WagnerModel

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1 Wagner model

Angel Villalba-Rodríguez - A00828035@itesm.mx Constanza Álvarez-López - A00829469@itesm.mx Osamu Katagiri-Tanaka - A01212611@itesm.mx Juan Jesús Rocha-Cuervo - A01752555@itesm.mx

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[1]:
```
# PYTHON LIBRARIES
%matplotlib inline

import numpy as np;
import pandas as pd;
import warnings
warnings.filterwarnings('ignore')
import matplotlib as mpl
import matplotlib.pyplot as plt
plt.rc('xtick', labelsize=18)
plt.rc('ytick', labelsize=18)
import statistics as stat

from scipy import special, optimize
```

2 Instructions

Using the experiemntal data, fit the Wagner model to find the transient shear viscosity at different shear rates (1, 10, and 100 $1/s$). Also, using the Wagner fitting parameters, obtain the stady state first normal stress difference curve.

3 Available Data

Starting values for λ_i, a_i, f_1, f_2, n_1, and n_2

30 shear rate vs shear viscosity experimental measurements

A cross model fitting data to the experiental measurements

A shear viscosity vs. time data (a.k.a. transient shear viscosity) at one shear rate (0.01 $1/s$)

4 Assumptions

The fitting will be done with 8 Maxwell elements, assuming that those are enough to achive a good model fit.

5 Algorithm

Define the shear viscosity function, given by the Wagner model

Define the steady state shear viscosity function at $t = \infty$

Compute the fitting curve with the Wagner model

Plot the Wagner fit and get the fitting parameters

Obtain the transient shear viscosity at 1, 10, and 100 $1/s$ shear rates

Define the steady state first normal stress difference function

Obtain the steady state 1st normal stress difference plot

6 Solution

6.1 Fit viscosity measurements

6.1.1 Read CSV data

[2]:
```
filename = "./experimentdata.csv";
df_data = pd.read_csv(filename, sep=',');
display(df_data.head())
```

	Shear rate 1/s	Viscosity Pa.s
0	0.031416	3376.02
1	0.062832	3296.92
2	0.125664	3150.91
3	0.251328	3010.33
4	0.376992	2853.87

6.2 Compute fitting curve with the Wagner model

6.2.1 Shear viscosity as a function of a given shear rate $\dot{\gamma}_o$

6.2.2

$$\eta(t, \dot{\gamma}_o) = f_1 \sum_{i=1}^{n} \frac{a_i}{{\alpha_i}^2} \left(1 - e^{1-\alpha_i t}(1 - \dot{\gamma}_o n_1 \lambda_i \alpha_i t)\right) + f_2 \sum_{i=1}^{n} \frac{a_i}{{\beta_i}^2} \Big(1 - e^{1-\beta_i t}(1 - \dot{\gamma}_o n_2 \lambda_i \beta_i t)\Big)$$

where:

$$f_2 = 1 - f_1$$

$$\alpha_i = \frac{1 + n_1 \lambda_i \dot{\gamma}_o}{\lambda_i}$$

$$\beta_i = \frac{1 + n_2 \lambda_i \dot{\gamma}_o}{\lambda_i}$$

$\eta(t, \dot{\gamma}_o)$ = shear viscosity t = time $\dot{\gamma}_o$ = shear rate a_i = the i^{th} elastic value of the Maxwell element λ_i = the i^{th} characteristic time of the Maxwell element f_1, f_2, n_1, n_2 are fitting parameters

