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Use of Least Square Procedures and Ansys Polyflow Software to Select Best Viscosity Model for Polypropylene

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Abstract* — This work was intended to select the best viscosity model of polypropylene (PP) data using the percentage root-mean-square error function (PRMSE) and ansys package. Eleven samples of polypropylene (KPC - PP113) were tested at different loads and constant temperature 230°C using melt flow index tester (SUST plastic laboratory) and the results for each sample were recorded. Different viscosity models (viscosity versus shear rate) were checked using polyflow and the best of them was selected using PRMSE function. It was found that PP 113 shear stress versus shear rate was Non-Newtonian and PRMSE beside easy to apply get an accurate model to quote viscosity.

***Index Terms*- Ansys Polyflow, Ansys Polyman, PRMSE, Viscosity Model.**

I. INTRODUCTION

Viscosity is the most important flow property, and it is the resistance to shearing, it can be measured by either capillary or rotational viscometers. In capillary viscometers like (Melt Flow Index Tester), the shear stress is determined from the pressure applied by a piston. The shear rate is determined from the flow rate [1].
MFI represents a point at specific shear rate and shear stress values on the viscosity versus shear rate curve at constant load and temperature [2]. Melt index is the amount of melt which flows through the capillary of the measuring instrument under a defined time scale at a given temperature and pressure, the fig. 1, shows the schema of shows the schema of capillary plastometer.

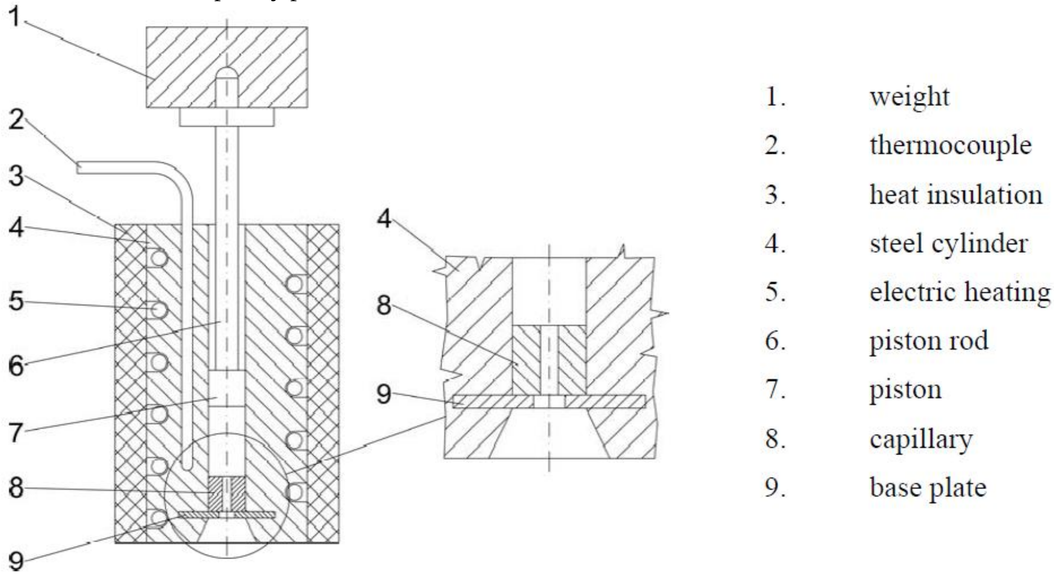

Fig. 1. Schema of capillary plastometer [3]

By measuring the mass of melt, we can calculate the Melt Flow Index (MFI)

$$MFI_{[T,F]} = m.S/t \quad ...(1)$$

Where
MFI [g/10min] melt flow index
T [^{0}C] test temperature
F [dyne] weigh force

