Propriétés des verres silicatés issues des bases de données et de la modélisation statistique

Exemple d'application : viscosité, Tg

Damien PERRET

CEA Marcoule ; DEN/DE2D/SEVT/LDMC

Atelier TherMatHT USTV, Marcoule
11/10/2019

TALK OBJECTIVES

Give researchers and engineers in glass science:

- A brief description of possible approaches for glass property modeling
- Basics on statistical modeling in formulation
  - Design of experiments, mixture designs
- Knowledge on database and Machine Learning for property prediction
  - Application example: viscosity and glass transition temperature prediction
- Information on where to find glass property data

Three approaches to model a property

- Theoretical, cognitive approach

Based on our intrinsic knowledge of the phenomenon, on the fundamental laws of physics and chemistry (conservation of energy, momentum, equations of diffusion, thermodynamics,…)

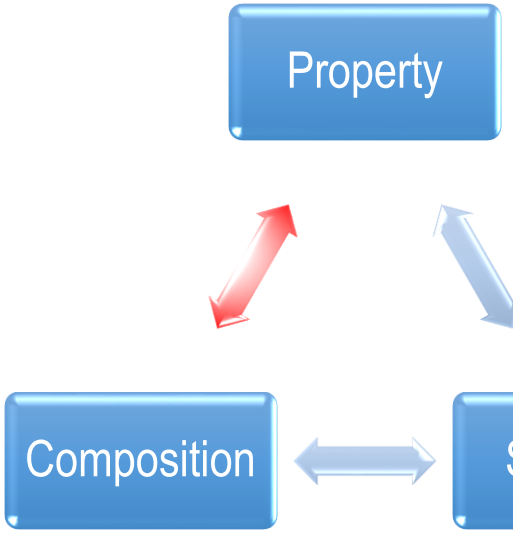
- Empirical approach

Based on a set of experimental data (*data-driven* models). Mathematical, statistical approach, which ignores any physicochemical knowledge of the phenomenon

- Mixed approach

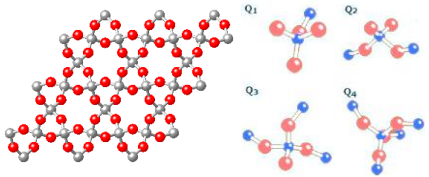
Combination of the two previous approaches

- For these three classes of models, there are different types: linear or non-linear, static or dynamic, deterministic or stochastic, continuous or discrete,…



- Physical properties: viscosity, density, Tg, electrical conductivity,…
- Optical properties
- Chemical durability
- Glass homogeneity
- …

Oxides	Composition (wt. (%))SiO_2
SiO_2	59.39
Al_2O_3	13.57
ZrO_2	15.61
Li_2O	8.64
K_2O	0.31
Na_2O	0.70
TiO_2	0.09
Fe_2O_3	0.22
CaO	0.62
P_2O_5	0.82



Available resources in glass science and technology

- First attempt for the calculation of glass properties from their composition proposed by Winckelmann and Schott at the end of the 19th century
- Monograph by Volf in 1988 that describes best known methods [1]
- Since 1988 methods have been proposed for viscosity calculation (Lakatos, Lyon, Mazurin, Hrma, Priven, Okhotin, Fluegel,…)

[1] M.B. Volf, *Mathematical approach to glass*, Elsevier Science Publishers, Amsterdam (1988)

Theoretical Principle of Additivity

M.B. Volf, *Mathematical Approach to Glass*, Elsevier Science Publishiers, 1988

- If glass were a simple mixture of the individual oxides, the **additive equation** would be generally valid:

$$G = \sum g(G)_i \, x_i$$

G is the property of the glass
$g(G)_i$ is the additive factor for oxide i and property G
x_i is the amount of oxide i

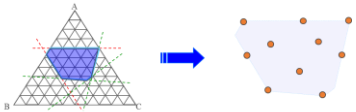
- But glass is not a mixture of oxides... Errors in additive calculation could be due to the degree of cross-linking, anomalies in the cross-linked structure, phase separation, interaction between ions,…
- However, on investigating a suitably narrow composition range, where the more complex interactions can be neglected, **one can express the effect of the individual components on a certain property by the additive equation.**

Two strategies for statistical property modeling

- Design of Experiments
- Database and Machine Learning

Two strategies for statistical property modeling

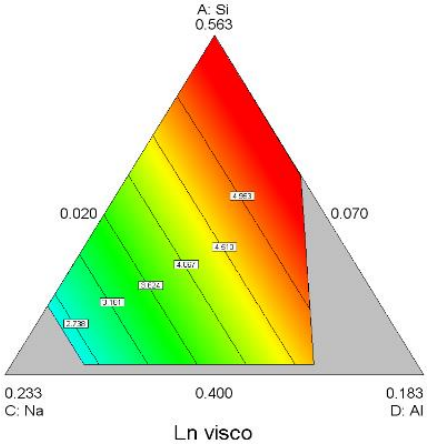
- Design of Experiments
  - Models based on the additivity equation $\hat{y}_i = \sum_{i=1}^{q} a_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} a_{ij} x_i x_j$
  - Very robust on *small* domains of composition
  - Key points:
    - Domain boundaries definition
    - Definition of the optimal number of runs
    - Model fit – avoid overfitting
    - Model validation

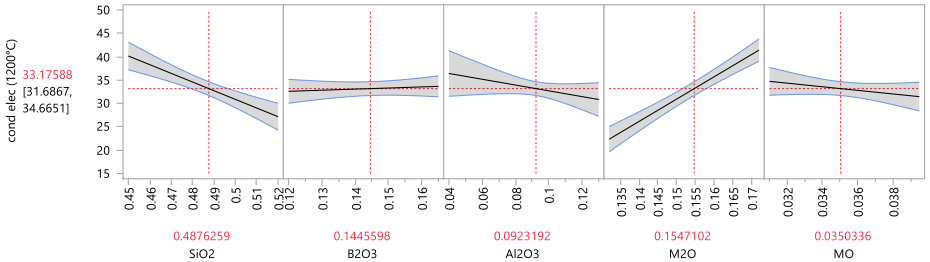


  - Nice examples in nuclear glass formulation: viscosity, electrical conductivity, density, initial rate of dissolution

Two strategies for statistical property modeling

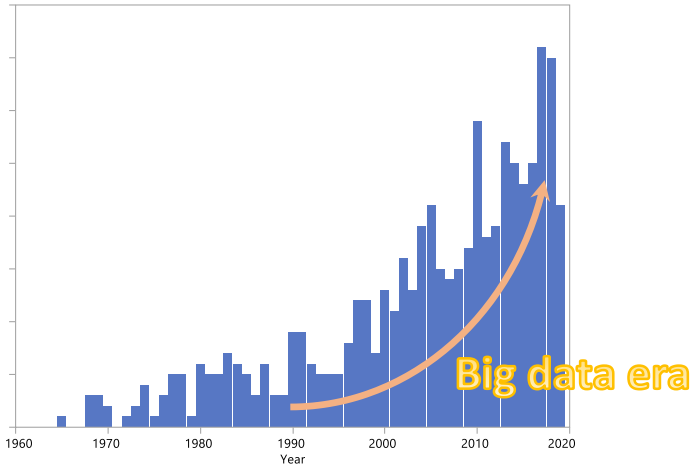
- Design of Experiments



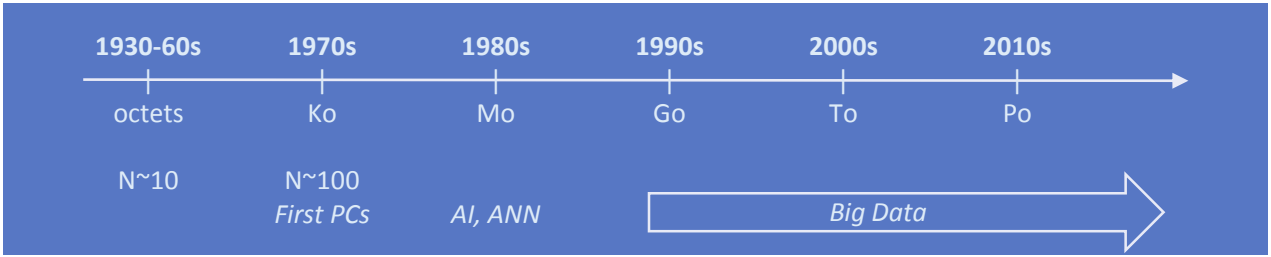


- Database and Machine Learning

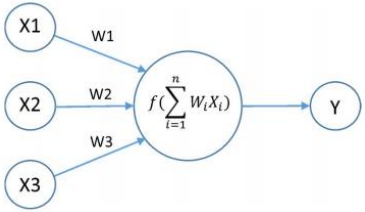
Published literature in the field of glass property prediction

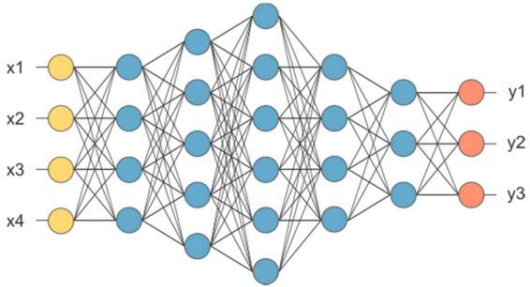


From Web of Science
« glass » and « prediction » in publication title



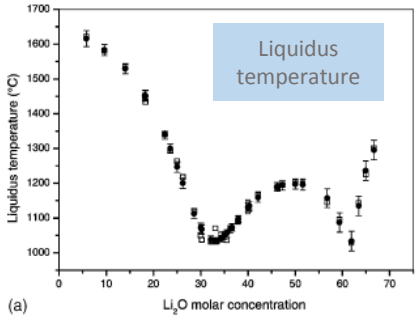
- Machine learning has seen growing application in material property determination
- Artificial Neural Networks (ANN) use interconnected mathematical nodes, or neurons, to form a network that can model complex functional relationships



