

1. Identify objective for the simulation
2. Draw a schematic diagram, labeling process variables
3. List all assumptions
4. Determine spatial dependence
   * yes = Partial Differential Equation (PDE)
   * no = Ordinary Differential Equation (ODE)
5. Write dynamic balances (mass, species, energy)

Mass balance (to obtain volume):

Species balance no reaction (to obtain concentration):

Energy balance (to obtain temperature):

Where the enthalpy is :

Where the mass is and is constant and equal to zero:

If the volume is not constant, the first derivative should be addressed with the chain rule:

Got to keep in the left and move everything else to the right (and consider that and are zero):

Also remember that mass flow rate is :

1. Other relations (thermo, reactions, geometry, etc.)
2. Degrees of freedom, does number of equations = number of unknowns?
3. Classify inputs as
   * Fixed values
   * Disturbances
   * Manipulated variables
4. Classify outputs as
   * States
   * Controlled variables
5. Simplify balance equations based on assumptions
6. Simulate steady state conditions (if possible)
7. Simulate the output with an input step