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Report
1990 Fischer Standard Study

Gordon J. Roubik

September 12, 1990

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SCOPE

Develop a set of Titanium areal density standards for calibration and maintenance of the Fischer's X-ray Fluorescence measurement system characterization curve program.

ABSTRACT

The electron microprobe was calibrated for Titanium films on ceramic substrates using an existing set of laboratory standards (Quantity: 6 Range: 0.310 to 1.605). Fourteen source assemblies were measured and assigned values. These values are based on a mean calculation, of five separate readings, from best curve fit equations developed from the plot of the laboratory standards areal density (Source Measure) versus electron microprobe measurement (reading). The best fit equations were determined using the SAS General Linear Modeling (GLM) procedure. Four separate best fit equations were evaluated (Linear, Quadratic, Cubic and Exponential). Areal density values for the Fischer Standards appear below ordered by best fit equation based on maximum R^2 .

FISCHER STANDARD	AREAL DENSITY (Mean[5] +/- One Standard Deviation)			
	CUBIC	QUADRATIC	EXPONENTIAL	LINEAR
0002	0.58 +/- 0.01	0.55 +/- 0.01	0.55 +/- 0.01	0.56 +/- 0.01
0003	0.83 +/- 0.02	0.82 +/- 0.02	0.80 +/- 0.02	0.85 +/- 0.02
0004	0.88 +/- 0.01	0.87 +/- 0.01	0.86 +/- 0.01	0.90 +/- 0.01
0005	0.94 +/- 0.06	0.95 +/- 0.07	0.93 +/- 0.06	0.98 +/- 0.07
0006	1.21 +/- 0.07	1.22 +/- 0.07	1.21 +/- 0.08	1.24 +/- 0.07
1072	1.31 +/- 0.02	1.32 +/- 0.04	1.32 +/- 0.04	1.33 +/- 0.04
1239	1.38 +/- 0.02	1.40 +/- 0.01	1.40 +/- 0.01	1.40 +/- 0.01
1053	1.40 +/- 0.03	1.41 +/- 0.03	1.40 +/- 0.03	1.41 +/- 0.02
1054	1.39 +/- 0.04	1.41 +/- 0.04	1.40 +/- 0.04	1.41 +/- 0.03
0999	1.47 +/- 0.05	1.48 +/- 0.04	1.48 +/- 0.05	1.47 +/- 0.04
1137	1.50 +/- 0.04	1.51 +/- 0.03	1.51 +/- 0.04	1.49 +/- 0.03
* 1087	1.71 +/- 0.06	1.68 +/- 0.05	1.70 +/- 0.05	1.63 +/- 0.04
* 1189	1.73 +/- 0.04	1.69 +/- 0.03	1.72 +/- 0.04	1.65 +/- 0.03
* 1089	1.78 +/- 0.03	1.73 +/- 0.03	1.76 +/- 0.03	1.68 +/- 0.02

NOTE(*): These standards are beyond the upper limit of the highest laboratory standard (1.605) used to develop the calibration curve from which these density values were calculated.

The areal density values for the Fischer Standards have been rounded to two significant digits after the decimal point.

Based on review of the best fit equation data plots (see Appendix) with individuals familiar with the physics of X-ray measurements and their characteristic curves, the best equation to use is the QUADRATIC.

The best curve fit for x-ray data is an exponential curve described by the equation:

$$y = a + b (1 - e^{-ux})$$

This exponential equation cannot be modeled through a linear regression formula. The exponential equation used by the SAS GLM procedure was a general exponential described by the equation:

$$y = a e^{bx}$$

Based on the previous exponential equation, this is not the best exponential equation to use.

The cubic regression is the best fit linear equation by R^2 analysis, however, it appears the best because it is capable of picking up data points not falling in the curvature of an exponential curve typical of X-ray data. In the plot of the laboratory standard curves, STD-124 is slightly out of a uniform curve with the other standards, which could be the result of measurement technique. If sufficient readings could be taken and averaged, this standard would most likely come into alignment with the others. The cubic equation specifically makes an effort to pickup the outlying 124 standard.

The linear regression is not applicable at all due to the curvature of X-ray readings.

A handwritten signature in cursive script, appearing to read "Gordon J. Roubik".

Gordon J. Roubik

Advanced Quality Assurance Engineer

MS017 FTS 848-6245

APPENDIX

Source Measure vs Readings

Laboratory Standards – 1990 Study

Group 1: Fischer Stds 6, 0999 and 1054

STANDARD x x x 105 * * * 11 + + + 124 □ □ □ 74 ◇ ◇ ◇ 93 △ △ △ 97

LINEAR: $SM = 0.0096 + 2.0820 (R)$

QUADRATIC: $SM = 0.1072 + 1.5063 (R) + 0.6429 (R^2)$

CUBIC: $SM = -0.0131 + 2.7292 (R) - 2.5700 (R^2) + 2.4280 (R^3)$

EXPONENTIAL: $SM = -1.1567 + 1.3095 \text{ EXP } (R)$

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The SAS System 1
14:27 Tuesday, September 11, 1990

OBS	STANDARD	POS	OP	SM	READING	GROUP	R2	R3	ER
1	74	4	1	0.310	0.1334	1	0.01780	0.00237	1.14271
2	74	4	2	0.310	0.1323	1	0.01750	0.00232	1.14145
3	74	4	3	0.310	0.1338	1	0.01790	0.00240	1.14316
4	124	8	1	0.679	0.3189	1	0.10170	0.03243	1.37561
5	124	8	2	0.679	0.3191	1	0.10182	0.03249	1.37589
6	124	8	3	0.679	0.3213	1	0.10323	0.03317	1.37892
7	105	9	1	0.950	0.4710	1	0.22184	0.10449	1.60159
8	105	9	2	0.950	0.4697	1	0.22062	0.10362	1.59951
9	105	9	3	0.950	0.4719	1	0.22269	0.10509	1.60304
10	11	7	1	1.207	0.5926	1	0.35117	0.20811	1.80868
11	11	7	2	1.207	0.5901	1	0.34822	0.20548	1.80417
12	11	7	3	1.207	0.5889	1	0.34680	0.20423	1.80201
13	93	6	1	1.484	0.7043	1	0.49604	0.34936	2.02243
14	93	6	2	1.484	0.7045	1	0.49632	0.34966	2.02284
15	93	6	3	1.484	0.7071	1	0.49999	0.35354	2.02810
16	97	5	1	1.605	0.7459	1	0.55637	0.41499	2.10834
17	97	5	2	1.605	0.7482	1	0.55980	0.41884	2.11319
18	97	5	3	1.605	0.7483	1	0.55995	0.41901	2.11340

14:27 Tuesday, September 11, 1990

General Linear Models Procedure

Number of observations in data set = 18

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.63236734	4054.78	0.0001
Error	16	0.01433316		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.996070	2.880221	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63236734	4054.78	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	3.63236734	4054.78	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.009560157	0.54	0.5953	0.01764113
READING	2.082046125	63.68	0.0001	0.03269689

The SAS System⁴
14:27 Tuesday, September 11, 1990

General Linear Models Procedure

Number of observations in data set = 18

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	2	3.64315062	7697.07	0.0001
Error	15	0.00354988		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999027	1.480389	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63236734	15348.6	0.0001
R2	1	0.01078329	45.56	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.07103647	300.16	0.0001
R2	1	0.01078329	45.56	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.107148482	6.28	0.0001	0.01706532
READING	1.506255931	17.33	0.0001	0.08693988
R2	0.642907795	6.75	0.0001	0.09524323

The SAS System⁶
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General Linear Models Procedure

Number of observations in data set = 18

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	3	3.64638052	53179.2	0.0001
Error	14	0.00031998		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999912	0.460060	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63236734	100000	0.0001
R2	1	0.01078329	471.79	0.0001
R3	1	0.00322989	141.32	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.01504850	658.41	0.0001
R2	1	0.00204210	89.35	0.0001
R3	1	0.00322989	141.32	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-0.013080732	-1.15	0.2712	0.01141995
READING	2.729156633	25.66	0.0001	0.10636071
R2	-2.569966714	-9.45	0.0001	0.27188667
R3	2.428007562	11.89	0.0001	0.20424683

The SAS System 8
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General Linear Models Procedure

Number of observations in data set = 18

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.64013325	8868.58	0.0001
Error	16	0.00656725		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.998199	1.949604	1.03916667

Source	DF	Type I SS	F Value	Pr > F
ER	1	3.64013325	8868.58	0.0001

Source	DF	Type III SS	F Value	Pr > F
ER	1	3.64013325	8868.58	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-1.156748598	-48.60	0.0001	0.02380179
ER	1.309471869	94.17	0.0001	0.01390494

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S T A N D A R D S P M				R E A D I N G U P				S M L C L C				S M C L C				S M C L C			
1	74	4	1	0.310	0.1334	1	0.28731	0.31952	0.31102	0.33959									
2	74	4	2	0.310	0.1323	1	0.28501	0.31768	0.30863	0.33795									
3	74	4	3	0.310	0.1338	1	0.28814	0.32020	0.31189	0.34019									
4	124	8	1	0.679	0.3189	1	0.67352	0.65288	0.67463	0.64458									
5	124	8	2	0.679	0.3191	1	0.67394	0.65326	0.67500	0.64494									
6	124	8	3	0.679	0.3213	1	0.67852	0.65748	0.67902	0.64891									
7	105	9	1	0.950	0.4710	1	0.99020	0.95922	0.95592	0.94049									
8	105	9	2	0.950	0.4697	1	0.98750	0.95647	0.95342	0.93777									
9	105	9	3	0.950	0.4719	1	0.99208	0.96112	0.95766	0.94238									
10	11	7	1	1.207	0.5926	1	1.24338	1.22553	1.20699	1.21167									
11	11	7	2	1.207	0.5901	1	1.23818	1.21986	1.20140	1.20576									
12	11	7	3	1.207	0.5889	1	1.23568	1.21715	1.19872	1.20293									
13	93	6	1	1.484	0.7043	1	1.47595	1.48691	1.48251	1.49157									
14	93	6	2	1.484	0.7045	1	1.47636	1.48739	1.48305	1.49210									
15	93	6	3	1.484	0.7071	1	1.48177	1.49367	1.49015	1.49899									
16	97	5	1	1.605	0.7459	1	1.56256	1.58836	1.60036	1.60406									
17	97	5	2	1.605	0.7482	1	1.56735	1.59403	1.60716	1.61042									
18	97	5	3	1.605	0.7483	1	1.56756	1.59428	1.60745	1.61069									

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T

----- STANDARD=105 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.4708667	0.0011060	0.4697000
SM	3	0.9500000	0	0.9500000
SM_LCALC	3	0.9899263	0.0023028	0.9874972
SM_QCALC	3	0.9589373	0.0023355	0.9564740
SM_CCALC	3	0.9556677	0.0021277	0.9534236
SM_ECALC	3	0.9402162	0.0023191	0.9377703

Variable	Maximum
READING	0.4719000
SM	0.9500000
SM_LCALC	0.9920777
SM_QCALC	0.9611195
SM_CCALC	0.9576560
SM_ECALC	0.9423834

----- STANDARD=11 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.5905333	0.0018877	0.5889000
SM	3	1.2070000	0	1.2070000
SM_LCALC	3	1.2390778	0.0039302	1.2356771
SM_QCALC	3	1.2208453	0.0042774	1.2171451
SM_CCALC	3	1.2023731	0.0042191	1.1987247
SM_ECALC	3	1.2067865	0.0044630	1.2029264

Variable	Maximum
READING	0.5926000
SM	1.2070000
SM_LCALC	1.2433807
SM_QCALC	1.2255287
SM_CCALC	1.2069934
SM_ECALC	1.2116734

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----- STANDARD=124 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.3197667	0.0013317	0.3189000
SM	3	0.6790000	0	0.6790000
SM_LCALC	3	0.6753291	0.0027726	0.6735247
SM_QCALC	3	0.6545375	0.0025540	0.6528754
SM_CCALC	3	0.6762184	0.0024372	0.6746322
SM_ECALC	3	0.6461418	0.0024017	0.6445789

Variable	Maximum
READING	0.3213000
SM	0.6790000
SM_LCALC	0.6785216
SM_QCALC	0.6574783
SM_CCALC	0.6790247
SM_ECALC	0.6489073

----- STANDARD=74 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.1331667	0.000776745	0.1323000
SM	3	0.3100000	0	0.3100000
SM_LCALC	3	0.2868193	0.0016172	0.2850149
SM_QCALC	3	0.3191327	0.0013028	0.3176791
SM_CCALC	3	0.3105109	0.0016889	0.3086263
SM_ECALC	3	0.3392453	0.0011618	0.3379490

