Supplementary Material

Isothermal Oxidation Kinetics of Industrial South African Chromite Concentrates in Air

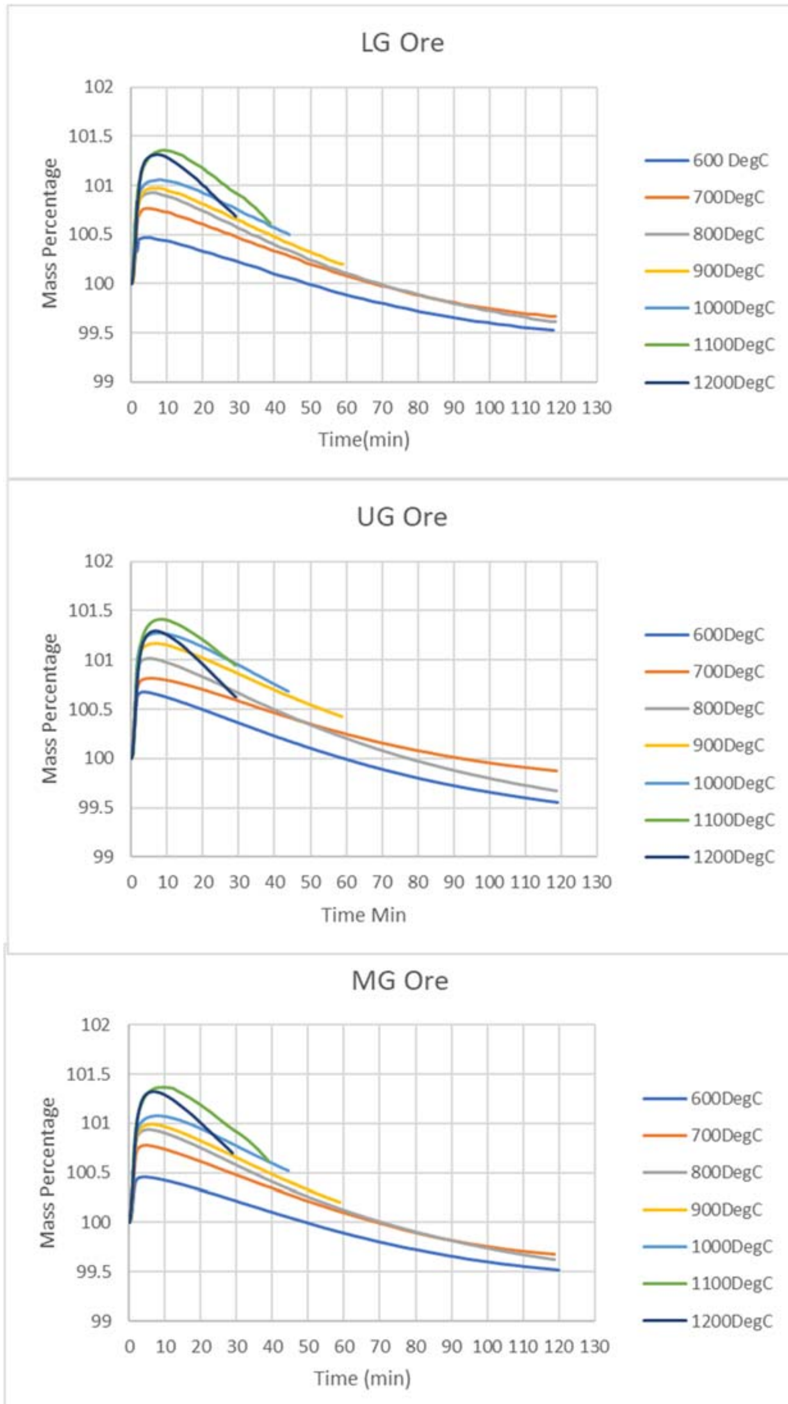


Figure S1: Mass percentage recorded from start of isothermal run for the three concentrates

