Using Microsoft Excel to efficiently generate Buckingham π sets.

In our course, *The scale-up of chemical processes – getting it right the first time*[1], we describe the use of Buckingham π theory[2] to generate dimensionless groups. According to the theory, dimensionless groups are invariant not only to the system of units selected to calculate them but more importantly they are invariant to the size of the system. Thus these dimensionless groups are the parameters which, if they are the same in the plant batch as in the lab or pilot batch, will ensure that the small system is a valid model of the large system.

The application of Buckingham π theory to the scale-up of chemical processes is the focus of the fine book *Scale-up in Chemical Engineering*[3] by Prof. Marko Zlokarnik, which contains numerous case studies of the use of dimensionless numbers in scale-up. In this book, Prof. Zlokarnik describes a null-matrix procedure for systematically generating dimensionless groups. While effective, Zlokarnik's procedure is a bit tedious. Presented here is a method using the matrix-math functionality built into Microsoft Excel to efficiently achieve the same result.

The procedure is best demonstrated by example. Assume we wish to scale-up a mixing process and decide the relevant parameters are: liquid density, agitator diameter, agitator speed, agitator power, viscosity and gravitational acceleration:

Property	Symbol	Units	Dimensionality
Density	ρ	kg m^{-3}	ML^{-3}
Agitator diameter	D	m	L
Agitator Speed	N	sec^{-1}	T^{-1}
Agitator Power	P	kg m^2 sec^{-3}	$ML^{-2}T^{-3}$
Viscosity	μ	kg m^{-1} sec^{-1}	$ML^{-1}T^{-1}$
Gravitational acceleration	g	m sec^{-2}	LT^{-2}

The dimensions of the system are mass (M), Length (L) and Time (T). Since this system has 3 dimensions and 6 relevant parameters, Buckingham's theory states there will be 6 – 3 = 3 dimensionless groups. Zlokarnik's matrix solution to the problem of finding these dimensionless groups is as follows:

Create a matrix with the dimensions as the rows and the process variables as the columns; each matrix element containing the exponent of the dimensionality:

	Core matrix			Residual matrix		
	ρ	D	N	P	μ	g
M	1	0	0	1	1	0
L	-3	1	0	2	-1	1
T	0	0	-1	-3	-1	-2

This matrix is partitioned into a core matrix and a residual matrix. The dimensionless numbers resulting from the analysis will be the ratio of the parameters which make up residual matrix to the product of those which make up the core matrix raised to the power of the mapped elements in the solved residual matrix.

Zlokarnik's procedure requires solving the system by performing elementary row operations on the above system until the core matrix equals the identity matrix, like so:

	Core matrix			Residual matrix		
	ρ	D	N	P	μ	g
M	1	0	0	1	1	0
3M-L	0	1	0	5	2	1
-T	0	0	1	3	1	2

We see here that the parameters of the core matrix (ρ, D, and N) are mapped to their exponents in the solved residual matrix. There will be one dimensionless group corresponding to each parameter of the residual matrix, and its denominator will be the product of the parameters in the core matrix raised to their mapped exponents. Row 1 contains the exponents of the density, row 2 the exponents of the diameter and so on. The π-set for this system, consists of the following 3 dimensionless numbers:

$$\pi_1 = \frac{P}{D^5 N^3 \rho} \equiv N_p \equiv \text{Power number}$$

$$\pi_2 = \frac{\mu}{DN^2 \rho} \equiv N_{\text{Re}}^{-1} \equiv \text{ Reynolds Number}$$

$$\pi_3 = \frac{g}{DN^2} \equiv N_{\text{Fr}} \equiv \text{ Froude Number}$$

The example above, which is the example used in the course, is a nice example in that it is relatively easy to solve and yields the dimensionless groups which have well known physical interpretations. In practice however, the pursuit of innovative projects would require us to deal with more complex, non-textbook examples. For instance, if we were to consider heat transfer as well, we would need to add Temperature (Θ) to the dimensionality, resulting in 4 dimensions. We would also add several columns to the residual matrix, for example thermal conductivity or heat capacity making the above procedure yet more tedious. Likewise, the above example is somewhat contrived in that a problem was selected which was known to yield the textbook dimensionless groups above. Additionally, just because the procedure produces a complete π-set, does not mean it produces a unique set. Occasionally, one finds that an unfortunate partitioning of parameters in the matricies yields a π-set contains, for instance, two numbers whose quotient is the Reynolds number, or some other familiar number. Frequently with a big problem, changing the parameters from one partition to the other yields a more useful, or at least more insightful, π set.

That having been said it is useful to have a procedure which allows us to do this calculation quickly, so we might experiment with which parameters should comprise the core and residual matrices. In order to do this, we should examine more closely what Prof. Zlokarnik is trying to achieve.

