

RheoPower

Usable results of the linear relation between MWD, RED and viscoelastic properties.

RheoPower software package for polymers

RheoAnalyzer

RheoDeveloper

The work with RheoPower chemometrics software family gives you following benefits:

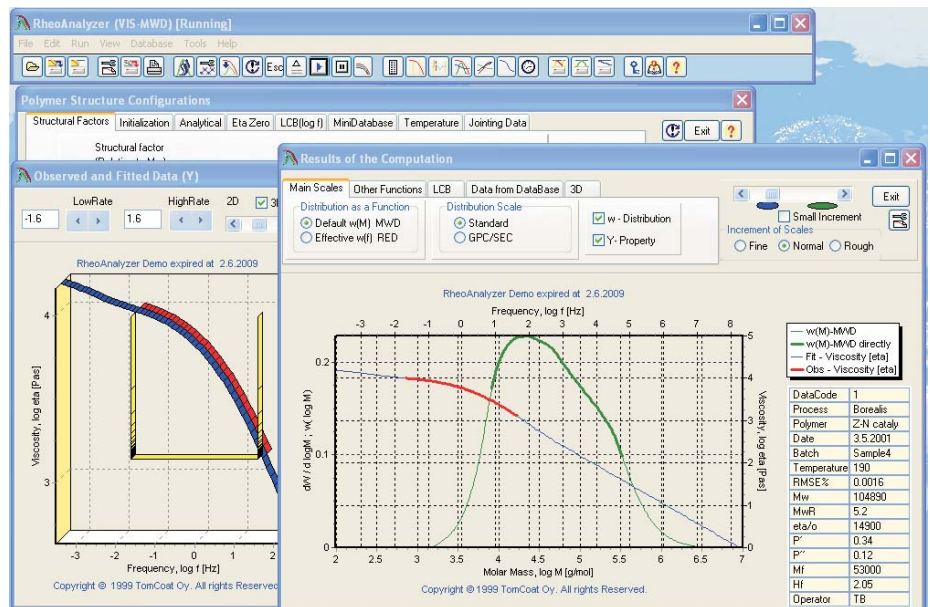
- * It is the fastest way to analyse viscoelastic material.
- * It accelerates your material development and design of polymerization, extrusion and injection moulding processes.
- * MWD (Molecular Weight Distribution) analyses and accurate wide viscoelastic fits are generated as viscosity, dynamic properties, relaxation modulus and transient effects even impossible to measure.
- * Impressive charts, research and new standpoints can be generated by the published principle starting on chain dimensions, Control Theory and new introduced RED (Rheologically Effective Distribution).
- * RED has similarities with the elugram of chromatogram technologies as GPC/SEC.

The software family

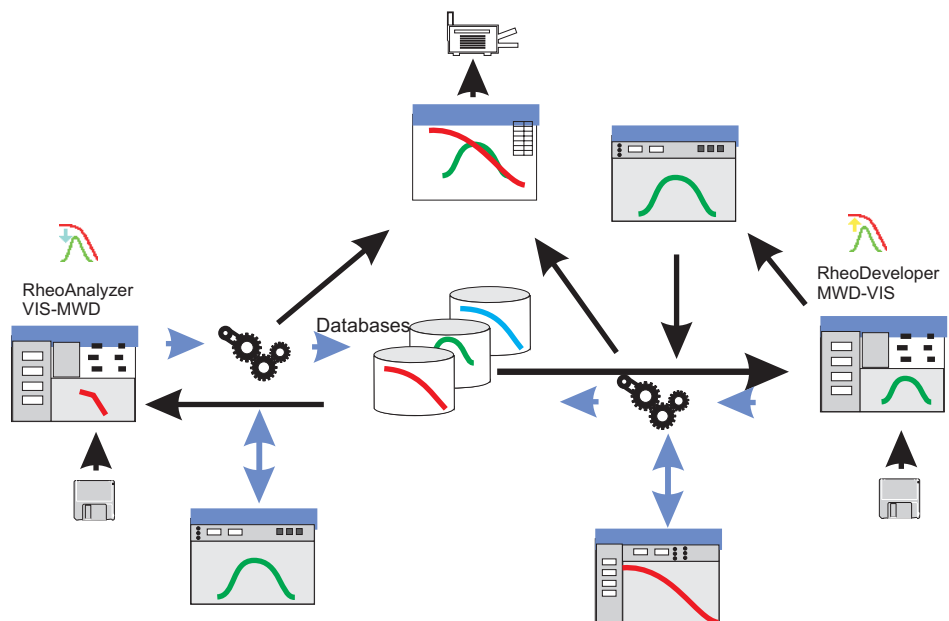
* RheoAnalyzer, RheoDeveloper and SQL database architecture present the backbone for the software family.