[3]:
```
dot_gamma_o = 1 # make it global

# Let's model with 8 Maxwell elements
def _eta_gamma(t, *p):
    a_          = p[0:8]
    lambda_     = p[8:16]
    f_1         = p[16]
    f_2         = 1 - f_1
    n_1         = p[17]
    n_2         = p[18]

    sum_1 = 0
    for i in range(0, 8, 1):
        alpha = _alpha(n_1, lambda_[i], dot_gamma_o)
        frac = a_[i] / alpha**2
        expo = np.exp(- alpha*t)
        prod = dot_gamma_o*n_1*lambda_[i]*alpha*t
        res_1 = frac*(1 - expo * (1 - prod))
        sum_1 = sum_1 + res_1

    sum_2 = 0
    for i in range(0, 8, 1):
        beta  = _beta(n_2, lambda_[i], dot_gamma_o)
        frac = a_[i] / beta**2
        expo = np.exp(- beta*t)
        prod = dot_gamma_o*n_2*lambda_[i]*beta*t
        res_2 = frac*(1 - expo * (1 - prod))
        sum_2 = sum_2 + res_2

    res = (f_1 * sum_1) + (f_2 * sum_2)

    return res/10
```

```python
def _alpha(n_1, lambda_, dot_gamma_o):
    nume = 1 + n_1*lambda_*dot_gamma_o
    deno = lambda_
    res = nume / deno
    return res

def _beta(n_2, lambda_, dot_gamma_o):
    nume = 1 + n_2*lambda_*dot_gamma_o
    deno = lambda_
    res = nume / deno
    return res
```

6.2.3 The Wagner model gives the shear viscosity vs. time of a single shear rate . . . now let's caculate the steady state shear viscocity at several shear rates at $t = \infty$

$$\eta(t = \infty, \dot{\gamma}_o) = f_1 \sum_{1=1}^{n} \frac{a_i}{{\alpha_i}^2} + f_2 \sum_{1=1}^{n} \frac{a_i}{{\beta_i}^2}$$

[4]:
```python
def _eta_infty(dot_gamma, *p):
    a_          = p[0:8]
    lambda_     = p[8:16]
    f_1         = p[16]
    f_2         = 1 - f_1
    n_1         = p[17]
    n_2         = p[18]

    sum_1 = 0
    for i in range(0, 8, 1):
        alpha = _alpha(n_1, lambda_[i], dot_gamma)
        res_1 = a_[i] / alpha**2
        sum_1 = sum_1 + res_1

    sum_2 = 0
    for i in range(0, 8, 1):
        beta  = _beta(n_2, lambda_[i], dot_gamma)
        res_2 = a_[i] / beta**2
        sum_2 = sum_2 + res_2

    res = (f_1 * sum_1) + (f_2 * sum_2)

    return res/10
```

Compute the fitting curve with the Wagner model

[5]:
```
def _fit_eta(t, eta):
    # Initial guess
    ai      = [0.0000006, 0.0003, 0.28, 30, 10000, 2000000, 40000000, 200000000]
    lambdai = [3000, 600, 100, 10, 1, 0.1, 0.01, 0.001]
    f1 = [0.57]
    n1 = [2.8]
    n2 = [0.07]
    p = ai + lambdai + f1 + n1 + n2

    # Fit the model
    upbound    = [np.inf]*16 + [1] + [np.inf]*2
    model      = optimize.curve_fit(_eta_infty, t, eta, p, bounds=(0, upbound));
 ↪ #bounds=(0, [3., 1., 0.5])
    parameters = model[0]

    # Show the fitting parameters
    print(parameters)

    return parameters
```

