Conversion, Yield and Selectivity of a Reactor

Conversion of a reactant, yield of the wanted product and its selectivity over a by-product, from the moles fed, unreacted and formed.

Method: Definitions of conversion; yield and selectivity (Fogler, Elements of Chemical Reaction Engineering)

Input parameters

Unit system: SI

Parameter	Value	Unit
Reactant A fed	0.10000	kmol
Reactant A leaving (unreacted)	0.015000	kmol
Wanted product formed	0.070000	kmol
By-product formed	0.015000	kmol
Moles of A per mole of P	1.0000	

Calculated results

Parameter	Value	Unit
Conversion of A	85.000	%
Yield of P on A fed	70.000	%
Fractional selectivity (on A reacted)	82.353	%
Selectivity P over D (moles)	4.6667	

Notes for this case

- Yield = conversion × fractional selectivity.

Formula and method

$$X = \frac{n_{A0} - n_A}{n_{A0}}, \quad Y = \frac{\nu n_P}{n_{A0}}, \quad S_f = \frac{\nu n_P}{n_{A0} - n_A}, \quad S_{P/D} = \frac{n_P}{n_D}$$

Variables

n_{A0}	Reactant A fed	mol
n_A	Reactant A leaving (unreacted)	mol
n_P	Wanted product formed	mol
n_D	By-product formed	mol
ν	Moles of A per mole of P	-
X	Conversion of A	-
Y	Yield of P on A fed	-
S_f	Fractional selectivity (on A reacted)	-
$S_{P/D}$	Selectivity P over D (moles)	-

Method and standards

Definitions.

Assumptions and limits

- Single key reactant.
- Product formed that would need more A than has reacted is rejected, so the yield never exceeds the conversion.

References

- Definitions of conversion
- yield and selectivity (Fogler, Elements of Chemical Reaction Engineering)

Report details

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Release checks	2 reference cases of this calculator, computed independently, are checked on every release

Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/chemical/reactors/conversion-yield-selectivity

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.