* The daily quality control at polymerization plants and design aid for new tailored polymers are given first consideration.

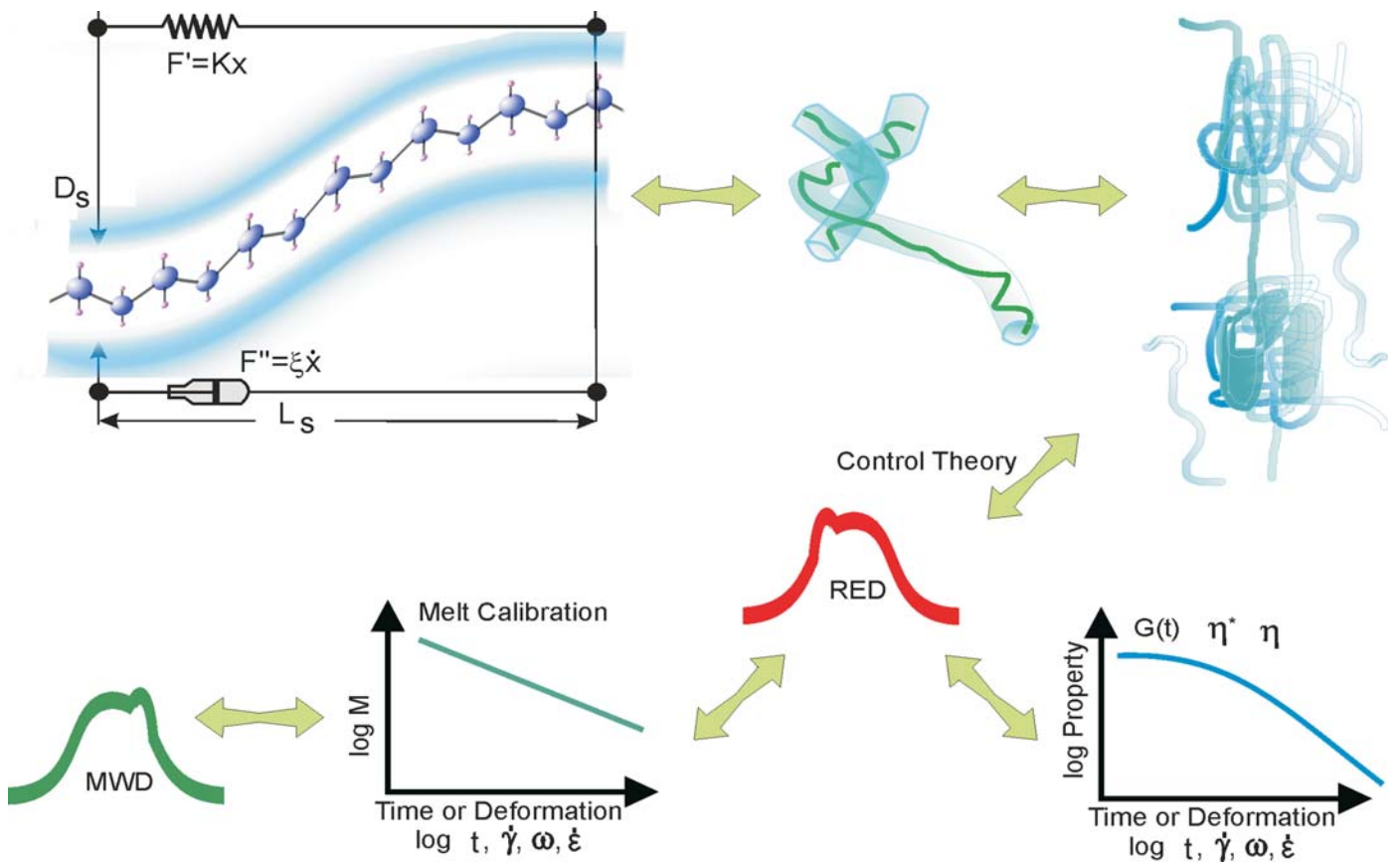
* Modern flexible technique offers scalability for special applications of new technologies.