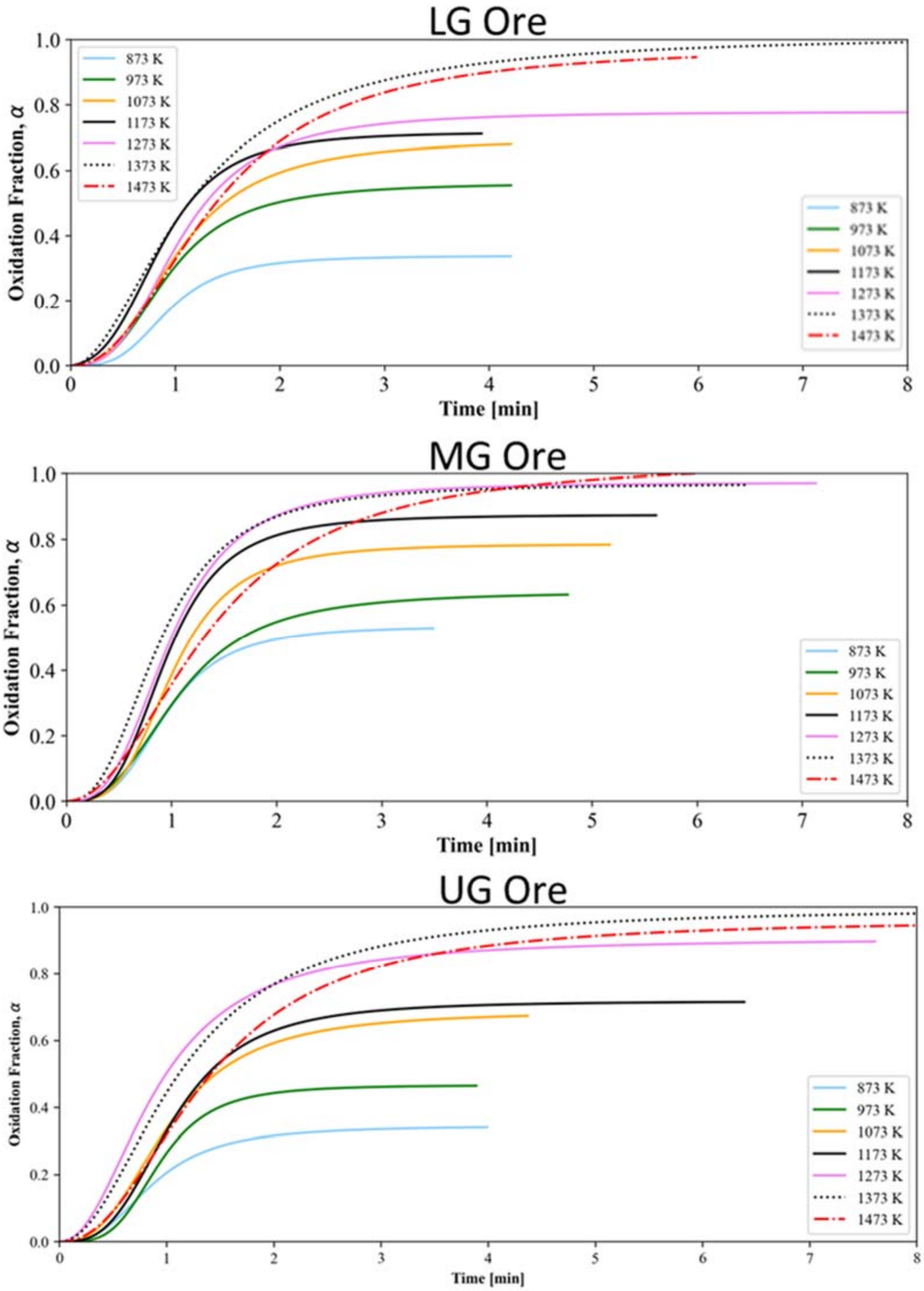


Figure S2: Extended time frame view for oxidation fraction over time
(plots only shown up to the point where the first derivative started exhibiting negative values indicating a turning point in the curve)

