

Perfectly stirred reactor

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Correction

1°) We start with the thermal balance:

$$\frac{d}{dt} \int_V \rho c_p T dV = \int_V -q_p R_{Fu} dV - \int_{S_1} \rho c_p T \mathbf{v} \cdot \mathbf{n} dS - \int_{S_2} \rho c_p T \mathbf{v} \cdot \mathbf{n} dS \quad (1)$$

c_p is constant and the mixture is homogeneous in space

$$M c_p \frac{dT}{dt} = \int_V -q_p R_{Fu} dV - \int_{S_1} \rho c_p T \mathbf{v} \cdot \mathbf{n} dS - \int_{S_2} \rho c_p T \mathbf{v} \cdot \mathbf{n} dS \quad (2)$$

q_p is a constant and $R_{Fu} = -k_0 e^{-\frac{T_{act}}{T}} \rho_{Fu} = -k_0 e^{-\frac{T_{act}}{T}} Y_{Fu} \rho$

$$M c_p \frac{dT}{dt} = -q_p \tilde{R}_{Fu} M - \int_{S_1} \rho c_p T \mathbf{v} \cdot \mathbf{n} dS - \int_{S_2} \rho c_p T \mathbf{v} \cdot \mathbf{n} dS \quad (3)$$

Finally, using the definitions of T_{fr} and T_{br} ,

$$M c_p \frac{dT}{dt} = -q_p \tilde{R}_{Fu} M + c_p \dot{m} T_{fr} - c_p \dot{m} T_{br} \quad (4)$$

which gives, using the definition of τ_s ,

$$\frac{dT}{dt} = -\frac{q_p}{c_p} \tilde{R}_{Fu} - \frac{(T_{br} - T_{fr})}{\tau_s} \quad (5)$$

The first term on the right hand side of Eq. (5) represents heat generated from the chemical reaction and the second term represents heat evacuated by convection (replacement of gases at T_{br} by gases at T_{fr}). Equation (5) tells that if you generate more heat by chemistry than you evacuate by convection, temperature in the PSR will increase and conversely. If the two terms are equal, then there is a steady state for temperature in the PSR.

2°) Simply start with the mass balance for the fuel

$$\frac{d}{dt} \int_V \rho Y_{Fu} dV = \int_V R_{Fu} dV - \int_{S_1} \rho Y_{Fu} \mathbf{v} \cdot \mathbf{n} dS - \int_{S_2} \rho Y_{Fu} \mathbf{v} \cdot \mathbf{n} dS \quad (6)$$

and proceed the same way as in the previous question to get the result

$$\frac{dY_{Fu}}{dt} = \tilde{R}_{Fu} + \frac{(Y_{Fu,fr} - Y_{Fu,br})}{\tau_s} \quad (7)$$

3°) The system being in steady state, we have from Eq. (7):

$$\frac{dY_{Fu}}{dt} = 0 \Rightarrow \tilde{R}_{Fu} = -\frac{(Y_{Fu,fr} - Y_{Fu,br})}{\tau_s} \quad (8)$$

Introducing this in Eq. (5) in steady state ($\frac{dT}{dt} = 0$), we get

$$c_p(T_{br} - T_{fr}) = q_p(Y_{Fu,fr} - Y_{Fu,br}) \quad (9)$$

4°) The adiabatic combustion temperature T_{ad} is the maximum temperature one can reach in a combustion system. It is defined by considering a complete and total combustion of the fuel, so that no fuel remains in the end (otherwise you could still increase the temperature by making this remaining fuel burn). This means that, to reach the adiabatic combustion temperature in the PSR, one should have $Y_{Fu,br} = 0$.

Introducing this condition in Eq. (9), we get:

$$T_{ad} = T_{fr} + \frac{q_p}{c_p} Y_{Fu,fr} \quad (10)$$

5°) We now have a relationship between $Y_{Fu,fr}$ and T_{ad} which we will use to introduce T_{ad} in the general problem. Simply use Eq. (10) to express $Y_{Fu,fr}$ as a function of T_{ad} and plug it into Eq. (9) to get:

$$\frac{c_p}{q_p}(T_{ad} - T_{br}) = Y_{Fu,br} \quad (11)$$

6°) The first term on the right hand side of Eq. (5) is the chemical term:

$$-\frac{q_p}{c_p} \tilde{R}_{Fu} \quad (12)$$

Using the definition of \tilde{R}_{Fu} , we can express it as a function of $Y_{Fu,br}$

$$\frac{q_p}{c_p} k_0 e^{-\frac{T_{act}}{T_{br}}} Y_{Fu,br} \quad (13)$$

Finally, using Eq. (11) and $k_0 = \frac{1}{\tau_{ch}}$, we get:

$$\frac{1}{\tau_{ch}}(T_{ad} - T_{br})e^{-\frac{T_{act}}{T_{br}}} \quad (14)$$

7°) See the provided Matlab correction script to trace the curves.

We want to find the steady state operating temperatures, that is the temperatures for which the two curves (which represent the chemical term producing heat and the convective term removing heat) cross. Depending on the value of τ_s , several behaviours can be witnessed.

For the lowest value of τ_s , only one crossing point can be found and its temperature is really low. It means that the only possible solution is that almost no reaction occurs. The reactants flow through the PSR too fast for anything to happen.

For the highest value of τ_s , only one crossing point can be found as well but its temperature is now quite high and close to T_{ad} . It means that the residence time in the PSR is long enough for combustion to occur inside it, bringing its temperature to a high value.

