DEGREES OF FREEDOM OF EQUIPMENT AND PROCESSES

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ABSTRACT

Simple equations are derived to carry out degree of freedom analyses quickly and almost mechanically, using easily countable physical entities. It is shown that the outlet stream freedom does not depend on the number of component substances, and in many cases not on the number of phases. The concept of phase constraint is introduced to facilitate the degree of freedom analysis.
A frequent problem facing chemical engineering students, practicing engineers dealing with an unfamiliar process, and persons writing computer process simulations, is that of calculating the number of degrees of freedom of a process. Only when this has been done can the following questions be answered:

- How many operating conditions or desired outputs can we specify? In fact, can we specify anything at all or do we have to accept whatever the equipment will give us?
- Is the process as described self-maintaining and stable, or does it need feedback control? How many control loops are required?
- Can we optimise the process by changing some of the operating conditions?

Stephanopoulos (1984) stressed the importance of d.o.f. analysis: "The desired control of a process will be achieved when and only when all the degrees of freedom have been specified. Sloppy modelling of a process may lead to a model that does not include all the relevant equations and variables or include redundant equations and variables. In either case we have an erroneous determination of the d.o.f."

A typical d.o.f. analysis, such as found in Smith (1963), Westerberg et al (1979), Coulson et al (1983) or Stephanopoulos (1984), starts by listing the number of component substances and the number of relationships between them. These relationships include, according to Smith (1963): inherent restrictions (e.g. thermal and pressure equilibrium between streams in close contact), material balances, energy balances, phase distributions, and chemical equilibria. Their number is not always obvious, and double-counting or omission of equations and variables is always a danger, especially when the number is large (Kwauk, 1956). Westerberg et al (1979) give an example of a process consisting of seven components, with 16 degrees of freedom. To arrive at this results, these authors subtracted 48 equations from 64 variables. Westerberg et al stated that determining these numbers is "very straightforward", nevertheless it is clear that the process is tedious and considerable care is needed to avoid errors. As will be seen, general formulæ can be derived that dispense with the need for most of this information, and allow the number of degrees of freedom to be calculated from a small number of easily countable quantities.

**THEORY**

The number of degrees of freedom, or simply freedom of a process (which may consist of a single piece of equipment), consists of operating freedom and design freedom. The latter consist of all the possible choices we make at the design stage, which may be very large and ill-defined: geometry, design details, relative size of components, wall thickness, flow layout, material of construction, etc. We shall in this paper ignore design freedom and assume that we are dealing with an existing plant. Furthermore, we shall consider only the static and not the dynamic degrees of freedom (Dixon, 1972).

The operating freedom depends, among other things, on the number of process streams. If the inlet streams are completely specified, as is usually the case, then we need only deal with the exit streams. Let us call this the outlet freedom, $F_O$. This is a convenient quantity to deal with, because in a complex plant, streams leaving one module will either leave the plant or enter another module, and the plant’s outlet freedom must equal the sum of the modules’ outlet freedoms (no matter how "module" is defined). This enables
independent checking of the freedom calculations. Additional freedom due to unspecified inlet stream details can be added at a later stage, together with design freedom if any.

Consider the multiple-circuit system of Figure 1 and let

\[ K = \text{number of separate circuits, where a circuit is a set of streams that are connected at some point inside the plant being considered. A heat exchanger, for example, would normally consist of two circuits, while a distillation column consist of a single circuit. It will be seen that splitting the process streams into circuits is important when the number of phases in each circuit is different, such as when a heating oil is used to partially evaporate a process fluid.} \]

\[ S_k = \text{number of stream splits in the k-th circuit. Every time a stream splits into two, to provide bypassing, recycle or a separate product stream, add 1 to } S_k. \text{ If there is only one circuit, then let } S_1 = S. \]

\[ C_k = \text{number of material components in the k-th circuit. If there is only one circuit, then let } C_1 = C. \]

\[ P_k = \text{number of phases in the outlet streams of the k-th circuit (a saturated fluid is considered to have two phases). If there is only one circuit then let } P_1 = P. \text{ It is important to note that in each circuit, each phase is counted once only, no matter how many outlet streams there are. Thus for a flash vessel or distillation column, } P=2 \text{ no matter the number of product streams.} \]