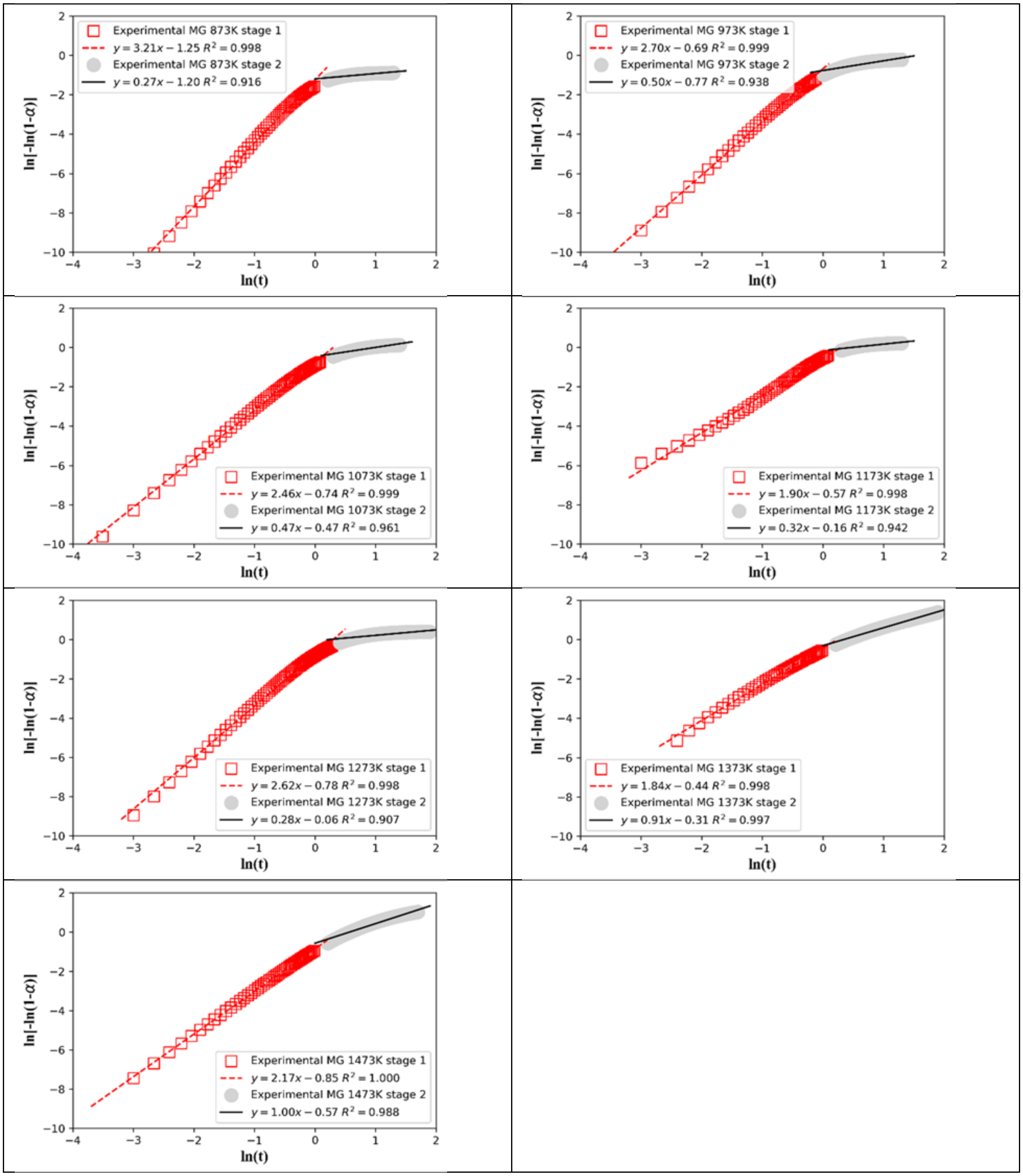


Figure 3S: Full set of Avrami plots for MG ore

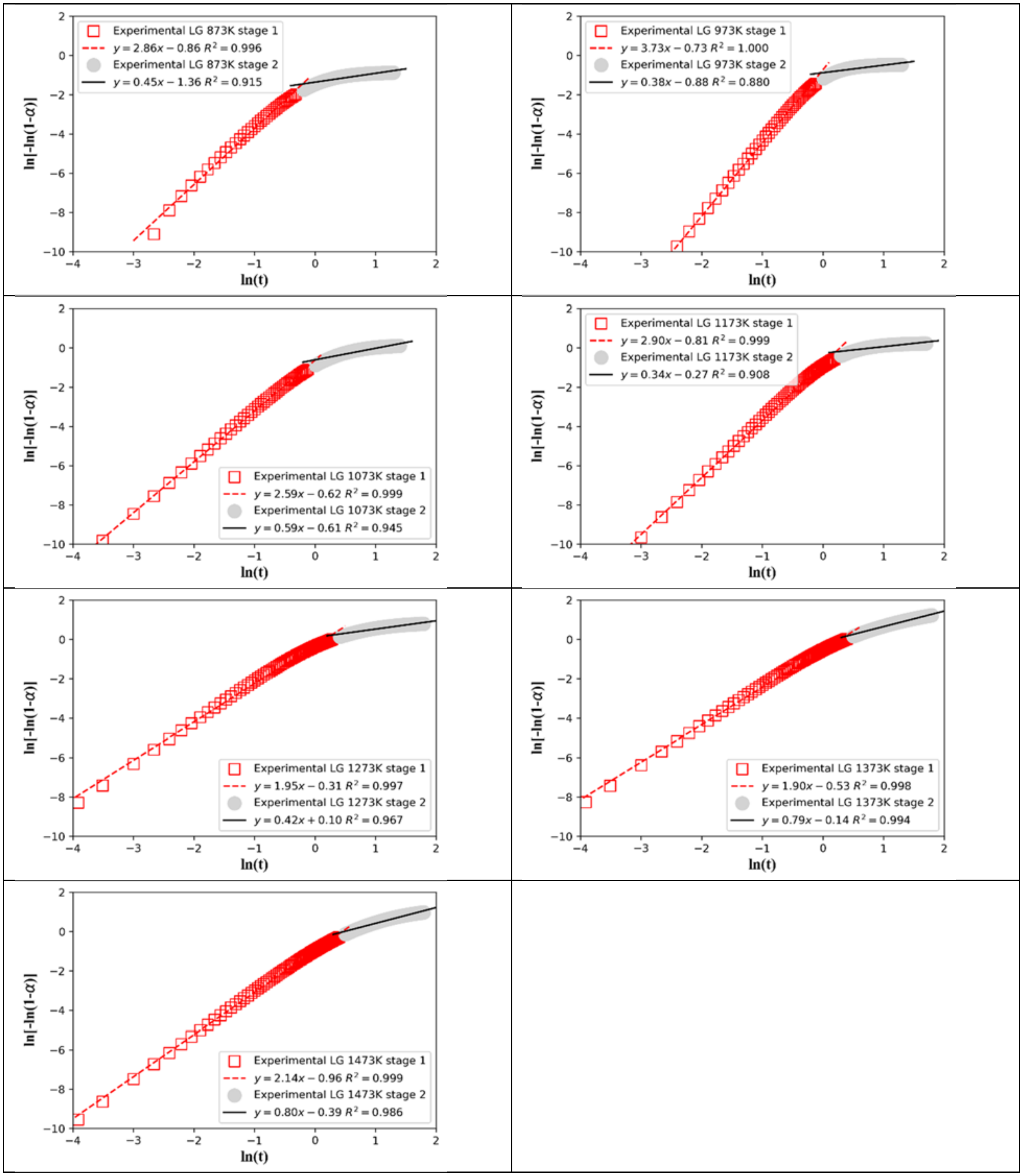


Figure S4: Full set of Avrami plots for LG ore