The red measured viscosity function and yellow marked range in use. The blue fit viscosity function has a wider range. Also on right is shown the computation results as MWD and data label of polymer.



The RheoPower software family. RheoAnalyzer and RheoDeveloper programs are integrated by open SQL database architecture.



Graphical demonstration of the system by Control Theory and nanostructure model of polymer melt. Relative diameters of the statistical tube yields the correct Rheologically Effective Distribution (RED), which is converted to the MWD by melt calibration.

Benefits

You get more advantages at low cost not even possible to gain before.

The main features

Viscoelastic properties are modelled by the distributions related to the material structure. MWD and Rheologically Effective Distribution (RED) are converted from each other by melt calibration.

The principle

The *analytical* model is based on Control Theory of dynamic systems and fast *characteristic* model gives simple equations for a dynamic system. New melt calibration gives the relation between time, frequency and shear rate scales and the molecular

weight. This procedure has similarities with the chromatogram and elugram technologies.

Formulas join viscosity, modulus and other flow properties with polymer structure. The best proofs of the principle are computation results and published complete theory [1-5].

- [1] T. Borg, E. J. Pääkkönen, Linear viscoelastic models: Part I. Relaxation modulus and melt calibration, *J. Non-Newtonian Fluid Mech.* 156 (2009) 121-128.
- [2] T. Borg, E. J. Pääkkönen, Linear viscoelastic models: Part II. Recovery of the molecular weight distribution using viscosity data, *J. Non-Newtonian Fluid Mech.* 156 (2009) 129-138.
- [3] T. Borg, E. J. Pääkkönen, Linear viscoelastic models: Part III. Start-up and transient flow effects from the molecular weight distribution, *J. Non-Newtonian Fluid Mech.* 159 (2009) 17-25.
- [4] T. Borg, E. J. Pääkkönen, Linear viscoelastic models: Part IV. From molecular dynamics to temperature and viscoelastic relations using control theory, *J. Non-Newtonian Fluid Mech.*, 165 (2010) 2431.
- [5] T. Borg, E. J. Pääkkönen, Linear viscoelastic model for elongational viscosity by control theory, *Rheologica Acta*, (2011) Doi: 10.1007/s00397-011-0598-2.

The practice

RheoPower runs on 32-bit

and 64-bit Windows XP/Vista/7. Whilst the underlying principle is simple, the use of the numerically sensitive and labile recursive exponent formulas require accurate data together with fluent software to achieve high computing accuracy. Also datafiles can be used by DataPower Server.

Technical background

Modern principles and tools are used in numerical computation to maintain reasonable computation times. Software is applicable for the use of complex viscosity, shear viscosity, dynamic moduli and relaxation modulus, or extension, temperature and other time depend models.

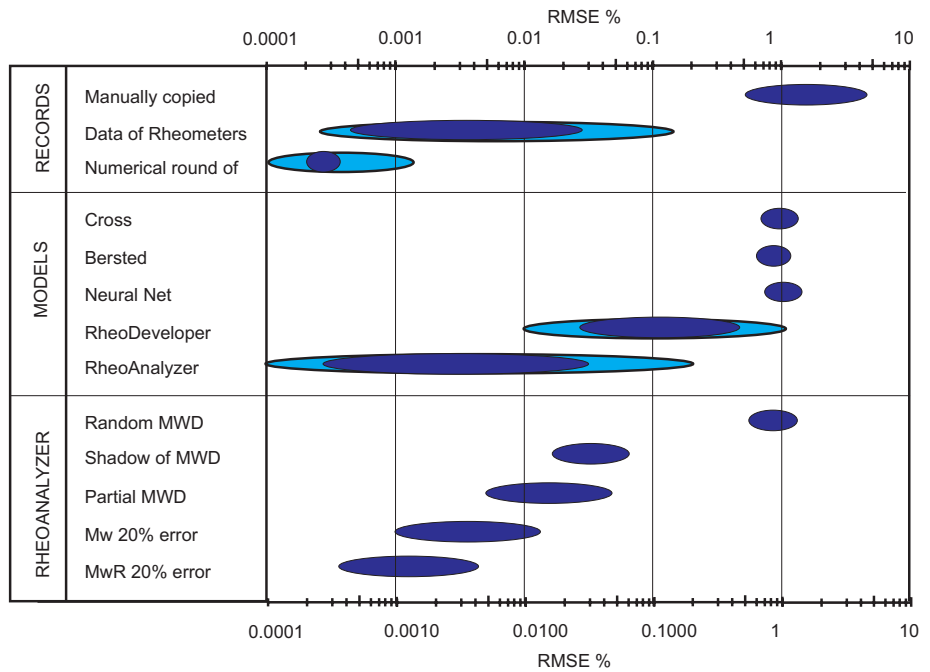
Accurate results

The quality of fit is evaluated by calculating the percent root mean square error %RMSE [1].