\[ E = \text{number of energy streams (heat input or removal, compressor/pump power) that materially affect the operation, and that can be varied by the operator. A pump or compressor’s contribution to the d.o.f. can be entered via } E \text{ (the compressor’s power) or } M \text{ (the speed or flow or other adjustment), but not both.} \]

\[ M = \text{number of other influential variables that may be manipulated: throttle valves, fluid levels (in heat exchangers or condensers), etc. If some feed stream is insufficiently specified, then the number of feed stream variables less than } C+2 \text{ may be included here. An influential variable needs not be a directly manipulated variable, but may be the setpoint of a controller. Care must be exercised in avoiding double-counting } S \text{ and } M: \text{ if a manipulated variable (e.g. a valve) is used to control a flow or flow ratio in a stream split, then it should not count towards } M, \text{ since it has already been counted under } S. \]

\[ N = \text{number of phase constraints, i.e. number of streams that are forced to be single-phase, or possess a predetermined phase ratio } L/V, \text{ although more than one phase is available. (e.g. in a separator, the V stream is pure vapour and L stream pure liquid, so } N = 2. \)
(b) An energy stream adds to \( E \) only if it can be varied by the operator or designer. Energy streams that cannot be changed by any practical means, such as the sun’s intensity in a solar heater or evaporative cooling from a cooling pond, do not count towards \( E \).

(c) A phase constraint can in practice be enforced by the design of the equipment (such as a steam trap or float valve causing the separation of liquid and vapour), or by a feedback loop which ensures that the \( L/V \) ratio is kept at a certain value. In both cases \( N \) is increased by 1. However, if the feedback loop crosses the boundaries (say by receiving an external setpoint or error signal), \( M \) will also increase by 1.

(d) A phase constraint exists when, and only when, a stream is forced to take on a certain phase ratio \( L/V \) although another \( L/V \) value is possible. For example, if there is only one exit stream (\( S=0 \)), then that exit stream has to carry whatever \( L \) and \( V \) are supplied to it and there is no possibility to vary \( L/V \), therefore no phase constraint. In a three-phase system, each single-phase outlet contributes two phase constraints (Phase 2/Phase 1 = 0 and Phase 3/Phase 1 = 0).

The total number of equations relating the operating variables is:

- Heat balance: 1 equation.
- Mass balance: Each material component, when present in a circuit \( k \), adds one mass balance equation (inlet flow rate = outlet flow rate) to the total. The total contribution from this source is therefore

\[
\sum_{k=1}^{K} C_k
\]

- Equilibrium or mass transfer relationship: Consider each circuit separately. The chemical potential of each component \( i \) in two connected outlet streams of circuit \( k \) will be equal if the two streams are in equilibrium. If there are \( C_k \) components in the two streams, there will be \( C_k-1 \) such relationships, since the \( C \)-th component does not contribute an independent relationship (the concentrations of each component in this stream can be determined by subtraction). Each additional stream (i.e. each increase in \( S_k \)) will add \( C_k-1 \) relationships. If the circuit has \( S_k+1 \) streams, therefore, the number of equilibrium relationships will be \( S_k(C_k-1) \). For \( K \) circuits, the number of equilibrium relationships will be

\[
\sum_{k=1}^{K} S_k(C_k-1)
\]

If two connected streams are not in equilibrium, they still obey mass transfer relationships. Each of these is an equilibrium relationship combined with a rate equation into a single expression. The total number of equations is still the same.

- Mechanical balance (pressure) relationship: \( \sum(S_k+1) \) equations, one per exit stream (downstream pressures depend on upstream pressures and flows).
- Phase constraint: \( N \) equations, each specifying a phase ratio.
- Thermal equilibrium between connected fluids: each additional single phase stream adds one thermal equilibrium relationship, each additional two-phase or saturated stream adds none since its temperature is specified by the saturation condition; hence the number of thermal equilibria is \( S_k(2-P_k) \) for the \( k \)-th circuit, or...
for all circuits. A saturated fluid is counted as two-phase \( (P=2) \), even though the amount in the second phase may be infinitesimal.