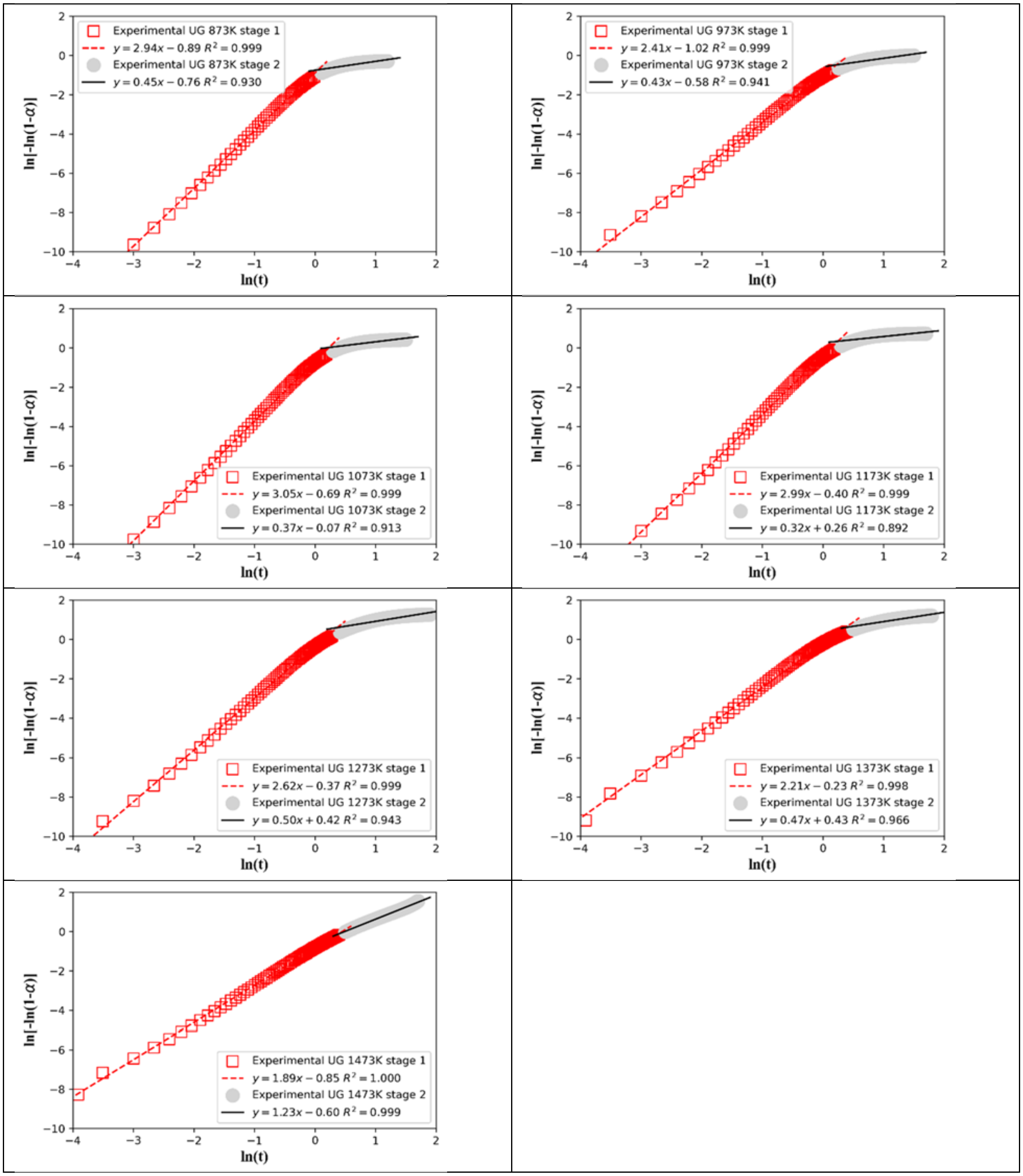


Figure S5: Full set of Avrami plots for UG ore

Fe^{2+} and Fe^{3+} calculation

$Fe^{2+/3+}$ calculations from average SEM-EDS results based on Droop, G. (1987). A general equation for estimating Fe^{3+} concentrations in ferromagnesian silicates and oxides from microprobe analyses, using stoichiometric criteria. Mineralogical magazine, 51(361), 431-435.

