



Universidad de Zaragoza

Escuela de Ingeniería y Arquitectura

Anexos - Caracterización de la cristalización del xilitol para su uso como material de cambio de fase mediante técnicas reológicas

Trabajo Fin de Grado

Grado de Ingeniería de Tecnologías Industriales

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Julio 2024

Anexo 1

0.1. Extracción de datos

```
1 import pandas as pd;
2 import numpy as np;
3 from matplotlib import pyplot as plt;
4 import seaborn as sns;
5 from lmfit.models import StepModel, LinearModel;
6 import os;
7
8 Induction_Time = [];
9 Initial_Viscosity = [];
10 Final_Viscosity = [];
11 Temperature = [];
12 Gap = [];
13 Shear_Rate = [];
14 Stress = [];
15 Normal_Stress = [];
16 File = [];
17 GAP_ref = [];
18 Temperature_ref = [];
19 Shear_Rate_ref = [];
20
21 ubic = 'C:\\Users\\Marta Martí\\OneDrive\\Escritorio\\TFG\\ENSAYOS';
22 for root, dirs, files in os.walk(ubic):
23     for file in files:
24         df = pd.read_excel(ubic + '\\\\' + file, sheet_name='Peak hold -
↪ 1', header=[0, 1, 2]);
25         print(file);
26
27         df = df.droplevel(level=0, axis=1);
28         df = df.droplevel(level=1, axis=1);
29
30         log_visc = np.log(df['Viscosity']);
31         df['Log_visc'] = log_visc;
32
33         plt.plot(df['Viscosity'], label='Viscosity');
34         plt.yscale('log');
35         plt.title(file);
36         plt.legend();
37         plt.show();
38
39         index = int(input('cortar: '));
40         if len(df) > index:
41             df = df.iloc[:index];
42
43         step_mod = StepModel(form='logistic', prefix='step_');
44         line_mod = LinearModel(prefix='line_');
45         step2_mod = StepModel(form='arctan', prefix='step2_');
46         pars = step2_mod.guess(df['Log_visc'], x=df.index) +
↪ line_mod.guess(df['Log_visc'], x=df.index) +
↪ step_mod.guess(df['Log_visc'], x=df.index);
47         mod = step2_mod + line_mod + step_mod;
```

```
48     out = mod.fit(df['Log_visc'], pars, x=df.index);
49
50     Ajuste = out.best_fit;
51     derivada_Ajuste = np.gradient(Ajuste, df.index);
52
53     x = [2 * i for i in range(len(Ajuste))]
54     f, ax1 = plt.subplots()
55     ax2 = ax1.twinx()
56     ax1.plot(x, Ajuste, label='Ajuste')
57     ax1.plot(x, df['Log_visc'], label='Viscosity')
58     ax2.plot(x, derivada_Ajuste, label='Deriv', c='r')
59     ax1.set_xlabel('Step time [s]')
60     ax1.set_ylabel('Logarithmic Viscosity')
61     ax2.set_ylabel('Derivative')
62     ax1.legend(loc='upper left')
63     ax2.legend(loc='upper right')
64     plt.show()
65
66
67     y_der_inflex = np.max(derivada_Ajuste);
68     x_inflex = np.argmax(derivada_Ajuste);
69
70     log_visc_inflex = df['Log_visc'][x_inflex];
