Degrees of freedom analysis for process control

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Abstract

In defining the control structure of a system it is very important to know how many variables we can regulate. The degrees of freedom (DOF) analysis of the system allows establishing the maximum variables that need to be fixed to have a completely determined system. Of all the DOF some of them will be disturbances (i.e. they are fixed externally) and the rest indicates the maximum number of variables to control. The procedure developed in this paper is based on, and extends and generalizes, the one presented by Ponton (Degrees of freedom analysis in process control.).

The procedure presented derives, from the analysis of a general unit (system), a formula to compute the DOF. This formula is then generalised to be applied to any process.

Keywords: Process control, degrees of freedom.

1. Introduction

The degrees of freedom analysis is used in the development of control (and plantwide control) strategies. Writing all the equations for a process and counting the variables is a tedious and error prone process, so it is important to have a simple but generic method to compute the degrees of freedom for control of a whole process. The first approach in this direction was developed by Kwauk [1] in the context of process design. The procedure developed in this paper follows somehow the one described by Ponton [2] but instead of applying the Kwauk method as in Ponton's it starts from a generic system and applies on it first principles equations..

Degrees of freedom (DOF) can be defined as:

DOF = Number of variables of the system – Number of equations of the system

The degrees of freedom are the variables that have to be set to have a completely determined system DOF can be set by the environment (disturbances) or by the control system. The following method will compute the overall DOF of the system and will differentiate between disturbances and control variables. An expression is deduced to compute in a simple way all the available DOF for control.

2. Degrees of freedom analysis

The degrees of freedom analysis will be performed on a generic system as the one described in figure 1. First the amount of system variables will be calculated and then the equations that can be applied to the system.

2.1. System variables (streams and unit)

* Input streams

There are S_i input streams, each stream has C variables corresponding to the components and one pressure and temperature, so the total amount of variables in input streams are:
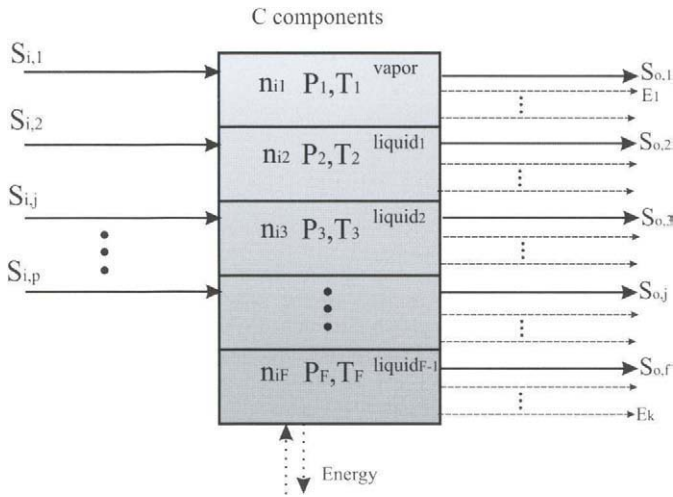
$S_i*(C+2)$

Fig 1. Generic system. Where S_i are the input streams, S_o are the output streams (one per phase), E are additional output streams from a phase, n_{ij} are the moles of component i in phase j, P_i and T_i are the pressure and temperature of phase i. The system has C different species and F different phases. One or more energy streams can interact with the system.

- Unit (system)

There are C variables corresponding to component accumulation and a pressure and a temperature in each phase. Total variables in the unit are:

$F*(C+2)$

- Output streams

We have So plus E output streams from the system, but the only new (not accounted for) variables that they add are the flows, because composition, pressure and temperatures have been taken into account in the unit (and they are the same as the composition , pressure and temperature of the outlet streams)

Total variables in output streams: S_o+E

- Energy stream

If there is an energy stream to (or out of) the system then an additional variable has to be taken into consideration. This energy flow can be thermal or mechanic... It only adds one variable (even if more than one energy stream exists) from a control point of view and it is the amount of energy that will be added in the propoer balance (this will affect to system temperature or pressure). If the energy is transferred inside the system boundaries as it happens with a process to process heat exchanger then this variable will not add any DOF..

To consider the energy a variable called H is added, which will take the value 1 if there is energy flow to (out of) the system and 0 otherwise.

Variables in the system: $S_i*(C+2) + F*(C+2) + S_{out} + H$

2.2. System equations

- Mass balance

There is one mass balance per component , so we have C equations.

- Energy balance

There is one energy balance to be applied to the system

- Momentum balance

Although the momentum balance is vectorial and three individual balances can be established, in the process industry only one of them is generally significant (in the flow line, Bernouilli's equation) so we have an additional equation (if more balances are applied more variables have to be considered so it doesn't affect to the degrees of freedom computation)

- Equilibrium or transport equations

We can have the system in equilibrium or not, in any case the same amount of equations arise.

If we have equilibrium we can establish composition, pressure and temperature equalities in the interfaces. If we don't have equilibrium we can establish in each interface C mass transport equations (Fick's law) for the compositions, one heat transport equation (Fourier's law) for temperature and one momentum (only one out of the three possible is generally meaningful) transport equation for pressure (Newton's law).

