# Mathematical Model Development for Well-Stirred Reactors

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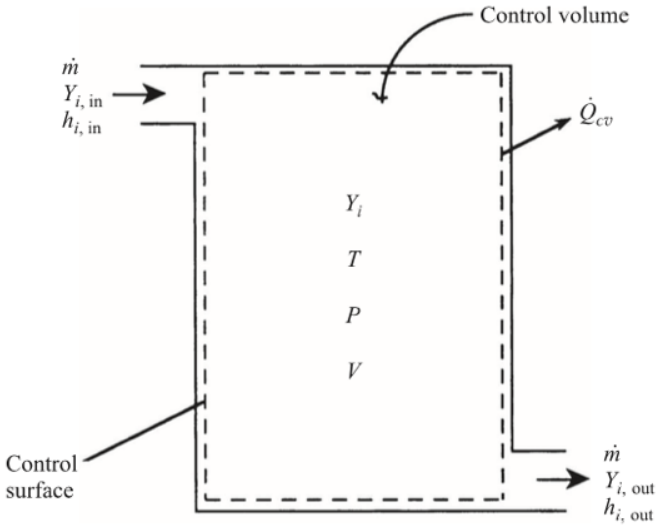
A well-stirred reactor (also known as a continuously-stirred reactor, perfectly-stirred reactor, etc.), is an ideal combustion model where perfect mixing is achieved within a reactor defined as a control volume. In this document, I'll derive the mathematical model for a well-stirred reactor, to be used in the implementation of a Cantera solver for reactors of this type.




A schematic of a well-stirred reactor [Turns, 2012].

## Assumptions

1. Steady-state, steady flow
2. Perfect mixing is achieved within the reactor. This implies that all thermodynamic properties are constant at any point within the control volume, and that no diffusional flux will occur.
3. The properties at the outlet of the control volume are the same as those within the control volume.
4. Changes in kinetic and potential energy in flowing through the reactor are negligible.

## Required Inputs

- A defined gas to flow into the reactor (a Cantera `Solution` object will likely be used).
- The volume of the reactor, $V$.
- The mass flowrate through the reactor, $\dot{m}$.
- The rate of heat loss, $\dot{Q}$ (if the reactor isn't adiabatic).

## Mathematical Model

### *Derivation*

Begin with the mass conservation equation for an individual chemical species inside of a control volume. For an arbitrary species *i*:

$$\frac{\mathrm{d}m_{i,cv}}{\mathrm{d}t} = \dot{m}_i'''V + \dot{m}_{i,\mathrm{in}} - \dot{m}_{i,\mathrm{out}} \quad [1]$$

*Terms utilized in the above equation are defined as follows:*

| | |
|---|---|
| $\frac{\mathrm{d}m_{i,cv}}{\mathrm{d}t}$ | The rate at which the total mass of species *i* accumulates within the control volume. |
| $\dot{m}_i'''V$ | The total mass generation rate of species *i* through chemical reactions within the control volume. |
| $\dot{m}_i'''$ | The mass generation rate per unit volume of species *i* through chemical reactions. |
| $V$ | The amount of volume defined within the reactor's control volume. |
| $\dot{m}_i$ | The mass flowrate of species *i* at some location. |
| $\dot{m}_{i,\mathrm{in}}$ | The mass flowrate of species *i* through the inlet of the reactor. |
| $\dot{m}_{i,\mathrm{out}}$ | The mass flowrate of species *i* through the outlet of the reactor. |

To make the mass conservation equation more usable, the following equivalencies are presented:

$$\dot{m}_i''' = \dot{\omega}_i MW_i \quad [2]$$

$$\dot{m}_{i,\mathrm{in}} = \dot{m}Y_{i,\mathrm{in}} \quad [3]$$

$$\dot{m}_{i,\mathrm{out}} = \dot{m}Y_{i,\mathrm{out}} \quad [4]$$

*Terms utilized in the above equations are as follows:*

| | |
|---|---|
| $\dot{\omega}_i MW_i$ | The mass generation rate per unit volume of species *i* through chemical reactions. |
| $\dot{\omega}_i$ | The total molar generation rate per unit volume of species *i* through chemical reactions. |
| $MW_i$ | The molar weight of species *i*. |
| $\dot{m}Y_i$ | The mass flowrate of species *i* at some location. |
| $\dot{m}$ | The total mass flowrate through the reactor. |
| $Y_{i,\mathrm{in}}$ | The fraction made up by species *i* of the total mass of the gaseous mixture entering the reactor. |
| $Y_{i,\mathrm{out}}$ | The fraction made up by species *i* of the total mass of the gaseous mixture exiting the reactor. |