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S [s] factor of standard time (10 minutes=600s), S=600
t [s] time needed for V amount of materials to flow through the capillary
m [g] amount of materials flowing through the capillary under t time [3].
Where dimensions as per ASTM D1238:
Piston radius $R_p = 0.4775cm$
Capillary radius $R_C = 0.10475cm$
Capillary length $L_C = 0.8cm$
Weigh force F = test load $L\ (kg) \times 9.80665 \times 10^5$ dyn ... (2)
The equations for master curve from MFI tester
Mass flow rate [2]

$$\dot{m}\ (g/s) = MFI/600 \quad \dots (3)$$

Melt density [4]

$$\rho_m\ (g/cm^3) = m/\pi R_p{}^2 l \quad \dots (4)$$

Where
m [g] amount of materials flowing through the capillary under t time.
l [cm] distant of piston move down during materials flowing through the capillary under t time.
Volume flow rate [2]

$$Q(cm^3/s) = \dot{m}/\rho_m \quad \dots (5)$$

Shear rate [2]

$$\dot{\gamma}\ (s^{-1}) = 4Q/\pi R_c{}^3 \quad \dots (6)$$

Shear stress [2]

$$\tau(dyne/cm^2) = R_c F/2\pi R_p{}^2 L_c \quad \dots (7)$$

viscosity [2]

$$\mu\ (dyne/cm^2.s) = \frac{\tau}{\dot{\gamma}} \quad \dots (8)$$

ANSYS POLYFLOW can be used to solve several types of models, ranging from Newtonian in elastic to non-Newtonian viscoelastic. Several shear-rate-dependent, temperature-dependent, and temperature-independent viscosity models are supplied.

ANSYS POLYMAN is an environment layer built on top of the programs used in the ANSYS POLYFLOW package, it package is an interactive graphical program that allows to visualize material data, including steady shear viscosity and steady elongational viscosity. It computes material properties from constitutive equations and numerical parameters, for isothermal and non-isothermal generalized Newtonian, differential viscoelastic, and integral viscoelastic fluids. It can also compare them with experimental curves (i.e., fitting). Several viscosity laws are available for generalized Newtonian flows. The isothermal viscosity laws (Constant, Power Law, Bird-Carreau Law, Cross Law, Modified Cross Law, Bingham Law, Modified Bingham Law, Herschel-Bulkley Law, Modified Herschel-Bulkley Law, Log-Log Law and Carreau-Yasuda Law)[5].

Least-square procedures are widely used in numerical computations. Here the quality of the fit between the observed η^*_{obs} and predicted η^*_{fit} viscosity values was quantified using a modified least square procedure called the percentage root-mean-square error function (%RMSE):

$$\%RMSE = \frac{100}{N}\sqrt{\sum_{i=1}^{N}\left(\frac{\eta^*_{obs} - \eta^*_{fit}}{\eta^*_{obs}}\right)^2} \quad \dots (9)$$

Where N is the number of data points:
The best-fit is used to find the smallest error (based on the %RMSE value) between viscosity measurements and the modeled viscosity [6]. Several authors have shown that a master curve can be generated especially for many individual types of polymers by plotting $\mu \times$MFI versus $\dot{\gamma}$ /MFI on a log-log scale [7].
In this work, a new easy technique has been developed to use Polyflow software and PRMSE method to choose a best viscosity curve fitting the experimental data (viscosity versus shear rate) obtained from MFI test. The technique to help designers and engineers to design or simulate the plastic machines and molds or dies in order to get accurate results.

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II. MATERIALS AND METHODS

Polypropylene properties (MFI =2 - 4 g/10min 2.16kg/230^{0}C), manufactured by Khartoum petrochemical company for extrusion applications was used in this work. The eleven samples with average 5 grams weighting, the different MFI values were obtained at loads from 0.74kg to 8.165kg and constant temperature 230^{0}C.

