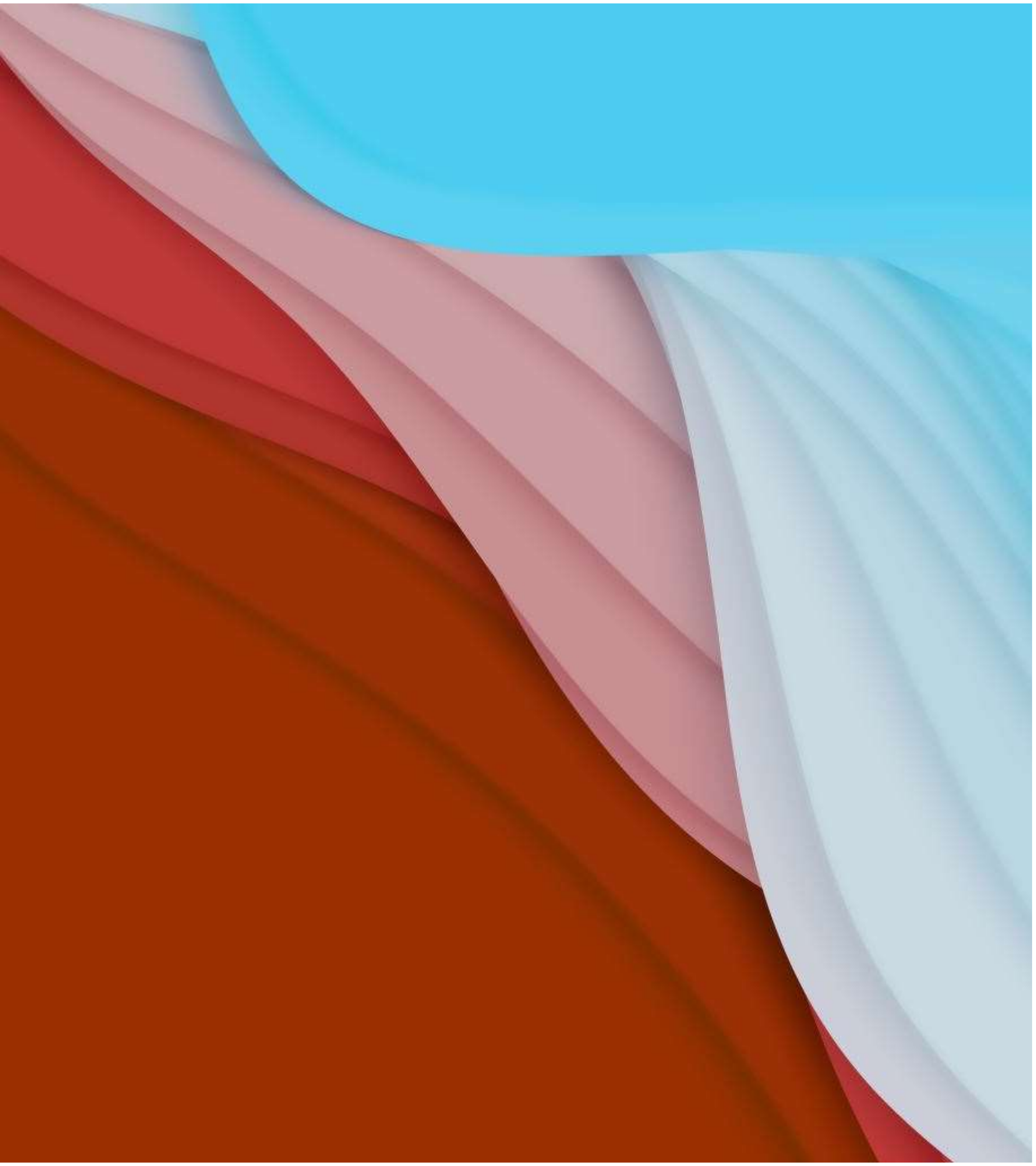

CEN4417
PROCESS DESIGN I

2.2 Predicting Trends

In this method, there are four possible modifiers to a term in an equation.

1. ¢: value remains constant.
2. ↑: value increases.
3. ↓: value decreases.
4. ?: value change not known.

Each variable in an expression has one of these identifiers appended. If x is a constant then x → x(¢).

Example

For a bimolecular, elementary, gas-phase reaction, the rate expression is known to be $-r_A = kC_AC_B$.

a. What is the effect on the reaction rate of increasing the reaction pressure by 10% while maintaining constant temperature?

b. What is the effect on the reaction rate of increasing the reaction temperature by 10% while maintaining constant pressure?

SOLUTION :

The goal is to determine the effect of increasing pressure on the reaction rate. The equation containing the unknown value, which is the reaction rate, r_A, is given. We need a relationship between pressure and at least one variable in the equation.

We have information, from the ideal gas law, that tells us that

$C_i = P_i/RT$,

where i is A or B.

Now that we have the necessary relationships, an intuitive understanding can be obtained by predicting trends.

a)

Ci(↑) = yi(¢)P(↑)/R(¢)T(¢) = Pi(↑)/R(¢)T(¢)

Moving to the rate expression, the resulting trend is predicted by

rA(↑) = k(¢)CA(↑)CB(↑)

which means that the reaction rate increases.

b)

$$C_i(\downarrow) = y_i(\text{¢})P(\text{¢})/R(\text{¢})T(\uparrow) = P_i(\text{¢})/R(\text{¢})T(\uparrow)$$

From the rate expression,

$$r_A(?) = k(\uparrow)C_A(\downarrow)C_B(\downarrow)$$

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