71     log_visc_ini = df['Log_visc'][3];
72
73     C_inflex = log_visc_inflex - x_inflex * y_der_inflex;
74
75     x_ind = (log_visc_ini - C_inflex) / y_der_inflex;
76     x_ind = round(x_ind);
77
78     t_ind = df['Step time'][x_ind];
79
80     plt.plot(df['Step time'], df['Log_visc']);
81     plt.axvline(t_ind, color='grey', ls='--', alpha=0.8);
82     plt.title(file);
83     plt.show();
84
85     File.append(file);
86     Induction_Time.append(t_ind);
87     Initial_Viscosity.append(df['Viscosity'][3]);
88     Final_Viscosity.append(df['Viscosity'][x_ind]);
89     Temperature.append(df['Temperature'][x_ind]);
90     Gap.append(df['Gap'][x_ind]);
91     Shear_Rate.append(df['Shear rate'][x_ind]);
92     Stress.append(df['Stress'][x_ind]);
93     Normal_Stress.append(df['Normal stress'][x_ind]);
94
95     if df['Gap'][x_ind] > 750:
96         GAP_ref.append(2);
97     else:
98         GAP_ref.append(1);
99
100     if 68 < df['Temperature'][x_ind] < 72:
101         Temperature_ref.append(70);
102     elif 73 < df['Temperature'][x_ind] < 77:
103         Temperature_ref.append(75);
104     elif 78 < df['Temperature'][x_ind] < 82:
105         Temperature_ref.append(80);
```

```

106         elif 83 < df['Temperature'][x_ind] < 87:
107             Temperature_ref.append(85);
108         elif 88 < df['Temperature'][x_ind] < 92:
109             Temperature_ref.append(90);
110
111         if df['Shear rate'][x_ind] > 98:
112             Shear_Rate_ref.append(100);
113         elif df['Shear rate'][x_ind] < 5:
114             Shear_Rate_ref.append(1);
115         elif 5 < df['Shear rate'][x_ind] < 50:
116             Shear_Rate_ref.append(10);
117
118     print(Temperature_ref);
119
120     df_salida = pd.DataFrame();
121     df_salida['File'] = File;
122     df_salida['Induction_Time'] = Induction_Time;
123     df_salida['Initial_Viscosity'] = Initial_Viscosity;
124     df_salida['Final_Viscosity'] = Final_Viscosity;
125     df_salida['Temperature'] = Temperature;
126     df_salida['Gap'] = Gap;
127     df_salida['Shear_Rate'] = Shear_Rate;
128     df_salida['Stress'] = Stress;
129     df_salida['Normal_Stress'] = Normal_Stress;
130     df_salida['GAP_ref'] = GAP_ref;
131     df_salida['Temperature_ref'] = Temperature_ref;
132     df_salida['Shear_Rate_ref'] = Shear_Rate_ref;
133
134     print(df_salida);
135
136     with pd.ExcelWriter('C:\\Users\\Marta
137         ↪ Martí\\OneDrive\\Escritorio\\TFG\\df_salida_rep.xlsx', mode='a',
138         ↪ if_sheet_exists='overlay') as writer:
139         df_salida.to_excel(writer, sheet_name='datos',
140             ↪ startrow=writer.sheets['datos'].max_row, index=False,
141             ↪ header=False);

