Degrees of Freedom

To determine the degrees of freedom (the number of variables whose values may be independently specified) in our model we could simply count the number of independent variables (the number of variables which remain on the right- hand side) in our modified equations.

This suggests a possible definition:

degrees of freedom = # variables - # equations

Definition:

The degrees of freedom for a given problem are the number of independent problem variables which must be specified to uniquely determine a solution.

In our distillation example, there are:

16 equations

16 variables (recall that F and X_F are fixed by upstream processes).

This seems to indicate that there are no degrees of freedom.

Degrees of Freedom

Consider the three equations relating Q_C, Q_R, and q_{vapour}:

$$Q_R - Q_C = 0$$
$$Q_R - \Delta H_{vap}\, q_{vapour} = 0$$
$$Q_C - \Delta H_{vap}\, q_{vapour} = 0$$

Notice that if we subtract the last from the second equation:

$$\begin{array}{rl} & Q_R - \Delta H_{vap}\, q_{vapour} = 0 \\ - & \underline{Q_C - \Delta H_{vap}\, q_{vapour} = 0} \\ & Q_R - Q_C = 0 \end{array}$$

the result is the first equation.

It seems that we have three different equations, which contain no more information than two of the equations. In fact any of the equations is a linear combination of the other two equations.

We require a clearer, more precise definition for degrees of freedom.

Degrees of Freedom

A More Formal Approach:

Suppose we have a set of "m" equations:

$$\mathbf{h}(\mathbf{v}) = \mathbf{0}$$

in the set of variables **v** ("*n+m*" elements). We would like to determine whether the set of equations can be used to solve for some of the variables in terms of the others.

In this case we have a system of "*m*" equations in "*n+m*" unknown variables. The Implicit Function Theorem states that if the "*m*" equations are linearly independent, then we can divide our set of variables **v** into "*m*" dependent variables **u** and "*n*" independent variables **x**:

$$\mathbf{v} = \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix}$$

The Implicit Function Theorem goes on to give conditions under which the dependent variables **u** may be expressed in terms of the independent variables **x** or:

$$\mathbf{u} = \mathbf{g}(\mathbf{x})$$

Degrees of Freedom

Usually we don't need to find the set of equations $\mathbf{u} = \mathbf{g}(\mathbf{x})$, we only need to know if it is possible. Again the Implicit Function Theorem can help us out:

> if *rank* $[\nabla_{\mathbf{v}}\mathbf{h}] = m$, all of the model equations are linearly independent and it is possible (at least in theory) to use the set of equations $\mathbf{h}(\mathbf{v}) = \mathbf{0}$ to determine values for all of the "*m*" dependent variables **u** given values for the "*n*" independent variables **x**.

Alternatively we could say that the number of degrees of freedom in this case are the number of independent variables. (Recall that there are "n" variables in **x**).

We know that:

$$\text{rank } [\nabla_{\mathbf{v}}\mathbf{h}] \leq m.$$

What does it mean if:

$$\text{rank } [\nabla_{\mathbf{v}}\mathbf{h}] < m?$$

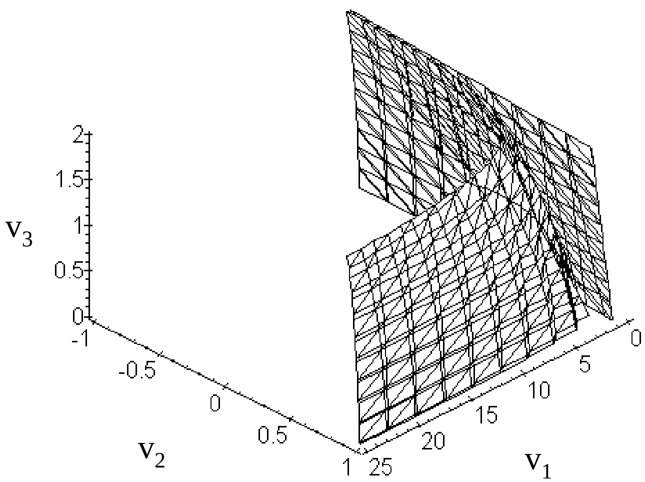
Degrees of Freedom

Let’s investigate a simple set of equations:

$$\mathbf{h}(\mathbf{v}) \equiv \begin{bmatrix} v_1 - v_1 v_2 - \alpha e^{v_3} \\ v_1 - v_2 - v_3 \end{bmatrix} = \mathbf{0}$$

with α=1/e. (This could be the material balances for a reactor.)

