Examples of Use

Contents

Notes

1) Parts where some operation or check is required are encircled with the following colors in each window.

Selection or input	:	
Operation of button or icon	:	
Check	:	

2) Refer the User's Manual for detailed operation. The corresponding chapters and sections are indicated under each example's title.

3) Number of searched data (Total Number) and data content in the [Data List of Property or Structure] window are different depending on the Version of INTERGLAD. So when the user tries the same example, the Total Number and the content may be different from those of the example described here. Ver.8.2.0.2 of INTERGLAD (with GP_42_2020.mdb and GS_37_2020.mdb) is used for these examples.

Search and Analysis of Property Data

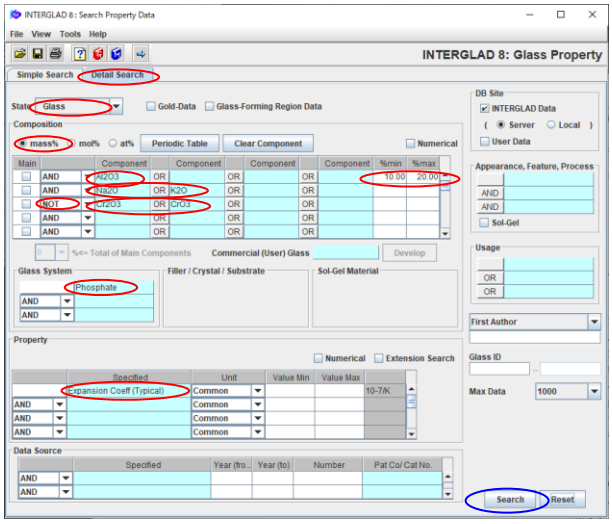
1. Search with a complicated composition – Thermal expansion coefficient of phosphate glasses

Search thermal expansion coefficient data of phosphate glasses with Al_2O_3 of 10-20 mass%, containing Na_2O or K_2O, and not containing Cr Oxides.

<Refer to B of Chapter 3 and 2 of Chapter 4>

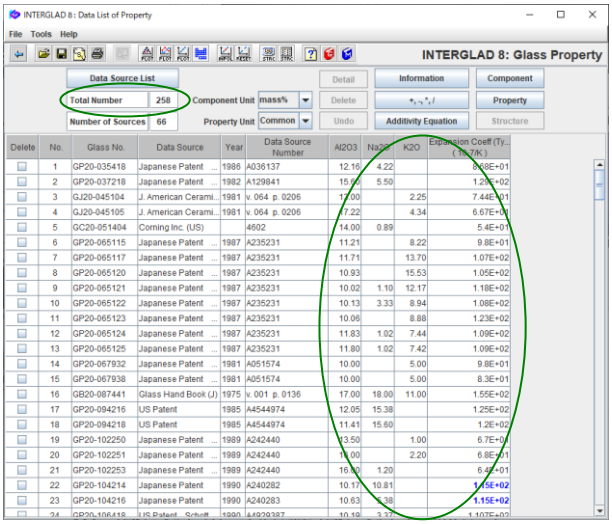
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search



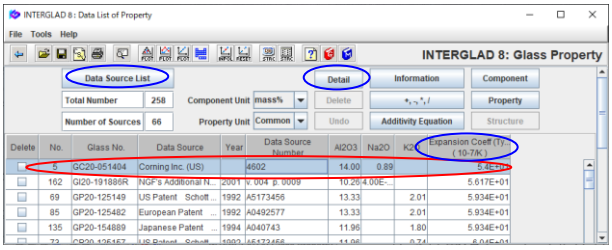
- Open the [Search Property Data] window by clicking the [Search Property Data] button in the [Main] window, select the [Detail Search] tub, and specify search conditions.
- Select 'mass%' for the unit of composition. The default of the unit is mol%.
- Select 'Na2O' and 'K2O' in the same row with connection of 'OR.' In this case the simultaneous selection of Na_2O and K_2O is not available on the periodic table.
- Cr Oxides can be selected by selecting 'Cr: O' on the Periodic Table.
- The order of selection for search conditions is free.
- More the search conditions become complex, longer the search time.
- 'Expansion Coeff (Typical)' is selected for the [Specified] of the [Property] column. The selection of 'Linear Expansion Coeff' (a middle category item, boldtype) brings the same result.

