 6 other nodes with a distance of Δh between each cubic node. Applying Fourier's second law, the heat flux into an interior node is:

$$\begin{aligned}\Delta Q &= k\Delta V \lim_{h \rightarrow 0} \left\{ \frac{[T(x + \Delta h, y, z, t) - T(x, y, z, t)] - [T(x, y, z, t) - T(x - \Delta h, y, z, t)]}{(\Delta h)^2} \right. \\ &\quad + \frac{[T(x, y + \Delta h, z, t) - T(x, y, z, t)] - [T(x, y, z, t) - T(x, y - \Delta h, z, t)]}{(\Delta h)^2} \\ &\quad \left. + \frac{[T(x, y, z + \Delta h, t) - T(x, y, z, t)] - [T(x, y, z, t) - T(x, y, z - \Delta h, t)]}{(\Delta h)^2} \right\}\end{aligned}$$

For small values of Δh , this can be simplified to:

$$\Delta Q = \frac{k\Delta V}{(\Delta h)^2} \sum_i^6 T_i - T_0 \quad \dots (1)$$

Where T_0 is the temperature of the node
and T_i is the temperature of the i^{th} neighbour

For a boundary node, there is additional heat flux from the surroundings. A generalised formula of equation 1 is summarised below:

$$\Delta Q = \frac{k\Delta V}{(\Delta h)^2} \left(\sum_i^n T_i - T_0 \right) + h(\Delta h)^2 \left(\sum_j^{6-n} T_j - T_0 \right) \quad \dots (2)$$

Where n is the number of neighbouring nodes,
 h is the thermal contact conductance between the material and its surroundings
and T_{out} is the temperature of the surroundings.

Substituting $Q = mc(T) \frac{\Delta T}{\Delta t}$, the updated temperature of all nodes on the pipe after a time interval Δt may be found using equation 3. A Python programme was subsequently used to implement this equation to obtain the temperature profile across the external surface of the pipe and along the downstream surface of the catalyst.

$$\begin{aligned}\Delta mc(T) \frac{\Delta T}{\Delta t} &= \frac{k\Delta V}{(\Delta h)^2} \left(\sum_i^n T_i - T_0 \right) + h(\Delta h)^2 \left(\sum_j^{6-n} T_j - T_0 \right) \\ \frac{\Delta T}{\Delta t} &= \frac{1}{\Delta mc(T)} \left[\frac{k\Delta V}{(\Delta h)^2} \left(\sum_i^n T_i - T_0 \right) + \frac{h\Delta V}{\Delta h} \left(\sum_j^{6-n} T_j - T_0 \right) \right] \\ \frac{\Delta T}{\Delta t} &= \frac{1}{\rho c(T) \Delta h} \left[\frac{k}{\Delta h} \left(\sum_i^n T_i - T_0 \right) + h \left(\sum_j^{6-n} T_j - T_0 \right) \right] \\ T' &= T_0 + \frac{\Delta t}{\rho c(T) \Delta h} \left[\frac{k}{\Delta h} \left(\sum_i^n T_i - T_0 \right) + h \left(\sum_j^{6-n} T_j - T_0 \right) \right] \quad \dots (3)\end{aligned}$$

where T_0 and T' is the temperature of the node at present and at a step Δt into the future,
 ρ is the density of the material
and c is its specific heat capacity

1.2 Determining the speed of the gas through the pipe

The reduction in area in the region where the catalyst is present will increase the velocity of the gas, since the volume flow rate is constant across the pipe. Discretisation of the pipe into cubes of 0.5 mm lengths allows for the determination of the area fraction occupied by the catalyst in one segment of the pipe interior.

$$\text{Area fraction occupied by catalyst} = \frac{822}{2315} = 35.5\%$$

For the volume flow rate of the gas to be constant, the velocity of the gas must hence be increased. The velocity of the gas through the hollow pipe and the pipe with the catalyst is calculated as follows.

$$\text{Gas velocity through hollow pipe} = \frac{0.05}{\pi(27 \times 10^{-3})^2} = 21.8 \text{ m s}^{-1}$$

$$0.05 \text{ m}^3 \text{ s}^{-1} = \text{Gas velocity through pipe with catalyst} \times \text{Reduced area}$$

$$\text{Gas velocity through pipe with catalyst} = \frac{0.05}{(1 - 0.355) \times \pi(27 \times 10^{-3})^2} = 33.8 \text{ m s}^{-1}$$

1.3 Determining the amount of CO extracted by catalyst

Since carbon monoxide is assumed to have an infinite diffusion coefficient in the radial direction while it has a diffusion coefficient of zero in the longitudinal direction, the removal of CO only occurs along the downstream surface area of the catalyst, and not at the first instance when the gas is incident on the catalyst. The time taken for exhaust gas particles in one slice of the catalyst filled pipe, to travel one discretised length is presented below.

$$t_c = \frac{0.5 \times 10^{-3}}{33.8} = 0.0000148 \text{ s} \quad \dots (4a)$$

Where t_c is the time taken for one cross sectional segment of the discretised gas to travel one discretised length in the region of the pipe with the catalyst

The surface area of one face of one discretised catalyst element is as follows.

$$A = (0.5 \times 10^{-3})^2 = 2.5 \times 10^{-7} \text{ m}^2 \quad \dots (4b)$$

The number of CO molecules removed by 1 discretised surface of the catalyst may be derived using equations 4a, 4b and 4c.