Since steady-state operation of the reactor has been assumed, the mass of any species *i* within the control volume must remain constant over time:

$$\frac{\mathrm{d}m_{i,cv}}{\mathrm{d}t} = 0 \quad [5]$$

Considering equation [5], substituting the presented equivalencies [2 – 4] into equation [1], and then simplifying the result gives the final mass conservation equation for some arbitrary species *i* within the reactor:

$$0 = \dot{\omega}_i MW_i V + \dot{m}(Y_{i,\text{in}} - Y_{i,\text{out}}) \qquad [6]$$

All terms used in this equation have been defined previously. It should be noted that in traditional solutions of a well-stirred reactor problem, each species production rate, $\dot{\omega}_i$, may be independently calculated as a function of the molar concentration of *i* within the reactor and the global reactor temperature, *T*. However, in the implementation of this solver, production rates will likely be obtained via a Cantera `Solution` object that iteratively models the gas mixture within the reactor based on successive estimates of reactor temperature.

Equation [6] will be applied once for each of the *N* chemical species present, which will result in *N* equations with a combined total of $N+1$ unknown values (namely, $Y_{1,\text{out}}$, $Y_{2,\text{out}}$, …, $Y_{N,\text{out}}$, $T$). One more equation will be required to find a unique solution set for the model. For this, the steady-state, steady-flow conservation of energy equation will be applied to the reactor:

$$\dot{Q} = \dot{m}(h_{\text{out}} - h_{\text{in}}) \qquad [7]$$

*Terms utilized in the above equation are as follows:*

| | |
|---|---|
| $\dot{Q}$ | The rate that heat is lost to the surroundings via heat transfer through the reactor walls. This will rate be equal to zero in adiabatic reactors. |
| $\dot{m}$ | The total mass flowrate through the reactor. |
| $h_{\text{out}}$ | The total enthalpy of the gaseous mixture leaving the reactor. |
| $h_{\text{in}}$ | The total enthalpy of the gaseous mixture entering the reactor. |

It should be noted that in traditional solutions of a well-stirred reactor problem, the total enthalpy of a gaseous mixture may be calculated by summing the products of each species' standardized enthalpy with its mass fraction. However, in the implementation of this solver, total enthalpies will likely be obtained via Cantera `Solution` objects that model the gases entering and leaving the reactor.

***Final Model***

The final mathematical model of a well-stirred reactor to be used in the implementation of this solver is as follows:

$$\begin{gathered}
0 = \dot{\omega}_1 MW_1 V + \dot{m}(Y_{1,\text{in}} - Y_{1,\text{out}}) \\
0 = \dot{\omega}_2 MW_2 V + \dot{m}(Y_{2,\text{in}} - Y_{2,\text{out}}) \\
\cdots \\
0 = \dot{\omega}_N MW_N V + \dot{m}(Y_{N,\text{in}} - Y_{N,\text{out}}) \\
0 = \dot{m}(h_{\text{out}} - h_{\text{in}}) - \dot{Q}
\end{gathered}$$

In the above equations, a numerical subscript $i \in \{1, 2, \ldots, N\}$ indicates a property specific to chemical species *i*, where a total of *N* species are present in the reactor. These $N+1$ nonlinear algebraic equations will need to be solved simultaneously using a capable numerical analysis technique, such as Newton's method. Once the system has converged to a solution, all properties of the combustion reaction within the well-stirred reactor can easily be derived.

## References

S. R. Turns, *An Introduction to Combustion: Concepts and Applications*, 3rd ed. New York: McGraw-Hill, 2012.