III. RESULTS AND DISCUSSION

Table (1) lists all calculated equations from Eq (1) to Eq (8).The experimental data on shear stress is plotted against shear rate, (Fig.1). It is obvious that the plastic melt is non Newton fluid. In case is plotted against viscosity at log scale (Fig. 2). It is obvious that the viscosity decrease with increase shear rate. Experimental viscosity (obs) with fitted viscosity (fit) for ten non Newton viscosity models fitting in POLYMAT against experimental shear rate lists in Table (2) and. Fig. 3, the method of PRMSE Eq (9) was described in Table (3), it is obvious that the best model (Carreau-Yasuda law) according to PRMSE method. Fig. 4, without taking into account the slight differences between it and (log log law and cross law).

Table (1): Experimental data for PP113 from MFI

Sample	t(s)	load (g)	load(kg)	m(g)	MFI (g/10 min)	load F (dyne)	distance of piston *l* (cm)	Melt density (g/cm^3)	Flow rate Q (cm^3/s)	shear rate at wall (s^{-1})	Shear Stress (dyne/cm^2)	Viscosity (dyne/cm^2.s)
1	150	325+415	0.74	0.1778	0.711	725692.1	0.325	0.76	0.001551553	1.719	66326.91541	38590.037
2	150	325+875	1.2	0.33	1.32	1176798	0.587	0.78	0.002803131	3.105	107557.1601	34637.603
3	150	325+960	1.335	0.335	1.34	1309187.775	0.688	0.68	0.003285442	3.640	119657.3406	32877.404
4	150	325+1640	1.965	0.6423	2.56	1927006.725	1.256	0.71	0.005976364	6.620	176124.8497	26603.303
5	150	325+875+960	2.16	0.765	3.06	2118236.4	1.51	0.71	0.007210781	7.988	193602.8882	24237.147
6	150	325+875+1200	2.4	0.8805	3.52	2353596	1.646	0.75	0.007855765	8.702	215114.3202	24719.108
7	150	325+875+1640	2.84	1.165	4.66	2785088.6	2.197	0.74	0.010491448	11.622	254551.9456	21902.464
8	150	325+960+1640	2.925	1.2225	4.9	2868445.125	2.416	0.71	0.011560843	12.807	262170.5778	20471.347
9	150	325+875+968+1640	3.8	1.839	7.36	3726527	3.666	0.70	0.017515959	19.404	340597.6737	17553.339
10	150	325+875+969+1640 +1200	5	2.974	11.9	4903325	5.894	0.70	0.028155387	31.190	448154.8338	14368.736
11	30	325+875+969+1640 +1200+3165	8.165	1.7692	42.48	8007129.725	3.497	0.71	0.100241737	111.044	731836.8437	6590.489

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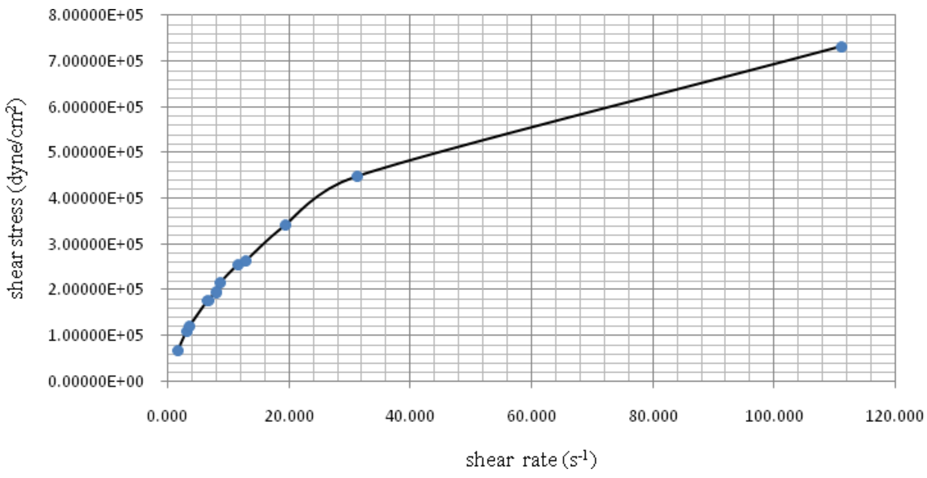