Variable	Maximum
READING	0.1338000
SM	0.3100000
SM_LCALC	0.2881379
SM_QCALC	0.3201951
SM_CCALC	0.3118877
SM_ECALC	0.3401927

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----- STANDARD=93 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.7053000	0.0015620	0.7043000
SM	3	1.4840000	0	1.4840000
SM_LCALC	3	1.4780273	0.0032523	1.4759452
SM_QCALC	3	1.4893251	0.0037703	1.4869115
SM_CCALC	3	1.4852394	0.0042639	1.4825104
SM_ECALC	3	1.4942190	0.0041428	1.4915672

Variable	Maximum
READING	0.7071000
SM	1.4840000
SM_LCALC	1.4817750
SM_QCALC	1.4936698
SM_CCALC	1.4901528
SM_ECALC	1.4989929

----- STANDARD=97 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.7474667	0.0013577	0.7459000
SM	3	1.6050000	0	1.6050000
SM_LCALC	3	1.5658202	0.0028268	1.5625584
SM_QCALC	3	1.5922221	0.0033492	1.5883573
SM_CCALC	3	1.6049905	0.0040115	1.6003616
SM_ECALC	3	1.6083912	0.0037528	1.6040608

Variable	Maximum
READING	0.7483000
SM	1.6050000
SM_LCALC	1.5675553
SM_QCALC	1.5942779
SM_CCALC	1.6074530
SM_ECALC	1.6106947

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	S T A N D A R D S		R E A D I N G	G R O U P	S M L C	S M Q C L C	S M C A L C	S M E C A L C
1	6	1	0.6260	1	1.31292	1.30200	1.28389	1.29211
2	6	2	0.5465	1	1.14740	1.12233	1.10715	1.10497
3	6	3	0.5842	1	1.22589	1.20652	1.18829	1.19186
4	6	4	0.5805	1	1.21819	1.19818	1.18013	1.18319
5	6	5	0.6209	1	1.30230	1.29023	1.27187	1.27966
6	0999	1	0.7174	1	1.50322	1.51862	1.51862	1.52649
7	0999	2	0.7223	1	1.51342	1.53053	1.53235	1.53967
8	0999	3	0.6832	1	1.43201	1.43631	1.42619	1.43627
9	0999	4	0.6880	1	1.44201	1.44777	1.43881	1.44875
10	0999	5	0.6891	1	1.44430	1.45040	1.44172	1.45162
11	1054	1	0.6763	1	1.41765	1.41988	1.40824	1.41844
12	1054	2	0.6788	1	1.42285	1.42583	1.41472	1.42489
13	1054	3	0.6551	1	1.37351	1.36980	1.35448	1.36442
14	1054	4	0.6538	1	1.37080	1.36675	1.35125	1.36115
15	1054	5	0.6883	1	1.44263	1.44849	1.43960	1.44953

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----- STANDARD=0999 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.7000000	0.0183378	0.6832000
SM_LCALC	5	1.4669924	0.0381802	1.4320141
SM_QCALC	5	1.4767254	0.0442021	1.4363076
SM_CCALC	5	1.4715363	0.0498308	1.4261878
SM_ECALC	5	1.4805594	0.0485133	1.4362732

Variable	Maximum
READING	0.7223000
SM_LCALC	1.5134221
SM_QCALC	1.5305333
SM_CCALC	1.5323547
SM_ECALC	1.5396685

----- STANDARD=1054 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.6704600	0.0152923	0.6538000
SM_LCALC	5	1.4054888	0.0318392	1.3708019
SM_QCALC	5	1.4061508	0.0361986	1.3667524
SM_CCALC	5	1.3936589	0.0390501	1.3512528
SM_ECALC	5	1.4036870	0.0391157	1.3611481

Variable	Maximum
READING	0.6883000
SM_LCALC	1.4426325
SM_QCALC	1.4484864
SM_CCALC	1.4395997
SM_ECALC	1.4495314

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----- STANDARD=6 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.5916200	0.0326107	0.5465000
SM_LCALC	5	1.2413403	0.0678970	1.1473984
SM_QCALC	5	1.2238535	0.0737917	1.1223296
SM_CCALC	5	1.2062650	0.0727329	1.1071481
SM_ECALC	5	1.2103579	0.0769317	1.1049676

Variable	Maximum
READING	0.6260000
SM_LCALC	1.3129210
SM_QCALC	1.3020048
SM_CCALC	1.2838882
SM_ECALC	1.2921146

```

GOPTIONS DEV=HP7550 HANDSHAKE=XONXOFF
      HPOS=100 VPOS=40 AUTOFEED NOPROMPT HBY=2;
* GOPTIONS DEV=HP2627X HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT241 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT240 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=TEK4115;
* GOPTIONS DEV=tek4107e HPOS=100 VPOS=40 NOCELL;
* options ls=79;

***** OUTPUT FILE FOR LATER DISPLAY *****;
* goptions gsfmode=append nocell noprompt nodisplay
      gsfname=mc1081;
  goptions gsfmode=replace nocell noprompt nodisplay
      gsfname=gout1;
  goptions colors=(black red green blue yellow purple orange teal);
* goptions colors=(white red green blue magenta yellow cyan);
* goptions colors=(white dgray ltgray); *vt240 colors;
  options ls=64 ps=51;
  libname perm 'us2:[gjroubi.fr1081_std]';

*****;
**** Input of Laboratory Standard's "SM" and "Reading" Values for ****;
**** Calibration Curve Generation for Calculating 1990 Souce Standards ****;
**** for the Fisher X-ray Fluoresence Measurement system ****;
*****;

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_std.dat';
DATA LABSTD;
INFILE INDATA;
INPUT  @1
      standard $ 3. +1
      pos      $ 1. +1
      op       $ 1. +1
      sm
      reading
      group
      ;

*      if group = 1 then delete;
*      if group = 2 then delete;
*      if group = 3 then delete;
*      if group = 4 then delete;
*      if group = 5 then delete;

*proc print data=labstd;

*****;

*endsas;

*****;
**** Calculating Best Fit Equations from Data above using ****;
**** the General Linear Model Procedure to Determine the ****;
**** Maximum Equation Coefficients. ****;
**** ****;
**** Polynomial: ****;
**** ****;
****  $y = b_0 + (b_1)X + (b_2)X^2 + (b_3)X^3$  ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Linear Coefficient ****;
**** b2 = Quadratic Coefficient ****;
**** b3 = Cubic Coefficient ****;
**** ****;
**** Exponential: ****;
**** ****;

```



```

**** y = b0 + (b1)EXP[X] ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Exponential Coefficient ****;
*****;

data labstd_1;
    set labstd;
        R2=reading*reading;
        R3=reading*reading*reading;
        ER=exp(reading);

proc print data=labstd_1;

** Calculate Linear Best fit Equation **;

proc glm data=labstd_1;
    model sm=reading;

** Calculate Quadratic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2;

** Calculate Cubic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2 R3;

** Calculate Exponential Best Fit Equation **;

proc glm data=labstd_1;
    model sm=ER;

*****;

*endsas;

*****;
**** Calculation of SM values for Laboratory Standards using ****;
**** Best Fit Equations ****;
*****;

data labstd;
    set labstd;
        sm_Lcalc = 0.009560157
            + (2.082046125*reading);

        sm_Qcalc = 0.107148482
            + (1.506255931*reading)
            + (0.642907795*reading*reading);

        sm_Ccalc = -0.013080732
            + (2.729156633*reading)
            + (-2.569966714*reading*reading)
            + (2.428007562*reading*reading*reading);

        sm_Ecalc = -1.156748598 + 1.309471869*exp(reading);

proc print data=labstd;

proc sort data=labstd;
    by standard;

proc means data=labstd;
    var reading sm sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;

```

```

        by standard;

*****;

endsas;

*****;
**** Calculation of SM values for Fisher Standards using Best ****;
**** Best Fit Equations ****;
*****;

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_scstd.dat';
DATA SCSTD;
INFILE INDATA;
INPUT @1
      standard $ 4. +1
      op $ 1. +1
      reading
      group
      ;

*      if group = 1 then delete;
      if group = 2 then delete;
      if group = 3 then delete;
      if group = 4 then delete;
      if group = 5 then delete;

proc print data=scstd;

data scstd;
    set scstd;
        sm_Lcalc = 0.009560157
                + (2.082046125*reading);

        sm_Qcalc = 0.107148482
                + (1.506255931*reading)
                + (0.642907795*reading*reading);

        sm_Ccalc = -0.013080732
                + (2.729156633*reading)
                + (-2.569966714*reading*reading)
                + (2.428007562*reading*reading*reading);

        sm_Ecalc = -1.156748598 + 1.309471869*exp(reading);

proc print data=scstd;

proc sort data=scstd;
    by standard;

proc means data=scstd;
    var reading sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;
    by standard;

*****;

endsas;

*****;
**** Plot Routine for Laboratory Standard's "SM" and "Reading" ****;
**** Calibration Calculation Curve ****;
*****;

proc sort data=labstd;
    by standard;

```

```

PROC GPLOT data=labstd;

  PLOT  sm*reading=standard /  vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000;
  plot2 sm*reading=7
        sm*reading=8
        sm*reading=9
        sm_Ecalc*reading=10 /  overlay
                                vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000
                                noaxes;

  TITLE1 h=1.5 f=complex 'Source Measure vs Readings' ;
  title2 h=1.5 f=complex 'Laboratory Standards - 1990 Study';
  title3 h=1.0 f=complex 'Group 1: Fischer Stds 6, 0999 and 1054';

  axis1 order=(0 to 1.7 by .1)
        label=(f=complex h=1.5 c=blue a=90 'SM units')
        value=(h=.6 f=simplex c=blue a=0);

  SYMBOL1 v=x          c=black;
  SYMBOL2 v=star        c=black;
  SYMBOL3 v=plus        c=black;
  SYMBOL4 v=square      c=black;
  SYMBOL5 v=diamond     c=black;
  SYMBOL6 v=triangle    c=black;

  symbol7 v=none c=red    h=1 i=rl;      * linear regression;
  symbol8 v=none c=blue   h=1 i=rq;      * quad regression;
  symbol9 v=none c=green  h=1 i=rc;      * cubic regression;
  symbol10 v=none c=orange h=1 i=stdj;    * exponential plot;

  FOOTNOTE1 J=R C=RED
    'LINEAR: SM = 0.0096 + 2.0820 (R)';

  FOOTNOTE2 J=R C=BLUE
    'QUADRATIC: SM = 0.1072 + 1.5063 (R) + 0.6429 (R^2)';

  FOOTNOTE3 J=R C=GREEN
    'CUBIC: SM = -0.0131 + 2.7292 (R) - 2.5700 (R^2) + 2.4280 (R^3)';

  FOOTNOTE4 J=R C=ORANGE
    'EXPONENTIAL: SM = -1.1567 + 1.3095 EXP (R)';

  FOOTNOTE5 J=R 'GJR ' "&sysdate";

  *****;

endsas;

```

Source Measure vs Readings

Laboratory Standards – 1990 Study

Group 2: Fischer Stds 3, 1053 and 1137

A22

STANDARD x x x 105 * * * 11 + + + 124 □ □ □ 74 ◇ ◇ ◇ 93 △ △ △ 97

LINEAR: $SM = 0.0064 + 2.1192 (R)$

QUADRATIC: $SM = 0.0879 + 1.6371 (R) + 0.5432 (R^2)$

CUBIC: $SM = 0.0255 + 2.2801 (R) - 1.1681 (R^2) + 1.3092 (R^3)$

EXPONENTIAL: $SM = -1.1860 + 1.3374 \text{ EXP } (R)$

GJR 11SEP90

The SAS System 1
14:29 Tuesday, September 11, 1990

OBS	STANDARD	POS	OP	SM	READING	GROUP	R2	R3	ER
1	74	4	1	0.310	0.1321	2	0.01745	0.00231	1.14122
2	74	4	2	0.310	0.1325	2	0.01756	0.00233	1.14168
3	74	4	3	0.310	0.1325	2	0.01756	0.00233	1.14168
4	124	8	1	0.679	0.3197	2	0.10221	0.03268	1.37671
5	124	8	2	0.679	0.3229	2	0.10426	0.03367	1.38113
6	124	8	3	0.679	0.3197	2	0.10221	0.03268	1.37671
7	105	9	1	0.950	0.4606	2	0.21215	0.09772	1.58502
8	105	9	2	0.950	0.4589	2	0.21059	0.09664	1.58233
9	105	9	3	0.950	0.4527	2	0.20494	0.09278	1.57255
10	11	7	1	1.207	0.5753	2	0.33097	0.19041	1.77766
11	11	7	2	1.207	0.5837	2	0.34071	0.19887	1.79266
12	11	7	3	1.207	0.5757	2	0.33143	0.19080	1.77837
13	93	6	1	1.484	0.6959	2	0.48428	0.33701	2.00551
14	93	6	2	1.484	0.6925	2	0.47956	0.33209	1.99871
15	93	6	3	1.484	0.6985	2	0.48790	0.34080	2.01073
16	97	5	1	1.605	0.7399	2	0.54745	0.40506	2.09573
17	97	5	2	1.605	0.7351	2	0.54037	0.39723	2.08569
18	97	5	3	1.605	0.7438	2	0.55324	0.41150	2.10392