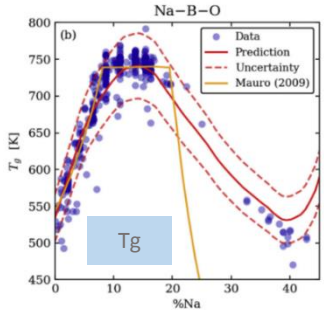


- This technique is particularly suited to problems that involve the manipulation of multiple parameters and non-linear interpolation

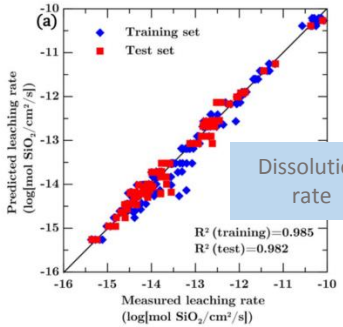
Examples of NN application to glass property prediction



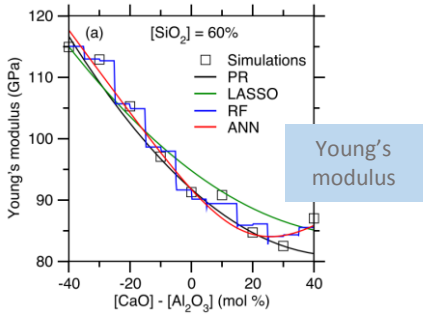
C. Dreyfus, G. Dreyfus / Journal of Non-Crystalline Solids 318 (2003) 63–78



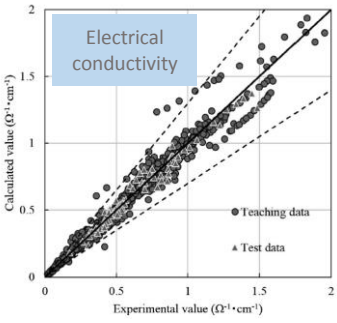
D.R. Cassar et al., Acta Materiala, 159 249-256 (2018)



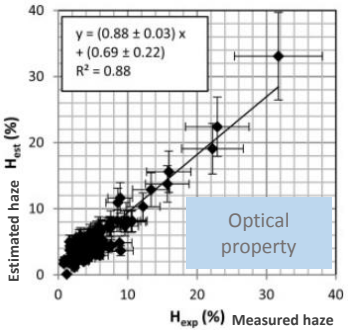
N.M. Anoop Krishnan et al.
Journal of Non-Crystalline Solids 487 (2018) 37–45



K. Yang et al.., Scientific Reports, 8739, 9 (2019)



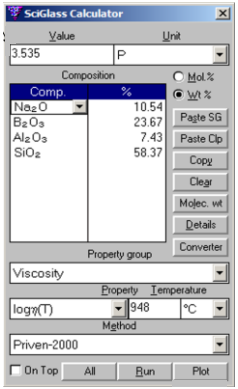
Y. Haraguchi et al., ISIJ International, Vol. 58 (2018), No. 6, pp. 1007–1012

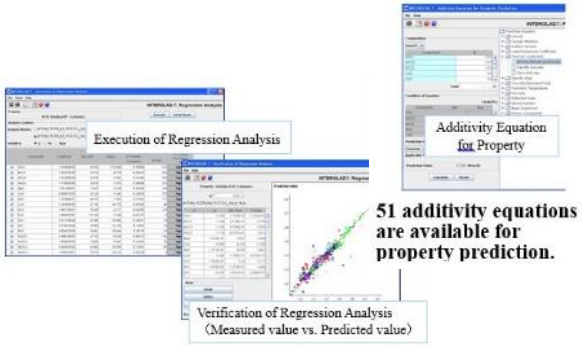


A. Verney-Caron et al., Atmospheric Environment, 54 141-148 (2012)

Available resources in glass science and technology

- SciGlass and Interglad Information Systems
  - Data collected from the published literature
  - Embedded property calculation tools
  - More than 300 000 glasses





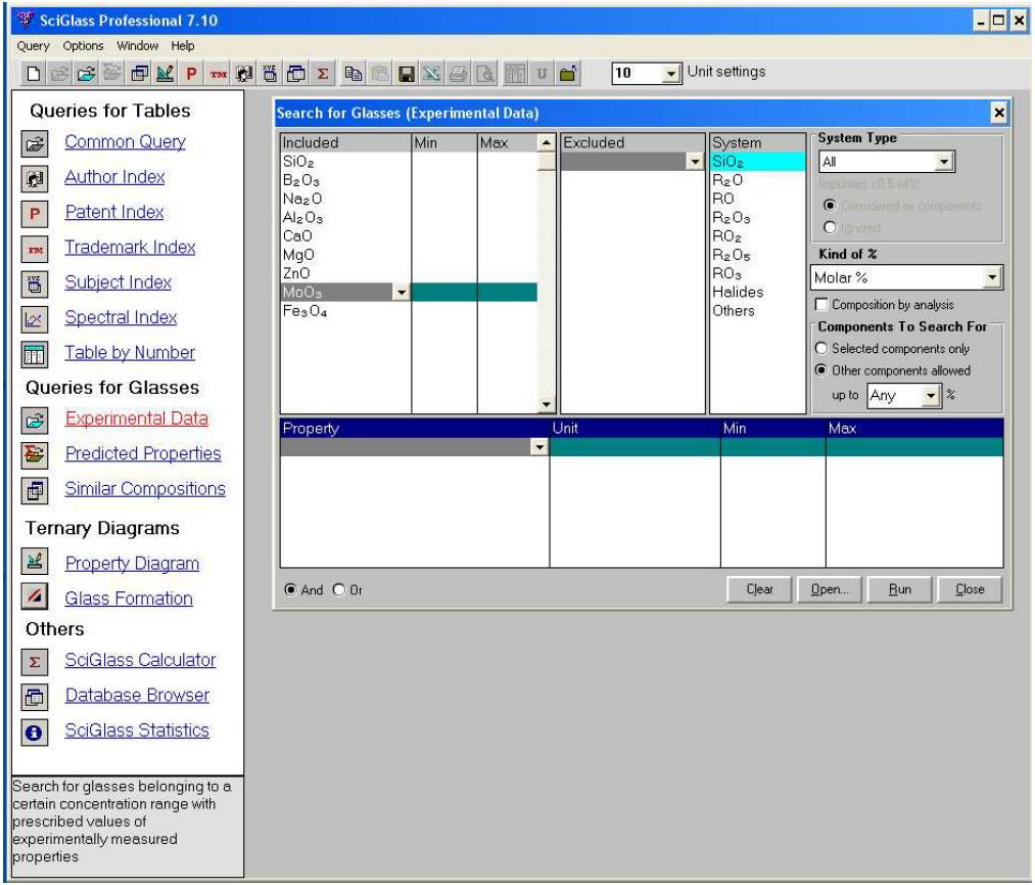
			Count
Number of glasses			374 405
By Number of Components			
	One-component		4 785
	Binary		64 689
	Ternary		156 401
	Four-component		46 658
	Others		101 872
By Systems			
	Oxide		278 477
		Silicate (>=45 mol.% SiO_2)	115 423
		Borate (>=45 mol.% B_2O_3)	37 158
		Germanate (>=45 mol.% GeO_2)	10 558
		Phosphate (>=40 mol.% P_2O_5)	23 334
		Tellurite (>=30 mol.% TeO_2)	17 004
	Halide		17 137
	Chalcogenide		37 460

By Properties	Count
Acoustical properties	282
Chemical durability	34 290
Crystallization	26 577
Density	82 459
Density at 20°C	77 133
Density at 800°C	772
Density at 1000°C	1 066
Density at 1200°C	837
Density at 1400°C	987
Molar/spec. volume at 20°C	77 133
Dielectric properties	11 219
Diff., permeat., & solub. of gases	2 120
Elastic properties	14 748
Electrical resistivity	42 490
logr at 20°C	14 767
logr at 100°C	14 361
logr at 150°C	15 256
logr at 300°C	12 058
logr at 800°C	2 072
logr at 1000°C	2 632
logr at 1200°C	2 227
logr at 1400°C	2 218
TK-100	12 934
Glass formation	74 081

By Properties	Count
Heat capacity	3 357
C_p at 20°C	926
C_p at 200°C	675
C_p at 400°C	511
C_p at 800°C	320
C_p at 1000°C	201
C_p at 1200°C	186
C_p at 1400°C	140
Internal friction	1 499
Ion diffusion	2 090
M_g	18 040
Magnetic properties	4 725
Microhardness	13 746
Optical properties	71 613
Stress-optic coef.	1 231
Strength	3 663
Surface tension	5 128
s at $T>T_g$	4 318
s at 900°C	771
s at 1200°C	951
s at 1300°C	1 384
s at 1400°C	830
T_{liq}	53 517
T_g	74 759
Thermal expansion coefficient	57 975
Thermal conductivity	1 700
Thermal diffusivity	901
Thermal endurance	1 117

	Count
Visc. standard points	17 542
Littleton Point	3 771
Annealing Point	3 907
Strain Point	5 948
Softening Point	7 763
Viscosity	37 205
T_1 (log[h,P]=1)	4 377
T_2 (log[h,P]=2)	5 653
T_3 (log[h,P]=3)	10 247
T_4 (log[h,P]=4)	9 746
T_5 (log[h,P]=5)	5 673
T_6 (log[h,P]=6)	5 260
T_7 (log[h,P]=7)	4 911
T_8 (log[h,P]=8)	5 236
T_9 (log[h,P]=9)	5 495
T_{10} (log[h,P]=10)	6 044
T_{11} (log[h,P]=11)	6 512
T_{12} (log[h,P]=12)	6 330
T_{13} (log[h,P]=13)	5 141