Fig. 1. Relation between Shear Stress and Shear Rate for (PP113)

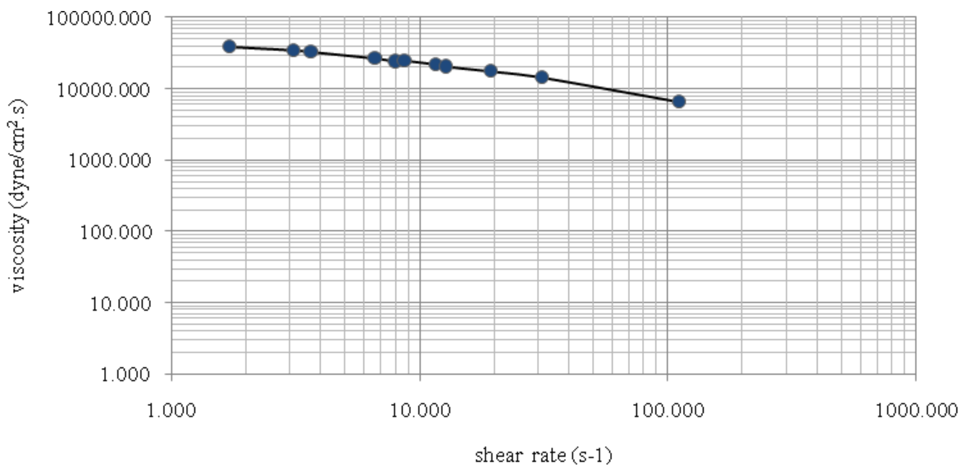

Fig. 2.Viscosity vs. shear rate curve for (PP113)

Table (2): Experimental (obs) with fitted (fit) viscosity for ten non Newton viscosity models

Exp	Power Low	Bird-Carreau Law	Cross Law	Log log law	Bingham law	Herschel-Bulkley law	modified Cross law	modified Bingham law	modified Herschel-Bulkley law	Carreau Yasuda law
38590.03724	45412.01182	37573.25705	38697.0458	38889.31757	34529.45607	37530.28061	38292.33019	36028.939	39884.70614	39049.84588
34637.6035	35427.97961	34582.28711	33900.29594	33895.84207	32914.25153	34842.51188	34028.3507	33395.295	33483.00355	33816.96347
32877.40406	33143.96077	33371.08834	32505.06136	32461.14219	32291.81347	33806.7486	32696.29091	32460.852	31941.30352	32369.08665
26603.30264	25783.08705	27570.69962	27014.40648	26920.01629	28819.08725	28027.98518	27198.15378	27950.197	26572.23246	26866.71516
24237.14692	23829.02123	25556.84069	25264.84754	25184.99908	27226.03045	25591.05334	25394.11631	26222.710	24983.60784	25155.0276
24719.1	22987.3	24640.1	24469.9	24400.4	26393.6	24543.3	24570.7	25392.7	24268.0	24380.9

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0775	4758	176	8772	2528	5634	5487	8419	55	2355	7127
21902.46398	20358.6245	21629.16973	21823.80309	21800.45089	22992.2191	21312.10258	21824.68595	22445.814	21881.05526	21812.45384
20471.34659	19545.83395	20664.28149	20955.34341	20949.76869	21612.1279	20326.27542	20924.63428	21426.022	21087.79172	20970.24093
17553.33874	16417.70576	16878.04388	17400.43453	17468.07348	16081.55464	16596.3475	17267.43118	17107.529	17729.05332	17510.00873
14368.73577	13452.10314	13287.17992	13760.88578	13876.43806	11999.83161	13165.44343	13597.07635	12823.126	14034.49033	13915.77655
6590.489347	7894.104651	6918.799807	6692.019625	6659.555721	7167.423352	7085.08718	6736.920983	6804.221	6615.603709	6648.867404