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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 3
 14:29 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.63751555	6336.48	0.0001
Error	16	0.00918495		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.997481	2.305649	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63751555	6336.48	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	3.63751555	6336.48	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.006399191	0.45	0.6572	0.01414993
READING	2.119221906	79.60	0.0001	0.02662271

The SAS System

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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 5
14:29 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	2	3.64500267	16101.4	0.0001
Error	15	0.00169783		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999534	1.023803	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63751555	32136.7	0.0001
R2	1	0.00748711	66.15	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.08303260	733.58	0.0001
R2	1	0.00748711	66.15	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.087902603	7.43	0.0001	0.01182805
READING	1.637115248	27.08	0.0001	0.06044449
R2	0.543180430	8.13	0.0001	0.06678650

The SAS System⁶
14:29 Tuesday, September 11, 1990

General Linear Models Procedure

Number of observations in data set = 18

The SAS System 7
14:29 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	3	3.64585975	20236.6	0.0001
Error	14	0.00084075		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999769	0.745736	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63751555	60571.0	0.0001
R2	1	0.00748711	124.67	0.0001
R3	1	0.00085708	14.27	0.0020

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.01010165	168.21	0.0001
R2	1	0.00039479	6.57	0.0225
R3	1	0.00085708	14.27	0.0020

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.025465498	1.37	0.1934	0.01863812
READING	2.280105751	12.97	0.0001	0.17580412
R2	-1.168136017	-2.56	0.0225	0.45559603
R3	1.309184856	3.78	0.0020	0.34654576

The SAS System⁸
14:29 Tuesday, September 11, 1990

General Linear Models Procedure

Number of observations in data set = 18

The SAS System 9
14:29 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.63903099	7591.69	0.0001
Error	16	0.00766951		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.997897	2.106874	1.03916667

Source	DF	Type I SS	F Value	Pr > F
ER	1	3.63903099	7591.69	0.0001

Source	DF	Type III SS	F Value	Pr > F
ER	1	3.63903099	7591.69	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-1.186007735	-45.52	0.0001	0.02605463
ER	1.337421517	87.13	0.0001	0.01534968

The SAS System 10
14:29 Tuesday, September 11, 1990

	S						S	S	S	S
	T						M	M	M	M
	A						L	Q	C	E
	N						C	C	C	C
	D						A	A	A	A
O	A	P					L	L	L	L
B	R	O	O	S			C	C	C	C
S	D	S	P	M						
1	74	4	1	0.310	0.1321	2	0.28635	0.31364	0.30930	0.34029
2	74	4	2	0.310	0.1325	2	0.28720	0.31436	0.31012	0.34090
3	74	4	3	0.310	0.1325	2	0.28720	0.31436	0.31012	0.34090
4	124	8	1	0.679	0.3197	2	0.68391	0.66681	0.67780	0.65524
5	124	8	2	0.679	0.3229	2	0.69070	0.67316	0.68399	0.66114
6	124	8	3	0.679	0.3197	2	0.68391	0.66681	0.67780	0.65524
7	105	9	1	0.950	0.4606	2	0.98251	0.95719	0.95579	0.93384
8	105	9	2	0.950	0.4589	2	0.97891	0.95356	0.95233	0.93024
9	105	9	3	0.950	0.4527	2	0.96577	0.94034	0.93973	0.91716
10	11	7	1	1.207	0.5753	2	1.22559	1.20951	1.19987	1.19148
11	11	7	2	1.207	0.5837	2	1.24339	1.22855	1.21873	1.21153
12	11	7	3	1.207	0.5757	2	1.22644	1.21042	1.20076	1.19243
13	93	6	1	1.484	0.6959	2	1.48117	1.49022	1.48770	1.49621
14	93	6	2	1.484	0.6925	2	1.47396	1.48209	1.47902	1.48710
15	93	6	3	1.484	0.6985	2	1.48668	1.49645	1.49435	1.50319
16	97	5	1	1.605	0.7399	2	1.57441	1.59657	1.60332	1.61686
17	97	5	2	1.605	0.7351	2	1.56424	1.58487	1.59039	1.60344
18	97	5	3	1.605	0.7438	2	1.58268	1.60610	1.61388	1.62781

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----- STANDARD=105 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.4574000	0.0041581	0.4527000
SM	3	0.9500000	0	0.9500000
SM_LCALC	3	0.9757313	0.0088120	0.9657709
SM_QCALC	3	0.9503667	0.0088691	0.9403426
SM_CCALC	3	0.9492840	0.0084493	0.9397345
SM_ECALC	3	0.9270779	0.0087779	0.9171576

Variable	Maximum
READING	0.4606000
SM	0.9500000
SM_LCALC	0.9825128
SM_QCALC	0.9571949
SM_CCALC	0.9557895
SM_ECALC	0.9338384

----- STANDARD=11 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.5782333	0.0047385	0.5753000
SM	3	1.2070000	0	1.2070000
SM_LCALC	3	1.2318039	0.0100419	1.2255876
SM_QCALC	3	1.2161598	0.0107410	1.2095115
SM_CCALC	3	1.2064551	0.0106399	1.1998703
SM_ECALC	3	1.1984801	0.0113142	1.1914780

Variable	Maximum
READING	0.5837000
SM	1.2070000
SM_LCALC	1.2433890
SM_QCALC	1.2285514
SM_CCALC	1.2187301
SM_ECALC	1.2115330

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----- STANDARD=124 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.3207667	0.0018475	0.3197000
SM	3	0.6790000	0	0.6790000
SM_LCALC	3	0.6861749	0.0039153	0.6839144
SM_QCALC	3	0.6689244	0.0036695	0.6668058
SM_CCALC	3	0.6798651	0.0035748	0.6778012
SM_ECALC	3	0.6572073	0.0034072	0.6552401

Variable	Maximum
READING	0.3229000
SM	0.6790000
SM_LCALC	0.6906959
SM_QCALC	0.6731615
SM_CCALC	0.6839929
SM_ECALC	0.6611415

----- STANDARD=74 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.1323667	0.000230940	0.1321000
SM	3	0.3100000	0	0.3100000
SM_LCALC	3	0.2869135	0.000489413	0.2863484
SM_QCALC	3	0.3141191	0.000411268	0.3136442
SM_CCALC	3	0.3098449	0.000471063	0.3093009
SM_ECALC	3	0.3406948	0.000352553	0.3402877

Variable	Maximum
READING	0.1325000
SM	0.3100000
SM_LCALC	0.2871961
SM_QCALC	0.3143566
SM_CCALC	0.3101169
SM_ECALC	0.3408983

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----- STANDARD=93 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.6956333	0.0030089	0.6925000
SM	3	1.4840000	0	1.4840000
SM_LCALC	3	1.4806006	0.0063765	1.4739604
SM_QCALC	3	1.4895859	0.0071991	1.4820905
SM_CCALC	3	1.4870238	0.0076873	1.4790225
SM_ECALC	3	1.4955017	0.0080667	1.4871048

Variable	Maximum
READING	0.6985000
SM	1.4840000
SM_LCALC	1.4866757
SM_QCALC	1.4964466
SM_CCALC	1.4943530
SM_ECALC	1.5031916

----- STANDARD=97 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.7396000	0.0043578	0.7351000
SM	3	1.6050000	0	1.6050000
SM_LCALC	3	1.5737757	0.0092350	1.5642392
SM_QCALC	3	1.5958440	0.0106344	1.5848655
SM_CCALC	3	1.6025271	0.0117653	1.5903874
SM_ECALC	3	1.6160382	0.0122079	1.6034397

Variable	Maximum
READING	0.7438000
SM	1.6050000
SM_LCALC	1.5826764
SM_QCALC	1.6060972
SM_CCALC	1.6138783
SM_ECALC	1.6278138

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O B S	S T A N D A R D S	O P	R E A D I N G	G R O U P	S M	S M	S M	S M
					$\bar{L}$ C A L C	$\bar{Q}$ C A L C	$\bar{C}$ C A L C	$\bar{E}$ C A L C
1	3	1	0.4002	2	0.85451	0.83007	0.83479	0.80959
2	3	2	0.3875	2	0.82760	0.80385	0.80978	0.78441
3	3	3	0.3868	2	0.82611	0.80241	0.80840	0.78303
4	3	4	0.4036	2	0.86172	0.83712	0.84151	0.81639
5	3	5	0.4052	2	0.86511	0.84044	0.84467	0.81959
6	1137	1	0.6943	2	1.47777	1.48639	1.48361	1.49192
7	1137	2	0.7150	2	1.52164	1.53613	1.53710	1.54793
8	1137	3	0.6854	2	1.45891	1.46515	1.46103	1.46819
9	1137	4	0.6985	2	1.48668	1.49645	1.49435	1.50319
10	1137	5	0.7188	2	1.52970	1.54531	1.54707	1.55834
11	1053	1	0.6810	2	1.44959	1.45468	1.44995	1.45654
12	1053	2	0.6573	2	1.39936	1.39866	1.39128	1.39465
13	1053	3	0.6575	2	1.39979	1.39913	1.39177	1.39516
14	1053	4	0.6564	2	1.39746	1.39654	1.38908	1.39233
15	1053	5	0.6523	2	1.38877	1.38691	1.37911	1.38178

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----- STANDARD=1053 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.6609000	0.0114318	0.6523000
SM_LCALC	5	1.4069929	0.0242264	1.3887676
SM_QCALC	5	1.4071840	0.0270096	1.3869136
SM_CCALC	5	1.4002371	0.0282589	1.3791071
SM_ECALC	5	1.4040911	0.0298165	1.3817769

Variable	Maximum
READING	0.6810000
SM_LCALC	1.4495893
SM_QCALC	1.4546840
SM_CCALC	1.4499500
SM_ECALC	1.4565400

----- STANDARD=1137 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.7024000	0.0141204	0.6854000
SM_LCALC	5	1.4949407	0.0299242	1.4589139
SM_QCALC	5	1.5058856	0.0339002	1.4651530
SM_CCALC	5	1.5046325	0.0364161	1.4610257
SM_ECALC	5	1.5139154	0.0381444	1.4681929

Variable	Maximum
READING	0.7188000
SM_LCALC	1.5296959
SM_QCALC	1.5453079
SM_CCALC	1.5470721
SM_ECALC	1.5583403

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The SAS System

----- STANDARD=3 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.3966600	0.0088706	0.3868000
SM_LCALC	5	0.8470098	0.0187988	0.8261142
SM_QCALC	5	0.8227785	0.0183336	0.8024063
SM_CCALC	5	0.8278295	0.0174801	0.8084042
SM_ECALC	5	0.8026004	0.0176196	0.7830272

Variable	Maximum
READING	0.4052000
SM_LCALC	0.8651079
SM_QCALC	0.8404449
SM_CCALC	0.8446698
SM_ECALC	0.8195928

```

GOPTIONS DEV=HP7550 HANDSHAKE=XONXOFF
      HPOS=100 VPOS=40 AUTOFEED NOPROMPT HBY=2;
* GOPTIONS DEV=HP2627X HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT241 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT240 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=TEK4115;
* GOPTIONS DEV=tek4107e HPOS=100 VPOS=40 NOCELL;
* options ls=79;

***** OUTPUT FILE FOR LATER DISPLAY *****;
* goptions gsfname=append nocell noprompt nodisplay
      gsfname=mc1081;
  goptions gsfname=replace nocell noprompt nodisplay
      gsfname=gout1;
  goptions colors=(black red green blue yellow purple orange teal);
* goptions colors=(white red green blue magenta yellow cyan);
* goptions colors=(white dgray ltgray); *vt240 colors;
  options ls=64 ps=51;
  libname perm 'us2:[gjrubi.fr1081_std]';

*****;
**** Input of Laboratory Standard's "SM" and "Reading" Values for ****;
**** Calibration Curve Generation for Calculating 1990 Souce Standards ****;
**** for the Fisher X-ray Fluoresence Measurement system ****;
*****;

FILENAME INDATA 'us2:[gjrubi.fr1081_std]lab_std.dat';
DATA LABSTD;
INFILE INDATA;
INPUT @1
      standard $ 3. +1
      pos $ 1. +1
      op $ 1. +1
      sm
      reading
      group
      ;

      if group = 1 then delete;
*      if group = 2 then delete;
      if group = 3 then delete;
      if group = 4 then delete;
      if group = 5 then delete;

*proc print data=labstd;

*****;

*endsas;

*****;
**** Calculating Best Fit Equations from Data above using ****;
**** the General Linear Model Procedure to Determine the ****;
**** Maximum Equation Coefficients. ****;
**** ****;
**** Polynomial: ****;
**** ****;
****  $y = b_0 + (b_1)X + (b_2)X^2 + (b_3)X^3$  ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Linear Coefficient ****;
**** b2 = Quadratic Coefficient ****;
**** b3 = Cubic Coefficient ****;
**** ****;
**** Exponential: ****;
**** ****;

