

Chapter 3. State variables and functions

3.1 Conservation equations and the state variables

The conservation of mass and energy are the basis for all reactor models. As a starting point, there is one equation for each molecular species and one equation for energy (for a non-isothermal reactor). The dependent variables in the conservation equations are the state variables, i.e. the variables that determine the state of the system.

Temperature is used as a state variable in the energy balance. Pressure is also required as a state variable. It is either assumed constant or it is calculated from a mechanical energy balance.

There are several possibilities for the composition state variable...molar concentrations, mole fractions, mass fractions, partial pressures. The mass fractions of each species are used in this book.

All other variables, such as heats of reaction, molar concentration, and reaction rates are functions of these state variables.

Why use mass fractions and not molar concentrations?

If molar concentrations are used, then the molar expansion or contraction must be explicitly calculated in order to modify the velocity through the reactor. The use of mass fractions simplifies the mass balances, allowing an implicit tracking of the molar change through the change in total molecular weight and, in turn, the change in density. This will be explained in more detail in the Ch. 7.

Why use mass fractions and not extents of reaction?

Decades ago, extents of reaction were beneficial for some reaction systems because their use could reduce the number of equations to be solved. With the improved computer speed, the need for extents of reaction has largely diminished.

The use of extents of reaction, in the author's opinion, adds an unnecessary step in the development of the models. The use of mass fractions also retains the features of the mass conservation balances in a more direct manner. Multiple feeds and effluents are readily modeled using mass fractions.

Why use mass fractions and not molar fluxes?

Molar fluxes are often used in steady state models of fixed bed reactors. However, they are not used in models of other reactor types such as batch or CSTR. Also, fluxes cannot be used in the accumulation term in a dynamic model, and therefore they are not convenient for dynamic models. In contrast, mass fractions may be used for models of all reactor types, and in dynamic models. Therefore, using mass fractions results in a more unified approach and saves time when comparing reactor types during the conceptual design stage.

3.2 Expressing functions in terms of the state variables

Some functions can be defined using either state or non-state (intermediate) variables.

Suppose:

Y is a state vector

r is a function of the state vector, Y

f is a function of Y and r , as shown below

$$f(Y, r) = \exp^{\frac{-a}{R \cdot Y_{10}}} \cdot r \quad r(Y) = Y_0 \cdot (Y_2)^2$$

If f and r are defined as above, f would eventually be used in a model as shown below:

$f(Y, r(Y))$ so the state variable, Y , would be used repeatedly in the function "call" for f .

As functions become functions of other functions, the argument list of the last definition can become large. Using the state variable approach, f would be defined as follows, no matter how many intermediate functions (such as r) are involved in its definition:

$$f(Y) = \exp^{\frac{-a}{R \cdot Y_{10}}} \cdot r(Y)$$

In this course and examples, the state variables (mass fraction vector, temperatures and pressure) are normally kept separate instead of combined into a single state vector. This makes it easy to change the reaction temperature from a fluid temperature to a catalyst temperature. This separation also makes the models easier to understand. The above example would then become:

$$f(\omega, T, p) = \exp^{\frac{-a}{R \cdot T}} \cdot r(\omega, p)$$

ω = weight fraction vector

T = temperature

p = pressure