Table (3): Apply PRMSE for experimental (obs) and fitted (fit) viscosity models

	Exp	Power Low	Bird-Carreau Law	Cross Law	Log log law	Bingham law	Herschel-Bulkley law	modified Cross law	modified Bingham law	modified Herschel-Bulkley law	Carreau-Yasuda law
	0	0.031251423	0.000694231	7.6893E-06	6.01459E-05	0.011071998	0.000754157	5.95152E-05	0.004404556	0.001125556	0.000141972
	0	0.000520681	2.55042E-06	0.000453108	0.000458599	0.002475439	3.49964E-05	0.000309385	0.001286362	0.001111136	0.000561319
	0	6.57331E-05	0.000225478	0.00012826	0.000160302	0.000317244	0.000799022	3.03462E-05	0.000160525	0.000810681	0.000239042
	0	0.000950572	0.001322325	0.000238799	0.00014173	0.006937196	0.002867907	0.000499972	0.00256328	1.36401E-06	9.80396E-05
	0	0.000283547	0.002964718	0.00179792	0.00152939	0.015207401	0.003120429	0.002278666	0.006711266	0.00094853	0.001434199
	0	0.004908061	1.02113E-05	0.000101567	0.000166208	0.004589125	5.05521E-05	3.60043E-05	0.000742676	0.000333004	0.000187119
	0	0.00496842	0.000155695	1.28983E-05	2.16933E-05	0.002475551	0.000726524	1.26104E-05	0.000615423	9.55423E-07	1.68887E-05
	0	0.002043958	8.88237E-05	0.000558975	0.000546172	0.00310536	5.02192E-05	0.000490292	0.002174795	0.000906768	0.000593915
	0	0.004185588	0.001480019	7.58786E-05	2.35953E-05	0.007030217	0.002972326	0.000265297	0.000645031	0.000100207	6.09338E-06
	0	0.004069617	0.005665794	0.001789599	0.001173866	0.027180526	0.007013022	0.002884126	0.011570775	0.00054112	0.000993759
	0	0.039125831	0.002481613	0.000237332	0.000109824	0.00766332	0.005632084	0.000493667	0.001051729	1.45214E-05	7.84628E-05
PRMSE	**0**	**2.762999791**	**1.116793623**	**0.668167867**	**0.602441657**	**2.697617225**	**1.408980586**	**0.779906843**	**1.624360456**	**0.697921528**	**0.599642512**

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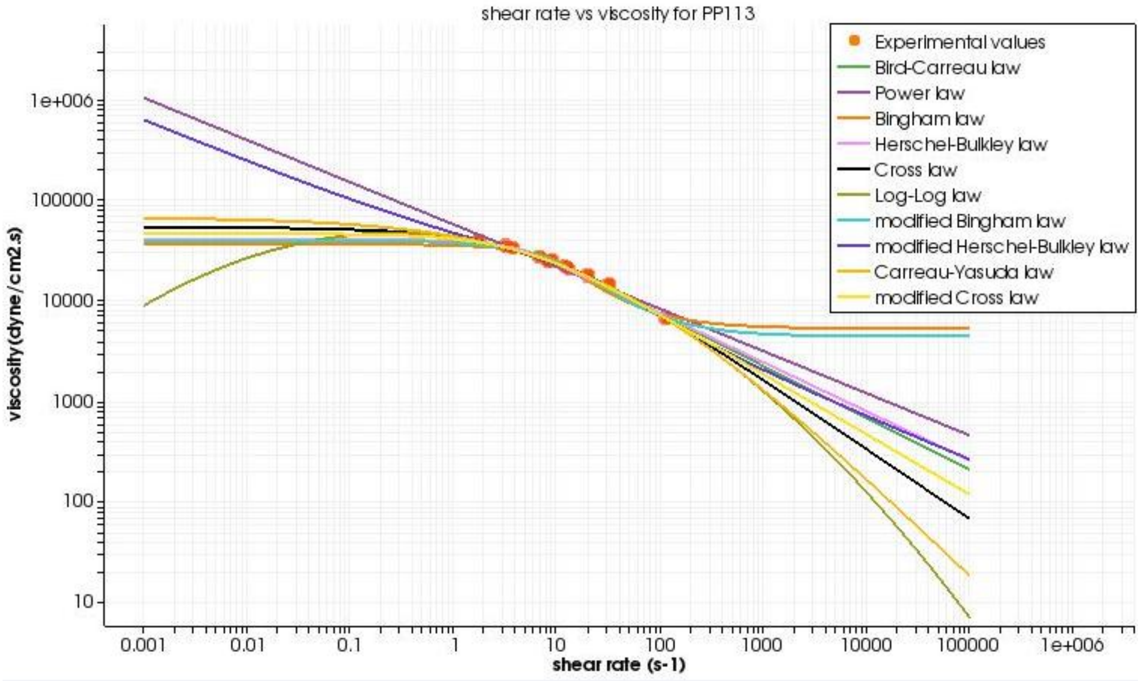