```

```

**** y = b0 + (b1)EXP[X] ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Exponential Coefficient ****;
**** ****;
**** ****;

data labstd_1;
    set labstd;
        R2=reading*reading;
        R3=reading*reading*reading;
        ER=exp(reading);

proc print data=labstd_1;

** Calculate Linear Best fit Equation **;

proc glm data=labstd_1;
    model sm=reading;

** Calculate Quadratic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2;

** Calculate Cubic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2 R3;

** Calculate Exponential Best Fit Equation **;

proc glm data=labstd_1;
    model sm=ER;

*****;

*endsas;

*****;
**** Calculation of SM values for Laboratory Standards using ****;
**** Best Fit Equations ****;
**** ****;

data labstd;
    set labstd;
        sm_Lcalc = 0.006399191
            + (2.119221906*reading);

        sm_Qcalc = 0.087902603
            + (1.637115248*reading)
            + (0.543180430*reading*reading);

        sm_Ccalc = 0.025465498
            + (2.280105751*reading)
            + (-1.168136017*reading*reading)
            + (1.309184856*reading*reading*reading);

        sm_Ecalc = -1.186007735 + 1.337421517*exp(reading);

proc print data=labstd;

proc sort data=labstd;
    by standard;

proc means data=labstd;
    var reading sm sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;

```

```

by standard;

*****;

endsas;

*****;
**** Calculation of SM values for Fisher Standards using Best ****;
**** Best Fit Equations ****;
*****;

FILENAME INDATA 'us2:[gjroubi.frl081_std]lab_scstd.dat';
DATA SCSTD;
INFILE INDATA;
INPUT @1
      standard $ 4. +1
      op $ 1. +1
      reading
      group
      ;

      if group = 1 then delete;
*      if group = 2 then delete;
      if group = 3 then delete;
      if group = 4 then delete;
      if group = 5 then delete;

proc print data=scstd;

data scstd;
set scstd;
      sm_Lcalc = 0.006399191
              + (2.119221906*reading);

      sm_Qcalc = 0.087902603
              + (1.637115248*reading)
              + (0.543180430*reading*reading);

      sm_Ccalc = 0.025465498
              + (2.280105751*reading)
              + (-1.168136017*reading*reading)
              + (1.309184856*reading*reading*reading);

      sm_Ecalc = -1.186007735 + 1.337421517*exp(reading);

proc print data=scstd;

proc sort data=scstd;
by standard;

proc means data=scstd;
var reading sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;
by standard;

*****;

endsas;

*****;
**** Plot Routine for Laboratory Standard's "SM" and "Reading" ****;
**** Calibration Calculation Curve ****;
*****;

proc sort data=labstd;
by standard;

```

```

PROC GPLOT data=labstd;

PLOT sm*reading=standard / vaxis=axis1
                             haxis=0.1000 to 0.9000 by 0.1000;
plot2 sm*reading=7
      sm*reading=8
      sm*reading=9
      sm_Ecalc*reading=10 / overlay
                           vaxis=axis1
                           haxis=0.1000 to 0.9000 by 0.1000
                           noaxes;

TITLE1 h=1.5 f=complex 'Source Measure vs Readings' ;
title2 h=1.5 f=complex 'Laboratory Standards - 1990 Study';
title3 h=1.0 f=complex 'Group 2: Fischer Stds 3, 1053 and 1137';

axis1 order=(0 to 1.7 by .1)
      label=(f=complex h=1.5 c=blue a=90 'SM units')
      value=(h=.6 f=simplex c=blue a=0);

SYMBOL1 v=x c=black;
SYMBOL2 v=star c=black;
SYMBOL3 v=plus c=black;
SYMBOL4 v=square c=black;
SYMBOL5 v=diamond c=black;
SYMBOL6 v=triangle c=black;

symbol7 v=none c=red h=1 i=rl; * linear regression;
symbol8 v=none c=blue h=1 i=rq; * quad regression;
symbol9 v=none c=green h=1 i=rc; * cubic regression;
symbol10 v=none c=orange h=1 i=stdj; * exponential plot;

FOOTNOTE1 J=R C=RED
          'LINEAR: SM = 0.0064 + 2.1192 (R)';

FOOTNOTE2 J=R C=BLUE
          'QUADRATIC: SM = 0.0879 + 1.6371 (R) + 0.5432 (R^2)';

FOOTNOTE3 J=R C=GREEN
          'CUBIC: SM = 0.0255 + 2.2801 (R) - 1.1681 (R^2) + 1.3092 (R^3)';

FOOTNOTE4 J=R C=ORANGE
          'EXPONENTIAL: SM = -1.1860 + 1.3374 EXP (R)';

FOOTNOTE5 J=R 'GJR' "&sysdate";

*****;

endsas;

```


Source Measure vs Readings

Laboratory Standards - 1990 Study

Group 3: Fischer Stds 4 and 1072

GJR 11SEP90

The SAS System 1
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OBS	STANDARD	POS	OP	SM	READING	GROUP	R2	R3	ER
1	74	4	1	0.310	0.1290	3	0.01664	0.00215	1.13769
2	74	4	2	0.310	0.1266	3	0.01603	0.00203	1.13496
3	74	4	3	0.310	0.1278	3	0.01633	0.00209	1.13633
4	124	8	1	0.679	0.3117	3	0.09716	0.03028	1.36574
5	124	8	2	0.679	0.3169	3	0.10043	0.03182	1.37287
6	124	8	3	0.679	0.3106	3	0.09647	0.02996	1.36424
7	105	9	1	0.950	0.4541	3	0.20621	0.09364	1.57476
8	105	9	2	0.950	0.4473	3	0.20008	0.08949	1.56408
9	105	9	3	0.950	0.4478	3	0.20052	0.08980	1.56487
10	11	7	1	1.207	0.5708	3	0.32581	0.18597	1.76968
11	11	7	2	1.207	0.5807	3	0.33721	0.19582	1.78729
12	11	7	3	1.207	0.5725	3	0.32776	0.18764	1.77269
13	93	6	1	1.484	0.6853	3	0.46964	0.32184	1.98437
14	93	6	2	1.484	0.6773	3	0.45874	0.31070	1.96856
15	93	6	3	1.484	0.6810	3	0.46376	0.31582	1.97585
16	97	5	1	1.605	0.7229	3	0.52258	0.37778	2.06040
17	97	5	2	1.605	0.7260	3	0.52708	0.38266	2.06680
18	97	5	3	1.605	0.7259	3	0.52693	0.38250	2.06659

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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 3
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General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.63318696	4301.69	0.0001
Error	16	0.01351354		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.996294	2.796658	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63318696	4301.69	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	3.63318696	4301.69	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.010851561	0.63	0.5349	0.01710965
READING	2.148739511	65.59	0.0001	0.03276155

The SAS System⁴
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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 5
14:31 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	2	3.64323910	7893.99	0.0001
Error	15	0.00346140		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999051	1.461825	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63318696	15744.4	0.0001
R2	1	0.01005213	43.56	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.07434250	322.16	0.0001
R2	1	0.01005213	43.56	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.104329313	6.23	0.0001	0.01675043
READING	1.579163944	17.95	0.0001	0.08798105
R2	0.656670447	6.60	0.0001	0.09949444

The SAS System⁶
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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 7
14:31 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	3	3.64568349	16728.6	0.0001
Error	14	0.00101701		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999721	0.820188	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63318696	50013.9	0.0001
R2	1	0.01005213	138.38	0.0001
R3	1	0.00244439	33.65	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.01380360	190.02	0.0001
R2	1	0.00146087	20.11	0.0005
R3	1	0.00244439	33.65	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.002140980	0.11	0.9161	0.01996646
READING	2.662269228	13.78	0.0001	0.19313207
R2	-2.297348244	-4.48	0.0005	0.51229506
R3	2.312562076	5.80	0.0001	0.39866353

The SAS System 8
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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 9
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General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.64014917	8890.16	0.0001
Error	16	0.00655133		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.998203	1.947240	1.03916667

Source	DF	Type I SS	F Value	Pr > F
ER	1	3.64014917	8890.16	0.0001

Source	DF	Type III SS	F Value	Pr > F
ER	1	3.64014917	8890.16	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-1.221788650	-49.97	0.0001	0.02444905
ER	1.371764871	94.29	0.0001	0.01454872

The SAS System 10
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	S T A N D A R D S	P O O S P M		R E A D I N G	G R O U P	S M L C	S M Q C	S M C	S M E C
1	74	4 1	0.310	0.1290	3	0.28804	0.31897	0.31231	0.33885
2	74	4 2	0.310	0.1266	3	0.28288	0.31478	0.30706	0.33511
3	74	4 3	0.310	0.1278	3	0.28546	0.31687	0.30968	0.33698
4	124	8 1	0.679	0.3117	3	0.68061	0.66035	0.67880	0.65169
5	124	8 2	0.679	0.3169	3	0.69179	0.67071	0.68870	0.66146
6	124	8 3	0.679	0.3106	3	0.67825	0.65817	0.67671	0.64963
7	105	9 1	0.950	0.4541	3	0.98659	0.95684	0.95389	0.93841
8	105	9 2	0.950	0.4473	3	0.97198	0.94207	0.94029	0.92377
9	105	9 3	0.950	0.4478	3	0.97306	0.94316	0.94129	0.92484
10	11	7 1	1.207	0.5708	3	1.23735	1.21967	1.20334	1.20580
11	11	7 2	1.207	0.5807	3	1.25862	1.24279	1.22627	1.22995
12	11	7 3	1.207	0.5725	3	1.24100	1.22363	1.20725	1.20993
13	93	6 1	1.484	0.6853	3	1.48338	1.49493	1.49196	1.50030
14	93	6 2	1.484	0.6773	3	1.46619	1.47513	1.46994	1.47861
15	93	6 3	1.484	0.6810	3	1.47414	1.48428	1.48008	1.48862
16	97	5 1	1.605	0.7229	3	1.56418	1.58907	1.59977	1.60460
17	97	5 2	1.605	0.7260	3	1.57084	1.59692	1.60899	1.61337
18	97	5 3	1.605	0.7259	3	1.57062	1.59666	1.60869	1.61309

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T

----- STANDARD=105 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.4497333	0.0037899	0.4473000
SM	3	0.9500000	0	0.9500000
SM_LCALC	3	0.9772113	0.0081435	0.9719827
SM_QCALC	3	0.9473565	0.0082287	0.9420742
SM_CCALC	3	0.9451561	0.0075832	0.9402885
SM_ECALC	3	0.9290036	0.0081600	0.9237661

Variable	Maximum
READING	0.4541000
SM	0.9500000
SM_LCALC	0.9865942
SM_QCALC	0.9568376
SM_CCALC	0.9538935
SM_ECALC	0.9384056

----- STANDARD=11 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.5746667	0.0052937	0.5708000
SM	3	1.2070000	0	1.2070000
SM_LCALC	3	1.2456605	0.0113748	1.2373521
SM_QCALC	3	1.2286945	0.0123644	1.2196676
SM_CCALC	3	1.2122853	0.0122687	1.2033352
SM_ECALC	3	1.2152269	0.0129182	1.2057993

Variable	Maximum
READING	0.5807000
SM	1.2070000
SM_LCALC	1.2586246
SM_QCALC	1.2427873
SM_CCALC	1.2262705
SM_ECALC	1.2299517

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----- STANDARD=124 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.3130667	0.0033650	0.3106000
SM	3	0.6790000	0	0.6790000
SM_LCALC	3	0.6835503	0.0072305	0.6782501
SM_QCALC	3	0.6630786	0.0067013	0.6581682
SM_CCALC	3	0.6814014	0.0064057	0.6767055
SM_ECALC	3	0.6542615	0.0063183	0.6496325