```

0.2. Tasa de nucleación con tiempo de inducción

```

1 import pandas as pd;
2 import numpy as np;
3 from matplotlib import pyplot as plt;
4 import seaborn as sns;
5 from lmfit.models import StepModel, LinearModel;
6 import os;
7 import math;
8
9 x = 1000;
10
11 if x == 300:
12     df3 = pd.read_excel('C:\\Users\\Marta
13         ↪ Martí\\OneDrive\\Escritorio\\TFG\\df_salida.xlsx',
14         ↪ sheet_name='datos', header=[0]);
15 elif x == 600:
16     df3 = pd.read_excel('C:\\Users\\Marta
17         ↪ Martí\\OneDrive\\Escritorio\\TFG\\df_salida_600.xlsx',

```

```

    ↪ sheet_name='datos', header=[0]);
15 elif x == 1000:
16     df3 = pd.read_excel('C:\\Users\\Marta
    ↪ Martí\\OneDrive\\Escritorio\\TFG\\df_salida_rep.xlsx',
    ↪ sheet_name='datos', header=[0]);
17
18 df_aux = pd.DataFrame();
19 df2 = pd.DataFrame();
20 df2_600 = [];
21 df2_300 = [];
22 df2_rep = [];
23 w = 1;
24 gap = 1;
25 print('Número de ensayos tratados:', len(df3));
26
27 G = 3.5 * 10**(-6);
28 pi = math.pi;
29 i = 0;
30 mu = 2.67;
31 alpha_max = 0.57;
32
33 for j in range(12):
34     alpha_crist = [];
35     Nucleation_rate = [];
36     temp = [];
37     nucl = [];
38
39     if j <= 2:
40         df2 = df3.drop(df3[df3['Shear_Rate_ref'] != w].index);
41         df2 = df2.reset_index(drop=True);
42         print('Shear Rate:', w);
43         w *= 10;
44     elif 2 < j <= 4:
45         df2 = df3.drop(df3[df3['GAP_ref'] != gap].index);
46         df2 = df2.reset_index(drop=True);
47         print('GAP:', gap);
48         gap += 1;
49     elif 4 < j <= 10:
50         if w == 1000:
51             w = 1;
52         if gap == 3:
53             gap = 1;
54         df2 = df3.drop(df3[df3['GAP_ref'] != gap].index);
55         df2 = df2.drop(df2[df2['Shear_Rate_ref'] != w].index);
56         df2 = df2.reset_index(drop=True);
57         print('GAP:', gap, 'Shear rate:', w);
58         if w == 100:
59             gap += 1;
60         w *= 10;
61     elif j == 11:
62         df2 = df3;
63
64     for i in range(0, len(df2)):
65         alp = alpha_max * (1 - ((df2['Final_Viscosity'][i]) /
    ↪ df2['Initial_Viscosity'][i]) ** (-1 / (mu * alpha_max)));
66         alpha_crist.append(alp);
67         nucl = (3 * alp) / (G ** 3 * (df2['Induction_Time'][i]) ** 4 *
    ↪ pi);

```

```

68     Nucleation_rate.append(nucl);
69
70     df2['alpha_crist'] = alpha_crist;
71     df2['Nucleation_rate'] = Nucleation_rate;
72
73     df2 = df2.sort_values(by=['Temperature_ref', 'GAP_ref',
↪ 'Shear_Rate_ref']);
74
75     df_aux = df2.loc[df2['alpha_crist'] <= 0];
76     df2 = df2.drop(df2[df2['alpha_crist'] <= 0].index);
77
78     df2 = df2.reset_index(drop=True);
79
80     temp = df2['Temperature_ref'];
81     nucl = df2['Nucleation_rate'];
82
83     if not temp.empty and not nucl.empty:
84         if x == 300:
85             df2_300.append(df2);
86         elif x == 600:
87             df2_600.append(df2);
88         elif x == 1000:
89             df2_rep.append(df2);
90
91     if x == 300:
92         with pd.ExcelWriter("C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ experimentales\\df2_300_all.xlsx") as writer:
93             for i, df in enumerate(df2_300, 1):
94                 df.to_excel(writer, sheet_name="Sheet{}".format(i),
↪ index=False);
95         elif x == 600:
96             with pd.ExcelWriter("C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ experimentales\\df2_600_all.xlsx") as writer:
97                 for i, df in enumerate(df2_600, 1):
98                     df.to_excel(writer, sheet_name="Sheet{}".format(i),
↪ index=False);
99         elif x == 1000:
100             if df2_rep:
101                 with pd.ExcelWriter("C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ experimentales\\df2_rep_all.xlsx") as writer:
102                     for i, df in enumerate(df2_rep, 1):
103                         df.to_excel(writer, sheet_name="Sheet{}".format(i),
↪ index=False);
104
105     if not temp.empty and not nucl.empty:
106         fig, ax = plt.subplots();
107         ax.scatter(x=temp, y=nucl);
108         plt.yscale('log');
109         plt.xlabel('Temperatura');
110         plt.ylabel('Nucleation rate');
111         if j <= 2:
112             plt.title('Shear rate {}'.format(w / 10));
113         elif 2 < j <= 4:
114             plt.title('GAP {}'.format(gap - 1));
115         elif 4 < j <= 10:

```

```
116         plt.title('GAP and Shear Rate');
117     elif j == 11:
118         plt.title('ALL');
119     plt.show();
```