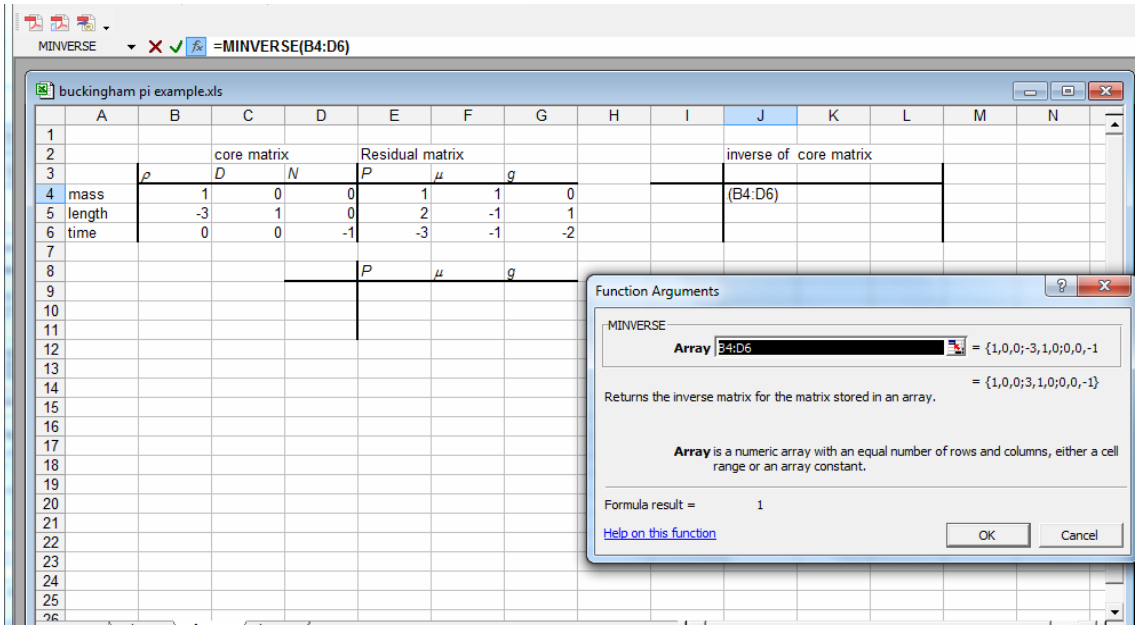
If we call the entire matrix **M**, we see that it is partitioned into a core matrix **C** and a residual matrix **R**, thus **M=C|R.** We then manipulate the matrix to a state **N** so that the partitions are the identity matrix **I** and the solved residual matrix **S**: **N=I|S.** This is equivalent to multiplying through matrix **M** by the inverse of the core matrix:

$$\mathbf{N} = \mathbf{C}^{-1}\mathbf{M}$$

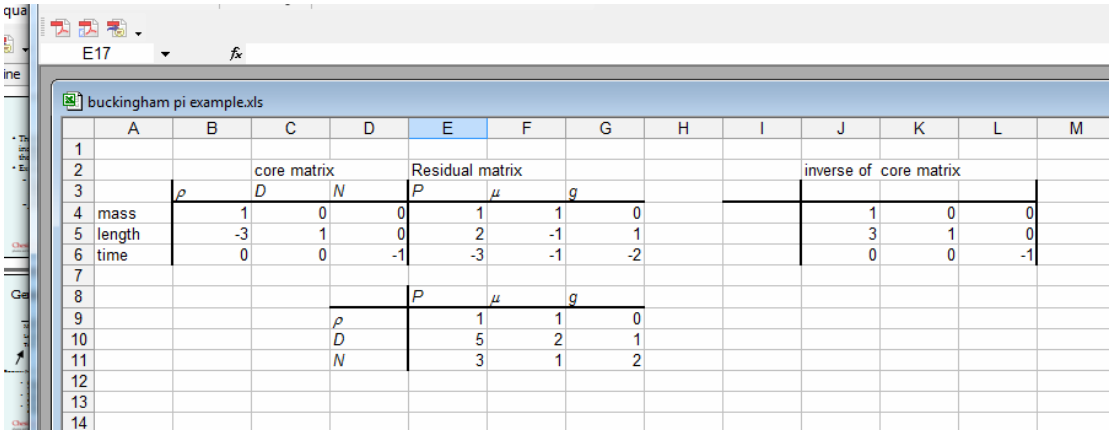
It then follows that the solved residual matrix is:

$$\mathbf{S} = \mathbf{C}^{-1}\mathbf{R}$$

We can automate this process using the matrix math functions in Microsoft Excel. To do so, set up a spreadsheet with the partitioned matrix as shown below. In this example J4:L6 are used to store the inverse of the core matrix B4:D6



Use the function MINVERSE in range J4:L6 to calculate the inverse of the matrix B4:D6. To do so one must enter that range as a matrix formula in the function by first highlighting the range J4:L6 selecting the MINVERSE function then highlighting B4:D6 and using CTRL+SHIFT+ENTER. Likewise, use the MMULT function in cells E9:G11 again entering ranges J4:L6 and E4:G6 as matrix arguments in that order (remember, matrix multiplication is not commutative so the order of the arguments matter. Finally one can use the TRANSPOSE function to place the column headings of the core matrix as the row headings of the solution matrix yielding a spreadsheet that looks like this:



Note that the TRANSPOSE function also requires highlighting the entire range of destination cells and entering a matrix argument using CTRL+SHIFT+ENTER.

The benefit of using a spreadsheet for this analysis is the same as the benefit of using a spreadsheet for any other analysis: one can set-up the math and quickly change the values one wishes to analyze. By trading parameters making up the columns in the core matrix with those in the residual matrix one can examine how to express a system through the most physically sensible set of dimensionless groups.

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[1] Guy Gloor and Roy Drayton *The scale-up of chemical processes – getting it right the first time* – A course in scale-up. For more information email: courses@chesilton.com

[2] Buckingham, E; *On physically similar systems; Illustrations in the use of dimensional equations*, Phys.Rev. **4**: 345–376 (1914)

[3] Zlokarnik, Marko; *Scale-up in Chemical Engineering*, Wiley-VCH (2006)