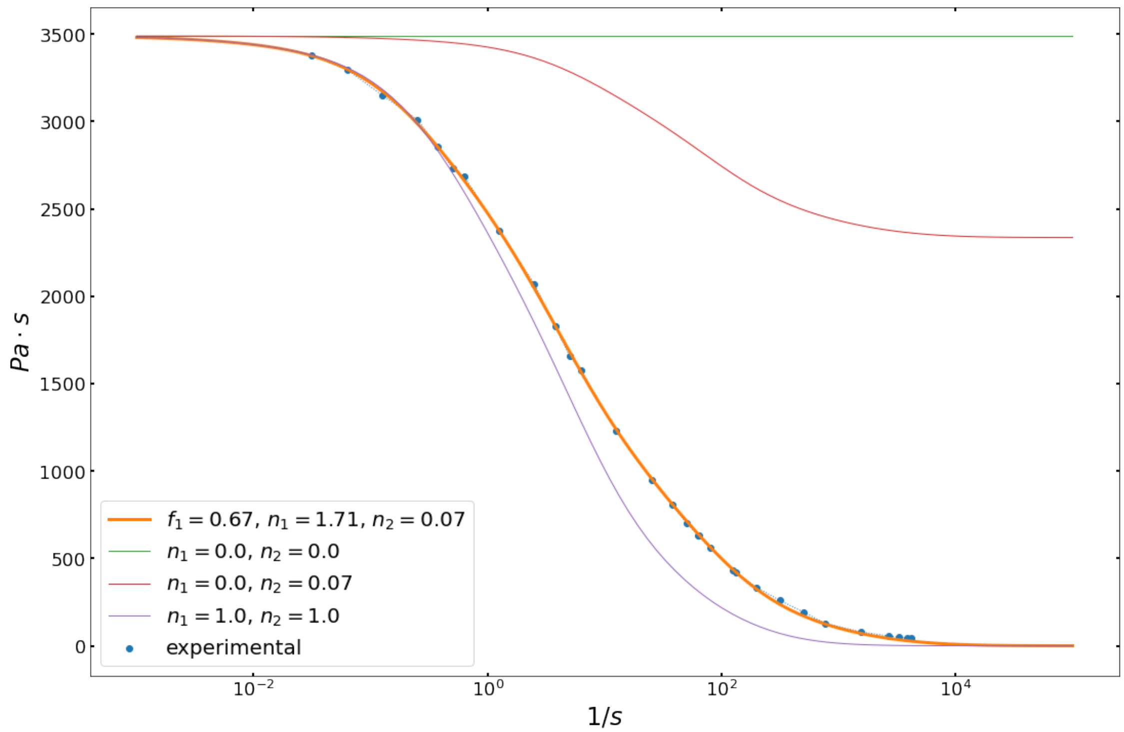
6.2.4 Plot the Wagner fit and get n_1, n_2

[6]:
```
parameters = _fit_eta(
    pd.Series(df_data['Shear rate 1/s']).dropna(),
    pd.Series(df_data['Viscosity Pa.s']).dropna())

# Draw plot canvas
scale = 6;
plotname = 'Wagner fit';
plt.subplots(figsize=(3*scale, 2*scale));
ax0 = plt.gca()

# plot dataset
t   = pd.Series(df_data['Shear rate 1/s']).dropna()
eta = pd.Series(df_data['Viscosity Pa.s']).dropna()
plt.scatter(t, eta, label='experimental')
plt.plot(t, eta, linewidth=1, linestyle=':')

# Plot fit
n_1 = parameters[17]
n_2 = parameters[18]
t = np.logspace(-3, 5, 100)
eta_fit = _eta_infty(t, *parameters)
```

```
plt.plot(t, eta_fit, linewidth=3, label = r'$f_1 = $' +␣
↪str(round(parameters[16],2)) + ', ' +
         r'$n_1 = $' + str(round(n_1, 2)) + ', ' +
         r'$n_2 = $' + str(round(n_2, 2)));

# Format and Display plots
ax0.tick_params(which='both', direction='in', width=2, bottom=True, top=True,␣
↪left=True, right=True);
plt.yscale('linear');
plt.xscale('log');

ax0.set(autoscale_on=False)
parameters[17] = 0
parameters[18] = 0
eta_fit = _eta_infty(t, *parameters)
plt.plot(t, eta_fit, linewidth=1, label = r'$n_1 = $' +␣
↪str(round(parameters[17],2)) + ', ' +
         r'$n_2 = $' + str(round(parameters[18],2)));
parameters[17] = 0
parameters[18] = n_2
eta_fit = _eta_infty(t, *parameters)
plt.plot(t, eta_fit, linewidth=1, label = r'$n_1 = $' +␣
↪str(round(parameters[17],2)) + ', ' +
         r'$n_2 = $' + str(round(parameters[18],2)));
parameters[17] = 1
parameters[18] = 1
eta_fit = _eta_infty(t, *parameters)
plt.plot(t, eta_fit, linewidth=1, label = r'$n_1 = $' +␣
↪str(round(parameters[17],2)) + ', ' +
         r'$n_2 = $' + str(round(parameters[18],2)));

# restore the saved the ns
parameters[17] = n_1
parameters[18] = n_2

plt.xlabel(r'$1/s$', fontsize=24);
plt.ylabel(r'$Pa \cdot s$', fontsize=24);
#plt.title(plotname, size=24);
plt.legend(prop={'size': 20});
plt.savefig('plt_' + plotname + '.png', dpi=300, bbox_inches='tight');
display(plt);
```

```
[3.96453361e-07 1.78460749e-04 1.46700609e-01 5.07620566e+01
 1.01527929e+04 1.88475089e+06 2.67036501e+07 2.12078861e+08
 2.22611145e+03 4.01589068e+02 5.10605560e+01 1.50384175e-01
 1.00911954e+00 9.64964058e-02 1.31382820e-02 3.05545551e-03
 6.69494901e-01 1.71085954e+00 6.80393423e-02]
```

```
<module 'matplotlib.pyplot' from 'C:\\Users\\oskat\\AppData\\Roaming\\Python\\Python37\\site-pa
```