The data for Cross, Bersted and Neural Net models have the same source.

If data is relatively accurate, it is possible to find the MWD and other structure properties.

[1] S. A.de Vries, L. T. Kale, T. Oswald, and T. P. Karjala, "Molecular structure - Linear viscoelastic properties modelling for constrained geometry catalyst polyolefin resins", XIth Int. Cong. on Rheology, Quebec (1996).



The typical %RMSE-errors of different known models and computation levels of RheoAnalyzer.

New winds for measurements

The RheoAnalyzer shows relatively absolute error, by which is possible to develop measuring methods and customs.

Software can be very sensitive to some measuring methods, such as start-up procedures.

Applications

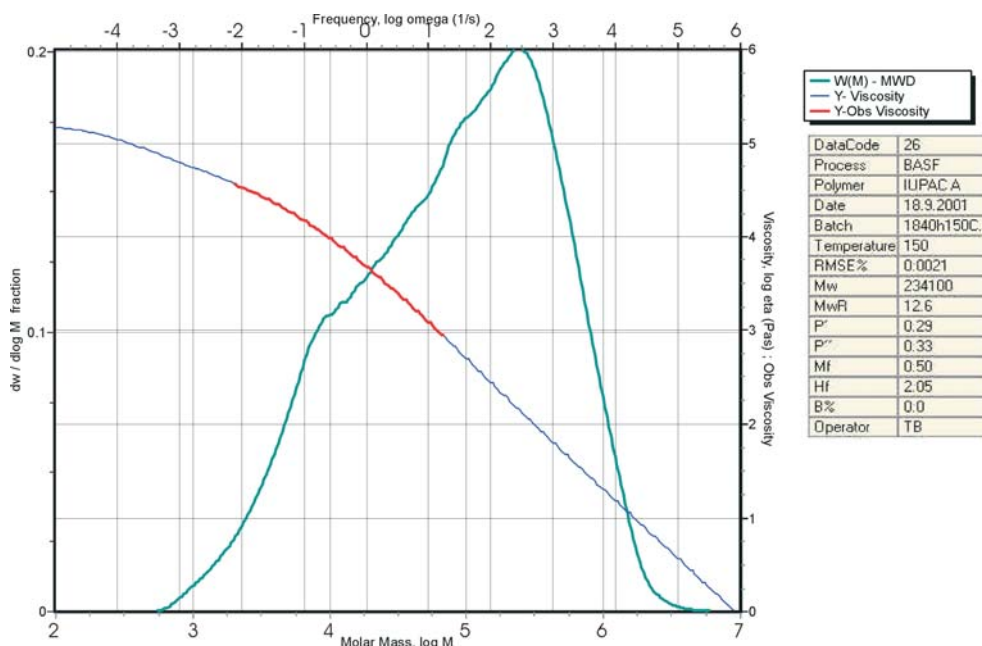
- * Control tool of polymerization can also be used with continuous on-line devices.
- * Easier to generate tailored polymers.
- * Design aid for extrusion dies and processes.

* Data feeder for injection mould design tools such as CAD/CFD software.

* General knowledge of relations and structure.

Top of iceberg

Shown properties are only a small portion of the system for additional different applications.



MWD of commercial Lupolen 1840H LDPE computed from viscosity data at 150°C provided by BASF. This material is the modern version from the classical IUPAC A LDPE.

Requirements for RheoAnalyzer

* Data in ASCII or IUPAC XML form of dynamic frequency sweep test (in energy, stress or strain controlled mode) or capillary data without Bagley or Rabinowitsch corrections.

* Optimally at log0.2 steps or more measured upwards.

* Already calibrated for PE, PP and PS and by customers for their own applications.

Requirements for RheoDeveloper

* P', P'', Mf and Hf values gained by RheoAnalyzer.