Variable	Maximum
READING	0.3169000
SM	0.6790000
SM_LCALC	0.6917871
SM_QCALC	0.6707129
SM_CCALC	0.6886985
SM_ECALC	0.6614597

----- STANDARD=74 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.1278000	0.0012000	0.1266000
SM	3	0.3100000	0	0.3100000
SM_LCALC	3	0.2854605	0.0025785	0.2828820
SM_QCALC	3	0.3168724	0.0020964	0.3147763
SM_CCALC	3	0.3096825	0.0026261	0.3070558
SM_ECALC	3	0.3369838	0.0018705	0.3351136

Variable	Maximum
READING	0.1290000
SM	0.3100000
SM_LCALC	0.2880390
SM_QCALC	0.3189691
SM_CCALC	0.3123079
SM_ECALC	0.3388547

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----- STANDARD=93 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.6812000	0.0040037	0.6773000
SM	3	1.4840000	0	1.4840000
SM_LCALC	3	1.4745729	0.0086030	1.4661928
SM_QCALC	3	1.4847799	0.0099053	1.4751350
SM_CCALC	3	1.4806582	0.0110201	1.4699375
SM_ECALC	3	1.4891732	0.0108556	1.4786066

Variable	Maximum
READING	0.6853000
SM	1.4840000
SM_LCALC	1.4833827
SM_QCALC	1.4949265
SM_CCALC	1.4919551
SM_ECALC	1.5002964

----- STANDARD=97 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.7249333	0.0017616	0.7229000
SM	3	1.6050000	0	1.6050000
SM_LCALC	3	1.5685445	0.0037853	1.5641754
SM_QCALC	3	1.5942182	0.0044579	1.5890727
SM_CCALC	3	1.6058165	0.0052402	1.5997681
SM_ECALC	3	1.6103511	0.0049866	1.6045953

Variable	Maximum
READING	0.7260000
SM	1.6050000
SM_LCALC	1.5708364
SM_QCALC	1.5969176
SM_CCALC	1.6089898
SM_ECALC	1.6133707

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S T A N D A R D O B S S		R E A D I N G		G R O U P		S M L C	S M Q C A L C	S M C A L C	S M E C A L C
1	4	1	0.4087	3	0.88904	0.85942	0.86434	0.84253	
2	4	2	0.4168	3	0.90645	0.87660	0.88012	0.85931	
3	4	3	0.4178	3	0.90859	0.87873	0.88207	0.86140	
4	4	4	0.4172	3	0.90731	0.87745	0.88090	0.86015	
5	4	5	0.4135	3	0.89936	0.86959	0.87368	0.85246	
6	1072	1	0.6301	3	1.36477	1.36008	1.34605	1.35411	
7	1072	2	0.6337	3	1.37251	1.36875	1.35516	1.36340	
8	1072	3	0.6132	3	1.32846	1.31959	1.30402	1.31094	
9	1072	4	0.5992	3	1.29838	1.28634	1.27005	1.27573	
10	1072	5	0.5986	3	1.29709	1.28492	1.26861	1.27423	

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----- STANDARD=1072 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.6149600	0.0165796	0.5986000
SM_LCALC	5	1.3322404	0.0356252	1.2970870
SM_QCALC	5	1.3239333	0.0395899	1.2849163
SM_CCALC	5	1.3087787	0.0408557	1.2686100
SM_ECALC	5	1.3156829	0.0421014	1.2742330

Variable	Maximum
READING	0.6337000
SM_LCALC	1.3725078
SM_QCALC	1.3687484
SM_CCALC	1.3551591
SM_ECALC	1.3633991

----- STANDARD=4 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.4148000	0.0037967	0.4087000
SM_LCALC	5	0.9021487	0.0081581	0.8890414
SM_QCALC	5	0.8723602	0.0080562	0.8594210
SM_CCALC	5	0.8762251	0.0073972	0.8643441
SM_ECALC	5	0.8551685	0.0078733	0.8425257

Variable	Maximum
READING	0.4178000
SM_LCALC	0.9085949
SM_QCALC	0.8787303
SM_CCALC	0.8820740
SM_ECALC	0.8613967


```

GOPTIONS DEV=HP7550 HANDSHAKE=XONXOFF
      HPOS=100 VPOS=40 AUTOFEED NOPROMPT HBY=2;
* GOPTIONS DEV=HP2627X HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT241 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT240 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=TEK4115;
* GOPTIONS DEV=tek4107e HPOS=100 VPOS=40 NOCELL;
* options ls=79;

***** OUTPUT FILE FOR LATER DISPLAY *****;
* goptions gsfname=append nocell noprompt nodisplay
      gsfname=mc1081;
  goptions gsfname=replace nocell noprompt nodisplay
      gsfname=gout1;
  goptions colors=(black red green blue yellow purple orange teal);
* goptions colors=(white red green blue magenta yellow cyan);
* goptions colors=(white dgray ltgray); *vt240 colors;
  options ls=64 ps=51;
  libname perm 'us2:[gjroubi.fr1081_std]';

*****;
**** Input of Laboratory Standard's "SM" and "Reading" Values for ****;
**** Calibration Curve Generation for Calculating 1990 Souce Standards ****;
**** for the Fisher X-ray Fluoresence Measurement system ****;
*****;

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_std.dat';
DATA LABSTD;
INFILE INDATA;
INPUT @1
      standard $ 3. +1
      pos      $ 1. +1
      op       $ 1. +1
      sm
      reading
      group
      ;

      if group = 1 then delete;
      if group = 2 then delete;
*      if group = 3 then delete;
      if group = 4 then delete;
      if group = 5 then delete;

*proc print data=labstd;

*****;

*endsas;

*****;
**** Calculating Best Fit Equations from Data above using ****;
**** the General Linear Model Procedure to Determine the ****;
**** Maximum Equation Coefficients. ****;
**** Polynomial: ****;
****          2      3 ****;
**** y = b0 + (b1)X + (b2)X + (b3)X ****;
**** ****;
**** where: b0 = Intercept ****;
****          b1 = Linear Coefficient ****;
****          b2 = Quadratic Coefficient ****;
****          b3 = Cubic Coefficient ****;
**** ****;
**** Exponential: ****;
**** ****;

```

```

**** y = b0 + (b1)EXP[X] ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Exponential Coefficient ****;
*****;

data labstd_1;
    set labstd;
        R2=reading*reading;
        R3=reading*reading*reading;
        ER=exp(reading);

proc print data=labstd_1;

** Calculate Linear Best fit Equation **;

proc glm data=labstd_1;
    model sm=reading;

** Calculate Quadratic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2;

** Calculate Cubic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2 R3;

** Calculate Exponential Best Fit Equation **;

proc glm data=labstd_1;
    model sm=ER;

*****;

*endsas;

*****;
**** Calculation of SM values for Laboratory Standards using ****;
**** Best Fit Equations ****;
*****;

data labstd;
    set labstd;
        sm_Lcalc = 0.010851561
            + (2.148739511*reading);

        sm_Qcalc = 0.104329313
            + (1.579163944*reading)
            + (0.656670447*reading*reading);

        sm_Ccalc = 0.002140980
            + (2.662269228*reading)
            + (-2.297348244*reading*reading)
            + (2.312562076*reading*reading*reading);

        sm_Ecalc = -1.221788650 + 1.371764871*exp(reading);

proc print data=labstd;

proc sort data=labstd;
    by standard;

proc means data=labstd;
    var reading sm sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;

```

```

        by standard;

*****

*endsas;

*****
**** Calculation of SM values for Fisher Standards using Best ****;
**** Best Fit Equations ****;
*****

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_scstd.dat';
DATA SCSTD;
INFILE INDATA;
INPUT @1
      standard $ 4. +1
      op $ 1. +1
      reading
      group
      ;

      if group = 1 then delete;
      if group = 2 then delete;
*      if group = 3 then delete;
      if group = 4 then delete;
      if group = 5 then delete;

*proc print data=scstd;

data scstd;
  set scstd;
      sm_Lcalc = 0.010851561
              + (2.148739511*reading);

      sm_Qcalc = 0.104329313
              + (1.579163944*reading)
              + (0.656670447*reading*reading);

      sm_Ccalc = 0.002140980
              + (2.662269228*reading)
              + (-2.297348244*reading*reading)
              + (2.312562076*reading*reading*reading);

      sm_Ecalc = -1.221788650 + 1.371764871*exp(reading);

proc print data=scstd;

proc sort data=scstd;
  by standard;

proc means data=scstd;
  var reading sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;
  by standard;

*****

*endsas;

*****
**** Plot Routine for Laboratory Standard's "SM" and "Reading" ****;
**** Calibration Calculation Curve ****;
*****

proc sort data=labstd;
  by standard;

```

```

PROC GPLOT data=labstd;

  PLOT  sm*reading=standard /  vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000;
  plot2 sm*reading=7
        sm*reading=8
        sm*reading=9
        sm_Ecalc*reading=10 /  overlay
                                vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000
                                noaxes;

  TITLE1 h=1.5 f=complex 'Source Measure vs Readings' ;
  title2 h=1.5 f=complex 'Laboratory Standards - 1990 Study';
  title3 h=1.0 f=complex 'Group 3: Fischer Stds 4 and 1072';

  axis1 order=(0 to 1.7 by .1)
        label=(f=complex h=1.5 c=blue a=90 'SM units')
        value=(h=.6 f=simplex c=blue a=0);

  SYMBOL1 v=x      c=black;
  SYMBOL2 v=star    c=black;
  SYMBOL3 v=plus    c=black;
  SYMBOL4 v=square  c=black;
  SYMBOL5 v=diamond c=black;
  SYMBOL6 v=triangle c=black;

  symbol17 v=none c=red   h=1 i=rl;      * linear regression;
  symbol18 v=none c=blue  h=1 i=rq;      * quad regression;
  symbol19 v=none c=green h=1 i=rc;      * cubic regression;
  symbol110 v=none c=orange h=1 i=stdj;  * exponential plot;

  FOOTNOTE1 J=R C=RED
    'LINEAR: SM = 0.0109 + 2.1487(R)';

  FOOTNOTE2 J=R C=BLUE
    'QUADRATIC: SM = 0.1043 + 1.5792(R) + 0.6567(R^2)';

  FOOTNOTE3 J=R C=GREEN
    'CUBIC: SM = 0.0021 + 2.6623(R) - 2.2973(R^2) + 2.3126(R^3)';

  FOOTNOTE4 J=R C=ORANGE
    'EXPONENTIAL: SM = -1.2218 + 1.3718 EXP(R)';

  FOOTNOTE5 J=R 'GJR ' "&sysdate";

  *****;

endsas;

```

Source Measure vs Readings

Laboratory Standards – 1990 Study

Group 4: Fischer Stds 2, 5 and 1239

STANDARD x x x 105 * * * 11 + + + 124 □ □ □ 74 ◇ ◇ ◇ 93 △ △ △ 97

LINEAR: $SM = 0.0104 + 2.2012 (R)$

QUADRATIC: $SM = 0.1109 + 1.5724 (R) + 0.7442 (R^2)$

CUBIC: $SM = -0.0612 + 3.4310 (R) - 4.4613 (R^2) + 4.1933 (R^3)$

EXPONENTIAL: $SM = -1.2782 + 1.4234 \text{ EXP } (R)$

GJR 11SEP90

The SAS System

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OBS	STANDARD	POS	OP	SM	READING	GROUP	R2	R3	ER
1	74	4	1	0.310	0.1249	4	0.01560	0.00195	1.13304
2	74	4	2	0.310	0.1272	4	0.01618	0.00206	1.13564
3	74	4	3	0.310	0.1263	4	0.01595	0.00201	1.13462
4	124	8	1	0.679	0.3061	4	0.09370	0.02868	1.35812
5	124	8	2	0.679	0.3021	4	0.09126	0.02757	1.35270
6	124	8	3	0.679	0.3012	4	0.09072	0.02733	1.35148
7	105	9	1	0.950	0.4388	4	0.19255	0.08449	1.55085
8	105	9	2	0.950	0.4365	4	0.19053	0.08317	1.54728
9	105	9	3	0.950	0.4357	4	0.18983	0.08271	1.54604
10	11	7	1	1.207	0.5867	4	0.34422	0.20195	1.79805
11	11	7	2	1.207	0.5665	4	0.32092	0.18180	1.76209
12	11	7	3	1.207	0.5642	4	0.31832	0.17960	1.75804
13	93	6	1	1.484	0.6604	4	0.43613	0.28802	1.93557
14	93	6	2	1.484	0.6626	4	0.43904	0.29091	1.93983
15	93	6	3	1.484	0.6571	4	0.43178	0.28372	1.92919
16	97	5	1	1.605	0.7063	4	0.49886	0.35234	2.02648
17	97	5	2	1.605	0.7088	4	0.50240	0.35610	2.03155
18	97	5	3	1.605	0.7009	4	0.49126	0.34432	2.01557