- Heat transfer between circuits: \( K=1 \). Heat transfer may be direct via a heat exchanger, or indirect via any number of intermediate fluids. It is assumed that transfer of heat or of another form of energy always take place between circuits, otherwise they would constitute independent, non-interacting processes.

Since each stream is completely specified by \( C_k + 2 \) variables (for example \( C_k \) flow rates + \( T \) and \( P \)), the total number of variables is

\[
n_v = \sum_{k=1}^{K} \left[ (S_k + 1) \ (C_k + 2) \right] + M + E \tag{1}
\]

The total number of relationships is

\[
n_r = 1 + \sum_{k=1}^{K} \left[ C_k + S_k (C_k - 1) + S_k + 1 + S_k (2 - P_k) \right] + N + K - 1
\]

\[
n_r = \sum_{k=1}^{K} \left[ (S_k + 1) \ (C_k + 2) - P_k \ S_k \right] + N \tag{2}
\]

and the outlet freedom is \( F_O = n_v - n_r \) or

\[
F_O = \sum_{k=1}^{K} \ P_k \ S_k \ + M + E - N \tag{3}
\]

Note that \( F_O \) is independent of the number of components \( C \) (or \( C_k \)). This has important consequences, as the freedom analysis can be made in terms of a single-component system.

Many processes (reactors, mass transfer equipment) consist of only one circuit, i.e. all streams are connected, and therefore \( K = 1 \), hence

\[
F_O = PS + M + E - N \tag{4}
\]

A frequent case in mass exchange equipment (flash tanks, distillation columns...) is that all outlet streams are single phases, in which case \( N = (S+1)(P-1) \) and the outlet freedom becomes (assuming further that \( K = 1 \))

\[
F_O = M + E + S + 1 - P \tag{5}
\]

If no circuit has more than one outlet stream, then the first term in eq.(3) vanishes, and also \( N = 0 \):

\[
F_O = M + E \tag{6}
\]

Closed-circuits systems, such as refrigeration cycles, whose only input and outputs are energy streams, have \( K = 0 \) and hence

\[
F_O = M + E \tag{7}
\]
APPLICATIONS
Elements and units
To calculate the number of degrees of freedom, one first identifies the circuits and adds up the products \( P_k S_k \). One then adds the degrees of freedom \( E \) from energy streams, \( M \) from influential variables and subtracts the number of phase constraints \( N \). If the inlets are not completely specified (less than \( C_k + 2 \) for each inlet stream), then further degrees of freedom will be added to the total, but only at the latest possible moment.

For example, consider the distillation column of Figure 2, with four outlet streams (\( S = 3 \)) all connected internally (\( K = 1 \)). There are two phases (\( P = 2 \)), two controllable energy streams at the condenser and reboiler (\( E = 2 \)) and four manipulable throttle valves (\( M = 4 \)). Assuming that the condenser is a total condenser, there is one phase constraint (bottoms must be all liquid). The total exit freedom is therefore \( 2(4-1) + 4 + 2 - 1 = 11 \), i.e. 11 variables can be specified. Normally the exit stream pressures are specified (by downstream process requirements), so one would have seven degrees of freedom to play with. The analysis tells us that we cannot specify two species concentrations per exit stream.

Table 1 shows how the above formulae can be applied to some other common units.

Processes
As an example of a process consisting of several units, consider that described by Westerberg et al (1979), p.128 (figure 3 of this paper). There are seven units (mixer, reactor, heat exchanger, valve, flash, stream splitter and compressor). Westerberg et al listed the variables and equations related to each unit, arriving at a total of 55 stream variables, 9 unit parameters (valve position, pressure drop, etc.) and 48 equations, from which

\[
\text{d.o.f.} = 55 + 9 - 48 = 16
\]

Of these, three (reaction heat, reactor pressure drop and compressor efficiency) are design rather than operating freedom, so the number of operating d.o.f. is 13 (including those related to inlet streams). Furthermore, this number also includes three variables for the cooling water stream (say flow, temperature and pressure), which we will ignore by considering that the heat exchanger consist of a single stream and a variable heat input (The argument is not affected by considering the heat input as a material stream.) Thus the total operating freedom is now reduced to 10.

