Appendix A: Dimensionless Groups

Dimensional analysis is a key step in modeling processes [1, 2]. There are usually fewer dimensionless groups than there are physical quantities (Buckingham's rule) [3]. When the model is evaluated or displayed, the dimensionless groups are the correct axes to choose (see, for example Fig. 4-18). It should be emphasized that dimensionless groups should always be used for exponential, logarithmic, or power law arguments since failure to do so may lead to pseudo-constants without physical significance [3].

Because of their ability to simplify complex modeling problems, dimensionless groups are frequently used in chemical engineering to solve complex equations of heat and mass transfer. In particular, equations of heat, mass and impulse transfer ubiquituously occuring in the description of plasma spray processes and numerical solutions of modeling approaches can be deduced from existing solutions of geometrically similar systems [4]. The term 'geometric similarity' refers to the interchangeability of streamlines and boundaries of systems of widely varying dimensional extention by linear scaling laws. Motion of fluids such as a plasma gas are dynamically similar when the solutions of the related dimensionless transfer equations are identical. For example, the simplified Navier–Stokes equation

$$\rho(\delta v/\delta t) = \rho(v \cdot \nabla)v - \nabla p + \eta\nabla^2 v + f, \tag{A-1}$$

where v = mass average velocity (barycentric velocity), p = plasma gas pressure, and η = plasma gas viscosity, can be transformed to its dimensionless version by using the free-stream plasma velocity V, a characteristic length L and a typical pressure p_0 to normalize $v(x, y, z)$ and p by setting

$$\begin{aligned} &\text{velocity} && W = v/V, \\ &\text{length} && X = x/L, \quad Y = y/L, \quad Z = z/L, \quad \text{and} \\ &\text{pressure} && P = p/p_0. \end{aligned} \tag{A-2}$$

Substituting the dimensionless ratios into Eq. (A-1) yields

$$\rho(V^2/L)(W \cdot \text{grad})\,W = -(p_0/L)\ \text{grad}(P) + (\eta V/L^2)\nabla^2 W \tag{A-3}$$

or

$$(W \cdot \text{grad})\,W = -(p_0/\rho V^2)\ \text{grad}(P) + \text{Re}^{-1}(\nabla^2 W), \tag{A-3a}$$

with $\text{Re} = VL/\eta$.

It should be noted that the second term on the right hand side of Eq. (A-3a) contains all the parameters that govern the fluid dynamics of a plasma jet. Dynamic similarity is assured if for two geometrically similar systems A and B, Re(A) = Re(B). The similarity principle was discovered by Reynolds and has overriding importance for any modeling approach in fluid dynamics [5].

The most important dimensionless groups used in modeling of plasma heat and mass transfer equations can be conveniently divided into groups describing momentum-, heat-, and mass transfer, and materials constants.

Momentum transfer

Reynolds number	$\mathrm{Re} = VL/\nu$ (inertia force/viscous force)
Euler number	$\mathrm{Eu} = \Delta p/\rho V^2$ (fluid friction)
Grashof number	$\mathrm{Gr} = L^3 g\gamma \Delta T/\nu^2$ (bouyancy force/viscous force)

Heat transfer

Fourier number	$\mathrm{Fo} = \kappa \Delta T/L^2$ (heat transfer by diffusion)
Péclet number	$\mathrm{Pe} = VL/\kappa = \mathrm{Re} \times \mathrm{Pr}$ (bulk heat transfer/conductive heat transfer)
Rayleigh number	$\mathrm{Ra} = L^3 g\gamma \Delta T/\nu\kappa = \mathrm{Gr} \times \mathrm{Pr}$ (free convection)
Nusselt number	$\mathrm{Nu} = hL/k = \mathrm{Re} \times \mathrm{St}$ (total heat transfer/conductive heat transfer)
Stefan number	$\mathrm{St} = \sigma LT^3/k$ (heat transfer by radiation)