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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 3
14:33 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.62324354	2471.42	0.0001
Error	16	0.02345696		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.993568	3.684602	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.62324354	2471.42	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	3.62324354	2471.42	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.010419598	0.46	0.6506	0.02257592
READING	2.201234767	49.71	0.0001	0.04427856

The SAS System

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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 5
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General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	2	3.63428531	2195.47	0.0001
Error	15	0.01241519		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.996596	2.768508	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.62324354	4377.59	0.0001
R2	1	0.01104177	13.34	0.0024

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.06655279	80.41	0.0001
R2	1	0.01104177	13.34	0.0024

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.110856674	3.43	0.0037	0.03230939
READING	1.572398253	8.97	0.0001	0.17535188
R2	0.744155996	3.65	0.0024	0.20373971

The SAS System⁶
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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 7
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General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	3	3.64110031	3034.15	0.0001
Error	14	0.00560019		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.998464	1.924652	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.62324354	9057.80	0.0001
R2	1	0.01104177	27.60	0.0001
R3	1	0.00681499	17.04	0.0010

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.02163821	54.09	0.0001
R2	1	0.00494342	12.36	0.0034
R3	1	0.00681499	17.04	0.0010

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-0.061199814	-1.29	0.2171	0.04735101
READING	3.430974710	7.35	0.0001	0.46649220
R2	-4.461325391	-3.52	0.0034	1.26907566
R3	4.193327637	4.13	0.0010	1.01592950

The SAS System⁸
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General Linear Models Procedure

Number of observations in data set = 18

The SAS System⁹
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General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.63310322	4275.09	0.0001
Error	16	0.01359728		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.996271	2.805310	1.03916667

Source	DF	Type I SS	F Value	Pr > F
ER	1	3.63310322	4275.09	0.0001

Source	DF	Type III SS	F Value	Pr > F
ER	1	3.63310322	4275.09	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-1.278215554	-35.41	0.0001	0.03610245
ER	1.423350211	65.38	0.0001	0.02176902

	S T A N D A R D S D	P R O D S P	O O S M	S M	R E A D I N G	G R O U P	S M L C	S M Q C	S M C	S M C
1	74	4	1	0.310	0.1249	4	0.28535	0.31886	0.30590	0.33449
2	74	4	2	0.310	0.1272	4	0.29042	0.32291	0.31167	0.33820
3	74	4	3	0.310	0.1263	4	0.28844	0.32132	0.30941	0.33675
4	124	8	1	0.679	0.3061	4	0.68422	0.66189	0.69128	0.65486
5	124	8	2	0.679	0.3021	4	0.67541	0.65379	0.68375	0.64715
6	124	8	3	0.679	0.3012	4	0.67343	0.65197	0.68206	0.64541
7	105	9	1	0.950	0.4388	4	0.97632	0.94411	0.93959	0.92918
8	105	9	2	0.950	0.4365	4	0.97126	0.93899	0.93514	0.92411
9	105	9	3	0.950	0.4357	4	0.96950	0.93722	0.93360	0.92235
10	11	7	1	1.207	0.5867	4	1.30188	1.28953	1.26294	1.28103
11	11	7	2	1.207	0.5665	4	1.25742	1.24044	1.21307	1.22985
12	11	7	3	1.207	0.5642	4	1.25236	1.23488	1.20753	1.22409
13	93	6	1	1.484	0.6604	4	1.46412	1.47382	1.46666	1.47677
14	93	6	2	1.484	0.6626	4	1.46896	1.47944	1.47334	1.48284
15	93	6	3	1.484	0.6571	4	1.45685	1.46539	1.45672	1.46770
16	97	5	1	1.605	0.7063	4	1.56515	1.59267	1.61402	1.60617
17	97	5	2	1.605	0.7088	4	1.57065	1.59923	1.62256	1.61339
18	97	5	3	1.605	0.7009	4	1.55327	1.57853	1.59576	1.59064

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----- STANDARD=105 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.4370000	0.0016093	0.4357000
SM	3	0.9500000	0	0.9500000
SM_LCALC	3	0.9723592	0.0035426	0.9694976
SM_QCALC	3	0.9401067	0.0035781	0.9372171
SM_CCALC	3	0.9361108	0.0031139	0.9335963
SM_ECALC	3	0.9252123	0.0035473	0.9223478

Variable	Maximum
READING	0.4388000
SM	0.9500000
SM_LCALC	0.9763214
SM_QCALC	0.9441089
SM_CCALC	0.9395938
SM_ECALC	0.9291801

----- STANDARD=11 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.5724667	0.0123800	0.5642000
SM	3	1.2070000	0	1.2070000
SM_LCALC	3	1.2705531	0.0272512	1.2523563
SM_QCALC	3	1.2549517	0.0300774	1.2348847
SM_CCALC	3	1.2278452	0.0305193	1.2075291
SM_ECALC	3	1.2449928	0.0313437	1.2240922

Variable	Maximum
READING	0.5867000
SM	1.2070000
SM_LCALC	1.3018840
SM_QCALC	1.2895338
SM_CCALC	1.2629406
SM_ECALC	1.2810323

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----- STANDARD=124 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.3031333	0.0026083	0.3012000
SM	3	0.6790000	0	0.6790000
SM_LCALC	3	0.6776872	0.0057415	0.6734315
SM_QCALC	3	0.6558867	0.0052806	0.6519739
SM_CCALC	3	0.6856943	0.0049072	0.6820558
SM_ECALC	3	0.6491402	0.0050304	0.6454132

Variable	Maximum
READING	0.3061000
SM	0.6790000
SM_LCALC	0.6842176
SM_QCALC	0.6618931
SM_CCALC	0.6912754
SM_ECALC	0.6548621

----- STANDARD=74 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.1261333	0.0011590	0.1249000
SM	3	0.3100000	0	0.3100000
SM_LCALC	3	0.2880687	0.0025513	0.2853538
SM_QCALC	3	0.3210284	0.0020398	0.3188581
SM_CCALC	3	0.3089948	0.0029050	0.3059027
SM_ECALC	3	0.3364812	0.0018712	0.3344903

Variable	Maximum
READING	0.1272000
SM	0.3100000
SM_LCALC	0.2904167
SM_QCALC	0.3229061
SM_CCALC	0.3116668
SM_ECALC	0.3382037

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----- STANDARD=93 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.6600333	0.0027683	0.6571000
SM	3	1.4840000	0	1.4840000
SM_LCALC	3	1.4633079	0.0060936	1.4568510
SM_QCALC	3	1.4728828	0.0070711	1.4653915
SM_CCALC	3	1.4655754	0.0083604	1.4567239
SM_ECALC	3	1.4757704	0.0076217	1.4676968

Variable	Maximum
READING	0.6626000
SM	1.4840000
SM_LCALC	1.4689578
SM_QCALC	1.4794411
SM_CCALC	1.4733380
SM_ECALC	1.4828409

----- STANDARD=97 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.7053333	0.0040377	0.7009000
SM	3	1.6050000	0	1.6050000
SM_LCALC	3	1.5630239	0.0088880	1.5532650
SM_QCALC	3	1.5901436	0.0105835	1.5785253
SM_CCALC	3	1.6107795	0.0136882	1.5957623
SM_ECALC	3	1.6034031	0.0116272	1.5906406

Variable	Maximum
READING	0.7088000
SM	1.6050000
SM_LCALC	1.5706548
SM_QCALC	1.5992346
SM_CCALC	1.6225577
SM_ECALC	1.6133943

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O B S	S T A N D A R D	O P	R E A D I N G	G R O U P	S M	S M	S M	S M
					$\bar{L}$ C A L C	$\bar{Q}$ C A L C	$\bar{C}$ C A L C	$\bar{E}$ C A L C
1	5	1	0.4609	4	1.02497	0.99366	0.98298	0.97851
2	5	2	0.3881	4	0.86472	0.83319	0.84352	0.82005
3	5	3	0.4451	4	0.99019	0.95816	0.95185	0.94313
4	5	4	0.4563	4	1.01484	0.98328	0.97385	0.96815
5	5	5	0.4486	4	0.99789	0.96599	0.95869	0.95092
6	2	1	0.2433	4	0.54598	0.53747	0.56986	0.53720
7	2	2	0.2514	4	0.56381	0.55319	0.58601	0.55196
8	2	3	0.2539	4	0.56931	0.55806	0.59096	0.55654
9	2	4	0.2420	4	0.54312	0.53496	0.56725	0.53484
10	2	5	0.2487	4	0.55787	0.54794	0.58065	0.54703
11	1239	1	0.6316	4	1.40072	1.40084	1.38264	1.39856
12	1239	2	0.6364	4	1.41129	1.41292	1.39622	1.41144
13	1239	3	0.6305	4	1.39830	1.39808	1.37955	1.39562
14	1239	4	0.6221	4	1.37981	1.37704	1.35622	1.37325
15	1239	5	0.6341	4	1.40622	1.40713	1.38969	1.40526

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----- STANDARD=1239 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.6309400	0.0054445	0.6221000
SM_LCALC	5	1.3992667	0.0119847	1.3798077
SM_QCALC	5	1.3992008	0.0136567	1.3770403
SM_CCALC	5	1.3808628	0.0152173	1.3562160
SM_ECALC	5	1.3968269	0.0145339	1.3732523

Variable	Maximum
READING	0.6364000
SM_LCALC	1.4112854
SM_QCALC	1.4129178
SM_CCALC	1.3962235
SM_ECALC	1.4114407

----- STANDARD=2 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.2478600	0.0051199	0.2420000
SM_LCALC	5	0.5560176	0.0112700	0.5431184
SM_QCALC	5	0.5463238	0.0099380	0.5349578
SM_CCALC	5	0.5789463	0.0102027	0.5672529
SM_ECALC	5	0.5455145	0.0093358	0.5348397

Variable	Maximum
READING	0.2539000
SM_LCALC	0.5693131
SM_QCALC	0.5580608
SM_CCALC	0.5909596
SM_ECALC	0.5565439

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----- STANDARD=5 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.4398000	0.0295630	0.3881000
SM_LCALC	5	0.9785226	0.0650751	0.8647188
SM_QCALC	5	0.9468554	0.0650592	0.8331904
SM_CCALC	5	0.9421783	0.0565000	0.8435157
SM_ECALC	5	0.9321521	0.0641932	0.8200549

Variable	Maximum
READING	0.4609000
SM_LCALC	1.0249687
SM_QCALC	0.9936552
SM_CCALC	0.9829845
SM_ECALC	0.9785066

```

GOPTIONS DEV=HP7550 HANDSHAKE=XONXOFF
      HPOS=100 VPOS=40 AUTOFEED NOPROMPT HBY=2;
* GOPTIONS DEV=HP2627X HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT241 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT240 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=TEK4115;
* GOPTIONS DEV=tek4107e HPOS=100 VPOS=40 NOCELL;
* options ls=79;

***** OUTPUT FILE FOR LATER DISPLAY *****;
* goptions gsfmode=append nocell noprompt nodisplay
      gsfname=mc1081;
  goptions gsfmode=replace nocell noprompt nodisplay
      gsfname=gout1;
  goptions colors=(black red green blue yellow purple orange teal);
* goptions colors=(white red green blue magenta yellow cyan);
* goptions colors=(white dgray ltgray); *vt240 colors;
  options ls=64 ps=51;
  libname perm 'us2:[gjroubi.fr1081_std]';

*****;
**** Input of Laboratory Standard's "SM" and "Reading" Values for ****;
**** Calibration Curve Generation for Calculating 1990 Souce Standards ****;
**** for the Fisher X-ray Fluoresence Measurement system ****;
*****;

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_std.dat';
DATA LABSTD;
INFILE INDATA;
INPUT  @1
      standard $ 3. +1
      pos      $ 1. +1
      op       $ 1. +1
      sm
      reading
      group
      ;

      if group = 1 then delete;
      if group = 2 then delete;
      if group = 3 then delete;
*      if group = 4 then delete;
      if group = 5 then delete;

*proc print data=labstd;

*****;

*endsas;

*****;
**** Calculating Best Fit Equations from Data above using ****;
**** the General Linear Model Procedure to Determine the ****;
**** Maximum Equation Coefficients. ****;
**** Polynomial: ****;
****          2          3 ****;
**** y = b0 + (b1)X + (b2)X + (b3)X ****;
**** where: b0 = Intercept ****;
****          b1 = Linear Coefficient ****;
****          b2 = Quadratic Coefficient ****;
****          b3 = Cubic Coefficient ****;
**** Exponential: ****;
**** ****;