The solution using this paper’s approach would go as follows:
(a) First, calculate and add up the outlet d.o.f. related to each unit (see Table 2). The total amounts to 6.
(b) To this is added 4 d.o.f. for the (two-component) feed stream, making a total of 10 operating d.o.f., in agreement with Westerberg et al.

DISCUSSION
The number of free variables in the last column of Table 1 is \( F_0 \). These free variables will be used up either by being given a desired value, or by an optimisation criterion (e.g. the intermediate pressure in a two-stage compression cycle may be specified by requiring that energy consumption be as low as possible).
While some of the results in the table are trivial, others are not. For a length of pipe, it is obvious that there is no freedom and the outlet conditions depend entirely on the inlet stream conditions. With a flash separator (Figure 4a), however, it is not immediately obvious that there is no freedom - at least not until control valves and/or heating are put in to throttle the flows and control the flashing pressure (Figure 4b).

It is not clear at first sight that a distillation column with partial condenser is less "free" than one with total condenser. Further thought, however, showed that with a total condenser, the reflux ratio can be controlled independently of the condensate flow, which will enable concentrations to be further manipulated, compared to the partial condenser situation.

Refrigeration plants operate on a closed cycle and therefore the number of circuits visible to the outside world is zero, $\Sigma P_k S_k = K = P = 0$. The fact that the fluid inside the closed cycle consists of a single circuit and two phases is irrelevant. The energy streams are two heat flows (heat removed at condenser and heat added at evaporator), plus one or more mechanical/electrical power inputs, depending on the number of compression stages. The two-stage compression refrigeration cycle has one more degree of freedom than single-stage, which can be used to optimise the intermediate pressure for minimum power input.

An actual compression refrigeration plant consists of several other auxiliary controls: thermostatic control, suction pressure control, delivery pressure control, oil pressure control. All these are normally completely inside the boundaries of the refrigeration plant and do not enter the degree of freedom analysis. Their role is to ensure that the various components work as designed. (A refrigeration system manufacturer, as opposed to a refrigeration user, may tackle the problem at a more detailed level and arrive at a different analysis.)

A (hypothetical) single-pass ultrafilter or other membrane equipment (Figure 5a) has two outlet streams, each of different phase, therefore $P = N = 2$. It may appear unclear at first that the permeate and concentrate are two different phases, since both are liquid; however, since the compositions of the two streams are related by an equilibrium/mass transfer relationship, they are by definition two different phases. Adding, say, a throttle to the concentrate outlet ($M = 1$) (Figure 5b) gives a degree of freedom, which can be used to specify the concentration or permeate flow rate; however, the pressure will remain uncontrolled and may rise to an intolerably high value. Adding a recycle pump (either $E=1$ or $M=1$, but not both) as well (Figure 5c) will enable both permeate flow and internal pressure to be controlled, and adding a controlled heat exchanger will allow temperature to be controlled as well.

A spray dryer and associated cyclone which separates the outlet stream into a powder stream and a gas stream has one degree of freedom, which is normally used to ensure a desired product moisture is obtained. In practice, the manipulated variable will be either the feed rate or the heater input. Again this is not obvious to someone unfamiliar with the equipment, who may assume that, for example, no control on the product moisture is possible, or that both product moisture and product temperature may be controlled.
Educational implications
From the educational point of view, the analysis points out some sources of confusion which often baffle students. Distillation columns are a case in point, because of their relatively complex structure. The present analysis shows that a distillation column, as depicted in Figure 6a, has only two degrees of freedom. Since distillation columns usually do not exist in isolation but are connected to other equipment, with their own feed pressure requirement, the two d.o.f. are used up in specifying distillate and bottoms pressures. Thus the distillation column of Figure 6a has no d.o.f. at all! Yet students are expected to specify two product concentrations and often the column pressure as well.

(That the distillation column as depicted has no freedom may seem counter-intuitive. However, a little thought will show that there is only one reboiler heating rate and one condenser cooling rate that will simultaneously ensure a saturated single-phase bottom stream and a saturated single-phase distillate stream. Increasing, say, the reboiler heating rate beyond that will cause the distillate to superheat or vapour to escape with the bottom product).