MG Ore:

	O	Mg	Al	Si	Ca	Ti	Cr	Fe	
Average Inputs :	57.19	6.63	8.73			0.19	16.82	10.45	42.81
	914.93	161.11	235.48	0.00	0.00	9.30	874.51	583.37	
	MgO	Al2O3	TiO2	Cr2O3	FeO	Fe2O3	Total		
Fe2+	9.62	16.01	0.56	46.00	27.01		99.19		
Fe2+/3+	9.62	16.01	0.56	46.00	20.26	7.50	99.94	Proceed with balance	
	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations (to 3)	0.46	0.61	0.01	1.18	0.73		3.00	(=T)	
Charge	0.93	1.83	0.05	3.54	1.46		7.82		
Nominal Oxygens	0.46	0.92	0.03	1.77	0.73		3.91	(=N)	
	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations	0.48	0.63	0.01	1.21	0.75		3.07	(=S)	
Charge	0.95	1.88	0.06	3.62	1.50		8.00		
Oxygens (to 4)	0.48	0.94	0.03	1.81	0.75		4.00	(=X)	
F = 2X (1-T/S)	Fe3+=	0.18	25.0%	<== Solution to equation					
Fe2+/FeTot			75%						
Normalised to formula	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations	0.47	0.61	0.01	1.18	0.55	0.18	3.00		
Charge	0.929	1.835	0.054	3.535	1.098	0.548	8.00		
Oxygens	0.465	0.917	0.027	1.768	0.549	0.274	4.00		

LG Ore:

	O	Mg	Al	Si	Ca	Ti	Cr	Fe	
Average Inputs :	57.14	6.71	9.27			0.03	17.24	9.61	42.86
	914.27	163.09	250.10	0.00	0.00	1.48	896.31	536.63	
	MgO	Al2O3	TiO2	Cr2O3	FeO	Fe2O3	Total		
Fe2+	9.79	17.11	0.09	47.43	25.00		99.42		
Fe2+/3+	9.79	17.11	0.09	47.43	19.79	5.79	100.00	Proceed with balance	
	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations (to 3)	0.47	0.65	0.00	1.21	0.67		3.00	(=T)	
Charge	0.94	1.95	0.01	3.62	1.35		7.86		
Nominal Oxygens	0.47	0.97	0.00	1.81	0.67		3.93	(=N)	
	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations	0.48	0.66	0.00	1.23	0.68		3.05	(=S)	
Charge	0.96	1.98	0.01	3.68	1.37		8.00		
Oxygens (to 4)	0.48	0.99	0.00	1.84	0.68		4.00	(=X)	
F = 2X (1-T/S)	Fe3+=	0.14	20.8%	<== Solution to equation					
Fe2+/FeTot			79.2%						
Normalised to formula	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations	0.47	0.65	0.00	1.21	0.53	0.14	3.00		
Charge	0.939	1.946	0.009	3.620	1.065	0.420	8.00		
Oxygens	0.470	0.973	0.004	1.810	0.532	0.210	4.00		

UG Ore:

	O	Mg	Al	Si	Ca	Ti	Cr	Fe	
Average Inputs :	56.87	6.99	9.50			0.32	15.92	10.40	43.13
	909.95	169.79	256.36	0.00	0.00	15.20	827.65	581.02	
	MgO	Al2O3	TiO2	Cr2O3	FeO	Fe2O3	Total		
Fe2+	10.20	17.55	0.92	43.83	27.08		99.58		
Fe2+/3+	10.20	17.55	0.92	43.83	20.06	7.80	100.36	Proceed with balance	
	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations (to 3)	0.49	0.66	0.02	1.11	0.72		3.00	(=T)	
Charge	0.97	1.98	0.09	3.32	1.45		7.81		
Nominal Oxygens	0.49	0.99	0.04	1.66	0.72		3.91	(=N)	
	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations	0.50	0.68	0.02	1.13	0.74		3.07	(=S)	
Charge	1.00	2.03	0.09	3.40	1.48		8.00		
Oxygens (to 4)	0.50	1.02	0.05	1.70	0.74		4.00	(=X)	
F = 2X (1-T/S)	Fe3+=	0.19	25.9%	<== Solution to equation					
Fe2+/FeTot			74.1%						
Normalised to formula	Mg2+	Al3+	Ti4+	Cr3+	Fe2+	Fe3+			
Cations	0.49	0.66	0.02	1.11	0.54	0.19	3.00		
Charge	0.972	1.983	0.088	3.322	1.072	0.563	8.00		
Oxygens	0.486	0.991	0.044	1.661	0.536	0.281	4.00		

Stepwise Linear regression methodology

Simple linear regression has a dependent variable (y), and independent variable (x) and includes a constant (c). The objective is then to establish a relationship between the dependent and independent variable by fitting a linear equation to the data of the form:

$$y = mx + c$$

With multiple linear regression, more than one independent variable is included which then gives the equation the general form:

$$y = m_1x_1 + m_2x_2 + \ldots\ldots + m_nx_n + c$$

For the current work the extent of oxidation (α) was considered as the dependent variable, the time(t) and temperature(T) as well as the cation compositions were considered as independent variables.

Examples of how this method is used can be found at:

van Staden, Yolindi, et al. "Damring formation during rotary kiln chromite pre-reduction: Effects of pulverized carbonaceous fuel selection and partial pellet melting." Metallurgical and Materials Transactions B 49 (2018): 3488-3503.

Du Preez, S. P., J. P. Beukes, and P. G. Van Zyl. "Cr (VI) Generation during flaring of CO-rich off-gas from closed ferrochromium submerged arc furnaces." Metallurgical and Materials Transactions B 46 (2015): 1002-1010.

It is also common to transform variables when non linear relationships are expected and instead of introducing the variable of temperature just as T it can also be considered in other forms such as 1/T, T^2, ln(T) etc. (Chung, Seokhyun, Young Woong Park, and Taesu Cheong. "A mathematical programming approach for integrated multiple linear regression subset selection and validation." Pattern Recognition 108 (2020): 107565.).