	Count
Viscosity	37 205
logh at 500°C	2 128
logh at 600°C	3 681
logh at 700°C	4 006
logh at 800°C	4 409
logh at 900°C	4 937
logh at 1000°C	5 403
logh at 1100°C	6 147
logh at 1200°C	7 424
logh at 1300°C	8 383
logh at 1400°C	8 831
logh at 1500°C	7 169
logh at 1600°C	3 703
logh at 1700°C	1 019
logh at 1800°C	396
logh at 2000°C	144
logh at 2200°C	44
logh at 2500°C	11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10 Unit settings
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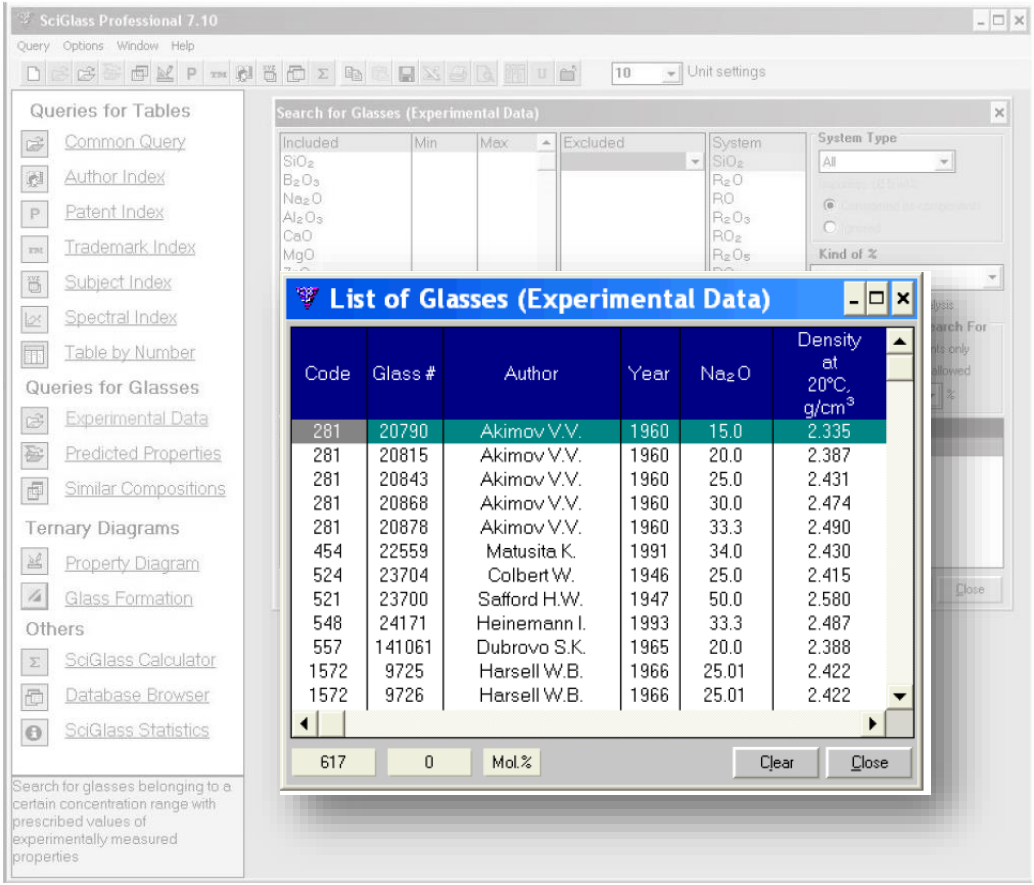
Common Query
Author Index
Patent Index
Trademark Index
Subject Index
Spectral Index
Table by Number
Queries for Glasses
Experimental Data
Predicted Properties
Similar Compositions
Ternary Diagrams
Property Diagram
Glass Formation
Others
SciGlass Calculator
Database Browser
SciGlass Statistics
Search for glasses belonging to a certain concentration range with prescribed values of experimentally measured properties
Search for Glasses (Experimental Data)
Included Min Max
SiO2
B2O3
Na2O
Al2O3
CaO
MgO
ZnO
MoO3
Fe3O4
Excluded
System
SiO2
R2O
RO
R2O3
RO2
R2O5
RO3
Halides
Others
System Type
All
Kind of %
Molar %
Composition by analysis
Components To Search For
Selected components only
Other components allowed
up to Any %
Property Unit Min Max
And Or
Clear Open... Run Close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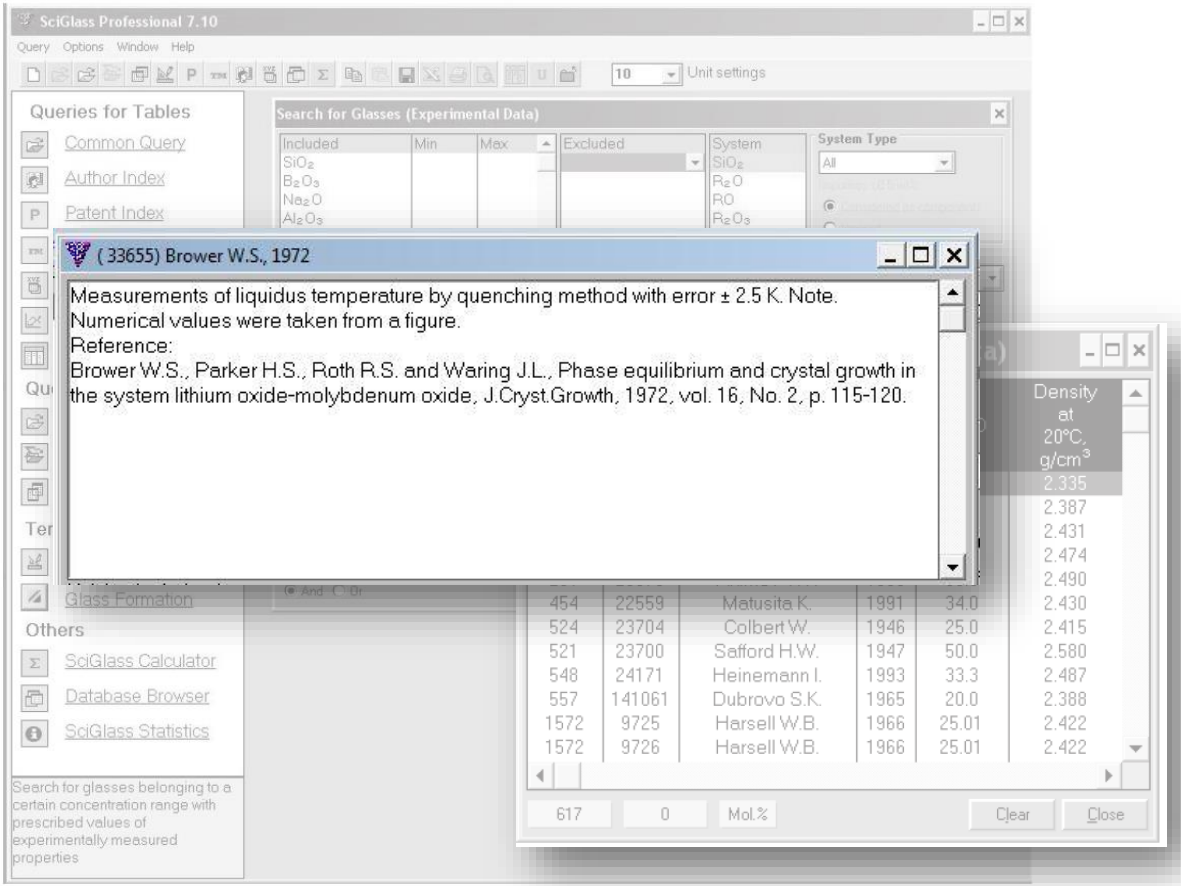
Search for glasses belonging to a certain concentration range with prescribed values of experimentally measured properties
Search for Glasses (Experimental Data)
Included
Min
Max
Excluded
System
System Type
Kind of %
List of Glasses (Experimental Data)
Code
Glass #
Author
Year
Na2O
Density at 20°C, g/cm3
281 20790 Akimov V.V. 1960 15.0 2.335
281 20815 Akimov V.V. 1960 20.0 2.387