$$\frac{\delta^2}{\delta A \delta t} N_{CO} = -C e^{-\frac{E}{RT}} \quad \dots (4c)$$

$$\begin{aligned} \Delta N_{CO} &= -C e^{-\frac{E}{RT}} \times (2.5 \times 10^{-7}) \times 0.0000148 \\ &= -4 \times 10^{27} \times 2.5 \times 10^{-7} \times 0.0000148 e^{-\frac{30000}{RT}} \\ &= -1.48 \times 10^{16} \times e^{-\frac{30000}{RT}} \end{aligned}$$

1.4 Finding the amount of CO removed in a discretised model

Using the discretisation of the pipe, the number of CO molecules removed by all catalyst elements in the pipe is summarised by the equation below. It should be noted that only some catalyst elements have an exposed surface to the gas and only these can contribute to the removal of CO.

$$\text{Total } \Delta N_{CO} = - \sum_{i=1}^n 1.48 \times 10^{16} \times e^{-\frac{30000}{RT}} \quad \dots (5)$$

Where n is the number of catalyst elements with an exposed surface area to the exhaust gas
T is the temperature of a particular exposed catalyst element

1.5 Determining the initial and target carbon monoxide emission rates

Volume and mass of exhaust gas in 1 slice of the discretised pipe filled with catalyst is as follows.

$$\begin{aligned} V(\text{gas}) &= \pi \times (27 \times 10^{-3})^2 \times 0.5 \times 10^{-3} \times (1 - 0.355) = 7.39 \times 10^{-7} \text{ m}^3 \\ \text{mass}(\text{gas}) &= 7.386 \times 10^{-7} \times 1.15 = 8.49 \times 10^{-7} \text{ kg} \end{aligned}$$

Before any CO was removed from the catalyst, the mass fraction of CO was found as follows (Taking molar mass of Carbon as 12 g mol⁻¹, Oxygen as 16 g mol⁻¹, nitrogen as 14 g mol⁻¹ and hydrogen as 1 g mol⁻¹).

$$\text{mass fraction of CO} = \frac{0.01 \times 28}{0.75 \times 28 + 0.15 \times 32 + 0.07 \times 44 + 0.02 \times 18 + 0.01 \times 28} = 0.00949$$

Mass and number of molecules of CO gas in 1 slice of the discretised pipe filled with catalyst can subsequently be calculated.

$$\text{Initial mass(CO)} = 0.00949 \times 8.4939 \times 10^{-7} = 8.06 \times 10^{-9} \text{ kg}$$

$$\text{Initial } N(\text{CO}) = \frac{8.06 \times 10^{-9}}{0.028} \times 6.02 \times 10^{23} = 1.73 \times 10^{17}$$

$$\text{Target } N(\text{CO}) = 1.73 \times 10^{17} \div 100 = 1.73 \times 10^{15}$$

The number of moles of carbon monoxide that needs to be extracted from one cross section to reach the target CO concentration can be found from the difference.

$$N(\text{CO}) \text{ to extract} = 1.73 \times 10^{17} - 1.73 \times 10^{15} = 1.7127 \times 10^{17}$$

The initial and target emission levels of CO per second can then be calculated as follows.

$$\text{Initial } N(\text{CO}) \text{ emitted per sec} = 1.73 \times 10^{17} \div 0.0000148 \text{ s} = 1.17 \times 10^{22} \text{ s}^{-1}$$

$$\text{Target } N(\text{CO}) \text{ emitted per sec} = 1.17 \times 10^{22} \div 100 = 1.17 \times 10^{20} \text{ s}^{-1}$$

Section 2: An overview of the python code

2.1 Modelling the pipe and the catalyst

To reduce the computational complexity of the pipe, only a quarter of the pipe is considered, because the rest of the data points may be extrapolated by symmetry. Using the RasterQuad() and RasterCat() functions, the pipe can be discretised into squares with sides of 0.5 mm. The discretised cross sections of the pipe with and without the catalyst is shown in figure 1.