Mass transfer

Fourier number	$\mathrm{Fo}^* = D\Delta T/L^2 = \mathrm{Fo}/\mathrm{Le}$ (unsteady state mass transfer)
Péclet number	$\mathrm{Pe}^* = VL/D = \mathrm{Re} \times \mathrm{Sc}$ (bulk mass transfer/diffusive mass transfer)
Grashof number	$\mathrm{Gr}^* = L^3 g\beta' \Delta x/\nu^2$ (mass transfer at free convection)
Nusselt number	$\mathrm{Nu}^* = kL/\rho D = \mathrm{Sh}$

Materials constants

Prandtl number	$\mathrm{Pr} = \nu/\kappa = \mathrm{Pe}/\mathrm{Re}$
Schmidt number	$\mathrm{Sc} = \nu/D = \mathrm{Pe}^*/\mathrm{Re}$
Lewis number	$\mathrm{Le} = \kappa/D = \mathrm{Sc}/\mathrm{Pr}$

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Appendix B: Calculation of Temperature Profiles of Coatings

The following treatment has been adapted from the work by Houben [1]. It provides the calculations required to arrive at the temperature profiles through Mo and AISI-316 coatings, respectively deposited onto a low carbon steel substrate as shown in Fig. 5-12. The calculations are based on the Neumann–Schwartz equation [2].

B.1 Heat Conduction Equations

For the three regions identified in the coordinate system of Fig. 5-10 the three heat conduction (Fourier) equations can be expressed by

$$\partial^2\Theta_0/\partial x^2 - (1/a_0)\partial\Theta_0/\partial t = 0 \quad \text{for } x \leq 0 \text{ (solid substrate)} \tag{B-1a}$$

$$\partial^2\Theta_1/\partial x^2 - (1/a_1)\partial\Theta_1/\partial t = 0 \quad \text{for } 0 \leq x \leq X(t) \text{ (solid deposit)} \tag{B-1b}$$

$$\partial^2\Theta_2/\partial x^2 - (1/a_2)\partial\Theta_2/\partial t = 0 \quad \text{for } x \geq X(t) \text{ (liquid deposit)}, \tag{B-1c}$$

where Θ = temperature and a = thermal diffusivity.

The boundary conditions are $\Theta_0 = T_{s0}$ (20 °C) as $x \to -\infty$,

$$\Theta_0 = \Theta_1 \quad \text{as } x = 0.$$

$$\Theta_1 = \Theta_2 \quad \text{as } x = X(t)$$

For thermal equilibrium conditions at the interfaces it follows that

$$k_0(\partial\Theta_0/\partial x) = k_1(\partial\Theta_1/\partial x) \quad \text{as } x = 0 \tag{B-3}$$

$$k_1(\partial\Theta_1/\partial x) - k_2(\partial\Theta_2/\partial x) = L\rho(\mathrm{d}X/\mathrm{d}t) \quad \text{as } x = X(t), \tag{B-4}$$

where L = latent heat of melting.

For the special case indicated in Fig. 5-10 ($\Theta_2 = T_3 = T_m$ for $x \geq 0$) the Eq. (B-4) simplifies to

$$k_1(\partial\Theta_1/\partial x) = L\rho(\mathrm{d}X/\mathrm{d}t) \quad \text{as } x = X(t). \tag{B-4a}$$

B.2 Solutions of the Equations

B.2.1 Substrate Temperature Profile

Assumption: $\Theta_0 = T_{s0} + \alpha[1 + \text{erf}(x/(4a_0t)^{1/2})]$. (B-5)

The quantity α is the so-called contact conductivity at the interface substrate/solid deposit ($x = 0$) and is defined as $\alpha = (k_1\rho_1c_1)^{1/2}$, where k = thermal conductivity, ρ = density, and c = specific molar heat. It should be emphasized that the solution shown in Eq. (B-5) satisfies both Eq. (B-1a) and, because of $\Theta_0 \to T_{s0}$ as $x \to -\infty$, the first boundary condition. The error function erf is as usually defined as erf $z = \int(2/\pi^{1/2}) \exp(-z^2)\,dz$.