281 20843 Akimov V.V. 1960 25.0 2.431
281 20868 Akimov V.V. 1960 30.0 2.474
281 20878 Akimov V.V. 1960 33.3 2.490
454 22559 Matusita K. 1991 34.0 2.430
524 23704 Colbert W. 1946 25.0 2.415
521 23700 Safford H.W. 1947 50.0 2.580
548 24171 Heinemann I. 1993 33.3 2.487
557 141061 Dubrovo S.K. 1965 20.0 2.388
1572 9725 Harsell W.B. 1966 25.01 2.422
1572 9726 Harsell W.B. 1966 25.01 2.422
617
0
Mol.%
Clear
Close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Others
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SciGlass Statistics
Search for glasses belonging to a certain concentration range with prescribed values of experimentally measured properties
Search for Glasses (Experimental Data)
Included
Min
Max
Excluded
System
System Type
(33655) Brower W.S., 1972
Measurements of liquidus temperature by quenching method with error ± 2.5 K. Note.
Numerical values were taken from a figure.
Reference:
Brower W.S., Parker H.S., Roth R.S. and Waring J.L., Phase equilibrium and crystal growth in the system lithium oxide-molybdenum oxide, J.Cryst.Growth, 1972, vol. 16, No. 2, p. 115-120.
Density at 20°C, g/cm3
454 22559 Matusita K. 1991 34.0 2.430
524 23704 Colbert W. 1946 25.0 2.415
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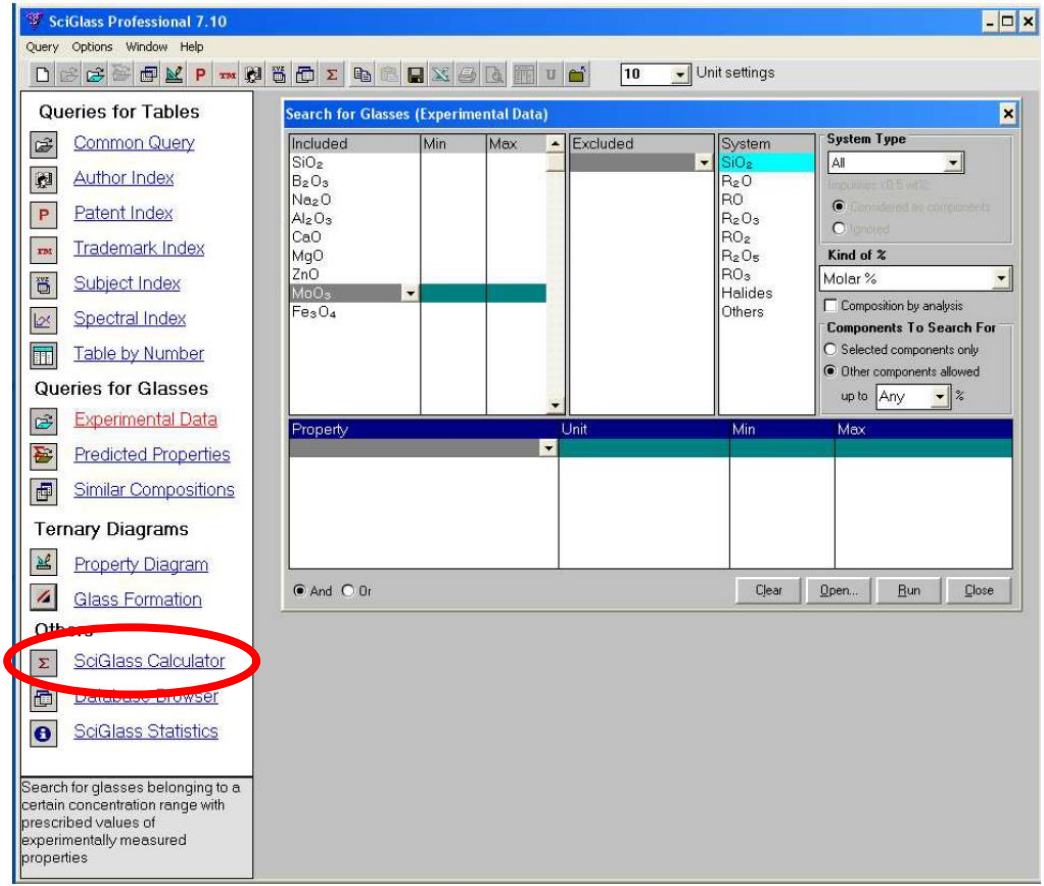
617
0
Mol.%
Clear
Close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System
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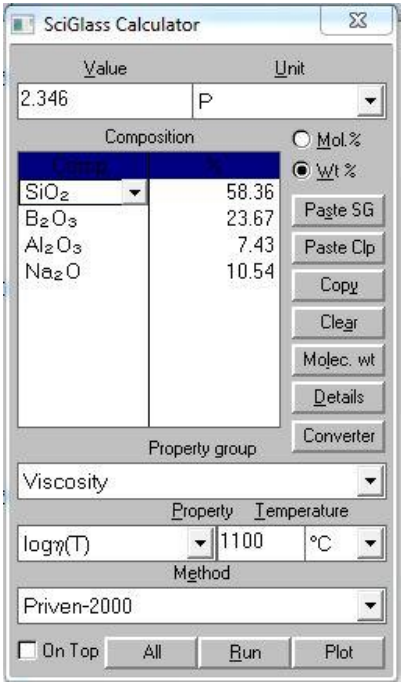
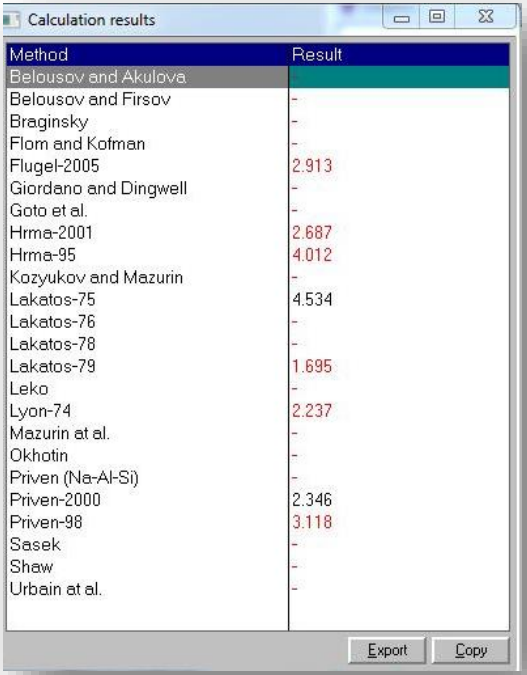
RO
R2O3
RO2
R2O5
RO3
Halides
Others
System Type
All
Considered as components
Ignored
Kind of %
Molar %
Composition by analysis
Components To Search For
Selected components only
Other components allowed
up to Any %
Property Unit Min Max
And Or
Clear Open... Run Close