Total equilibrium or transport equations (there are F-1 interfaces) : $(F-1)*(C+2)$

Equations in the system: $C+1+1+(F-1)*(C+2)$

(In the case of vapor phase we have an additional equation, the gas law, but we have another variable, V. so it doesn't change the degrees of freedom)

2.3. Degrees of freedom

The computation of the degrees of freedom using the above decomposition results in:

$DOF= S_i*(C+2) + F*(C+2) + S_{out} + H-[C+1+1+(F-1)*(C+2)]= S_i*(C+2) + S_{out} + H$

From these degrees of freedom in the input streams we can only act upon the flow so the remaining degrees of freedom of these streams are disturbances (from a control point of view). This results in:

$DOF= S_i + S_{out} + H$

Up to this point all the inventories have been considered, but many times we are not interested in or we cannot control them (like when a pipe is splitted into two or when the output of a tank is through a weir). We introduce now an additional variable, A. This variable is the amount of inventories (liquid or gas) that are not considered. This variable (A) removes one DOF if there is one process variable available to control the inventory that is not used (or cannot be used). For example if we have a tank with one input and one output and both are flow controlled then A does not remove any degree of freedom as the inventory is taken into account indirectly.
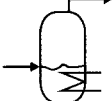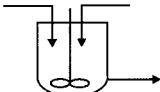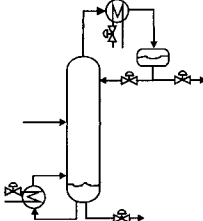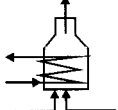
The final DOF equation is: $DOF= S_i + S_{out} + H-A$

We have not considered the case of the existence of a reaction as it does not vary the DOF analysis (it adds one variable the extent of the reaction, and one equation, the kinetic expression which is composed of variables that are already considered).

One final consideration must be noticed. In the system only a temperature, pressure,... is considered in each phase. This is true only in completely mixed systems, in the case where a gradient of variables exists it doesn't modify the DOF analysis. We can decompose each phase in N compartments, this will add N-1 new variables for temperature, pressure and each composition. But we can set an equation for each of the new N-1 interfaces for temperature, pressure and each composition through the transport laws, so the DOF is not altered as stated before.

2.4. Examples

The expression is applied to some common process units.

Table 1. Process units degrees of freedom

Unit		Degrees of freedom $S_i + S_{out} + H\text{-}A$
Heater		DOF=1 + 1 + 1 – 1 = 2
Process heat exchanger		DOF=2 + 2 + 0 – 2 = 2 (in this case the inventories in shell and tubes are not controlled) Energy is cero because the flow is between process streams.
Pump		DOF=1 + 1 + 1 – 1 = 2 [1]
Compressor		DOF=1 + 1 + 1 – 1 = 2 [2]
Vaporizer		DOF= 1 +1 + 1 – 0 = 3
CSTR		DOF= 2 +1 + 0 – 0 = 3
Distillation		Column: 1+3+0-2 = 2 Condenser: 1+2+1-0 = 4 Reboiler: 1+1+1-1 = 2 (pressure is not controlled) The distillation has been decomposed as a process so the general expression (next section) is applied: DOF= 1+[3-2]+[2+1]+[1+1-1]= 6
Furnace		DOF=3 + 2 + 0 – 1 = 4 The inventory in the tubes is not considered, and the energy term is cero because it both are considered process streams.

(1) Although it is possible to control (specify) two different variables in pumps, the flow and the head, it is not desirable from a process point of view. The speed of the pump and the impulsion valve can be manipulated to fix the flow and the head, but it doesn't make sense to work with other than the minimum necessary head so only one degree of freedom is used in pumps.

(2) The same happens to compressors. Usually the pressure is the only variable to control, but both pressure and flow can be controlled.

3. Degrees of freedom analysis of a process

3.1. DOF expression

The expression deduced can be extended to compute the degrees of freedom of a complete process. The total DOF of the process will be the sum of the DOF of the units, but removing all the DOF related to input streams but the inputs to the process (any input of a unit is the output of an upstream unit so it is already accounted for in the DOF expression).

The DOF expression for a complete process is:

$$DOF = S_{ip} + \Sigma^u (S_{out} + H\text{-}A)$$

Where S_{ip} are the inputs to the process, and Σ^u is the sum of all the units in the process. This is the maximum SISO control loops that can be established, although other process constraints can make this number lower. This expression is easily applied to any process, and it finally derives in counting all the process streams, adding all the energy flows (one per unit) and removing all the inventories not to be considered. Following the expression is applied to several processes.