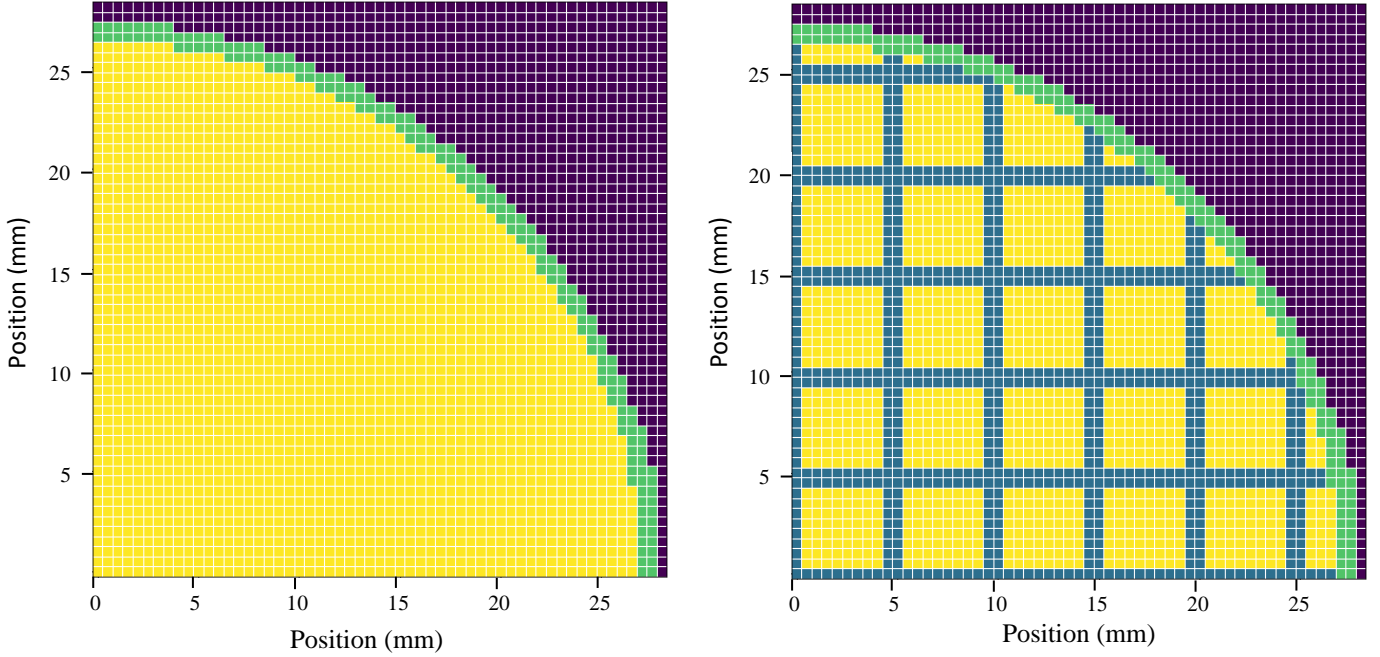
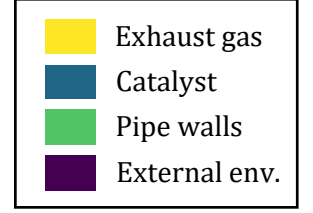


Figure 1: Discretised cross sections of a quarter of the pipe without the catalyst (Left) and with the catalyst (Right)

2.2 Discretisation of the pipe and the setting of temperature

A cartesian coordinate system was employed and a quarter of the pipe, with the surrounding environment, was discretised into squares with sides of 0.5 mm. A 3 dimensional numpy array (pipe [y, x, z]) was used to store these positions, and the initial temperature of all points were set to 298 K. In the RasterQuad() function, the maximum number of squares that could fit within the outer radius of the pipe was determined as follows.

$$S = \frac{R_o}{dx} = \frac{28 \text{ mm}}{0.5 \text{ mm}} = 56$$

Where S is the number of squares that can fit in the outer radius,
 R_o is the outer radius of the pipe
 and dx is the length of the discretised square

Knowing that (56 – 2) squares can fit in the y-direction of the pipe interior since the walls were 1 mm thick, the number of squares that can fit in the x direction was then determined at each y position. Trigonometry was used to determine the maximum number of squares that could fit in the x direction of the pipe interior for a particular value of y. This relationship is summarised by equation 6.

$$S_x(y) = \frac{R_i}{dx} \times \cos \theta \quad \dots (6)$$

Where S_x is the number of squares for a given y value,
 R_i is the inner radius of the pipe
 and $\theta = \sin^{-1}(y/R_i)$

A similar procedure was used to determine S_x for the outer radius, and the position and temperature of the corresponding pipe interior and pipe wall were saved into separate key value pairs (dictionaries of pipe_inner and pipe_nodes respectively). The temperature for the entire pipe interior was updated to 573K in the 3 dimensional pipe [y, x, z] array, because it was found that the linear speed of the gas was high and would have flowed through the gas pipe in less than one time step (time step set at 0.01 s).

$$\text{Gas linear speed} = \frac{0.05 \times 10^9}{\pi(27)^2} = 21800 \text{ mm s}^{-1}$$

$$\text{Time to pass through entire pipe} = \frac{100}{21800} \cong 0.00459 \text{ s}$$

Note: Gas would take less than 0.00459 s because of the reduced surface area in the catalyst, as explained in section 1.2

To model the catalyst, a blue grid representing the catalyst was superimposed onto a red circle representing the cross section of the pipe (not including the pipe walls), as shown in figure 2. The blue and green region consists of discretised squares that have a length of 0.5 mm. The position of the blue squares with an x and y coordinate > 0 is saved in the pos_cat_pos array as these squares may fall in the first quadrant of the circle.