SciGlass Calculator
Value
Unit
2.346
P
Composition
Mol.%
Wt %
Comp.
%
SiO2
58.36
B2O3
23.67
Al2O3
7.43
Na2O
10.54
Paste SG
Paste Clp
Copy
Clear
Molec. wt
Details
Converter
Property group
Viscosity
Property
Temperature
logγ(T)
1100
°C
Method
Priven-2000
On Top
All
Run
Plot


Calculation results
Method
Result
Belousov and Akulova
Belousov and Firsov -
Braginsky -
Flom and Kofman -
Flugel-2005 2.913
Giordano and Dingwell -
Goto et al. -
Hrma-2001 2.687
Hrma-95 4.012
Kozyukov and Mazurin -
Lakatos-75 4.534
Lakatos-76 -
Lakatos-78 -
Lakatos-79 1.695
Leko -
Lyon-74 2.237
Mazurin at al. -
Okhotin -
Priven (Na-Al-Si) -
Priven-2000 2.346
Priven-98 3.118
Sasek -
Shaw -
Urbain at al. -
Export
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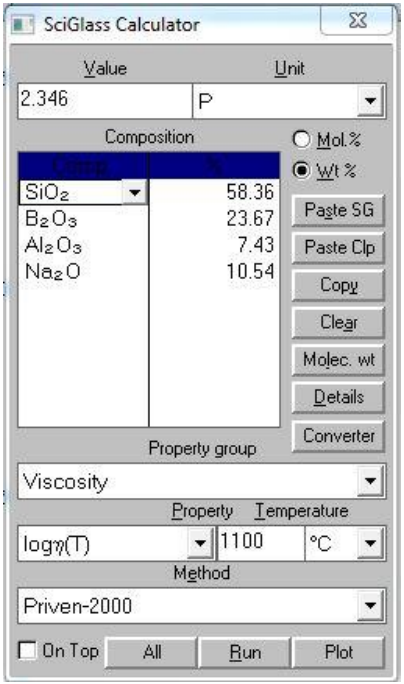
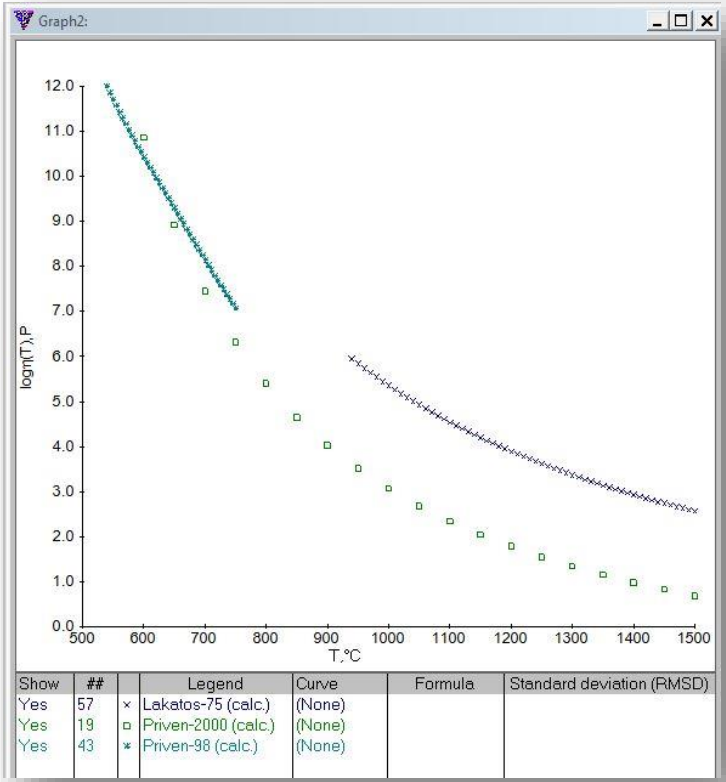
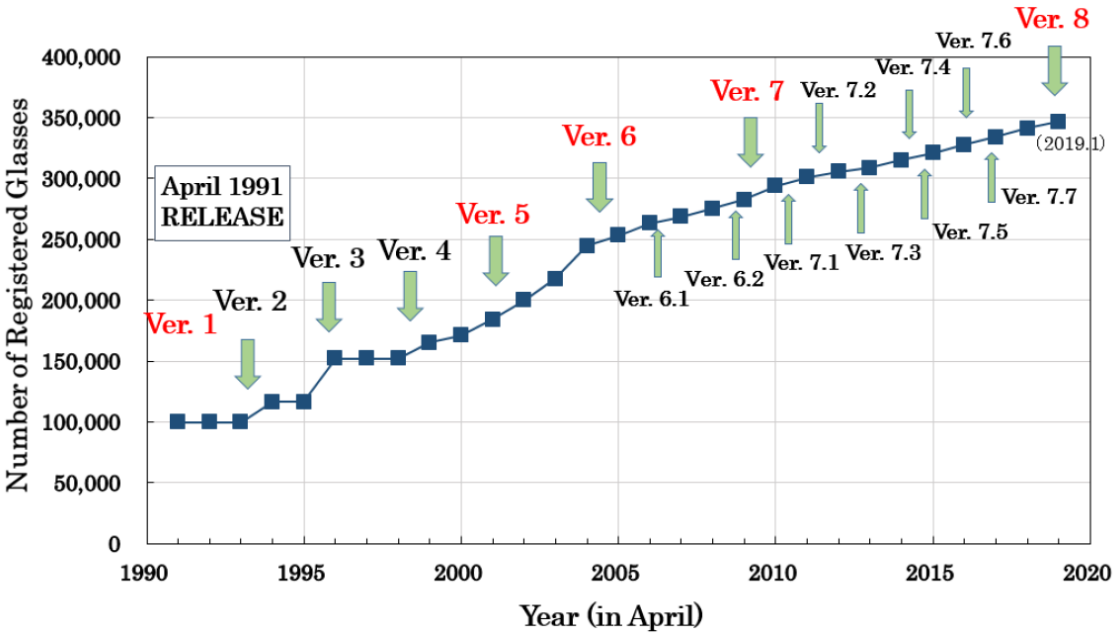
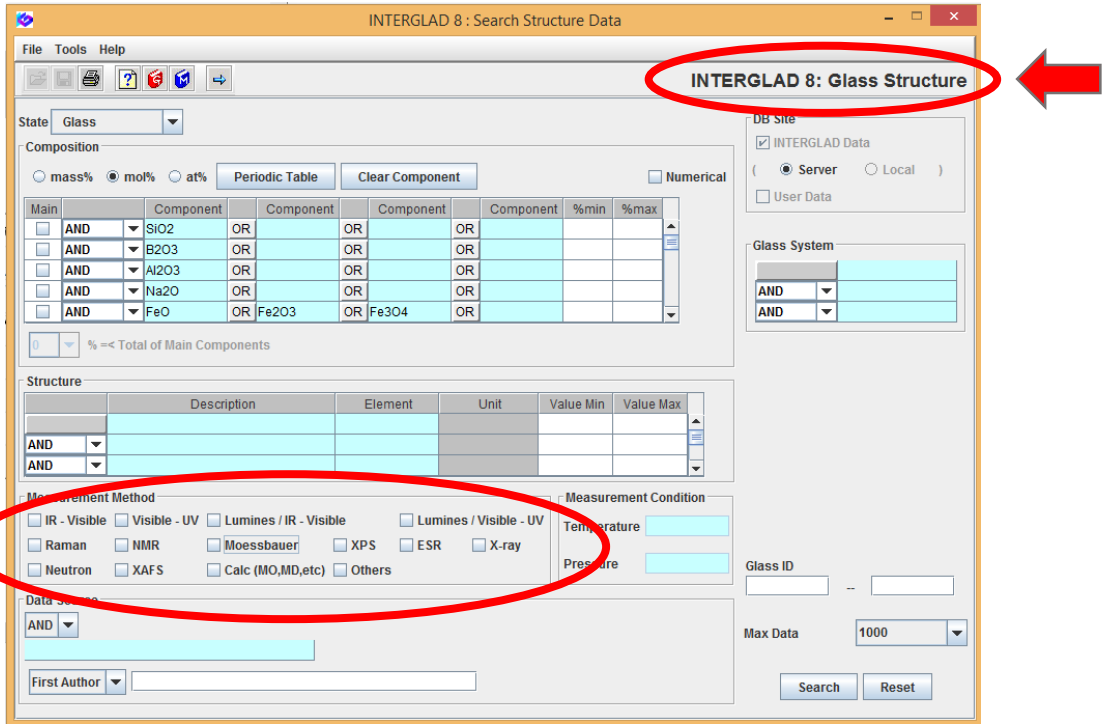

SciGlass Calculator
Value
Unit
2.346
P
Composition
Mol.%
Wt %
Comp.
%
SiO2
58.36
B2O3
23.67
Al2O3
7.43
Na2O
10.54
Paste SG
Paste Clp
Copy
Clear
Molec. wt
Details
Converter
Property group
Viscosity
Property
Temperature
logγ(T)
1100
°C
Method
Priven-2000
On Top
All
Run
Plot


Graph2:
logη(T),P
T,°C
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
500
600
700
800
900
1000
1100
1200
1300
1400
1500
Show
##
Legend
Curve
Formula
Standard deviation (RMSD)
Yes 57 Lakatos-75 (calc.) (None)
Yes 19 Priven-2000 (calc.) (None)
Yes 43 Priven-98 (calc.) (None)

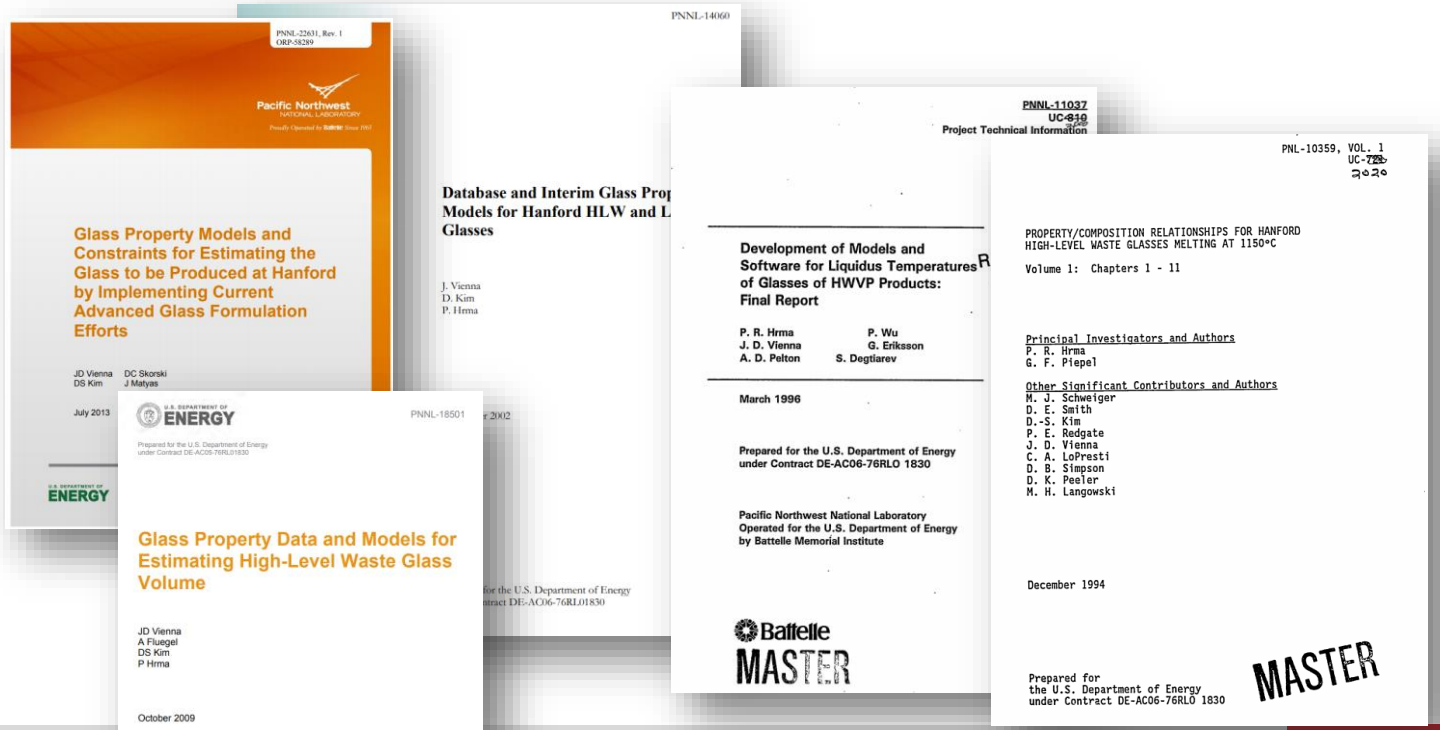

Number of Registered Glasses
400,000
350,000
300,000
250,000
200,000
150,000
100,000
50,000
0
1990
1995
2000
2005
2010
2015
2020
Year (in April)
April 1991
RELEASE
Ver. 1
Ver. 2
Ver. 3
Ver. 4
Ver. 5
Ver. 6
Ver. 6.1
Ver. 6.2
Ver. 7
Ver. 7.1
Ver. 7.2
Ver. 7.3
Ver. 7.4
Ver. 7.5
Ver. 7.6
Ver. 7.7
Ver. 8
(2019.1)

INTERGLAD Information System



Available resources for nuclear glass property data

- Published reports from Pacific Northwest National Laboratory (PNNL)



Big Data vs. Good Data

- Statistical modeling requires highly reliable experimental data
- Unfortunately the quality of published data differs from each other greatly

O.V. Mazurin / Journal of Non-Crystalline Solids 351 (2005) 1103–1112

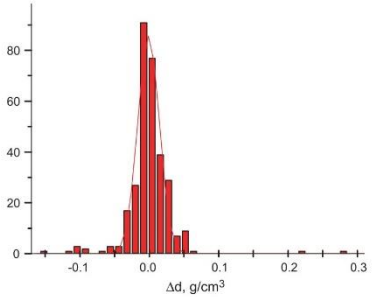


Fig. 2. A histogram of the differences between the values calculated by the equation describing the approximating curve in Fig. 1 and experimental values of density of sodium borate glasses. The solid line is the Gaussian approximation of the presented data.