B.2.2 Deposit Temperature Profile

Assumption: $\Theta_1 = T_{s0} + \beta + \gamma \text{ erf}(x/(4a_1t)^{1/2})$. (B-6)

The quantity β is the contact conductivity at the interface solid/liquid deposit ($x = X(t)$), and γ the 'contact' diffusivity at the free interface receiving a constant stream of molten particles. Eq. (B-6) satisfies Eq. (B-1b), and also satisfies the second boundary condition if $\beta = \alpha$ ($\Theta_0 = \Theta_1$ as $x = 0$). Then Eq. (B-6) can be rewritten as

$$\Theta_1 = T_{s0} + \alpha + \gamma \text{ erf}(x/(4a_1t)^{1/2}). \tag{B-6a}$$

To establish the required connection between α and γ the Eqs. (B-5) and (B-6) will be differentiated to yield

$$\begin{aligned}\partial\Theta_0/\partial x &= \alpha[[\partial/\partial x) \text{ erf}(x/(4a_0t)^{1/2})] \\ &= \alpha(2/\pi^{1/2}) \exp(-x^2/4a_0t)(1/(4a_0t)^{1/2}) \\ &= [\alpha/(\pi a_0t)^{1/2}] \exp(-x^2/4a_0t).\end{aligned} \tag{B-7}$$

For $x = 0$ it follows that

$$(\partial\Theta_0/\partial x)_{x=0} = \alpha/(\pi a_0t)^{1/2}. \tag{B-7a}$$

Analogously one obtains

$$(\partial\Theta_1/\partial x)_{x=0} = \gamma/(\pi a_1t)^{1/2}. \tag{B-7b}$$

Substituting Eqs. (B-7a) and (B-7b) into (B-3) yields

$$k_0(\alpha/(\pi a_0t)^{1/2}) = k_1(\gamma/(\pi a_1t)^{1/2}).$$

With $\alpha/\gamma = B$, and $a = k/\rho c$ one obtains

$$B = (k_1\rho_1 c_1)^{1/2}/(k_0\rho_0 c_0)^{1/2}. \tag{B-8}$$

With Eq. (B-8), Eq. (B-6a) can be expressed as

$$\begin{aligned}\Theta_1 &= T_{s0} + \gamma[(\alpha/\gamma) + \operatorname{erf}(x/(4a_1t)^{1/2})] \\ &= T_{s0} + \gamma[B + \operatorname{erf}(x/(4a_1t)^{1/2})].\end{aligned} \tag{B-9}$$

For $\Theta_1 = \Theta_2 = T_m$ (as $x \geq X(t)$) we obtain the explicit solution of the heat transfer equation at the interface liquid/solid deposit as

$$T_m - T_{s0} = \gamma[B + \operatorname{erf}(x/(4a_1t)^{1/2})]. \tag{B-10}$$

With the assumption

$$X = p(4a_1t)^{1/2} \quad \text{or} \quad t = X^2/4p^2a_1 \tag{B-10a}$$

(solution of the first-order differential equation of heat transfer) it follows that

$$\mathrm{d}X/\mathrm{d}t = p(a_1/t)^{1/2}. \tag{B-11}$$

With Eq. (B-7) for $x = X(t)$, Eq. (B-4a) can further be expressed by

$$k_1(\gamma/(\pi a_1t)^{1/2}) \exp(-X^2/4a_1t) = L\rho\,(\mathrm{d}X/\mathrm{d}t) \tag{B-12}$$

and with (Eq. B-11) as

$$k_1(\gamma/(\pi a_1t)^{1/2}) \exp(-X^2/4a_1t) = L\rho p(a_1/t)^{1/2}. \tag{B-13}$$