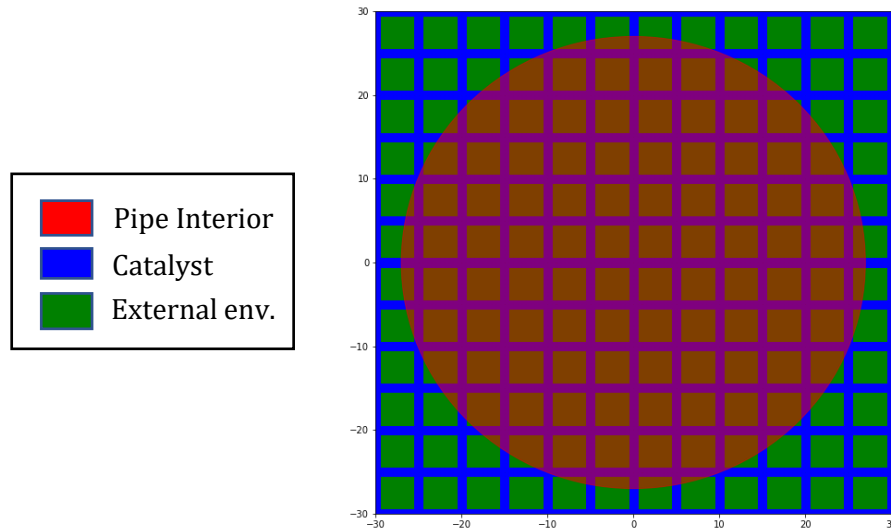


Figure 2: Superimposing a catalyst grid onto the cross section of the pipe

The data saved in pos_cat_pos was subsequently checked to ascertain whether they fall in the pipe_inner dictionary. If they did, the temperature at these positions were set to 298 K and their positions were saved in a separate pipe_cat dictionary.

2.3 Material Setup

Classes steel_ and catalyst_ were used to store the density, thermal conductivity and specific heat capacity of the stainless steel wall and the cordierite catalyst.

2.4 Fourier's 2nd Law

Implementation of Fourier's 2nd law is performed for both the pipe walls and the catalyst in the f2l_pipe() and f2l_pipe() functions. For each position on the pipe wall and the catalyst, the temperature of its neighbours is found.

In 3 dimensions, each point has 6 neighbours, and if it happens that the compared position is out of bounds from the 3 dimensional pipe[y, x, z] numpy array, the temperature of the point not in the numpy array would be extrapolated by logical deduction. In the case where the compared position is out of bounds in the x or y directions, then the temperature at the compared position is taken to be the same as the current position, because the same material extends outwards by symmetry. In the case when the compared position is out of bounds in the z direction, the temperature at the compared position is taken to be either 300 °C or 25 °C (The former if it is the side in contact with the manifold, the latter if it is the side in contact with air).

If the compared position is within the 3D array, then a cross check with the various dictionaries would be made to determine if the compared position is a point on the pipe wall, catalyst, interior gas or external environment. Compared positions are determined to be non-neighbours if their thermal contact conductance is not infinite.

Equation 3 is then used to determine the new temperature of the current point. This value is saved in a dictionary, and the new temperature would only be applied to the 3D numpy array when the new temperatures for all points are calculated.

2.5 Acquiring temperature profiles

Temperature profiles for task 2 and 3 were acquired by using the `tabulate_data()`, `plot_graph()` and `VisualiseXsect()` functions. In essence, `tabulate_data()` stores the required data for a specified range of points over a specified time interval. `Plot_graph()` processes the time, x-position, and temperature to provide a heatmap that allows one to visualise how the temperature profile of the desired section of the pipe varies with time. `VisualiseXsect()` allows one to visualise a specified cross section of the pipe.

2.6 Determining the area fraction of catalyst

The area fraction of the catalyst can be determined by finding the ratio of the number of elements in one cross section of the pipe over the total number of elements in the pipe interior.

2.7 Extraction of CO

If extraction of CO is enabled, the catalyst may be activated at the specific temperature set (`cat_work_temp`). Alternatively, assuming a smooth curve, this would not need to be used and can be set to zero. Using the equation derived in section 1.3, the amount of carbon monoxide removed by one catalyst element is calculated, if the temperature of the catalyst reaches its activation temperature.

This is repeated for all catalyst elements with an exposed surface to gas and the total amount of CO extracted is calculated (Equation 5). The carbon monoxide emission rate is subsequently calculated and checked if it has met the target emission rate, after which the simulation terminates (Refer to section 1.5).

2.8 User interface

To run a simulation, refer to the top of the second cell to adjust input parameters if required. Select the type of data to calculate in the 'functionalities' segment. To save images of the downstream surface of the catalyst, set `save_downstream_img` to True and create a file named `Surface_data` in the local folder directory. View the temperature profiles and graphs generated at the bottom or saved in the directory. Refer to comments in the code for further details.

Section 3: Solutions to Tasks

Task 1:

Calculate the time taken for the system to reach thermal equilibrium.

It was determined that equilibrium was reached when the following criteria was fulfilled for all discretised volume elements in the model.

$$\Delta T < 0.1K \text{ for } \Delta t > 1s$$

Since a time step of 0.01 s was used, a change in temperature of less than 0.001 K was required for thermal equilibrium to be achieved. It was found that this criterion was reached on the 76417th time step, indicating that it took 764.17 s for thermal equilibrium to be reached.

Task 2:

Prepare a temperature profile of the pipe's external surface along the length over this time period.

A straight line along the discretised, external surface of the pipe was chosen and the time interval was set to 0.01s. The temperature of each point along this straight line of the pipe was recorded at every time interval and plotted as shown in figure 3. This straight line is representative of the entire external surface, because heat conduction would be identical along any line due to the symmetry of the defect less and perfectly welded metal pipe.