3.2. Example 1. Vinyl Acetate process

The flowsheet of fig. 2 represents the industrial process for the vapor phase manufacture of vinyl acetate monomer. The process is based on the description in [3] and [4]. The process has three feeds: oxygen, ethylene and acetic acid. The main reaction takes place in a plug flow reactor and the heat is removed generating steam. This process is described by Luyben in [5] when exposing his methodology for plantwide control. He presents 26 degrees of freedom.
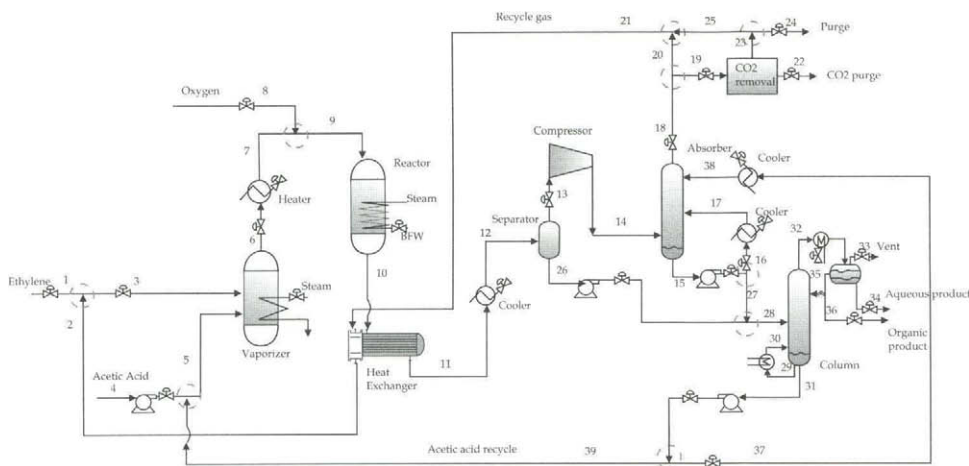

Figure 2. Vinyl acetate monomer process

Degrees of freedom:
Number of process streams: 39
Number of inventories not accounted: 20 (9 mixers or splitters, 4 heaters, 2 heat exchanger, reactor, CO_2 removal, 1 reboiler, 2 distillation column)
Number of energy streams: 8 (4 heaters, 1 vaporizer, 1 reactor, 1 reboiler, 1 condenser)

DOF=39-20+8=27 The difference with Luyben is the compressor. Usually (as in this case) only the pressure is controlled, so one degree of freedom is removed (as explained in the previous section when commenting the DOF of pumps and compressors). One possible set of manipulated variables is shown in the figure.

3.3. Example 2.Vinyl Chloride Monomer(VCM) process

Vinyl chloride (VCM), which is made from ethylene and chlorine, is used as feedstock in the production of the standard plastic material PVC. Figure 3 shows the balanced process with no net consumption or generation of HCl as described in [6] and [7]. It combines direct chlorination, ethylene dichloride (EDC) pyrolysis and oxychlorination (which consumes all the HCl generated in EDC pyrolysis. Chlorination and oxychlorination reactions takes place in tubular reactors and the pyrolysis takes place in a furnace type reactor.
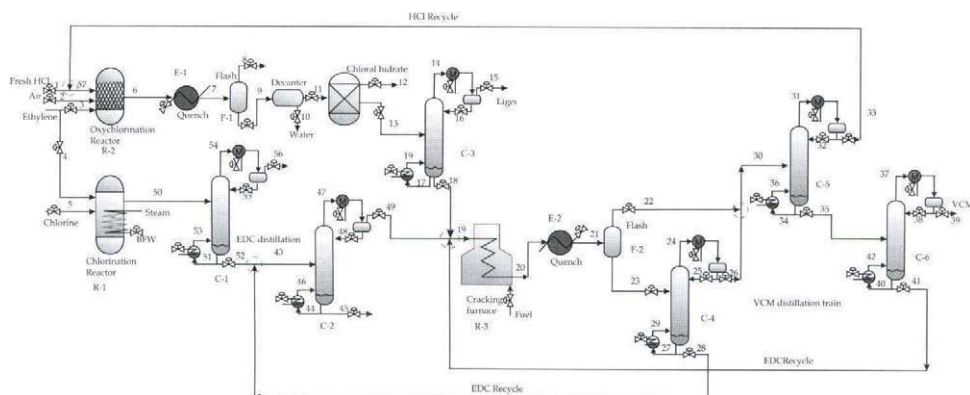
Figure 3. Vinyl chloride monomer process

Degrees of freedom:
Number of process streams: 57
Number of inventories not accounted: 24 (4 in mixers or splitters, 2 in heaters, 3 in reactors, 5 in reboilers, 10 (2*5) in distillation columns)
Number of energy streams: 14 (2 in reactors, 2 in heaters, 5 in reboilers, 5 in condensers)

DOF=57-24+14=47 One possible set of manipulated variables is shown in figure 3.

4. Conclusions

In this paper a simple expression to compute the (maximum) degrees of freedom available for control of any process. There is no need to write any equations as the expression has been obtained through a rigorous application of the available physicochemical equations (conservation laws, transport laws, equilibrium constraints) to a generic system. This method takes into consideration the inventories which are very important in establishing any control strategy for a process. The expression has been tested in numerous processes as the two presented in this paper. The expression is easily implemented in a software application and can be used as an initial step in any Plantwide control method. It can help to sort out the available controlled variables of the process.

This expression is currently implemented and is being used in a plantwide control methodology that is being developed by the authors and that will be presented elsewhere.

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