From Eqs. (B-10 and 10a) it follows that

$$\gamma = (T_m - T_{s0})/[B + \operatorname{erf}(X/(4a_1t)^{1/2})] = (T_m - T_{s0})/(B + \operatorname{erf} p). \tag{B-14}$$

Inserting Eqs. (B-14) and (B-10a) into Eq. (B-13) yields

$$(k_1/(\pi a_1t)^{1/2})[(T_m - T_{s0})/(B + \operatorname{erf} p)] \exp(-X^2/4a_1t) = L\rho p(a_1/t)^{1/2} \tag{B-15}$$

or

$$(k_1/(\pi a_1t)^{1/2})[(T_m - T_{s0})/(B + \operatorname{erf} p)] \exp(-p^2) = L\rho p(a_1/t)^{1/2}. \tag{B-15a}$$

If the density of the molten particles equals the density of the solid material ($\rho = \rho_1$), Eq. (B-15a) can be expressed as

$$(k_1/(\pi a_1t)^{1/2})[(T_m - T_{s0})/(B + \operatorname{erf} p)](1/(a_1/t)^{1/2}) = (L\rho_1 p) \exp(p^2), \tag{B-16}$$

and finally, because $c_1 = k_1/\rho_1 a_1$,

$$(B + \text{erf } p)p \exp(p^2) = c_1(T_m - T_{s0})/L(\pi)^{1/2}. \tag{B-17}$$

Eq. (B-17) can be used to determine the constant p from the energy balance at the solidification front. It can also be taken from a nomogram provided by Kuijpers and Zaat [2]. With this one can also determine the *real temperature profiles.*

B.3 Real Temperature Profiles

From Eq. (B-8) it follows that $\alpha = \gamma B$, and with Eq. (B-14) one obtains

$$\alpha = [B(T_m - T_{s0})]/[B + \text{erf } p)]. \tag{B-18}$$

Inserting Eq. (B-18) into Eq. (B-5) yields the *real substrate temperature profile*

$$\Theta_0 = T_{s0} + \{[B(T_m - T_{s0})]/[B + \text{erf } p]\}\{1 + \text{erf}(X/(4a_0t)^{1/2})\}. \tag{B-19}$$

Likewise, the *real solid deposit temperature profile* becomes

$$\Theta_1 = T_{s0} + \{(T_m - T_{s0})/[B + \text{erf } p]\}\{B + \text{erf}(X/(4a_1t)^{1/2})\}. \tag{B-20}$$

On rewriting the Eqs. (B-19) and (B-20) yield their final expressions:

$$(\Theta_0 - T_{s0})/(T_m - T_{s0}) = [B/(B + \text{erf } p)][1 + \text{erf } (X/(4a_0t)^{1/2})] \tag{B-19a}$$

and

$$(\Theta_1 - T_{s0})/(T_m - T_{s0}) = [1/(B + \text{erf } p)][B + \text{erf } (X/(4a_1t)^{1/2})]. \tag{B-20a}$$

These equations should be compared with the approximate expression obtained for transient heat conduction in solid spheres as shown earlier:

$$(T_m - T_R)/(T_m - T_1) = \text{f}(\text{Bi}, \text{Fo}) = \text{f}[\alpha\Theta/r^2] = \text{f}[a_1 t/r_0^2] \tag{4-23}$$

References

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Appendix C: Calculation of Factor Effects for a Fractional Factorial Design 2^{8-4}

In this example, calculations will be shown for estimating factor effects for the dependence of the thickness of a plasma-sprayed 88WC12Co coating on the eight selected plasma parameters and their ranges (Table C-1). To avoid bias (systematic) errors the 16 experimental runs to be performed were randomized. This randomized fractional two-level factorial design is shown in Table C-2.