The answer is obviously to put throttle valves (or compressors/pumps) on the two outlet streams, making \( M = 2 \) (Figure 6b). With the two d.o.f. that result, one can then specify two product concentrations. Putting another throttle or pump on the feed stream adds another d.o.f., which can be used to specify the column pressure. In the author’s opinion, leaving out throttling valves from sketches and flow diagrams is a frequent source of misunderstanding, particularly for unfamiliar pieces of equipment.

CONCLUSION
This paper has proposed a method of counting operational degrees of freedom that is considerably quicker and easier than the classical method of listing all variables and relationships. The classical method usually involves subtracting one large number from another, while the proposed method involves mainly adding the contributing factors. Obviously, the method does not mean one can do away with judgment, common sense or understanding of the process. In particular, care is still needed to determine which variables are "influential" and to avoid double-counting. However, by reducing the number of things to be counted (e.g. from 55+9+48 = 112 to 12 for the example process), the possibility for errors is much reduced.

REFERENCES
Table 1. D.o.f. analysis of some elementary units and processes. "x" indicates parameters that are irrelevant to d.o.f. Feed streams are assumed to be completely specified. Unless otherwise specified, the most basic equipment configuration is assumed.

<table>
<thead>
<tr>
<th>Equipment</th>
<th>S</th>
<th>K</th>
<th>M</th>
<th>E</th>
<th>P</th>
<th>N</th>
<th>F₀</th>
<th>Free variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pipe</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>x</td>
<td>0</td>
<td>0</td>
<td>-</td>
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<td>Variable stream splitter</td>
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<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>Flow ratio</td>
</tr>
<tr>
<td>Distillation tray. Adiabatic flash separator</td>
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<td>1</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>-</td>
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<tr>
<td>Tray with take-off. Adiabatic flash with three outlets</td>
<td>2</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>-</td>
<td>Take-off flow</td>
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<td>Heat exchanger</td>
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<td>2</td>
<td>0</td>
<td>0</td>
<td>x</td>
<td>0</td>
<td>0</td>
<td>-</td>
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<td>Non-adiabatic reactor</td>
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<td>1</td>
<td>0</td>
<td>1</td>
<td>x</td>
<td>0</td>
<td>1</td>
<td>Conversion</td>
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<td>2</td>
<td>1</td>
<td>1</td>
<td>Heat input</td>
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<td>1</td>
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<td>0</td>
<td>1</td>
<td>Degree of subcooling</td>
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<td>1</td>
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<td>1</td>
<td>Vapour/liquid ratio</td>
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<td>1</td>
<td>0</td>
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<td>2</td>
<td>2</td>
<td>2</td>
<td>Conc. and flow of one key component</td>
</tr>
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<td>Distillation column with partial condenser and side take-off</td>
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<td>0</td>
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<td>3</td>
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<td>1</td>
<td>3</td>
<td>Conc. and flow of one key component + column pressure</td>
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<td>Compression refrigeration cycle</td>
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<td>0</td>
<td>0</td>
<td>3</td>
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<td>Refrigeration load + evaporating temp.+ condensing temp.</td>
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<td>As single stage + intermediate pressure</td>
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<td>1</td>
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<td>2</td>
<td>1</td>
<td>Product moisture</td>
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Table 2. D.o.f. analysis of the process of Figure 3.

<table>
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<tr>
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<th>S</th>
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<th>N</th>
<th>F₀</th>
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<td>Reactor with heat input</td>
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<td>1</td>
<td>0</td>
<td>1</td>
<td>x</td>
<td>0</td>
<td>1</td>
<td>Heat input</td>
</tr>
<tr>
<td>Heat exchanger</td>
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<td>1</td>
<td>0</td>
<td>1</td>
<td>x</td>
<td>0</td>
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<td>Heat output</td>
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<td>Valve</td>
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<td>0</td>
<td>x</td>
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<td>Heat input</td>
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<td>6</td>
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</table>
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6. Distillation column (a) basic (b) throttles added.
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