```

```

**** y = b0 + (b1)EXP[X] ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Exponential Coefficient ****;
**** ****;
*****

data labstd_1;
    set labstd;
        R2=reading*reading;
        R3=reading*reading*reading;
        ER=exp(reading);

proc print data=labstd_1;

** Calculate Linear Best fit Equation **;

proc glm data=labstd_1;
    model sm=reading;

** Calculate Quadratic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2;

** Calculate Cubic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2 R3;

** Calculate Exponential Best Fit Equation **;

proc glm data=labstd_1;
    model sm=ER;

*****;

*endsas;

*****;
**** Calculation of SM values for Laboratory Standards using ****;
**** Best Fit Equations ****;
*****;

data labstd;
    set labstd;
        sm_Lcalc = 0.010419598
            + (2.201234767*reading);

        sm_Qcalc = 0.110856674
            + (1.572398253*reading)
            + (0.744155996*reading*reading);

        sm_Ccalc = -0.061199814
            + (3.430974710*reading)
            + (-4.461325391*reading*reading)
            + (4.193327637*reading*reading*reading);

        sm_Ecalc = -1.278215554 + 1.423350211*exp(reading);

proc print data=labstd;

proc sort data=labstd;
    by standard;

proc means data=labstd;
    var reading sm sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;

```

```

        by standard;

*****

endsas;

*****
**** Calculation of SM values for Fisher Standards using Best ****
**** Best Fit Equations ****
*****

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_scstd.dat';
DATA SCSTD;
INFILE INDATA;
INPUT @1
      standard $ 4. +1
      op $ 1. +1
      reading
      group
      ;

      if group = 1 then delete;
      if group = 2 then delete;
      if group = 3 then delete;
*      if group = 4 then delete;
      if group = 5 then delete;

proc print data=scstd;

data scstd;
  set scstd;
      sm_Lcalc = 0.010419598
              + (2.201234767*reading);

      sm_Qcalc = 0.110856674
              + (1.572398253*reading)
              + (0.744155996*reading*reading);

      sm_Ccalc = -0.061199814
              + (3.430974710*reading)
              + (-4.461325391*reading*reading)
              + (4.193327637*reading*reading*reading);

      sm_Ecalc = -1.278215554 + 1.423350211*exp(reading);

proc print data=scstd;

proc sort data=scstd;
  by standard;

proc means data=scstd;
  var reading sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;
  by standard;

*****

endsas;

*****
**** Plot Routine for Laboratory Standard's "SM" and "Reading" ****
**** Calibration Calculation Curve ****
*****

proc sort data=labstd;
  by standard;

```



```

PROC GPLOT data=labstd;

  PLOT  sm*reading=standard /  vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000;
  plot2 sm*reading=7
        sm*reading=8
        sm*reading=9
        sm_Ecalc*reading=10 /  overlay
                                vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000
                                noaxes;

  TITLE1 h=1.5 f=complex 'Source Measure vs Readings' ;
  title2 h=1.5 f=complex 'Laboratory Standards - 1990 Study';
  title3 h=1.0 f=complex 'Group 4: Fischer Stds 2, 5 and 1239';

  axis1 order=(0 to 1.7 by .1)
        label=(f=complex h=1.5 c=blue a=90 'SM units')
        value=(h=.6 f=simplex c=blue a=0);

  SYMBOL1 v=x          c=black;
  SYMBOL2 v=star        c=black;
  SYMBOL3 v=plus        c=black;
  SYMBOL4 v=square      c=black;
  SYMBOL5 v=diamond     c=black;
  SYMBOL6 v=triangle    c=black;

  symbol7 v=none c=red    h=1 i=rl;      * linear regression;
  symbol8 v=none c=blue   h=1 i=rq;      * quad regression;
  symbol9 v=none c=green  h=1 i=rc;      * cubic regression;
  symbol10 v=none c=orange h=1 i=stdj;    * exponential plot;

  FOOTNOTE1 J=R C=RED
    'LINEAR: SM = 0.0104 + 2.2012(R)';

  FOOTNOTE2 J=R C=BLUE
    'QUADRATIC: SM = 0.1109 + 1.5724(R) + 0.7442(R^2)';

  FOOTNOTE3 J=R C=GREEN
    'CUBIC: SM = -0.0612 + 3.4310(R) - 4.4613(R^2) + 4.1933(R^3)';

  FOOTNOTE4 J=R C=ORANGE
    'EXPONENTIAL: SM = -1.2782 + 1.4234 EXP(R)';

  FOOTNOTE5 J=R 'GJR' "&sysdate";

  *****;

endsas;

```

Source Measure vs Readings

Laboratory Standards – 1990 Study

Group 5: Fischer Stds 1087, 1089 and 1189

STANDARD x x x 105 * * * 11 + + + 124 □ □ □ 74 ◇ ◇ ◇ 93 △ △ △ 97

LINEAR: $SM = 0.0039 + 2.1145 (R)$

QUADRATIC: $SM = 0.1087 + 1.4897 (R) + 0.7061 (R^2)$

CUBIC: $SM = -0.0147 + 2.7684 (R) - 2.7125 (R^2) + 2.6264 (R^3)$

EXPONENTIAL: $SM = -1.1923 + 1.3381 \text{ EXP } (R)$

GJR 11SEP90

The SAS System 1
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OBS	STANDARD	POS	OP	SM	READING	GROUP	R2	R3	ER
1	74	4	1	0.310	0.1322	5	0.01748	0.00231	1.14134
2	74	4	2	0.310	0.1313	5	0.01724	0.00226	1.14031
3	74	4	3	0.310	0.1322	5	0.01748	0.00231	1.14134
4	124	8	1	0.679	0.3226	5	0.10407	0.03357	1.38071
5	124	8	2	0.679	0.3232	5	0.10446	0.03376	1.38154
6	124	8	3	0.679	0.3206	5	0.10278	0.03295	1.37795
7	105	9	1	0.950	0.4584	5	0.21013	0.09632	1.58154
8	105	9	2	0.950	0.4622	5	0.21363	0.09874	1.58756
9	105	9	3	0.950	0.4634	5	0.21474	0.09951	1.58947
10	11	7	1	1.207	0.5859	5	0.34328	0.20113	1.79661
11	11	7	2	1.207	0.5949	5	0.35391	0.21054	1.81285
12	11	7	3	1.207	0.5852	5	0.34246	0.20041	1.79535
13	93	6	1	1.484	0.6992	5	0.48888	0.34183	2.01214
14	93	6	2	1.484	0.6999	5	0.48986	0.34285	2.01355
15	93	6	3	1.484	0.6928	5	0.47997	0.33252	1.99931
16	97	5	1	1.605	0.7374	5	0.54376	0.40097	2.09049
17	97	5	2	1.605	0.7360	5	0.54170	0.39869	2.08757
18	97	5	3	1.605	0.7355	5	0.54096	0.39788	2.08652

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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 3
14:36 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.63013728	3506.70	0.0001
Error	16	0.01656322		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.995458	3.096187	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63013728	3506.70	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	3.63013728	3506.70	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.003910166	0.21	0.8400	0.01905629
READING	2.114470492	59.22	0.0001	0.03570692

The SAS System 4
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General Linear Models Procedure

Number of observations in data set = 18

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	2	3.64241296	6371.51	0.0001
Error	15	0.00428754		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.998824	1.626946	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63013728	12700.1	0.0001
R2	1	0.01227568	42.95	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.06718416	235.04	0.0001
R2	1	0.01227568	42.95	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	0.108703429	5.76	0.0001	0.01886727
READING	1.489683820	15.33	0.0001	0.09716706
R2	0.706077856	6.55	0.0001	0.10774281

The SAS System⁶
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General Linear Models Procedure

Number of observations in data set = 18

The SAS System 7
14:36 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	3	3.64574348	17777.6	0.0001
Error	14	0.00095702		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.999738	0.795630	1.03916667

Source	DF	Type I SS	F Value	Pr > F
READING	1	3.63013728	53104.4	0.0001
R2	1	0.01227568	179.58	0.0001
R3	1	0.00333052	48.72	0.0001

Source	DF	Type III SS	F Value	Pr > F
READING	1	0.01462703	213.98	0.0001
R2	1	0.00207282	30.32	0.0001
R3	1	0.00333052	48.72	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-0.014747209	-0.74	0.4720	0.01994825
READING	2.768359790	14.63	0.0001	0.18925212
R2	-2.712483806	-5.51	0.0001	0.49258649
R3	2.626400368	6.98	0.0001	0.37627137

The SAS System 8
14:36 Tuesday, September 11, 1990

General Linear Models Procedure

Number of observations in data set = 18

The SAS System⁹
 14:36 Tuesday, September 11, 1990

General Linear Models Procedure

Dependent Variable: SM

Source	DF	Sum of Squares	F Value	Pr > F
Model	1	3.64046857	9346.62	0.0001
Error	16	0.00623193		
Corrected Total	17	3.64670050		

R-Square	C.V.	SM Mean
0.998291	1.899180	1.03916667

Source	DF	Type I SS	F Value	Pr > F
ER	1	3.64046857	9346.62	0.0001

Source	DF	Type III SS	F Value	Pr > F
ER	1	3.64046857	9346.62	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > T	Std Error of Estimate
INTERCEPT	-1.192268680	-50.64	0.0001	0.02354522
ER	1.338140481	96.68	0.0001	0.01384122

S T A N D A R D S				R E A D I N G S				S M L C S				S M L C S				S M L C S				S M L C S			
O B S D				P O S S I B L E				S M L C S				S M L C S				S M L C S				S M L C S			
1	74	4	1	0.310	0.1322	5	0.28344	0.31798	0.30989	0.33500													
2	74	4	2	0.310	0.1313	5	0.28154	0.31647	0.30792	0.33363													
3	74	4	3	0.310	0.1322	5	0.28344	0.31798	0.30989	0.33500													
4	124	8	1	0.679	0.3226	5	0.68604	0.66276	0.68421	0.65532													
5	124	8	2	0.679	0.3232	5	0.68731	0.66392	0.68532	0.65643													
6	124	8	3	0.679	0.3206	5	0.68181	0.65887	0.68053	0.65163													
7	105	9	1	0.950	0.4584	5	0.97318	0.93994	0.93728	0.92406													
8	105	9	2	0.950	0.4622	5	0.98122	0.94807	0.94465	0.93211													
9	105	9	3	0.950	0.4634	5	0.98376	0.95065	0.94699	0.93466													
10	11	7	1	1.207	0.5859	5	1.24278	1.22389	1.20434	1.21184													
11	11	7	2	1.207	0.5949	5	1.26181	1.24480	1.22514	1.23358													
12	11	7	3	1.207	0.5852	5	1.24130	1.22227	1.20273	1.21016													
13	93	6	1	1.484	0.6992	5	1.48235	1.49548	1.49258	1.50026													
14	93	6	2	1.484	0.6999	5	1.48383	1.49721	1.49456	1.50215													
15	93	6	3	1.484	0.6928	5	1.46882	1.47965	1.47460	1.48308													
16	97	5	1	1.605	0.7374	5	1.56312	1.59113	1.60481	1.60510													
17	97	5	2	1.605	0.7360	5	1.56016	1.58759	1.60054	1.60119													
18	97	5	3	1.605	0.7355	5	1.55910	1.58633	1.59902	1.59979													

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Tt

----- STANDARD=105 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.4613333	0.0026102	0.4584000
SM	3	0.9500000	0	0.9500000
SM_LCALC	3	0.9793859	0.0055193	0.9731834
SM_QCALC	3	0.9462209	0.0055868	0.9399430
SM_CCALC	3	0.9429726	0.0050678	0.9372782
SM_ECALC	3	0.9302778	0.0055371	0.9240560

Variable	Maximum
READING	0.4634000
SM	0.9500000
SM_LCALC	0.9837558
SM_QCALC	0.9506458
SM_CCALC	0.9469871
SM_ECALC	0.9346641

----- STANDARD=11 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.5886667	0.0054096	0.5852000
SM	3	1.2070000	0	1.2070000
SM_LCALC	3	1.2486285	0.0114384	1.2412983
SM_QCALC	3	1.2303205	0.0125671	1.2222691
SM_CCALC	3	1.2107376	0.0125026	1.2027314
SM_ECALC	3	1.2185283	0.0130613	1.2101619

Variable	Maximum
READING	0.5949000
SM	1.2070000
SM_LCALC	1.2618087
SM_QCALC	1.2448015
SM_CCALC	1.2251446
SM_ECALC	1.2335788