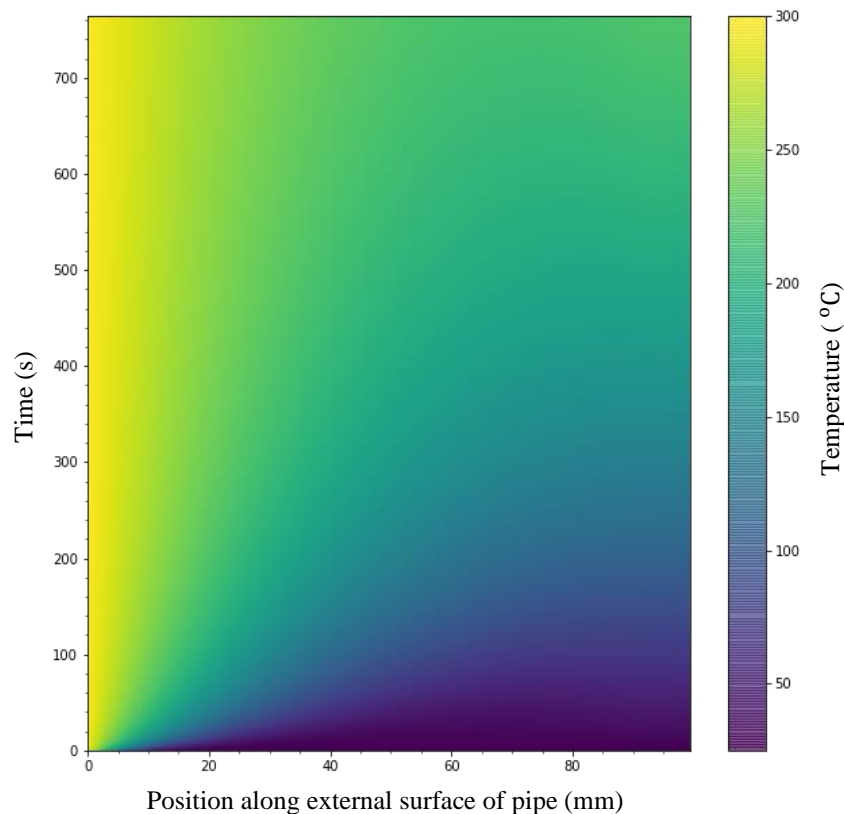


Figure 3: Temperature profile along the pipe's external surface.
The pipe node at a position of 0 mm is in contact with the manifold

It can be observed that in the region near the manifold, heat is constantly conducted away from the manifold to the rest of the pipe. Heat transfer in the pipe is predominantly by conduction between solids, otherwise the entire pipe should heat up at a more even rate. This computational result is logical because the thermal contact conductance between gas and solid ($2 \text{ Wm}^{-2}\text{K}^{-1}$) is much lower than that between solids (Taken to be infinite).

Additionally, a significantly longer time was taken to heat the external surface in the region between 90 and 100 mm. This is consistent with the fact that in this region, the catalyst was in thermal contact with the wall and would thus conduct heat away from the wall.

It should also be noted that at equilibrium, the temperature gradient observed along the external surface is expected, because heat is continuously loss to the environment and more loss is expected further from the manifold.

Task 3:

Prepare a temperature profile across the downstream surface of the catalyst over this time period.

The time interval was set to 0.01s. The temperature of each point on the downstream surface was recorded at every 0.5 s time interval and a selected plot is shown below. The remaining plots may be accessed through the movie file attached in the blackboard submission (Video plays at 50 Frames per second, with each frame representing a 0.5s time interval). It can be observed that the catalyst heats up symmetrically.

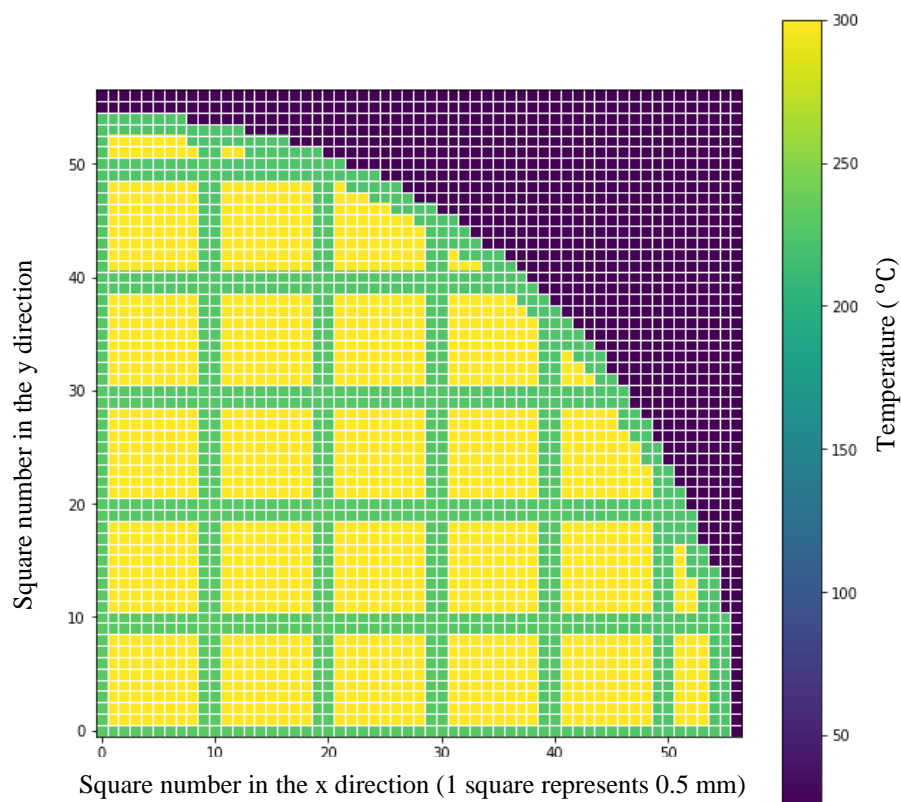


Figure 4: Final temperature profile along the downstream surface of the catalyst ($t = 764.17\text{s}$)

Task 4:

Calculate the time taken for exhaust gases exiting the system to contain 0.01mol% CO.