Performance of RheoAnalyzer

* MW distribution in respective data range and forecasts the forms in off-data areas.

* Wide range viscosity, relaxation modulus and spectrum by analytical and characteristic models.

* Additional new information of structure.

* At accurate data and frequency range $0.01/s < \omega < 100/s$ gives typically MWD's up to $MwR < 15$.

* Internal numerical error for viscosity fit typically $\%RMSE < 0.0002$. *For wider and not accurate data is needed to give priori knowledge about the MWD.*

System Requirements:

* Standard PC with Windows operating system.



RheoPower DataPower Software Packages

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RheoPower and DataPower Software packages for Polymerization, Extrusion and Injection Moulding business.

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Version 4.0

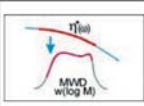
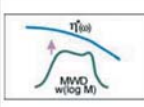

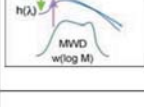

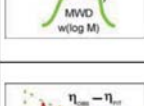

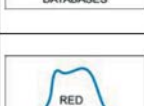
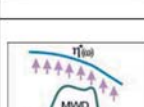
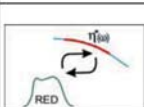
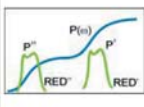

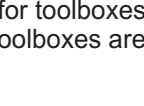
	RheoAnalyzer base module RheoAnalyzer (VIS-MWD) base module, databases for measured and computed data. Inputs: complex viscosity or storage and loss moduli. Outputs: MWD, wide viscosity fits and chart prints for results.	
	RheoDeveloper base module RheoDeveloper (MWD-VIS) base module, databases for measured and computed data. Inputs can be: MWD and complex viscosity data. Outputs are: wide viscosity fits and chart prints for results.	
	RheoPower Desktop Package RheoAnalyzer (VIS-MWD) and RheoDeveloper (MWD-VIS) base modules, databases for measured and computed data. Inputs can be: complex viscosity, storage and loss moduli and MWD data. Outputs are: MWD, wide viscosity fits and chart prints for results.	
	Relaxation Modulus and Spectrum Toolbox From MWD by control theory and using developed zero viscosity value for classical formula is generated relaxation modulus. By derivation is developed further wide relaxation spectrum. You can also import relaxation modulus data for MWD analyses.	A or D
	Exporting Results Toolbox Besides saving results on internal databases or printing charts, you can export dynamic and MWD results on ASCII *.txt files, to generate new *.xml files according to IUPAC XML standard or save charts and figures to *.wmf files.	A or D
	Drawing MWD Toolbox You can design own MWDs or piece of segments by a simple CAD drawing tool. On RheoDeveloper you can design complete MWDs and on RheoAnalyzer out of data range segments. Usable with developments of new polymers or mixtures.	A or D
	Error Chart This chart show absolute error between measured and modelled viscosity. Very usable for finding measurement error sources in developing data obtaining and recording routines.	A
	Complete DataBase System Must be with heavy using of software package. Gives possibilities to save on several databases and even by many users in intranet. It includes also MPDBAdmi and DataBase Desktop software programs. Developed for the use of polymerization plants, which are doing several analyses daily with several types of polymers.	A or D
	RED Distribution Rheologically Effective Distribution (RED) chart gives actually direct linear viscoelastic properties to the polymer melt and is related to the molecular weight distribution (MWD) by melt calibration. RED is essential in many polymer studies and mixtures of different chemical types.	A or D
	Analytical Model Toolbox Analytical formula of control theory is used for MWD (and RED) for computing wide viscosity fit curve and respective P' and P'' values.	A or D
	Best Fit (Go-Module) Toolbox This component finds best fit form of MWD by characteristic formula using least-square procedures between modelled and measured viscosity by comparing %RMSE values.	A
	Polymer Structure Function P and Orientation Function P is kernel of control theory for viscoelasticity. This chart toolbox shows the true core of the principle and is a fingerprint for behaviour of polymers. This function has important influence in modern polymer science and developments.	A or D
	RheoPower Premium Package This is complete collection of all earlier toolboxes and is designed for the use of polymerization plants or laboratories for daily use, but is usable for all kinds of polymer studies.	

Table shows partition of all packages and toolboxes available. Needed modules for toolboxes are: A = RheoAnalyzer and D = RheoDeveloper. Several additional toolboxes are ready for commercial process.