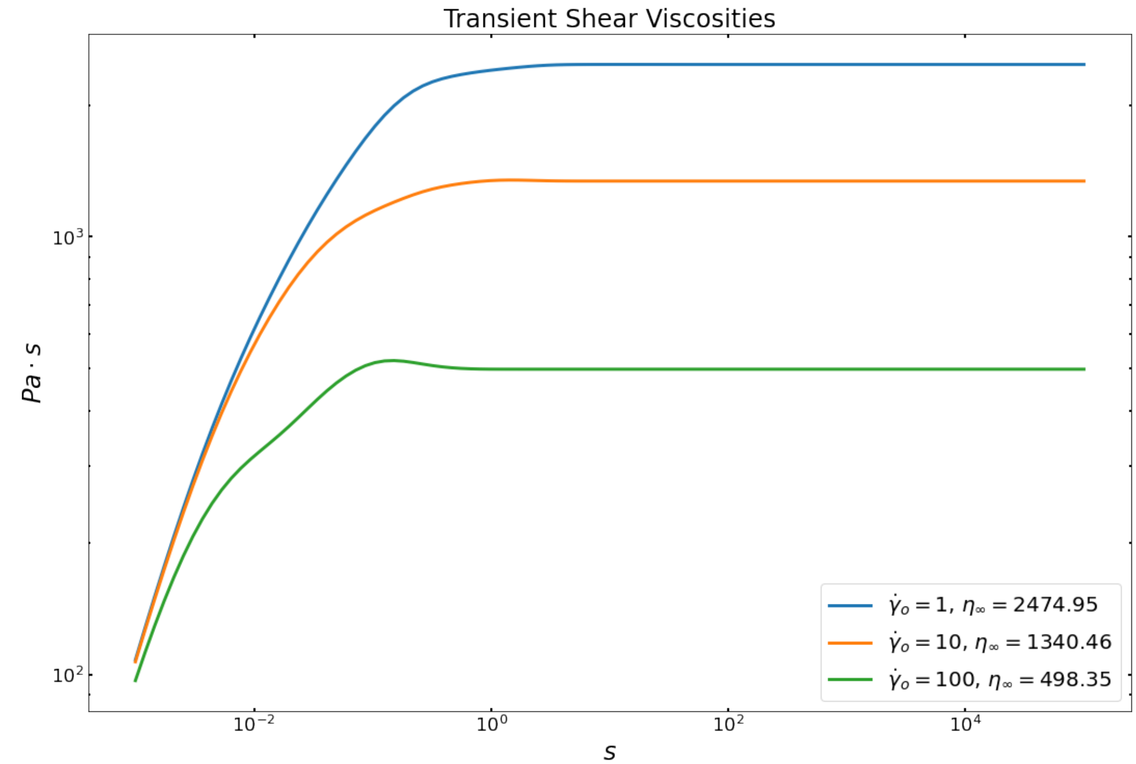
6.2.5 1.a) Obtain the Transient Shear Viscosity at 1, 10 and 100 1/s