31889 time steps passed before the exhaust gases exiting the system contained 0.01 mol% CO. It therefore took 318.89 s.

Task 5:

Prepare a plot of N_{CO} after passing through the exhaust against time over the direction of the time from task 4.

The graph requested is as shown in figure 5.

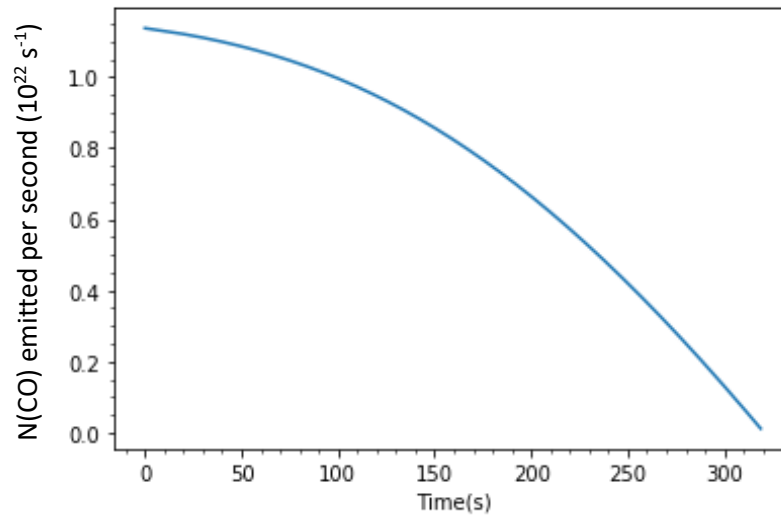


Figure 5: Graph of the amount of CO emitted per second over time

Section 4: Responses to Questions

Question 1:

What would happen if the exhaust gases were no longer considered incompressible?

Exhaust gas in the catalyst segment of the pipe have higher speeds compared to that in the rest of the pipe. As Bernoulli's principal states that higher fluid speeds lead to a decrease in pressure of the fluid, a pressure drop is expected across the length of the pipe.

If the gas was no longer incompressible, the exhaust gas would expand and occupy a larger volume due to the lower gas pressure nearer the outlet of the pipe. As gas particles are now further spaced apart, they will cool down. This is analogous to how fridges are cooled, which is by passing pressurised coolants from a higher pressure to a lower pressure. Reducing the temperature of the gas particles reaching the catalyst would cause the catalyst to be less efficient at removing CO since the catalyst will heat up slower and would hence cause less CO to be removed by the catalyst. This effect is not very significant since the thermal contact conductivity between air and solid is low.

Additionally, expansion of the gas must result in faster volume flow rate in the region of low pressure to maintain a constant mass flow rate. This suggests that the velocity of the gas particles in the catalyst region is even higher than that calculated previously. Since less time is now available for the exhaust gas particles to interact with the catalyst, the catalyst will be even less effective in removing CO.

Question 2:

How would you simulate the application of thermal insulation to the exterior of the pipe?

Perfect thermal insulation can be simulated by setting the thermal contact conductance to zero for all nodes (along the longitudinal direction of the pipe) that are one discretised distance away from the pipe exterior. More realistically, the thermal contact conductance for the thermal insulation should be set to some lower, arbitrary value, and depending on the thickness of the insulation, an appropriate number of nodes away from the pipe exterior can have that particular thermal contact conductance.

To implement this in the code, I would first create a new class containing information about the new insulation material. I would require the material density, specific heat capacity and thermal contact conductance. I would then raster the new material as a layer surrounding the exterior walls of the pipe and write a function similar to that described in `f2l_pipe()`. After which, the simulation can be run to obtain temperature profiles of the desired regions on the pipe, to observe the effect of the additional thermal insulation.

Question 3:

A new catalyst is developed that becomes operable at 125°C.

- Qualitatively discuss the impact of this change.
- Quantify the impact of this change. How long does it take for the scrubbed exhaust gases to achieve 0.01mol% CO? [Use the same rate formula as before, using $E = 28.5 \text{ kJ mol}^{-1}$]

Part (a):

It was previously determined from equation 5 that the number of carbon monoxide molecules removed from the exhaust gas is exponentially dependent on the value of E and proportional to the value of C .

$$\text{Total } \Delta N_{CO} = - \sum_{i=1}^n 3.7 \times 10^{-12} \times C e^{-\frac{E}{RT}}$$

For the catalyst to become operable at 125 °C, either C needs to be increased or E needs to be decreased, or a combination of the two. Since the operating temperature of the catalyst is lower, an appreciable reduction in carbon monoxide emissions may be achieved in a shorter frame of time. This is particularly useful for applications where the exhaust pipe system is started and cooled repeatedly, such as in cars that are likely to be stuck in traffic jams. Conversely, this change will have less of an impact if the system is constantly in operation and the temperature of the catalyst would reach temperatures much higher than 125 °C.