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----- STANDARD=124 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.3221333	0.0013614	0.3206000
SM	3	0.6790000	0	0.6790000
SM_LCALC	3	0.6850516	0.0028786	0.6818094
SM_QCALC	3	0.6618507	0.0026467	0.6588698
SM_CCALC	3	0.6833540	0.0025029	0.6805349
SM_ECALC	3	0.6544584	0.0025133	0.6516277

Variable	Maximum
READING	0.3232000
SM	0.6790000
SM_LCALC	0.6873070
SM_QCALC	0.6639249
SM_CCALC	0.6853150
SM_ECALC	0.6564281

----- STANDARD=74 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.1319000	0.000519615	0.1313000
SM	3	0.3100000	0	0.3100000
SM_LCALC	3	0.2828088	0.0010987	0.2815401
SM_QCALC	3	0.3174769	0.000870738	0.3164715
SM_CCALC	3	0.3092353	0.0011382	0.3079211
SM_ECALC	3	0.3345420	0.000793235	0.3336261

Variable	Maximum
READING	0.1322000
SM	0.3100000
SM_LCALC	0.2834432
SM_QCALC	0.3179796
SM_CCALC	0.3098924
SM_ECALC	0.3350000

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----- STANDARD=93 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.6973000	0.0039128	0.6928000
SM	3	1.4840000	0	1.4840000
SM_LCALC	3	1.4783304	0.0082735	1.4688153
SM_QCALC	3	1.4907815	0.0096757	1.4796539
SM_CCALC	3	1.4872461	0.0109973	1.4745991
SM_ECALC	3	1.4951632	0.0105039	1.4830833

Variable	Maximum
READING	0.6999000
SM	1.4840000
SM_LCALC	1.4838281
SM_QCALC	1.4972124
SM_CCALC	1.4945598
SM_ECALC	1.5021459

----- STANDARD=97 -----

Variable	N	Mean	Std Dev	Minimum
READING	3	0.7363000	0.000984886	0.7355000
SM	3	1.6050000	0	1.6050000
SM_LCALC	3	1.5607948	0.0020825	1.5591032
SM_QCALC	3	1.5883495	0.0024915	1.5863259
SM_CCALC	3	1.6014543	0.0030008	1.5990179
SM_ECALC	3	1.6020303	0.0027526	1.5997949

Variable	Maximum
READING	0.7374000
SM	1.6050000
SM_LCALC	1.5631207
SM_QCALC	1.5911323
SM_CCALC	1.6048062
SM_ECALC	1.6051048

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	S T A N D A R D S		O R D I N A L P		R E A D I N G		G R O U P		S M L C		S M Q C		S M C A L C		S M E C A L C
1	1087	1	0.7904	5	1.67519	1.72726	1.77567	1.75736							
2	1087	2	0.7763	5	1.64537	1.69066	1.72839	1.71607							
3	1087	3	0.7447	5	1.57856	1.60965	1.62725	1.62560							
4	1087	4	0.7581	5	1.60689	1.64383	1.66934	1.66361							
5	1087	5	0.7820	5	1.65743	1.70542	1.74734	1.73269							
6	1089	1	0.7945	5	1.68386	1.73795	1.78969	1.76948							
7	1089	2	0.8061	5	1.70838	1.76834	1.82998	1.80404							
8	1089	3	0.7898	5	1.67392	1.72570	1.77363	1.75560							
9	1089	4	0.7802	5	1.65362	1.70075	1.74133	1.72743							
10	1089	5	0.7866	5	1.66715	1.71737	1.76279	1.74618							
11	1189	1	0.7582	5	1.60710	1.64408	1.66966	1.66390							
12	1189	2	0.7736	5	1.63966	1.68368	1.71949	1.70822							
13	1189	3	0.7884	5	1.67096	1.72205	1.76888	1.75147							
14	1189	4	0.7847	5	1.66314	1.71243	1.75639	1.74060							
15	1189	5	0.7837	5	1.66102	1.70983	1.75303	1.73767							

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----- STANDARD=1087 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.7703000	0.0185816	0.7447000
SM_LCALC	5	1.6326868	0.0392902	1.5785563
SM_QCALC	5	1.6753617	0.0478114	1.6096463
SM_CCALC	5	1.7095984	0.0602999	1.6272546
SM_ECALC	5	1.6990676	0.0535549	1.6256004

Variable	Maximum
READING	0.7904000
SM_LCALC	1.6751876
SM_QCALC	1.7272591
SM_CCALC	1.7756743
SM_ECALC	1.7573649

----- STANDARD=1089 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.7914400	0.0097048	0.7802000
SM_LCALC	5	1.6773867	0.0205205	1.6536200
SM_QCALC	5	1.7300231	0.0253334	1.7007528
SM_CCALC	5	1.7794834	0.0332496	1.7413281
SM_ECALC	5	1.7605455	0.0287189	1.7274315

Variable	Maximum
READING	0.8061000
SM_LCALC	1.7083848
SM_QCALC	1.7683450
SM_CCALC	1.8299757
SM_ECALC	1.8040396

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----- STANDARD=1189 -----

Variable	N	Mean	Std Dev	Minimum
READING	5	0.7777200	0.0122122	0.7582000
SM_LCALC	5	1.6483762	0.0258223	1.6071017
SM_QCALC	5	1.6944146	0.0315216	1.6440827
SM_CCALC	5	1.7334904	0.0400920	1.6696594
SM_ECALC	5	1.7203729	0.0353984	1.6638996

Variable	Maximum
READING	0.7884000
SM_LCALC	1.6709587
SM_QCALC	1.7220502
SM_CCALC	1.7688826
SM_ECALC	1.7514715

```

GOPTIONS DEV=HP7550 HANDSHAKE=XONXOFF
      HPOS=100 VPOS=40 AUTOFEED NOPROMPT HBY=2;
* GOPTIONS DEV=HP2627X HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT241 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=VT240 HPOS=100 VPOS=40 NOCELL;
* GOPTIONS DEV=TEK4115;
* GOPTIONS DEV=tek4107e HPOS=100 VPOS=40 NOCELL;
* options ls=79;

***** OUTPUT FILE FOR LATER DISPLAY *****;
* goptions gsfmode=append nocell noprompt nodisplay
      gsfname=mc1081;
  goptions gsfmode=replace nocell noprompt nodisplay
      gsfname=gout1;
  goptions colors=(black red green blue yellow purple orange teal);
* goptions colors=(white red green blue magenta yellow cyan);
* goptions colors=(white dgray ltgray); *vt240 colors;
  options ls=64 ps=51;
  libname perm 'us2:[gjroubi.fr1081_std]';

*****;
**** Input of Laboratory Standard's "SM" and "Reading" Values for ****;
**** Calibration Curve Generation for Calculating 1990 Souce Standards ****;
**** for the Fisher X-ray Fluoresence Measurement system ****;
*****;

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_std.dat';
DATA LABSTD;
INFILE INDATA;
INPUT @1
      standard $ 3. +1
      pos $ 1. +1
      op $ 1. +1
      sm
      reading
      group
      ;

      if group = 1 then delete;
      if group = 2 then delete;
      if group = 3 then delete;
      if group = 4 then delete;
*      if group = 5 then delete;

*proc print data=labstd;

*****;

*endsas;

*****;
**** Calculating Best Fit Equations from Data above using ****;
**** the General Linear Model Procedure to Determine the ****;
**** Maximum Equation Coefficients. ****;
**** ****;
**** Polynomial: ****;
****  $y = b_0 + (b_1)X + (b_2)X^2 + (b_3)X^3$  ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Linear Coefficient ****;
**** b2 = Quadratic Coefficient ****;
**** b3 = Cubic Coefficient ****;
**** ****;
**** Exponential: ****;
**** ****;

```

```

**** y = b0 + (b1)EXP[X] ****;
**** ****;
**** where: b0 = Intercept ****;
**** b1 = Exponential Coefficient ****;
*****
data labstd_1;
    set labstd;
        R2=reading*reading;
        R3=reading*reading*reading;
        ER=exp(reading);

proc print data=labstd_1;

** Calculate Linear Best fit Equation **;

proc glm data=labstd_1;
    model sm=reading;

** Calculate Quadratic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2;

** Calculate Cubic Best Fit Equation **;

proc glm data=labstd_1;
    model sm=reading R2 R3;

** Calculate Exponential Best Fit Equation **;

proc glm data=labstd_1;
    model sm=ER;

*****;

*endsas;

*****;
**** Calculation of SM values for Laboratory Standards using ****;
**** Best Fit Equations ****;
*****;

data labstd;
    set labstd;
        sm_Lcalc = 0.003910166
            + (2.114470492*reading);

        sm_Qcalc = 0.108703429
            + (1.489683820*reading)
            + (0.706077856*reading*reading);

        sm_Ccalc = -0.014747209
            + (2.768359790*reading)
            + (-2.712483806*reading*reading)
            + (2.626400368*reading*reading*reading);

        sm_Ecalc = -1.192268680 + 1.338140481*exp(reading);

proc print data=labstd;

proc sort data=labstd;
    by standard;

proc means data=labstd;
    var reading sm sm_Lcalc sm_Qcalc sm_Ccalc sm_Ecalc;

```

```

        by standard;

*****

*endsas;

*****
**** Calculation of SM values for Fisher Standards using Best ****;
**** Best Fit Equations ****;
*****

FILENAME INDATA 'us2:[gjroubi.fr1081_std]lab_scstd.dat';
DATA SCSTD;
INFILE INDATA;
INPUT   @1
        standard $ 4. +1
        op       $ 1. +1
        reading
        group
        ;

        if group = 1 then delete;
        if group = 2 then delete;
        if group = 3 then delete;
        if group = 4 then delete;
*       if group = 5 then delete;

*proc print data=scstd;

data scstd;
    set scstd;
        sm_lcalc = 0.003910166
                + (2.114470492*reading);

        sm_qcalc = 0.108703429
                + (1.489683820*reading)
                + (0.706077856*reading*reading);

        sm_ccalc = -0.014747209
                + (2.768359790*reading)
                + (-2.712483806*reading*reading)
                + (2.626400368*reading*reading*reading);

        sm_escal = -1.192268680 + 1.338140481*exp(reading);

proc print data=scstd;

proc sort data=scstd;
    by standard;

proc means data=scstd;
    var reading sm_lcalc sm_qcalc sm_ccalc sm_escal;
    by standard;

*****

*endsas;

*****
**** Plot Routine for Laboratory Standard's "SM" and "Reading" ****;
**** Calibration Calculation Curve ****;
*****

proc sort data=labstd;
    by standard;

```

```

PROC Gplot data=labstd;

  PLOT  sm*reading=standard /  vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000;
  plot2 sm*reading=7
        sm*reading=8
        sm*reading=9
        sm_Ecalc*reading=10 /  overlay
                                vaxis=axis1
                                haxis=0.1000 to 0.9000 by 0.1000
                                noaxes;

  TITLE1 h=1.5 f=complex 'Source Measure vs Readings' ;
  title2 h=1.5 f=complex 'Laboratory Standards - 1990 Study';
  title3 h=1.0 f=complex 'Group 5: Fischer Stds 1087, 1089 and 1189';

  axis1 order=(0 to 1.7 by .1)
        label=(f=complex h=1.5 c=blue a=90 'SM units')
        value=(h=.6 f=simplex c=blue a=0);

  SYMBOL1 v=x          c=black;
  SYMBOL2 v=star       c=black;
  SYMBOL3 v=plus       c=black;
  SYMBOL4 v=square     c=black;
  SYMBOL5 v=diamond    c=black;
  SYMBOL6 v=triangle   c=black;

  symbol17 v=none c=red   h=1 i=r1;      * linear regression;
  symbol18 v=none c=blue  h=1 i=rq;      * quad regression;
  symbol19 v=none c=green h=1 i=rc;      * cubic regression;
  symbol110 v=none c=orange h=1 i=stdj;  * exponential plot;

  FOOTNOTE1 J=R C=RED
    'LINEAR: SM = 0.0039 + 2.1145(R)';

  FOOTNOTE2 J=R C=BLUE
    'QUADRATIC: SM = 0.1087 + 1.4897(R) + 0.7061(R^2)';

  FOOTNOTE3 J=R C=GREEN
    'CUBIC: SM = -0.0147 + 2.7684(R) - 2.7125(R^2) + 2.6264(R^3)';

  FOOTNOTE4 J=R C=ORANGE
    'EXPONENTIAL: SM = -1.1923 + 1.3381 EXP(R)';

  FOOTNOTE5 J=R 'GJR ' "&sysdate";

  *****;

endsas;

```