[7]:
```
parameters = _fit_eta(
    pd.Series(df_data['Shear rate 1/s']).dropna(),
    pd.Series(df_data['Viscosity Pa.s']).dropna())

# Draw plot canvas
scale = 6;
plotname = 'Transient Shear Viscosities';
plt.subplots(figsize=(3*scale, 2*scale));
ax0 = plt.gca()

# Plot fit
dot_gamma_o = 1
t = np.logspace(-3, 5, 100)
eta_fit = _eta_gamma(t, *parameters)
plt.plot(t, eta_fit, linewidth=3, label = r'$\dot{\gamma}_o = $' +␣
 ↪str(dot_gamma_o) + ", " +
```

```
        r'$\eta_{\infty} = $' + str(round(_eta_infty(dot_gamma_o,␣
↪*parameters),2)));
dot_gamma_o = 10
eta_fit = _eta_gamma(t, *parameters)
plt.plot(t, eta_fit, linewidth=3, label = r'$\dot{\gamma}_o = $' +␣
↪str(dot_gamma_o) + ", " +
        r'$\eta_{\infty} = $' + str(round(_eta_infty(dot_gamma_o,␣
↪*parameters),2)));
dot_gamma_o = 100
eta_fit = _eta_gamma(t, *parameters)
plt.plot(t, eta_fit, linewidth=3, label = r'$\dot{\gamma}_o = $' +␣
↪str(dot_gamma_o) + ", " +
        r'$\eta_{\infty} = $' + str(round(_eta_infty(dot_gamma_o,␣
↪*parameters),2)));

# Format and Display plots
ax0.tick_params(which='both', direction='in', width=2, bottom=True, top=True,␣
↪left=True, right=True);
plt.yscale('log');
plt.xscale('log');
plt.xlabel(r'$s$', fontsize=24);
plt.ylabel(r'$Pa \cdot s$', fontsize=24);
plt.title(plotname, size=24);
plt.legend(prop={'size': 20});
plt.savefig('plt_' + plotname + '.png', dpi=300, bbox_inches='tight');
display(plt);
```

```
[3.96453361e-07 1.78460749e-04 1.46700609e-01 5.07620566e+01
 1.01527929e+04 1.88475089e+06 2.67036501e+07 2.12078861e+08
 2.22611145e+03 4.01589068e+02 5.10605560e+01 1.50384175e-01
 1.00911954e+00 9.64964058e-02 1.31382820e-02 3.05545551e-03
 6.69494901e-01 1.71085954e+00 6.80393423e-02]
```

```
<module 'matplotlib.pyplot' from 'C:\\Users\\oskat\\AppData\\Roaming\\Python\\Python37\\site-pa
```



6.3 Steady state first normal stress difference $N1$ at $t = \infty$

6.3.1

$$N1(t, \dot{\gamma}_o) = \dot{\gamma}_o^2 \left\{ f_1 \sum_{i=1}^{n} a_i {\alpha_i}^3 \left(1 - e^{-\alpha_i t} \left[1 + \alpha_i t - {\alpha_i}^2 \left(n_1 \lambda_i \frac{\dot{\gamma}_o}{2}\right) t^2\right)\right] + f_2 \sum_{i=1}^{n} a_i {\beta_i}^3 \left(1 - e^{-\beta_i t} \left[1 + \beta_i t - \right.\right.\right.$$

6.3.2

$$N1(t = \infty, \dot{\gamma}_o) = \dot{\gamma}_o^2 \left\{ f_1 \sum_{i=1}^{n} a_i {\alpha_i}^3 + f_2 \sum_{i=1}^{n} a_i {\beta_i}^3 \right\}$$