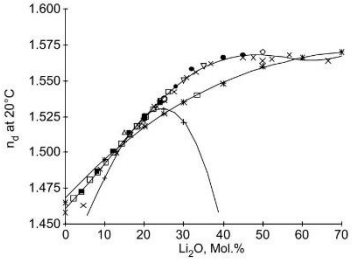


Fig. 8. Comparison of the curves approximating the composition dependencies of the refractive index for binary lithium borate glasses according to the data published by Conzone et al. [9] and Lorosch et al. [14] with the curve approximating the results for sets of data taken from papers published earlier [10–13]. (+): data by Conzone; (*): data by Lorosch.

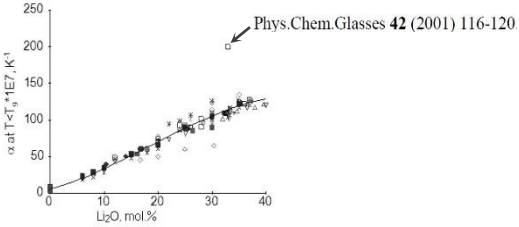


Fig.2. Thermal expansion coefficient of solid lithium silicate glasses

Big Data vs. Good Data

- Statistical modeling requires highly reliable experimental data
- Unfortunately the quality of published data differs from each other greatly

O.V. Mazurin / Journal of Non-Crystalline Solids 351 (2005) 1103–1112

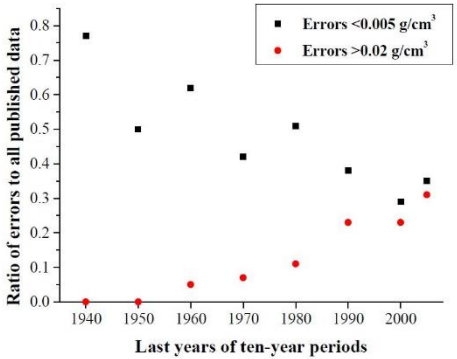


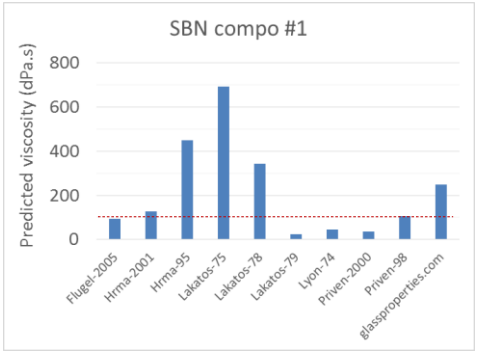
Table 3. Changes in number of co-authors of papers

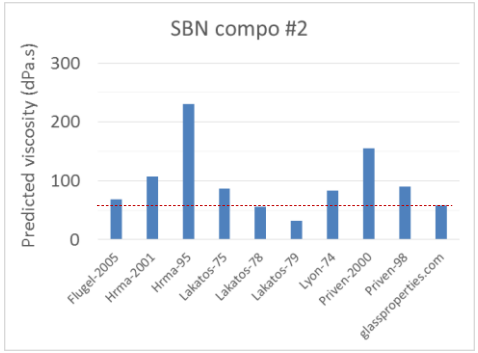
Year	1930	1950	1975	2000
Average number of co-authors	1.6	1.6	2.8	3.1
Maximal number of co-authors	4	4	9	10

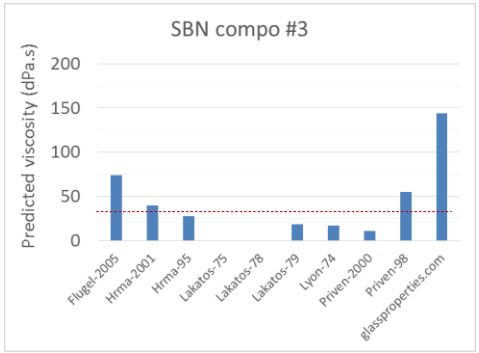
Viscosity prediction

Viscosity is a property which is difficult to calculate

- Example : Prediction using well-known literature models (from SciGlass) on simple SBN glass (1200°C)



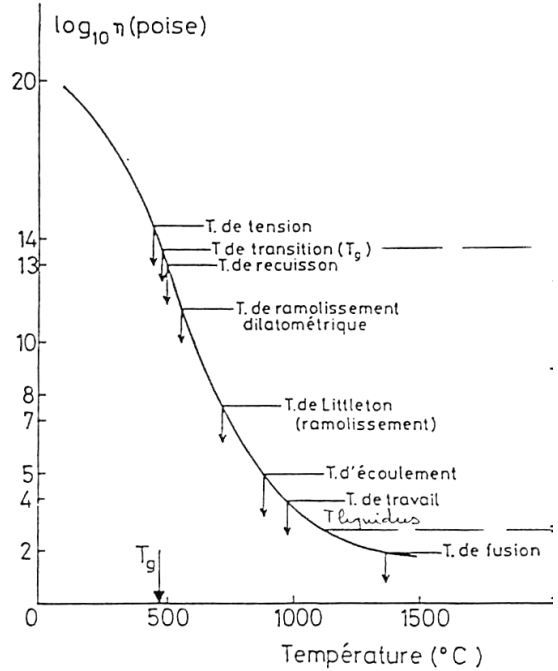




Measured

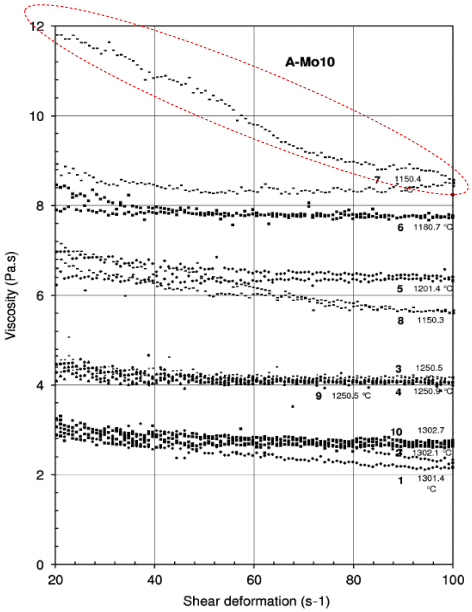
- Motivation for developing internal prediction tool

- Range of viscosity values is very wide vs temperature and vs composition



- Viscosity temperature dependence is highly sensitive to phase separation and crystallization

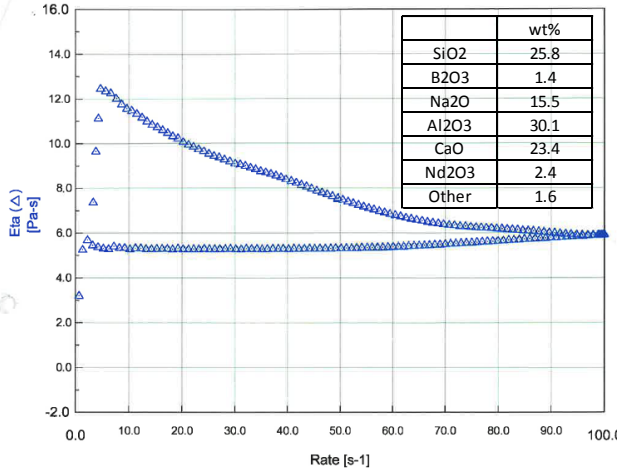
Phase separation



Oxide mol%	AMo10 batch no. 5052
SiO_2	46.5
Na_2O	11.0
B_2O_3	14.4
Li_2O	0.2
CaO	7.9
MoO_3	5.1
P_2O_5	1.6
Al_2O_3	5.4
ZnO	5.4
ZrO_2	2.0
Nd_2O_3	0.2
Minors	0.3
Sum	100.0

J. Am. Ceram. Soc., **94** [2] 447–454 (2011) –*Schuller et al.*

Crystallization



	wt%
SiO2	25.8
B2O3	1.4
Na2O	15.5
Al2O3	30.1
CaO	23.4
Nd2O3	2.4
Other	1.6

Our viscosity database

- Internal CEA database

(mainly borosilicate glass)

- SciGlass and Interglad Information Systems

(all types of glass)