0.3. Obtención de parámetros tasa de nucleación

```
1 import pandas as pd;
2 import numpy as np;
3 from matplotlib import pyplot as plt;
4 import seaborn as sns;
5 from lmfit.models import StepModel, LinearModel;
6 import os;
7 import math;
8 from sklearn.linear_model import LinearRegression;
9 from lmfit.models import LinearModel;
10
11 x = 600;
12 if x == 300:
13     df3 = pd.read_excel('C:\\Users\\Marta
14     ↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
15     ↪ experimentales\\df2_300_all.xlsx', sheet_name='Sheet12',
16     ↪ index_col=0);
17 elif x == 600:
18     df3 = pd.read_excel('C:\\Users\\Marta
19     ↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
20     ↪ experimentales\\df2_600_all.xlsx', sheet_name='Sheet8',
21     ↪ index_col=0);
22 elif x == 1000:
23     df3 = pd.read_excel('C:\\Users\\Marta
24     ↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
25     ↪ experimentales\\df2_rep_all.xlsx', sheet_name='Sheet4',
26     ↪ index_col=0);
27
28 A = [];
29 B = [];
30 df_aux_XY = pd.DataFrame();
31 Tm = 92.4;
32 ln = 0;
33 w = 1;
34 gap = 2;
35 df4 = pd.DataFrame(index=None);
36
37 for j in range(12):
38     X = [];
39     Y = [];
40
41     if j <= 2:
42         df4 = df3.drop(df3[df3['Shear_Rate_ref'] != w].index);
43         df4 = df4.reset_index(drop=True);
44         print(w);
45         w *= 10;
46     elif 2 < j <= 4:
47         df4 = df3.drop(df3[df3['GAP_ref'] != gap].index);
48         df4 = df4.reset_index(drop=True);
49         print(gap);
```



```

41     gap -= 1;
42 elif 4 < j <= 10:
43     if w == 1000:
44         w = 1;
45     if gap == 0:
46         gap = 2;
47     df4 = df3.drop(df3[df3['GAP_ref'] != gap].index);
48     df4 = df4.drop(df4[df4['Shear_Rate_ref'] != w].index);
49     df4 = df4.reset_index(drop=True);
50     print(gap, w);
51     if w == 100:
52         gap -= 1;
53     w *= 10;
54 elif j == 11:
55     df4 = df3;
56
57 print(df4);
58 print(len(df4));
59
60 for i in range(len(df4)):
61     T3 = df4['Temperature_ref'][i] * (Tm -
↪ (df4['Temperature_ref'][i]) ** 2);
62     X.append(T3);
63     ln = math.log((df4['Nucleation_rate'][i]) *
↪ (df4['Initial_Viscosity'][i]));
64     Y.append(T3 * ln);
65
66 line_mod = LinearModel(prefix='line_');
67 if X and Y:
68     pars = line_mod.guess(Y, x=X);
69     mod = line_mod;
70     out = mod.fit(Y, pars, x=X);
71     Ajuste = out.best_fit;
72     Slope = out.params['line_slope'].value;
73     term_ind = out.params['line_intercept'].value;
74
75 plt.scatter(X, Y, label='Datos Originales');
76 plt.plot(X, Ajuste, color='red', label='Ajuste Lineal');
77 plt.xlabel('X');
78 plt.ylabel('Y');
79 plt.legend();
80 if j <= 2:
81     plt.title('Shear rate');
82 elif 2 < j <= 4:
83     plt.title('GAP');
84 elif 4 < j <= 10:
85     plt.title('GAP and Shear Rate');
86 elif j == 11:
87     plt.title('ALL');
88 plt.show();
89
90 print(Slope);
91
92 A.append(math.exp(Slope));
93 B.append(-term_ind);
94
95 df_aux_XY['X'] = X;
96 df_aux_XY['Y'] = Y;