Fig. 3. Experimental viscosity (Obs) and fitted viscosity (fit) for ten non Newton viscosity models in POLYMAT against experimental shear rate

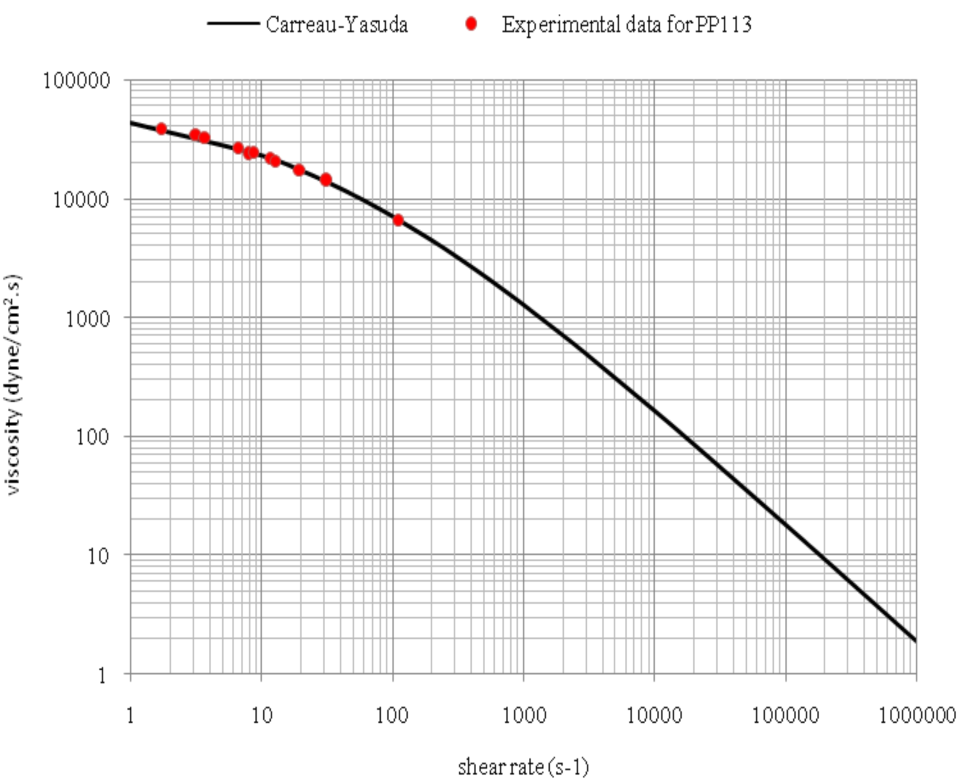

Fig. 4. Experimental viscosity (obs) with Carreau-Yasuda model

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IV. CONCLUSION

The shear stress vs. shear rate for PP113 is non Newton model, the viscosity decreases with increasing shear rate. Polymat in Ployflow software was good fitting experimental data. PRMSE was easy method and accurate result obtained. Finally viscosity model Carreau-Yasuda was best one from them.