A three dimensional plot of the equations looks like:

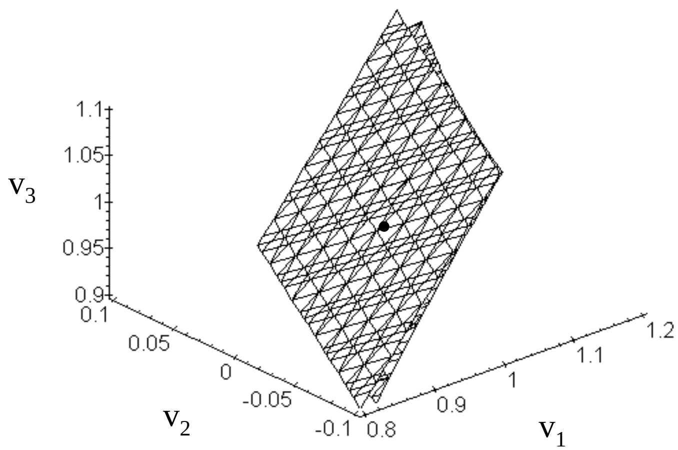


The solution of the equations lies at the intersection of the two surfaces, each described by one of the equations.

How many degrees of freedom does this problem have?

Degrees of Freedom

Take a closer look:



Examine the neighbourhood of the point:

$v_1=1,$

$v_2=0,$

$v_3=1.$

What is happening here?

Degrees of Freedom

The Jacobian of the equation set **h**(**v**) = **0** is:

$$\nabla_{\mathbf{v}}\mathbf{h} = \begin{bmatrix} 1 - v_2 & -v_1 & -\alpha e^{v_3} \\ 1 & -1 & -1 \end{bmatrix}$$

When α=1/e at the point **v**=$[1,0,1]^T$, then:

$$\nabla_{\mathbf{v}}\mathbf{h} = \begin{bmatrix} 1 & -1 & -1 \\ 1 & -1 & -1 \end{bmatrix}$$

What is the rank of this matrix?

Note that:

$$\text{rank } [\nabla_{\mathbf{v}}\mathbf{h}] = 1 < m = 2.$$

This tells us that, at the point **v**=$[1,0,1]^T$, our system contains only one linearly independent equation.

Then:

$$\text{degrees of freedom} = 3 \text{ variables} - 1 \text{ equation}$$
$$= 2.$$

∴ at the given point two variables must be specified to uniquely determine the solution to the problem.

This example was chosen because it was very easy to see the occurrence of linear dependence within the equation set. Of course the situation can be much more complex for real problems with many more equations and variables. So, clearly we cannot determine degrees of freedom by counting the number of equations in our problem.

As a result, we must modify our definition:

degrees of freedom = number of variables - number of linearly independent equations

Degrees of Freedom

In summary, determination of the degrees of freedom for a specific steady-state set of equations requires:

1) determination of rank [$\nabla_v \mathbf{h}$].

2) if rank [$\nabla_v \mathbf{h}$] =number of equations (m), then all of the equations are linearly independent and:

$$\text{d.o.f.} = \#\text{ variables} - \#\text{ equations.}$$

3) if rank [$\nabla_v \mathbf{h}$] <number of equations (m), then all of the equations are not linearly independent and:

$$\text{d.o.f.} = \#\text{ variables} - \text{rank}\ [\nabla_v \mathbf{h}].$$

<u>Remember:</u>

For sets of linear equations, the analysis has to be performed only once. Generally, for nonlinear equation sets, the analysis is only valid at the variable values used in the analysis.

Degrees of Freedom

Degrees of freedom analysis tells us the maximum number of variables which can be independently specified to uniquely determine a feasible solution to a given problem.

We need to consider degrees of freedom when solving many different types of problems. These include:

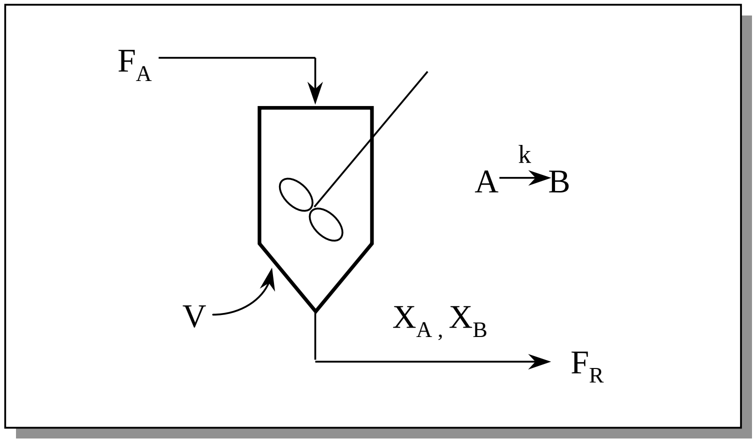
i) plant design,
ii) plant flowsheeting,
iii) model fitting,

⋮

and, of course, <u>optimization problems</u>.