The 2^{8-4} design chosen is a 1/16 replicate of a full 2^8 factorial of resolution IV that has the power to estimate the eight main factor effects X_i clear of each other, and clear of composite two-factor interactions E_i[1]. The effects of higher-order interactions can usually be safely neglected. Composite effects of the sum of four two-factor interactions, however, can be estimated from the unassigned factors. If only weak or no interactions exist, the effects of unassigned factors can be used to estimate the experimental (statistical) error, i.e. the minimum significant factor effect. The arrangement of the coded parameter levels in the design matrix (Table C-3) follows Yates' standard order.

Tables C-3 and C-4 show the numerical evaluation of the results for the main factor effects X_i and the composite two-factor interactions E_i. First the sum $\sum(+)$ of all responses Y (thickness of coating) on the '+' level is calculated. Then the $\sum(-)$ of all responses Y on the '−' level is calculated. The factor effect is the difference Δ of the two sums, divided by the number of '+' (or '−') signs in each column. The coefficients, C, of the parameters in the polynomial response equation are obtained by dividing

[1] The confounding pattern of the composite two-factor interactions E_i is as follows:

$$E_1 = X_1X_2 + X_3X_7 + X_4X_8 + X_5X_6 = 12 + 37 + 48 + 56$$
$$E_2 = 13 + 27 + 58 + 36$$
$$E_3 = 14 + 28 + 36 + 57$$
$$E_4 = 15 + 38 + 26 + 47$$
$$E_5 = 16 + 78 + 34 + 25$$
$$E_6 = 17 + 23 + 68 + 45$$
$$E_7 = 18 + 24 + 35 + 67$$

Table C-1. Plasma spray parameter and their ranges used to estimate the factor effects on coating thickness and microhardness.

	Plasma Spray Parameter	Ranges
X_1	Plasma arc current	700–900 A
X_2	Argon gas pressure	0.34–1.36 MPa
X_3	Helium gas pressure	0.34–1.36 MPa
X_4	Powder gas pressure	0.34–0.68 MPa
X_5	Powder feed rate	0.50–2 (scale value)
X_6	Powder grain size	$(-45+5)$–$(-75+45)$ μm
X_7	Number of passes 1st set	5–15
	2nd set	20–30
X_8	Spray distance	20–45cm

Table C-2. Fractional two-level factorial design in variables 1 to 8 and the response Y (coating thickness) and its standard deviation.

Run #	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	Resp. Y (μm)	σ (μm)
1	700	0.34	0.34	0.68	2	Coarse	20	45	118	79
2	900	0.34	0.34	0.34	0.5	Coarse	30	45	16	8
3	700	1.36	0.34	0.34	2	Fine	30	45	203	111
4	900	1.36	0.34	0.68	0.5	Fine	20	45	57	25
5	700	0.34	1.36	0.68	0.5	Fine	30	45	82	35
6	900	0.34	1.36	0.34	2	Fine	20	45	138	87
7	700	1.36	1.36	0.34	0.5	Coarse	20	45	30	12
8	900	1.36	1.36	0.68	2	Coarse	30	45	82	44
9	900	1.36	1.36	0.34	0.5	Fine	30	25	7	4
10	700	1.36	1.36	0.68	2	Fine	20	25	108	104
11	900	0.34	1.36	0.68	0.5	Coarse	20	25	65	30
12	700	0.34	1.36	0.34	2	Coarse	30	25	16	10
13	900	1.36	0.34	0.34	2	Corase	20	25	26	21
14	700	1.36	0.34	0.68	0.5	Coarse	30	25	9	12
15	900	0.34	0.34	0.68	2	Fine	30	25	30	13
16	700	0.34	0.34	0.34	0.5	Fine	20	25	22	19

the factor effect by two. Factor significance is checked against the minimum factor significance, $\{\min\} = \sigma_{FE} t_{\alpha,df}$ where $\sigma_{FE} = [(1/n)\sum E_i^2]^{1/2}$ with $t_{\alpha,df}$ = Student's t-value for a confidence level α of a double-sided significance test and df = degrees of freedom. All absolute factor effects larger than $\{\min\}$ are considered to be statistically significant.