APPENDIX

Appendix A: Equations and parameters from Polymat software

Power Low	Bird-Carreau Law
Power law f(g) = fac * (tnat*g)**(expo-1) fac = 0.1807456E+05 [auto] tnat = 0.6480288E-01 [auto] expo = 0.5802489E+00 [auto]	Bird-Carreau law f(g) = facinf + (fac-facinf) * [1+(tnat*g)**2]**((expo-1)/2) fac = 0.3939230E+05 [auto] tnat = 0.2607249E+00 [auto] expo = 0.4833018E+00 [auto] facinf = 0.3273708E-02 [auto]
Cross Law	**Log log law**
Cross law f(g) = fac/ (1 + (tnat*g)**expom) fac = 0.5356631E+05 [auto] tnat = 0.1473487E+00 [auto] expom = 0.6964472E+00 [auto]	Log-Log law f(g) = fac * 10**(a0 +a1*log(g/gcrit) +a11*log(g/gcrit)**2) a0 = -0.3965743E+00 [auto] a1 = 0.5546945E+00 [auto] a11 = -0.1229601E+00 [auto] fac = 0.2771846E+05 [auto] gcrit = 0.1456364E-02 [auto]
Bingham law	**Herschel-Bulkley law**
Bingham law f(g) = fac + ystr/g when g >= gcrit = fac + ystr/gcrit*(2-g/gcrit) when g < gcrit fac = 0.5279988E+04 [auto] ystr = 0.2095891E+06 [auto] gcrit = 0.1341293E+02 [auto]	Herschel-Bulkley law f(g) = fac1 / g + fac2 * (g/gcrit) ** (expo-1) when g > gcrit = fac1 * [2 - g/gcrit] / gcrit + fac2 * [(2-expo) + (expo-1) * g/gcrit] when g < gcrit fac1 = 0.5191806E-02 [auto] fac2 = 0.2746237E+05 [auto] expo = 0.5120642E+00 [auto] gcrit = 0.6912179E+01 [auto]
modified Cross law	**modified Bingham law**
modified Bingham law f(g) = fac + ystr*(1-exp(-m*g))/g where m = 3/gcrit fac = 0.4399646E+04 [auto] ystr = 0.2670147E+06 [auto] gcrit = 0.2265015E+02 [auto]	modified Bingham law f(g) = fac + ystr*(1-exp(-m*g))/g where m = 3/gcrit fac = 0.4399646E+04 [auto] ystr = 0.2670147E+06 [auto] gcrit = 0.2265015E+02 [auto]
modified Herschel-Bulkley law	**Carreau Yasuda law**
modified Herschel-Bulkley law f(g) = fac1 * (1 - exp(-3 * g / gcrit)) / g + fac2 * (g / gcrit) ** (expo-1) fac1 = 0.2262428E+06 [auto] fac2 = 0.6511587E+04 [auto] expo = 0.5786505E+00 [auto] gcrit = 0.4817822E+02 [auto]	Carreau-Yasuda law f(g) = facinf + (fac-facinf) * [1+(tnat*g)**expoa]**((expo-1)/expoa) fac = 0.6738002E+05 [auto] tnat = 0.3531332E-01 [auto] expo = 0.5375814E-05 [auto] facinf = 0.1445808E-01 [auto] expoa = 0.4534786E+00 [auto]

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Dr. Ahmed Ibrahim Ahmed Sidahmed Ahmed, had been the Examination Coordinator Faculty of Science and Technology U of G 1996 – 1997.Textile Technology Head department U of G 1997 -1999.Deputy Dean Faculty of Textiles U of G 1999 – 2000.Deputy Dean College of Engineering SUST (North Campus) April 2006 – June 2010.Deputy Dean College of Engineering SUST (Administration) July 2010 – Nov. 2010.Dean College of Engineering SUST Dec. 2010 June 2012(most important achievements are: restructuring of the college(13 departments, 8150 student) into six schools and signing Cooperation agreements with Belgrade University, Serbia and Reading University, UK) and right now guided more than 10 Ph.D students so far.