[8]:
```
def _N1(dot_gamma, *p):
    a_      = p[0:8]
    lambda_ = p[8:16]
    f_1     = p[16]
    f_2     = 1 - f_1
    n_1     = p[17]
    n_2     = p[18]

    print(p)
```

```
    sum_1 = 0
    for i in range(0, 8, 1):
        alpha = _alpha(n_1, lambda_[i], dot_gamma)
        res_1 = a_[i] * (alpha**3)
        sum_1 = sum_1 + res_1

    sum_2 = 0
    for i in range(0, 8, 1):
        beta  = _beta(n_2, lambda_[i], dot_gamma)
        res_2 = a_[i] * (beta**3)
        sum_2 = sum_2 + res_2

    res = dot_gamma**2 * (f_1*sum_1 + f_2*sum_2)

    return res/10
```

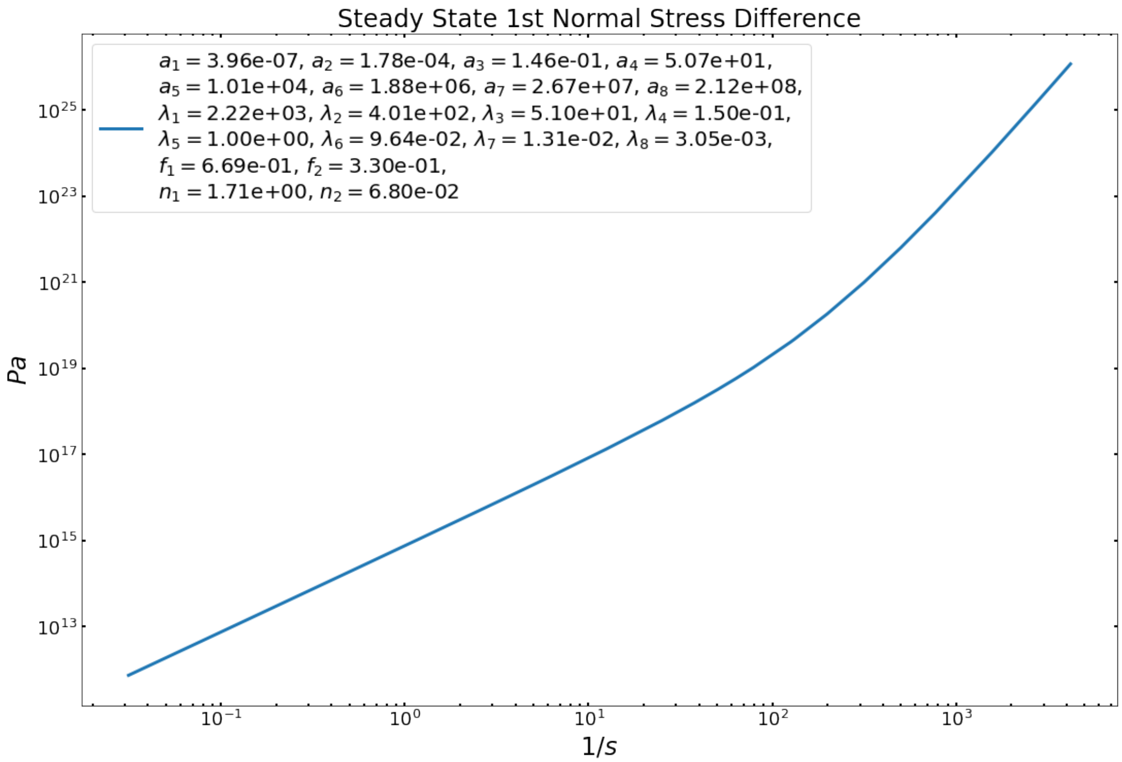
6.3.3 1.b) Obtain the steady state first normal stress dfference