- Pacific Northwest National Laboratory database

(borosilicate glass) *Grateful acknowledgement to J. Vienna from PNNL*

- About 16,000 data of composition and viscosity
- Temperature range: 900-1500°C

General database

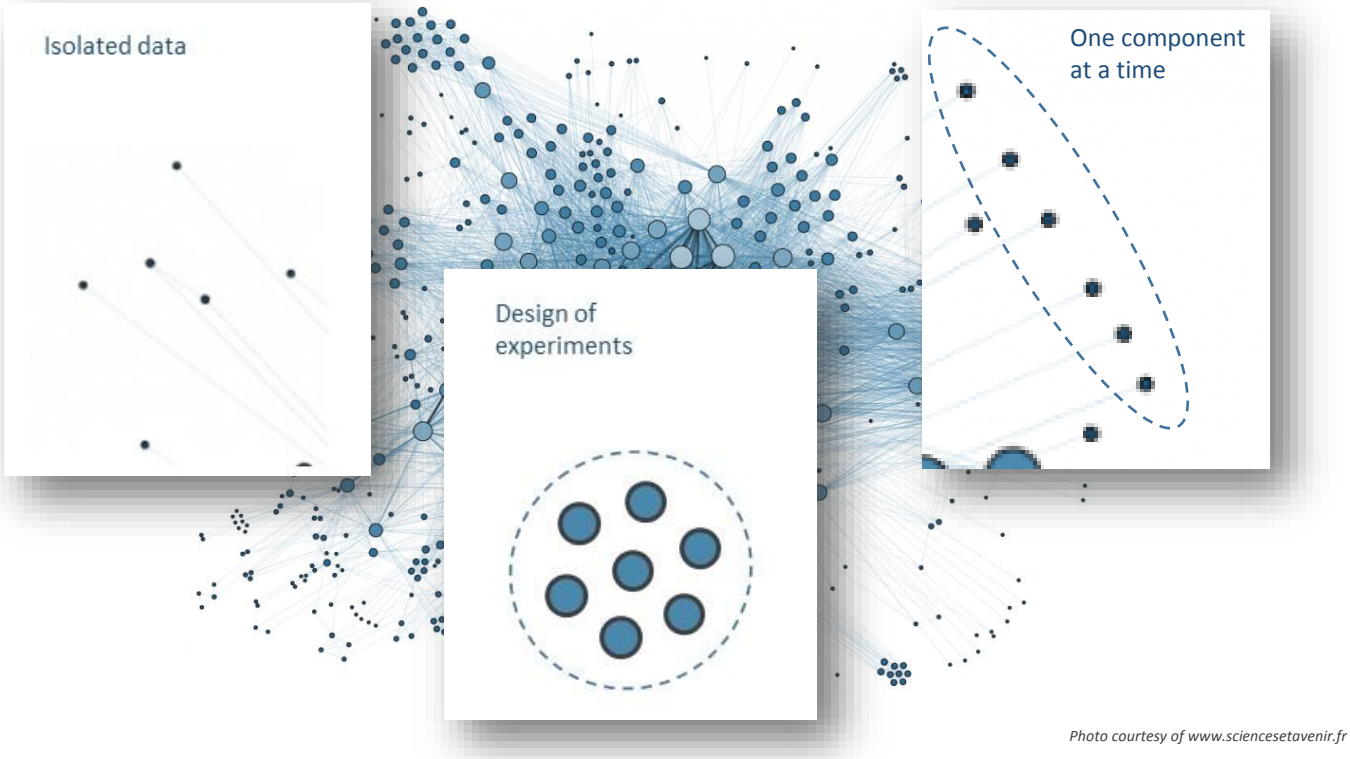
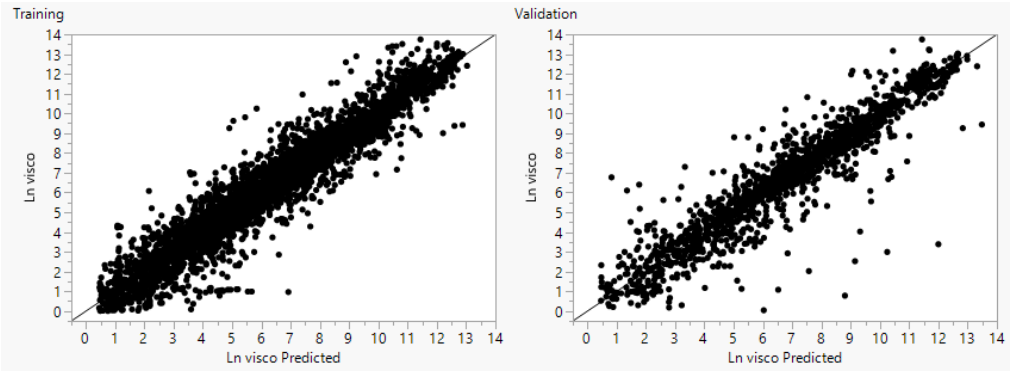


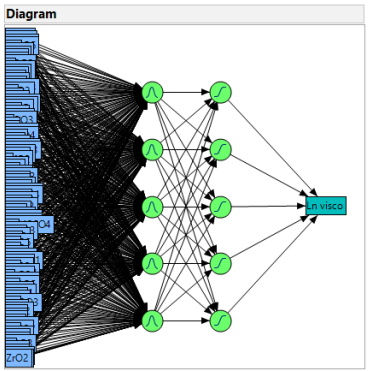
Photo courtesy of www.sciencesetavenir.fr

What we learnt from the past

- We applied several machine learning techniques to build viscosity models (neural nets, boosted tree, random forest,…)
- The **whole database** (about 16,000 data) was considered and partitioned into training set and validation set
- But at the end, **no statistical model** with acceptable predictive capability was found to predict the viscosity

- NN are unable to predict efficiently glass viscosity on big database…





Training

Ln visco	
Measures	**Value**
RSquare	0.9287269
RMSE	0.7518628
Mean Abs Dev	0.496624
-LogLikelihood	6435.0916
SSE	3208.6293
Sum Freq	5676

Validation

Ln visco	
Measures	**Value**
RSquare	0.8822247
RMSE	0.9682362
Mean Abs Dev	0.5912263
-LogLikelihood	2545.9066
SSE	1721.2158
Sum Freq	1836

Dynamic and *automatic* dataset for model training

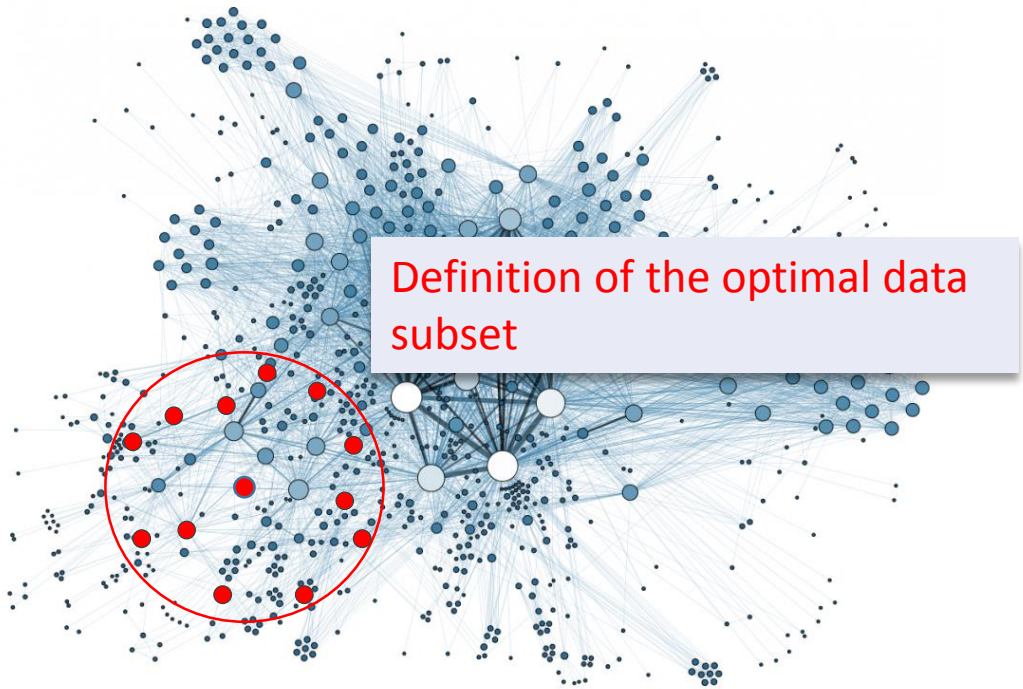
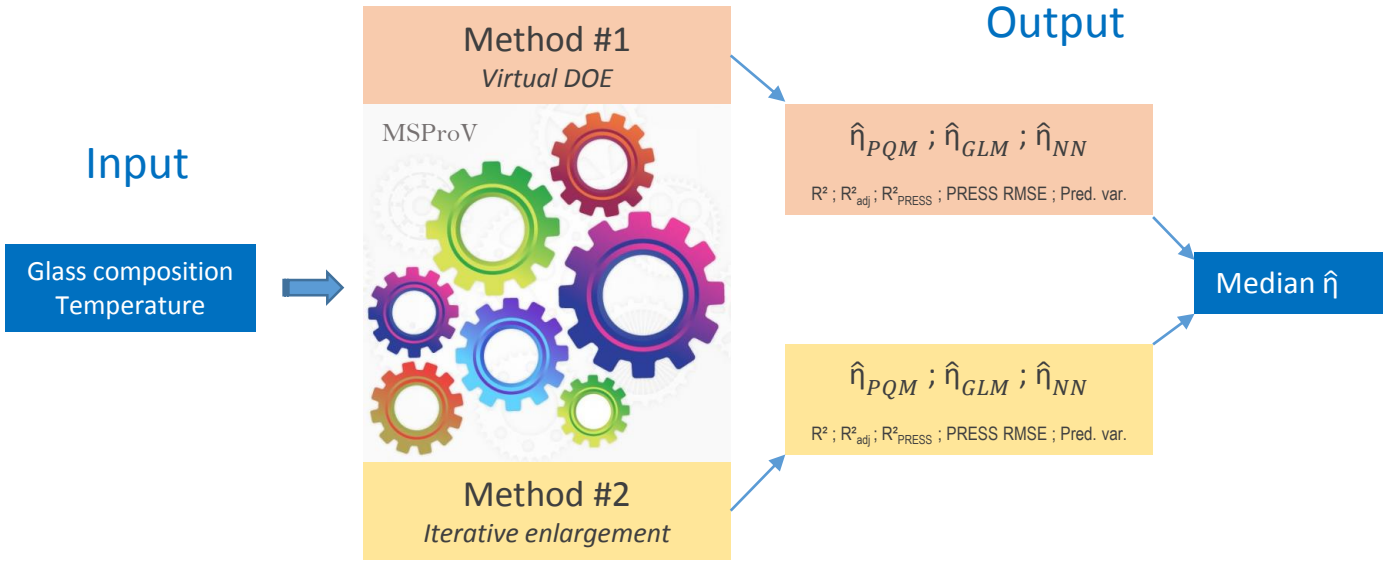


Photo courtesy of www.sciencesetavenir.fr

MSProV schematic diagram



Algorithms coded in JSL language (JMP software from SAS Institute)

