Supporting information

A process intensification methodology including economic, sustainability and safety considerations

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Methodology for the estimation of FEDI penalties

The damage potential is estimated as follows. For equipment that involves chemical reaction, equation 1 is used.

$$damage\ potential = [F1 * pn1 + F * pn2 + F4 * pn7 * pn8](pn3 * pn4 * pn5 * pn6) \quad (1)$$

For a piece of equipment that does not involve chemical reaction, the damage potential is estimated using equation 2.

$$damage\ potential = [F1 * pn1 + F * pn2](pn3 * pn4 * pn5 * pn6) \quad (2)$$

In both cases, the terms pn1 to pn6 refer to penalties related to process parameters. In the case of units involving chemical reactions, pn7 and pn8 are penalties related to the type of reaction and to the occurrence of undesirable side reactions, respectively. The value of F is determined from the severity of pressure, and it can take the value of F2 or F3, or the sum of both energy factors.

Estimation of penalties

The first penalty (pn1) is used to account for the effect of temperature. The procedure to estimate the value of pn1 compares the operating temperature to flash point, fire point and auto ignition temperature. The algorithm for the estimations is as follows.

If $(Temperature > Flash\ point < Fire\ point)$

$pn1 = 1.45$

Else if $(Temperature > Fire\ point < 0.75\ Auto\ ignition\ temperature)$

$pn1 = 1.75$

Else if $(Temperature > 0.75\ Auto\ ignition\ temperature)$

$pn1 = 1.95$

Else

$pn1 = 1.1$

The second penalty (pn2) is used to account for the effect of the operating pressure through a comparison to vapor and atmospheric pressures. The algorithm for the estimation of pn2 followed by the estimation of F is given.

If $(AP < VP < PP)$

$$pn2 = 1 + \left(\frac{PP-VP}{PP}\right) * 0.6$$

$$F = F2 + F3$$

Else

$$pn2 = 1 + \left(\frac{PP-VP}{PP}\right) * 0.4$$

$$F = F2$$

If $(VP < AP < PP)$

$$pn2 = 1 + \left(\frac{PP-VP}{PP}\right) * 0.2$$

$$F = F3$$

Otherwise

$pn2 = 1.1$ (A limiting value)

$$F = F3$$

For processes working at vacuum pressures, pn2 is computed using the relationship

$$pn2 = 1.6505 - 0.0044 * PP$$

which applies for pressures between 0.001 atm to 1 atm.

Penalty pn3 has to do with the quantity of chemical handled in the equipment unit. According to the National Fire Protection Association (NFPA) ranking for reactivity or flammability, whichever is higher, pn3 is estimated using one of the following equations,

$$pn3_{NR\ or\ NF=1} = 0.0025(tons\ of\ chemical) + 1$$

$$pn3_{NR\ or\ NF=2} = 0.005(tons\ of\ chemical) + 1$$

$$pn3_{NR\ or\ NF=3} = 0.0075(tons\ of\ chemical) + 1$$

$$pn3_{NR\ or\ NF=4} = 0.010(tons\ of\ chemical) + 1$$

Penalty pn4 considers the effects of reactivity and flammability using the NFPA reactivity (NR) and flammability (NF) ranks. The estimation of pn4 is done as follows,

$$pn4 = 1 + 0.25(NR + NF)$$

Penalties pn5 and pn6 account for factors regarding plant distribution and layout. For the application of FEDI at the conceptual stage of design, a value of 1 is assigned to both factors.

Finally, for equipment units that involve chemical reactions, penalties pn7 and pn8 are used depending on the type of reaction and on the presence of possible side reactions. Table S1 gives the values for these penalty factors.

Table S1. Penalty values due to type of reaction and side reactions

Type of reaction	*Penalty*
Oxidation	1.60
Electrolysis	1.20
Nitration	1.95
Esterification	1.25
Reduction	1.10
Aminolysis	1.40
Halogenation	1.45
Sulfonation	1.30
Hydrogenation	1.35
Alkylation	1.25
Polymerization	1.50
Pyrolysis	1.45

Undesirable side reaction	*Penalty*
Autocatalytic reaction	1.65
Non-auto-catalytic side reaction probable to occur at above normal reaction conditions	1.45
Non-auto-catalytic side reaction probable to occur at below normal reaction conditions	1.20