Degrees of Freedom

Consider the example isothermal reactor system:



The material balances are:

mass	$F_A - F_R = 0$
component A	$F_A - kX_AV\rho - X_A F_R = 0$
component B	$kX_AV\rho - X_B F_R = 0$

What other information do we have?

By definition, we also know:

$$1 - X_A - X_B = 0.$$

Degrees of Freedom

If we know the feed-rate (F_A = 5 kg/min.), reactor volume (V =2 litres), density of the reaction mixture (ρ=1 kg/l), and reaction rate constant (k=7 min^{-1}), then the material balances can be re-written:

$$5 - F_R = 0$$
$$5 - 14X_A - X_A F_R = 0$$
$$14X_A - X_B F_R = 0$$
$$1 - X_A - X_B = 0$$

Is this set of equations linear or nonlinear?

In our problem, there are:

3 variables (X_A, X_B, F_R)
4 equations (1 mass balance
2 component balances,
1 other equation).

What does this mean?

Degrees of Freedom

Consider what happens if we add:

$-1\times$mass balance	$-5 +$		$F_R = 0$
+component A	$5 - 14X_A - X_A F_R$		$= 0$
+component B	$14X_A -$	$X_B F_R$	$= 0$

$$F_R - X_A F_R - X_B F_R = 0$$

or:

$$F_R (1 - X_A - X_B) = 0$$

and since $F_R \neq 0$, then:

$$(1 - X_A - X_B) = 0$$

which is our fourth equation. Thus our four equations are not linearly independent.

Caution:

Care should be taken when developing a model to avoid this situation of specifying too many linearly dependent equations, since it often leads to difficulty in finding a feasible solution.

Degrees of Freedom

We need to eliminate one of the equations from our model. I would suggest eliminating:

$$(1 - X_A - X_B) = 0$$

This equation could then provide an easy check on any solution we find using the other equations.

Thus our model is reduced to:

$$\begin{aligned} 5 - F_R &= 0 \\ 5 - 14X_A - X_A F_R &= 0 \\ 14X_A - X_B F_R &= 0. \end{aligned}$$

How many degrees of freedom are there in this model?

Degrees of Freedom

For our reactor model:

$$\nabla_v \mathbf{h} = \begin{bmatrix} -1 & 0 & 0 \\ -X_A & -14-F_R & 0 \\ -X_B & 14 & -F_R \end{bmatrix}$$

What is the rank of this matrix?

(Suppose $F_R = 0$ or $F_R = -14$.)

We could determine the rank by:

1) using software (Maple, Matlab, Mathcad, ...)

2) examining the eigenvalues (which are displayed on the diagonal of a triangular matrix.

rank $[\nabla_v \mathbf{h}] = 3$ $\quad F_R \neq 0$ or -14

rank $[\nabla_v \mathbf{h}] = 2$ $\quad F_R = 0$ or -14

3) using the determinant:

$$|\nabla_v \mathbf{h}| = -F_R\,(14 + F_R)$$

rank $[\nabla_v \mathbf{h}] = 3$ $\quad (|\nabla_v \mathbf{h}| \neq 0,\ F_R \neq 0$ or $-14)$

rank $[\nabla_v \mathbf{h}] = 2$ $\quad (|\nabla_v \mathbf{h}| = 0,\ F_R = 0$ or $-14)$

Degrees of Freedom

Then for our reactor problem and realistic flowrates, we have:

3 variables (F_R, X_A, X_B)
3 linearly independent equations
(1 mass and 2 component balances).

Therefore:

degrees of freedom = 3 - 3 = 0

This says there are no degrees of freedom for optimization and the reactor problem is fully specified.

In fact the unique solution is:

$F_R = 5$ kg/min.
$X_A = 5/19$ wt. fraction
$X_B = 14/19$ wt. fraction

Degrees of Freedom

Until now, we have specified the feed-rate (F_A) in our reactor problem. Suppose we decide to include it as an optimization variable:

1) how many degrees of freedom are now available for optimization?

d.o.f = 4 variables - 3 equations
= 1

2) Can we re-introduce the fourth equation:

$$1 - X_A - X_B = 0$$

to reduce the degrees of freedom?

No, using F_A as an optimization variable does not change the linear dependence among the four equations.