```

```
97
98 AB = pd.DataFrame({'A': A, 'B': B});
99 print(AB);
100
101 if x == 300:
102     AB.to_excel("C:\\Users\\Marta
103     ↪ Martí\\OneDrive\\Escritorio\\TFG\\AB.xlsx", sheet_name="Sheet1");
104     df_aux_XY.to_excel("C:\\Users\\Marta
105     ↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
106     ↪ experimentales\\XY_300.xlsx", sheet_name="Sheet1");
107 elif x == 600:
108     AB.to_excel("C:\\Users\\Marta
109     ↪ Martí\\OneDrive\\Escritorio\\TFG\\AB_600.xlsx",
110     ↪ sheet_name="Sheet1");
111     df_aux_XY.to_excel("C:\\Users\\Marta
112     ↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
113     ↪ experimentales\\XY_600.xlsx", sheet_name="Sheet1");
114 elif x == 1000:
115     AB.to_excel("C:\\Users\\Marta
116     ↪ Martí\\OneDrive\\Escritorio\\TFG\\AB_rep.xlsx",
117     ↪ sheet_name="Sheet1");
118     df_aux_XY.to_excel("C:\\Users\\Marta
119     ↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
120     ↪ experimentales\\XY_rep.xlsx", sheet_name="Sheet1");
```

0.4. Tasa de nucleación en función de la temperatura

```
1 import pandas as pd;
2 import numpy as np;
3 from matplotlib import pyplot as plt;
4 import seaborn as sns;
5 from lmfit.models import StepModel, LinearModel;
6 import os;
7 import math;
8
9 x = 1000;
10 if x == 300:
11     params = pd.read_excel('C:\\Users\\Marta
12     ↪ Martí\\OneDrive\\Escritorio\\TFG\\AB.xlsx', sheet_name='Sheet1',
13     ↪ index_col=0);
14 elif x == 600:
15     params = pd.read_excel('C:\\Users\\Marta
16     ↪ Martí\\OneDrive\\Escritorio\\TFG\\AB_600.xlsx',
17     ↪ sheet_name='Sheet1', index_col=0);
18 elif x == 1000:
19     params = pd.read_excel('C:\\Users\\Marta
20     ↪ Martí\\OneDrive\\Escritorio\\TFG\\AB_rep.xlsx',
21     ↪ sheet_name='Sheet1', index_col=0);
22
23 T = np.linspace(60, 90, 31);
24 Tm = 92.4;
25
26 A = params['A'].tolist();
27 B = params['B'].tolist();
28 Jt = pd.DataFrame();
29 print("Longitud de parámetros:", len(params));
```

```

24
25 for j in range(len(params)):
26     A1 = A[j];
27     B1 = B[j];
28     J = [];
29
30     for i in range(len(T)):
31         mu = 0.0079 * 10**(-10) * math.exp(9955 / (T[i] + 273.15));
32         J.append((A1 / mu) * math.exp(-B1 / (T[i] * (Tm - T[i]) ** 2)));
33
34     Jt['Nucleation_Rate'] = J;
35     Jt['Temperature_ref'] = T;
36
37     plt.plot(T, J, label=f'Lista {j + 1}');
38
39     if x == 300:
40         Jt.to_excel("C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ teoricos\\df4_{}.xlsx".format(j + 1), index=False,
↪ sheet_name="Sheet1");
41     elif x == 600:
42         Jt.to_excel("C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ teoricos\\df4_600_{}.xlsx".format(j + 1), index=False,
↪ sheet_name="Sheet1");
43     elif x == 1000:
44         Jt.to_excel("C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ teoricos\\df4_rep_{}.xlsx".format(j + 1), index=False,
↪ sheet_name="Sheet1");
45
46 plt.xlabel('Índice');
47 plt.ylabel('Valor');
48 plt.yscale('log');
49 plt.title('Gráfico de 12');
50 plt.legend();
51 plt.show();

```

0.5. Comparación de las tasas de nucleación

```

1 import pandas as pd;
2 import numpy as np;
3 from matplotlib import pyplot as plt;
4 import seaborn as sns;
5 from lmfit.models import StepModel, LinearModel;
6 import os;
7 import math;
8
9 caso = 600;
10
11 def plot_data(file_type, rep):
12     if file_type == 300:
13         file_pattern = 'C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ experimentales\\df2_300_all.xlsx';
14     elif file_type == 600:

```

```

15     file_pattern = 'C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ experimentales\\df2_600_all.xlsx';
16
17     print(file_pattern);
18
19     for j in range(rep):
20         exp = pd.read_excel(file_pattern, sheet_name='Sheet{}'.format(j
↪ + 1));
21
22         if caso == 300:
23             teo = pd.read_excel('C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ teoricos\\df4_{}.xlsx'.format(j + 1), sheet_name='Sheet1');
24         elif caso == 600:
25             teo = pd.read_excel('C:\\Users\\Marta
↪ Martí\\OneDrive\\Escritorio\\TFG\\datos
↪ teoricos\\df4_600_{}.xlsx'.format(j + 1), sheet_name='Sheet1');
26
27         fig, ax = plt.subplots();
28         ax.scatter(x=exp['Temperature_ref'], y=exp['Nucleation_rate'],
↪ label='experimental');
29         ax.plot(teo['Temperature_ref'], teo['Nucleation_Rate'],
↪ color='red', label='teórico');
30         plt.yscale('log');
31         plt.xlabel('Temperatura');
32         plt.ylabel('Nucleation rate');
33
34         if caso == 300:
35             if j <= 2:
36                 plt.title('Shear rate');
37             elif 2 < j <= 4:
38                 plt.title('GAP');
39             elif 4 < j <= 10:
40                 plt.title('GAP and Shear Rate');
41             elif j == 11:
42                 plt.title('ALL');
43         elif caso == 600:
44             if j <= 2:
45                 plt.title('Shear rate');
46             elif j == 3:
47                 plt.title('GAP');
48             elif 4 <= j <= 6:
49                 plt.title('GAP and Shear Rate');
50             elif j == 7:
51                 plt.title('ALL');
52
53         plt.legend();
54         plt.show();
55
56 if caso == 300:
57     rep = 12;
58 elif caso == 600:
59     rep = 8;
60
61 plot_data(caso, rep);