Key parameters

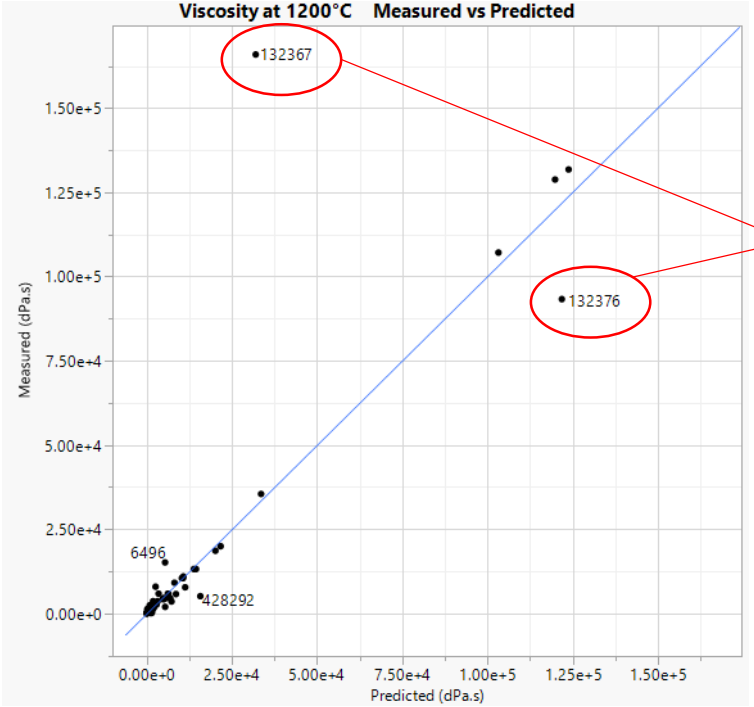
- Inputs from glass science experts on the nature and roles of oxides
- These inputs were implemented in MSProV algorithms
  - weights and type of distance calculation between *similar* glasses
- Origin and reliability of the data, viscosity measurement device

Results for viscosity prediction

- MSProV global database for viscosity prediction contains 15,569 glasses (all silica glass)
- 230 glasses extracted for testing MSProV capability to predict viscosity at 1200°C

Viscosity prediction relative error	Borosilicate glass for nuclear waste	Sodo alumino silica glass	Overall
	N=73	N=55	N=230
Quantile 50% (median)	11%	18%	17%
Quantile 75%	19%	35%	34%
Quantile 90%	37%	73%	77%

Results for viscosity prediction



Num	132367
Origin	SCIGLASS
Year	1994
	%wt
Al_2O_3	12,50
B_2O_3	7,50
BaO	20,00
CaO	2,50
SiO_2	57,50
Visc. exp. (dPa.s) 1200°C	165 959

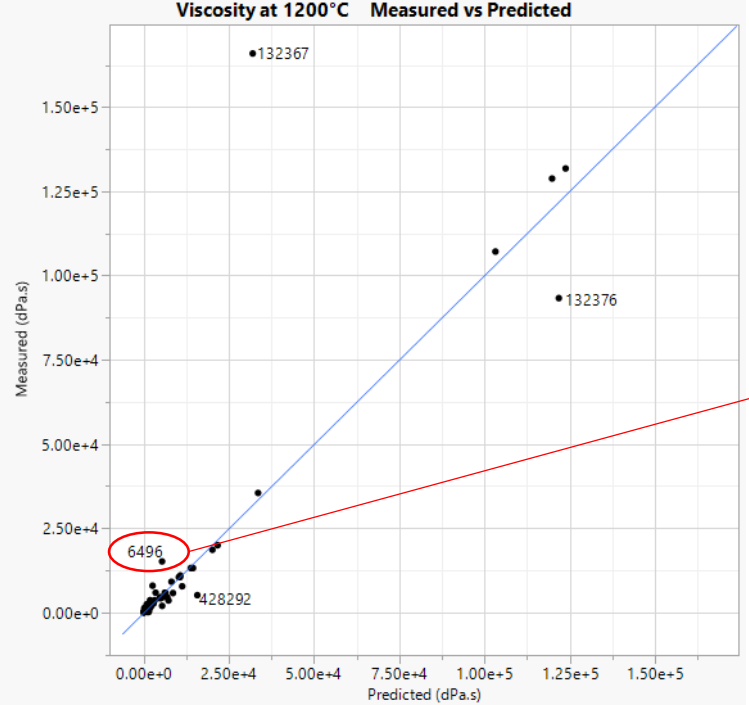
Num	132376
Origin	SCIGLASS
Year	1994
	%wt
Al_2O_3	19,01
B_2O_3	6,79
BaO	9,43
CaO	4,11
MgO	1,42
SiO_2	57,35
SrO	1,86
Visc. exp. (dPa.s) 1200°C	93 325

SciGlass reference: US Patent 5374595

Experimental error not mentioned

High %Al_2O_3 and/or %BaO

Results for viscosity prediction



Num	6496
Origin	SCIGLASS
Year	1968
	%wt
Al_2O_3	21,10
B_2O_3	7,40
BaO	3,50
CaO	13,50
SiO_2	54,50
Visc. exp. (dPa.s) 1200°C	15 136

Experimental device (1968)

High %Al_2O_3

Tg prediction

Prediction results

- MSProV global database for Tg prediction contains 20,201 glasses (all silica glass)
- 100 glasses extracted for testing MSProV capability

Tg prediction error	Borosilicate glass		Sodo alumino silica glass		Overall	
	N=80		N=20		N=100	
	Rel.	Abs.	Rel.	Abs.	Rel.	Abs.
Quantile 50% (median)	1,4%	7°C	1,7%	10°C	1,5%	7°C
Quantile 75%	2,8%	13°C	3,2%	17°C	2,9%	14°C
Quantile 90%	5,1%	29°C	4,2%	19°C	4,7%	26°C

General conclusion

GLASS PROPERTY MODELING - CONCLUSION

- When glass composition is too complex, properties can not be predicted from theoretical models
- In this case, statistical modeling using empirical data is an alternative way to predict glass properties
- Excellent predictive models can be obtained by using a Design of Experiments methodology, on small domains of composition
- Glass property information systems containing published data are commercially available
- Machine Learning has seen growing application in material property determination on big data sets
- Several physical and chemical glass properties can be well predicted by using Neural Nets

THANK YOU FOR YOUR ATTENTION

Acknowledgments

- Glass elaboration and characterization teams, R&D Scientist from CEA Marcoule

V. Ansault, T. Blisson, M. Chartier, V. Debono, V. Lemaitre, S. Mure, B. Penelon, J. Renard, C. Vallat, J.L. Dussossoy, M. Fournier, I. Giboire, I. Hugon, A. Laplace, M. Neyret, O. Pinet, E. Régnier, S. Schuller, S. Vaubaillon, F. Bart, J. Lacombe, C. Ladirat, S. Gin

- ORANO and EDF for financial support

- Pacific Northwest National Laboratory

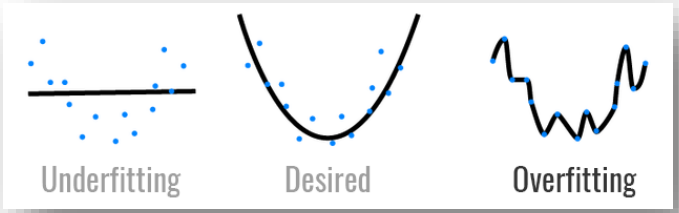
J. Vienna

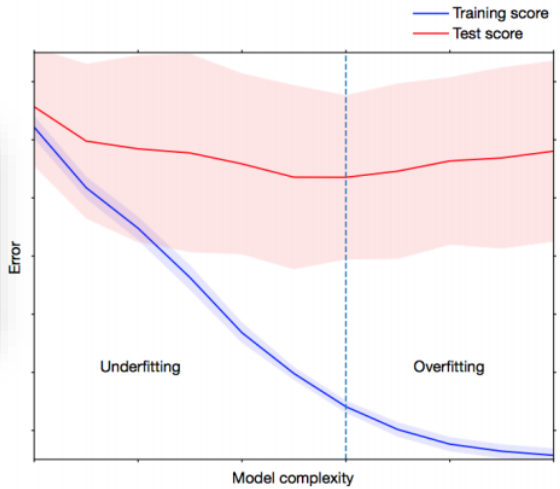
- JMP, SAS Institute

B. Jones

Advice when building predictive models

- Beware of overfitting (principle of parsimony)





from K. T. Butler et al. *Machine learning for molecular and materials science* Nature, 2018

SBN1

Component	Mol. %	Wt %
B_2O_3	18.04	20.23
SiO_2	67.73	65.56
Na_2O	14.23	14.21

SBN2

Component	Mol. %	Wt %
B_2O_3	8.467	9.61
SiO_2	67.73	66.34
Na_2O	23.8	24.05

SBN3

Component	Mol. %	Wt %
B_2O_3	19.57	21.86
SiO_2	60.86	58.68
Na_2O	19.57	19.46

Chemical composition range of R7T7 glasses produced in the AREVA - La Hague plant workshops

Oxides	Specified interval for the industry (wt%)		Average composition of industrial glasses (wt%)
	min	max	
SiO_2	42.4	51.7	45.6
B_2O_3	12.4	16.5	14.1
Al_2O_3	3.6	6.6	4.7
Na_2O	8.1	11.0	9.9
CaO	3.5	4.8	4.0
Fe_2O_3		< 4.5	1.1
NiO		< 0.5	0.1
Cr_2O_3		< 0.6	0.1
P_2O_5		< 1.0	0.2
Li_2O	1.6	2.4	2.0
ZnO	2.2	2.8	2.5
Oxides (PF + Zr + actinides) Fines suspension	7.5	18.5	17.0
Actinide oxides			0.6