For the middle value of τ_s , three crossing points are observed but only two are stable. Indeed, considering the middle crossing point, one can see that a small increase (resp. decrease) of temperature leads to the chemical term being higher (resp. lower) than the convective

term, therefore leading to a further increase (resp. decrease) of temperature until the next crossing point. So for this value of τ_s , two stable values for the temperature in steady state are possible, one corresponding to an ignited state of the PSR (high temperature) and the other corresponding to an extinguished state (low temperature). The choice of one or the other of these two points depends on the history of the PSR (ie, was it already ignited or not).

The remaining two values for τ_s correspond to specific cases where the convective term curve is tangent to the chemical term curves. They correspond to limit cases. The one with the highest τ_s corresponds to the ignition case. Starting from gases at temperature T_{fr} , it is the lowest possible value of τ_s to get a chemical term above the convective term everywhere until the crossing point close to T_{ad} . This means that, starting with fresh gases at T_{fr} and any higher value of τ_s , the system will see its temperature increase to reach an ignited state (high temperature). The other limit case corresponds to the extinction case. This time, starting from a ignited state, the corresponding value of τ_s is the lowest possible value to remain ignited. Any value lower than that brings the system to an extinguished state (low temperature).

8°) The S-curve represents the temperature of the intersection points between the two curves of the previous question as a function of the residence time τ_s . The central branch corresponds to the middle intersection point in the cases where there are three intersection points. As discussed previously, this middle intersection point is unstable and, while it is an acceptable solution mathematically, it is never witnessed in reality. So, the central branch does not really exist and stable points for these values of τ_s are only on the top or bottom branches depending on the history of the system (hysteresis effect).

When one blows a candle, one increases the mass flow rate \dot{m} to the candle. Therefore, close to the candle, the residence time decreases. The ignited candle corresponds to a solution on the top branch of the curve (high temperature). Decreasing the residence time makes the system follow the top branch until it reaches the point with a vertical tangent and jumps to the bottom branch which corresponds to an extinguished state.

To ignite a combustion chamber, one uses an electric spark plug that will create a spark to initiate the combustion reactions. The goal is to make sure that we will jump to an ignited state at high temperature. Therefore, we want to be all the way on the right side of the S-curve where the only solution is the ignited solution. This corresponds to large values of τ_s , so to a small mass flow rate to the system and therefore regions where the velocity is low, ie "calm" regions.

9°) As mentioned in question 7, the ignition and extinction cases correspond to values of τ_s where the convective term curve is tangent to the chemical term curve. This ignition and extinction temperatures therefore correspond to two conditions: the two curves have the same slope and they have the same value.

This gives the following equation system:

$$\frac{d}{dT} \left(\frac{1}{\tau_{ch}} (T_{ad} - T) e^{-\frac{T_{act}}{T}} \right) = \frac{d}{dT} \left(\frac{(T - T_{fr})}{\tau_s} \right) \quad (15)$$

$$\frac{1}{\tau_{ch}} (T_{ad} - T) e^{-\frac{T_{act}}{T}} = \frac{(T - T_{fr})}{\tau_s} \quad (16)$$

Deriving the first line and rearranging the second line, one obtains:

$$\frac{e^{-\frac{T_{act}}{T}}}{\tau_{ch}} \left(\frac{(T_{ad} - T) T_{act}}{T^2} - 1 \right) = \frac{1}{\tau_s} \quad (17)$$

$$\frac{e^{-\frac{T_{act}}{T}}}{\tau_{ch}} = \frac{(T - T_{fr})}{\tau_s (T_{ad} - T)} \quad (18)$$

Introducing the second line into the first, one can get rid of the exponential term and the residence times, to obtain

$$(T - T_{fr}) \left(\frac{T_{act}}{T^2} - \frac{1}{(T_{ad} - T)} \right) = 1 \quad (19)$$

which expands into the following second degree equation:

$$(T_{fr} - T_{ad} - T_{act})T^2 + (T_{fr}T_{act} + T_{ad}T_{act})T - T_{fr}T_{act}T_{ad} = 0 \quad (20)$$

10°) The provided Matlab script solves Eq. (20) and gives the value of the ignition and extinction temperatures. These values can then be entered into Eq. (18) to obtain the corresponding $\frac{\tau_{ch}}{\tau_s}$.

The ratio is maximum when ϕ is close to one, that is for the highest adiabatic flame temperatures. This indicates that the operating zone of the PSR is the largest for these conditions (any $\frac{\tau_{ch}}{\tau_s}$ below this value leads to a stable ignited system). As we move towards lower or higher equivalence ratios, the operating zone of the system decreases.

The curve shows that, in any case, there is a maximum value of $\frac{\tau_{ch}}{\tau_s}$ that one can reach and any value higher than that leads to an extinguished system. Given that $\frac{\tau_{ch}}{\tau_s} \propto \frac{\dot{m}}{Vp^n}$, if one wants to increase the output power (which means increasing the mass flow rate \dot{m}), one has to compensate using the volume V or the pressure p of the combustion system. Increasing the volume is why industrial furnaces or thermal power stations working at atmospheric pressure are so big. In aircraft engines, where space and weight constraints are drastic, the preferred solution is to increase the pressure inside the combustor (civilian aircraft engines have combustor pressure around 40 to 50 times the ambient pressure).