```

0.6. Método estadístico

```
1 import pandas as pd
2 import numpy as np
3 from matplotlib import pyplot as plt
4 import seaborn as sns
5 from sklearn.neighbors import KernelDensity
6 from matplotlib.patches import Patch
7 from matplotlib.lines import Line2D
8 from sklearn.linear_model import LinearRegression
9
10
11 ubic = 'C:\\Users\\GITSE\\Downloads\\TODOS_ANOVA.csv'
12 df = pd.read_csv(ubic, delimiter = ';')
13 pd.set_option('display.max_columns', None)
14
15 df = df.dropna(axis=0, how='all')
16
17
18
19
20 def indicator_function(x, y):
21     if x >= y:
22         return 1
23     else:
24         return 0
25
26 def curva_prob(tiempos_de_induccion):
27     min_tiempo = min(tiempos_de_induccion)-10
28     max_tiempo = max(tiempos_de_induccion)+200
29     probabilidades = []
30     current_tiempo_values = []
31     paso = (max_tiempo-min_tiempo)/1000
32     current_tiempo = min_tiempo
33     while current_tiempo <= max_tiempo:
34         suma_indicadores = sum(indicator_function(current_tiempo,
35 ↪ tiempo) for tiempo in tiempos_de_induccion)
36         probabilidad = suma_indicadores / len(tiempos_de_induccion)
37         probabilidades.append(round(probabilidad,4))
38         current_tiempo_values.append(current_tiempo)
39         current_tiempo += paso
40
41     probs = list(set(probabilidades))
42     probs.sort()
43     print(type(probs))
44     index_l=[]
45     times = []
46     for prob in probs:
47         index_l.append(probabilidades.index(prob))
48     for i in index_l:
49         times.append(current_tiempo_values[i])
50
51     return current_tiempo_values, probabilidades
52     #return times, probs
53
54 temperaturas = pd.unique(df['Temperature_ref'])
55 print(df.columns)
56 print(pd.unique(df['GAP_ref']))
```

```

56 print(pd.unique(df['Shear_Rate_ref']))
57 print(temperaturas)
58 color = ['r', 'b', 'g', 'k', 'purple']
59 i=0
60 J=[]
61 tg=[]
62 for temp in temperaturas:
63
64     if temp == 75:
65         i+=1
66         continue
67     if temp == 85:
68         i+=1
69         continue
70
71
72     df_filt = df[df['Temperature_ref']==temp]
73     df_filt = df_filt[df_filt['GAP_ref']==1]
74     df_filt = df_filt[df_filt['Shear_Rate_ref']==10]
75
76     tiempos_ind = np.array(df_filt['Induction_Time'])
77     tiempo,prob = curva_prob(tiempos_ind)
78
79     ##### Modelo #####
80     # Step 2: Calculate the ECDF
81     sorted_induction_times = sorted(tiempos_ind)
82     ecdf = np.arange(len(sorted_induction_times)) / len(tiempos_ind)
83
84     # Step 4: Transform the ECDF
85     y = -np.log(1 - ecdf)
86
87     # Create the design matrix X for linear regression
88     t_array = np.array(sorted_induction_times).reshape(-1, 1)
89     X = t_array
90
91     # Step 5: Fit the linear regression model
92     model = LinearRegression()
93     model.fit(X, y)
94
95     # The parameters A and B are now available in the model's
    ↪ coefficients
96     A = model.coef_[0]
97     B = -model.intercept_ / A
98
99     # Calculate the model
100     t_plot = tiempo
101     P_t_plot = 1 - np.exp(-A * (t_plot - B))
102     P_t_plot2 = [x if x>0 else 0 for x in P_t_plot]
103     J.append(-A)
104     tg.append(B)
105
106     #plt.plot(tiempo,prob, label = str(int(temp))+'$^{\circ}$C', color =
    ↪ color[i]) #Descomentar para la comparación
107     #plt.scatter(tiempo,prob,color = color[i])
108     plt.scatter(sorted_induction_times, ecdf, color = color[i])
109     plt.plot(t_plot, P_t_plot2, '-', color = color[i])
110     i+=1
111     sorted_data = np.sort(tiempos_ind)

```

```

112     cumulative_density = np.linspace(0, 1, len(sorted_data))
113     #plt.scatter(sorted_data, cumulative_density, label='CDF ' +
↪ str(int(temp))+'$^\circ$C')
114     #plt.plot(sorted_data, cumulative_density)
115     file = open("list"+str(temp)+".csv", "w")
116     for index in range(len(prob)):
117         file.write(str(tiempo[index]) + ";" + str(prob[index]) + "\n")
118 file.close()
119 print(J)
120 plt.grid()
121 custom_lines = [Line2D([0], [0], color='gray', lw=2, label='ECDF and
↪ data'),
122                 Line2D([0], [0], color=color[0],
↪ lw=2, label='70'+'$^\circ$C'),
123                 Line2D([0], [0], color=color[1],
↪ lw=2, label='75'+'$^\circ$C'),
124                 Line2D([0], [0], color=color[2],
↪ lw=2, label='80'+'$^\circ$C'),
125                 Line2D([0], [0], color=color[3],
↪ lw=2, label='85'+'$^\circ$C'),
126                 Line2D([0], [0], color=color[4],
↪ lw=2, label='90'+'$^\circ$C')]
127
128 custom_lines = [Line2D([0], [0], color=color[0],
↪ lw=2, label='70'+'$^\circ$C'),
129                 Line2D([0], [0], color=color[2],
↪ lw=2, label='80'+'$^\circ$C'),
130                 Line2D([0], [0], color=color[4],
↪ lw=2, label='90'+'$^\circ$C')]
131
132
133 plt.ylabel('Probabilidad')
134 plt.xlabel('Tiempo de inducción [s]')
135 plt.title('Probabilidad acumulada')
136 plt.legend(handles = custom_lines)
137 plt.show()

```