Note that the second half of the main effect design matrix (Table C-3) is the mirror image of the first half, and that the two halves of the composite two-factor inter-

Table C-3. Computing of main factor effects according to Yates' algorithm.

Run	Main	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	Y
1	+	−	−	−	+	+	+	−	+	118
2	+	+	−	−	−	−	+	+	+	16
3	+	−	+	−	−	+	−	+	+	203
4	+	+	+	−	+	−	−	−	+	57
5	+	−	−	+	+	−	−	+	+	82
6	+	+	−	+	−	+	−	−	+	138
7	+	−	+	+	−	−	+	−	+	30
8	+	+	+	+	+	+	+	+	+	82
9	+	+	+	+	−	−	−	+	−	7
10	+	−	+	+	+	+	−	−	−	108
11	+	+	−	+	+	−	+	−	−	65
12	+	−	−	+	−	+	+	+	−	16
13	+	+	+	−	−	+	+	−	−	26
14	+	−	+	−	+	−	+	+	−	9
15	+	+	−	−	+	+	−	+	−	30
16	+	−	−	−	−	−	−	−	−	22
$\sum(+)$	1009	421	522	528	551	721	362	445	726	
$\sum(-)$	0	588	487	481	458	288	647	564	283	
$\sum\sum$	1009	1009	1009	1009	1009	1009	1009	1009	1009	
Δ	1009	−167	35	47	93	433	−285	−119	443	
Effect	63	−21	4	6	12	54	−36	−15	55	
c	b_0	−11	2	3	6	27	−18	−8	28	

action design matrix are identical (Table C-4). From Table C-4 the minimum factor effect can be calculated as follows:

$$\sigma_{FE} = [(1/n)\sum E^2]^{1/2} = (3592/7)^{1/2} = 22.6 \tag{C-1a}$$

$$\{\min\} = \sigma_{FE} t_{\alpha=0.90;df=7} = 22.6 \times 1.895 = 43. \tag{C-1b}$$

Thus, all factor effects whose absolute values are larger than 43 are significant at a confidence level of 90%. From Table C-3 it follows that X_5 (powder feed rate) and X_8 (stand-off distance) are the only significant main factor effects. This holds true even when the confidence level is increased to 95%. There are no significant composite two-factor interactions (Table C-4). Both main factor effects have positive signs, i.e. the coating thickness increases with increasing powder feed rate and increasing spray distance. Hence the response polynomial can be roughly expressed by the equation

$$d[\mu m] = 63 + 27X_5 + 28X_8. \tag{C-2}$$

Table C-4. Computing of composite two-factor interactions.

Run	E_1	E_2	E_3	E_4	E_5	E_6	E_7	Y
1	+	+	−	−	−	+	−	118
2	−	−	−	−	+	+	+	16
3	−	+	+	−	+	−	−	203
4	+	−	+	−	−	−	+	57
5	+	−	−	+	+	−	−	82
6	−	+	−	+	−	−	+	138
7	−	−	+	+	−	+	−	30
8	+	+	+	+	+	+	+	82
9	+	+	−	−	−	+	−	7
10	−	−	−	−	+	+	+	108
11	−	+	+	−	+	−	−	65
12	+	−	+	−	−	−	+	16
13	+	−	−	+	+	−	−	26
14	−	+	−	+	−	−	+	9
15	−	−	+	+	−	+	−	30
16	+	+	+	+	+	+	+	22
$\sum(+)$	410	644	505	419	604	413	448	
$\sum(-)$	599	365	504	590	405	596	561	
$\sum\sum$	1009	1009	1009	1009	1009	1009	1009	
Δ	−189	279	1	−171	199	−183	−113	
Effect	−24	35	0	−21	25	−23	−14	
c	−12	18	0	−11	13	−12	−7	

Plasma- Spray Coating

by. Robert B. Heimann

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