Part (b):

Using $E = 28.5 \text{ kJ mol}^{-1}$, the new model predicts that after 24828 steps, or 248.28 s, the exhaust gas achieves 0.01 mol% CO.

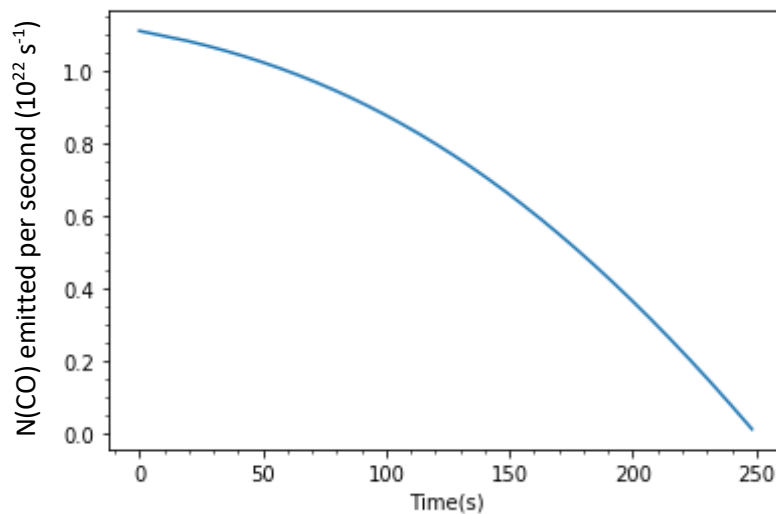


Figure 5: Graph of the amount of CO emitted per second over time

Question 4:

Consider the other assumptions given and highlight how the model would have to be altered to adjust for these changes.

Assumption: Laminar flow and boundary layers

The Reynolds number (Re) for air flowing in the pipe can be calculated according to equation 7.

$$Re = \frac{\rho v L}{\mu} \quad \dots (7)$$

Where ρ is the density of air,

v is the velocity of the air

L is the characteristic diameter of fluid flow

μ is the viscosity of the air

In the initial segment of the pipe, the Reynolds number can thus be calculated as follows. This suggests that the assumption that the exhaust undergoes laminar flow, with no turbulence is inconsistent with reality because the Reynolds number is much larger than 4000 ($Re > 4000$ is considered to result in turbulent flow for gases).

$$Re = \frac{1.15 \times \frac{0.05}{\pi(27 \times 10^{-3})^2} \times 54 \times 10^{-3}}{1.7 \times 10^{-5}} = 79800$$

Additionally, the assumption to ignore boundary layers was arbitrary because in incompressible fluid flow, air particles adjacent to the pipe walls would collide and lose some of their momentum to the wall. The decrease in momentum is analogous to friction acting on particles adjacent to the inner pipe walls. A velocity gradient would be set up, and as particles exchange momentums with particles further from the wall, the wall affected zone would grow until it fills the pipe interior.

The model can be changed to include the Navier-Stokes equations that account for the velocity and pressure of a fluid flow, with each component being broken down into a mean and a fluctuating part. Common computational models that can be used is the K-epsilon turbulence model (1). This can be done by implementing two partial differential equations involving turbulent kinetic energy and the dissipation of turbulent kinetic energy. Another method would be to implement multiscale models for computational fluid dynamics (2). This model is ideal for this problem as it is an efficient method to model the flow of fluids with a large range of Reynold numbers and small boundary layers.

Assumption: No pressure drop across the length of pipe, gas enters at atmospheric pressure

Unless a fan is present, it is unlikely that gas enters at atmospheric pressure because there would otherwise be no driving force for gas to flow in the direction assumed by the model. It is hence expected that gas enters at a pressure above atmospheric pressure, creating a pressure drop across the pipe.

In established laminar flow for incompressible air through a pipe, the rate of pressure drop across the length of the pipe is constant. This induces a maximum velocity for gas particles at the central axis, and a minimum velocity at the walls of the pipe. The equation described below may be used to determine the velocity of CO gas at various parts of the catalyst.

$$v = \frac{1}{4\mu} \cdot \frac{\Delta P}{L} (r_0^2 - r^2)$$

Where v is the velocity of the gas, μ is dynamic viscosity of the gas,

ΔP is the pressure drop across the pipe, r_0 is the radius of the pipe

r is the distance of gas from the centre

This formula may be implemented for each discretised element of gas in the pipe, to understand how a distribution of CO particle's x and y coordinates affects the overall interaction time with the catalyst. Successful implementation would hence affect the emission rate of CO.

Assumption: Thermal contact conductance is infinite between solids

The thermal contact conductance of metal plates is in the order of $10^2 \text{ Wm}^{-2}\text{K}^{-1}$ (3) and is far from being infinite. Since thermal contact conductance depends significantly on surface roughness, it would be useful to determine the manufacturing process of the cordierite and the stainless steel pipe and get a rough estimate of the surface roughness and their thermal contact conductance. This can be easily implemented by changing the calculation of thermal contact conductance in the steel_ and catalyst_ class defined in the code, and by considering the two material nodes as non-neighbours. It is likely that this would have little effect on any output, however, as the thermal contact conductance of these materials are still several magnitudes higher than that between air and steel.