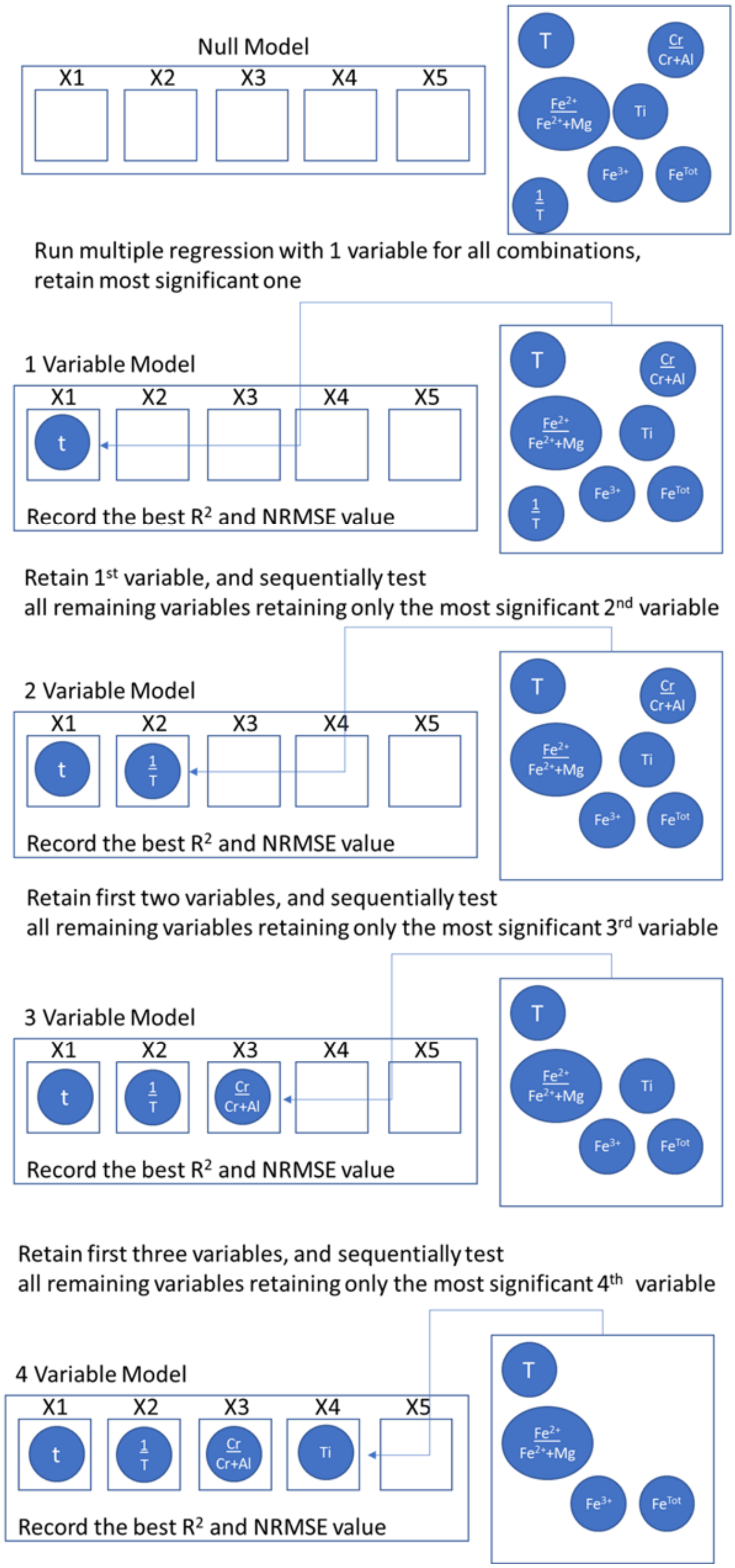
For the current work time and Temperature were investigated as straight linear variables but also in a number of standard transforms, with correlations using 1/T resulting in superior regression fits.

The methodology for the stepwise regression is visually illustrated on the next page, but is in essence an iterative process:

1) Compile a simple linear regression model for each variable on its own, and the variable that has regression parameters is retained as the first variable
2) Retain the first variable, then test all combinations with the remaining variables and similarly the variable with the best regression fitting parameters is retained as the 2^{nd} variable
3) The process of adding variables continues, until no more statistically significant variables (with a $p<0.05$ for the coefficient of the variable) can be added

In this instance only 4 variables could be added, and no further additional variables retained statistical significance if added to the equation :

$$\alpha = 1.98 + 1.82Ti - 2.06\left[\frac{Cr}{Cr + Al}\right] + 0.23t - 665.80\frac{1}{T}$$


Null Model
X1 X2 X3 X4 X5
T
Cr / Cr+Al
Fe2+ / Fe2++Mg
Ti
Fe3+
FeTot
1 / T
Run multiple regression with 1 variable for all combinations, retain most significant one
1 Variable Model
X1 X2 X3 X4 X5
t
Record the best R2 and NRMSE value
Retain 1st variable, and sequentially test all remaining variables retaining only the most significant 2nd variable
2 Variable Model
Record the best R2 and NRMSE value
Retain first two variables, and sequentially test all remaining variables retaining only the most significant 3rd variable
3 Variable Model
Record the best R2 and NRMSE value
Retain first three variables, and sequentially test all remaining variables retaining only the most significant 4th variable
4 Variable Model
Record the best R2 and NRMSE value