[9]:
```
# Format scientific notation
def format_e(n):
    a = '%E' % n
    numeric_part    = a.split('E')[0].rstrip('0').rstrip('.')
    int_part        = numeric_part.split('.')[0]
    decimal_part    = numeric_part.split('.')[1]
    scientific_part = a.split('E')[1]
    return int_part + '.' + decimal_part[0:2] + 'e' + scientific_part

# Draw plot canvas
scale = 6;
plotname = 'Steady State 1st Normal Stress Difference';
plt.subplots(figsize=(3*scale, 2*scale));
ax0 = plt.gca()

a_            = parameters[0:8]
lambda_       = parameters[8:16]
f_1           = parameters[16]
f_2           = 1 - f_1
n_1           = parameters[17]
n_2           = parameters[18]

# Plot fit
gamma = pd.Series(df_data['Shear rate 1/s']).dropna()
N1 = _N1(gamma, *parameters)
plt.plot(gamma, N1, linewidth=3, label =
        r'$a_1 = $' + format_e(a_[0]) + ", " +
```

```
         r'$a_2 = $' + format_e(a_[1]) + ", " +
         r'$a_3 = $' + format_e(a_[2]) + ", " +
         r'$a_4 = $' + format_e(a_[3]) + ",\n" +
         r'$a_5 = $' + format_e(a_[4]) + ", " +
         r'$a_6 = $' + format_e(a_[5]) + ", " +
         r'$a_7 = $' + format_e(a_[6]) + ", " +
         r'$a_8 = $' + format_e(a_[7]) + ",\n" +
         r'$\lambda_1 = $' + format_e(lambda_[0]) + ", " +
         r'$\lambda_2 = $' + format_e(lambda_[1]) + ", " +
         r'$\lambda_3 = $' + format_e(lambda_[2]) + ", " +
         r'$\lambda_4 = $' + format_e(lambda_[3]) + ",\n" +
         r'$\lambda_5 = $' + format_e(lambda_[4]) + ", " +
         r'$\lambda_6 = $' + format_e(lambda_[5]) + ", " +
         r'$\lambda_7 = $' + format_e(lambda_[6]) + ", " +
         r'$\lambda_8 = $' + format_e(lambda_[7]) + ",\n" +
         r'$f_1 = $' + format_e(f_1) + ", " +
         r'$f_2 = $' + format_e(f_2) + ",\n" +
         r'$n_1 = $' + format_e(n_1) + ", " +
         r'$n_2 = $' + format_e(n_2));

# Format and Display plots
ax0.tick_params(which='both', direction='in', width=2, bottom=True, top=True,␣
 ↪left=True, right=True);
plt.yscale('log');
plt.xscale('log');
plt.xlabel(r'$1/s$', fontsize=24);
plt.ylabel(r'$Pa$', fontsize=24);
plt.title(plotname, size=24);
plt.legend(prop={'size': 20});
plt.savefig('plt_' + plotname + '.png', dpi=300, bbox_inches='tight');
display(plt);
```

```
(3.9645336065341767e-07, 0.00017846074924745392, 0.1467006093305382,
50.76205659755287, 10152.792916261515, 1884750.889982305, 26703650.056959767,
212078861.3393067, 2226.111452881524, 401.58906791986004, 51.060555958380846,
0.15038417496012438, 1.0091195389204213, 0.09649640578894919,
0.013138282025652327, 0.0030554555092308466, 0.6694949010007502,
1.7108595354483316, 0.0680393422606903)
```

```
<module 'matplotlib.pyplot' from 'C:\\Users\\oskat\\AppData\\Roaming\\Python\\Python37\\site-pa
```



7 References

Bonilla-Rios Jaime, ESTIMATION OF THE FIRST NORMAL STRESS DIFFERENCE (N1) AND CREEP COMPLIANCE(J(t)) OF POLYPROPYLENE (PP) RESINS USING A CONSTITUTIVE EQUATION. (2020)

[10]:
```
## Recover matplotlib defaults
#mpl.rcParams.update(mpl.rcParamsDefault);
```