Assumption: External air temperature fixed at 25 °C

Assuming that the air outside the pipe maintains a constant 25 °C is also unrealistic as the heat loss by the external pipe surface would be transferred to the surrounding air, thereby heating it up. To improve the model, several layers of air nodes adjacent to the external surface of the pipe should be considered during the calculation of Fourier's Second law. This would not have a large effect as the thermal contact conductance of air with metal is low, and successful implementation of this would need to account for non-trivial convection currents that would probably have removed the excess heat from the air nodes adjacent to the pipe.

Assumption: Enthalpy of reaction is 0

It is likely that the catalyst provided a lower alternative reaction pathway that is energetically favourable. Removal of CO by the catalyst is thus likely to involve an exothermic reaction, and hence would be an additional heat source in the pipe. Accounting for the heat source requires an additional term in Fourier's second law, as described below. This can be implemented into the code by modifying equation 3 appropriately.

$$\frac{\delta T}{\delta t} = \frac{q}{\rho c} + \frac{k}{\rho c} \nabla^2 T(x, y, z, t)$$

Where q is the heat generation rate per unit volume of the material

The implication of this change would be that of an autocatalytic effect. As the catalyst is activated and generates heat, the temperature of the catalyst increases and rate of removal of carbon monoxide increases.

Assumption: Instant adsorption/desorption of and CO and lack of an upper limit on adsorption

In reality, time is required for CO molecules to diffuse and adsorb onto the catalytic surface. Additionally, there are finite catalytic sites and thus there would be a local limit on the amount of CO that can adsorb onto a particular surface.

The former assumption can be corrected by creating a model that simulates CO particles moving in random directions, but still flowing through a pipe. In this model, only CO molecules that land on the catalytic surface and stay for a certain period of time to allow for adsorption would undergo the reaction. Empirical data can be collected to determine the probability that a CO molecule successfully undergoes the catalytic reaction. Accounting for the fact that not all CO molecules would have the chance to react at the catalytic sites can provide a more realistic, reduced rate of catalytic conversion.

The latter assumption can be accounted for by assigning a maximum threshold to each catalytic element. When this threshold is reached, no further CO can adsorb onto the surface, even if it meets the 1st criterion. This effect would account for local saturation of the catalyst and similarly lead to a more realistic, reduced rate of catalytic conversion.

Assumption: Surface of catalyst is perfectly flat and homogeneous

A catalyst may purposefully have an uneven surface to increase its surface area and sites for catalytic conversion to take place. The additional surface area may be accounted for by using a smaller discretisation value (< 0.5 mm) to account for the small burrs or defects present on the surface. This would lead to a slight increase in catalytic conversion rates.

In addition, homogeneity is impossibly hard to achieve since small local differences in compositions would likely be introduced during the manufacture of the cordierite. As the composition would affect its effectiveness at catalysing the CO, if the compositional map of the catalyst is known, a fudge factor can be applied to equation 4, to account for the effects of compositional differences at each local catalytic element.

Assumption: Diffusion coefficient of CO in the exhaust gas is infinite in the radial direction and zero in the longitudinal direction

Firstly, this assumption ignores the fact that the chemical potential of CO would be reduced if diffusion were to occur in the longitudinal direction. Since the concentration of CO outside the pipe is lower than that in the pipe, a concentration gradient would be set up and diffusion of CO would occur in the direction of gas flow. Fick's first law may be used in the model, assuming that the concentration profile remains similar over time. Fick's second law may additionally be used if precise results are required and the concentration profile needs to be updated with time. Accounting for diffusion of CO in the longitudinal direction would increase the flow rate of CO out of the pipe and hence reduce the time CO molecules spend at the catalyst. This will consequently increase CO emission. Additionally, a non-zero diffusion in the longitudinal direction would mean that the CO that is incident on the XY surface of the catalyst can be adsorbed and the CO may be removed. This will increase the CO removal rate.

An infinite diffusion coefficient of CO in the radial direction assumes that all CO molecules would be able to diffuse to a catalytic site, regardless of its initial position in the catalytic segment of the pipe. A more realistic representation of diffusion would be to similarly use Fick's first and second laws to model the concentration gradient and how it changes with time. The diffusion rate of CO molecules and proportion of CO molecules that can diffuse to the catalyst before being ejected from the pipe may subsequently be calculated and used as a fudge factor to decrease the CO removal rate.

Assumption: Ideal gas

This assumption is incorrect, and the ideal gas law cannot be used in this task. A mathematical proof may be found below. As the ideal gas law was not applied in the code, no correction is required.

$$\text{Molar mass of gas} = 0.75 \times 28 + 0.15 \times 32 + 0.07 \times 44 + 0.02 \times 18 + 0.01 \times 28 = 29.52 \text{ g mol}^{-1}$$

$$PV = nRT \Rightarrow P = \frac{n}{V}RT \Rightarrow P = \frac{\rho}{M}RT$$

Where ρ is the density of the exhaust gas

M is the molar mass of the exhaust gas,

P is the pressure of the exhaust gas

V is the volume of the exhaust gas

and T is the temperature of the exhaust gas

$$P = \frac{1.15}{0.02952} \times 8.314 \times 573 = 185 \text{ kPa} \neq 100 \text{ kPa}$$

References

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