2) Search result ([Data List of Property] window)

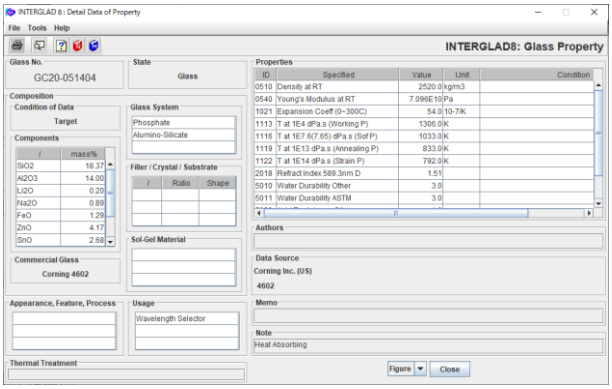


- Take notice of 'Total Number' of the Data Source, 258.
- A table with values of components, property data etc., which are specified as the search conditions, appears.

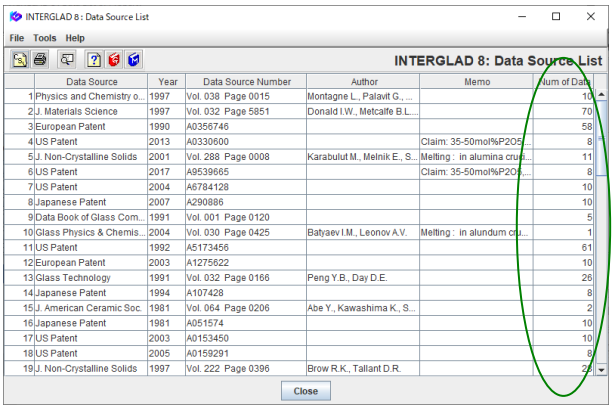
3) Utilization of the search result ([Detail Data of Property] window and [Data Source List] window)



- Sort of each column is available. Click an item label holding down the Ctrl key.
- In this example, by sorting 'Expansion Coeff' the glass with the expansion coefficient of the lowest value can be found. The detailed data of a glass can be checked by selecting its row and clicking the [Detail] button.



[Detail Data of Property] window



[Data Source List] window

- The [Data Source List] window opens by clicking the [Data Source List] button in the [Data List of Property] window.
- Number of glasses of each data source is shown in the [Num of Data] column.

- If necessary, analyze the result using Ternary Plot or XY Plot.

2. Ternary plot analysis of property data

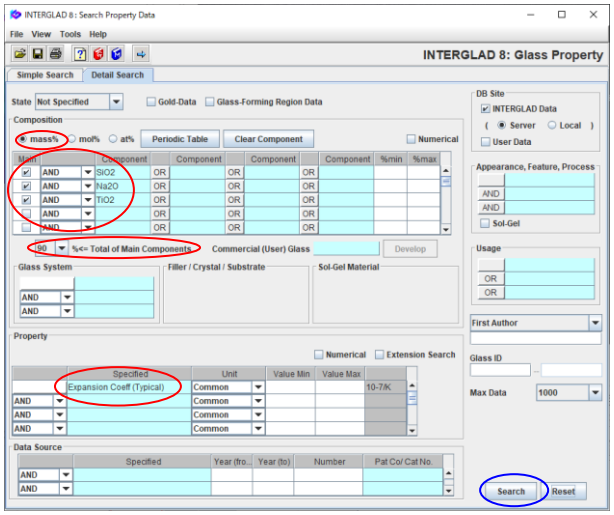
– Thermal expansion coefficient of SiO_2-Na_2O-TiO_2 glasses

Investigate relation between composition and thermal expansion coefficient on SiO_2-Na_2O -TiO_2 glasses.

<Refer to B and C.1 of Chapter 3, and 2 and 3.1 of Chapter 4>

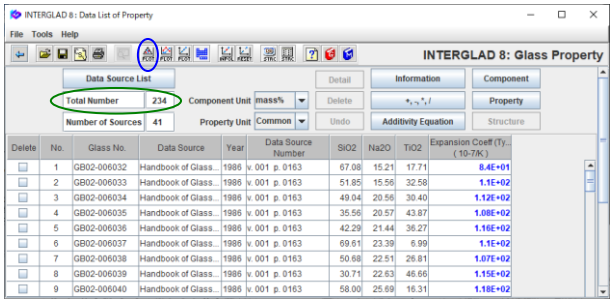
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search



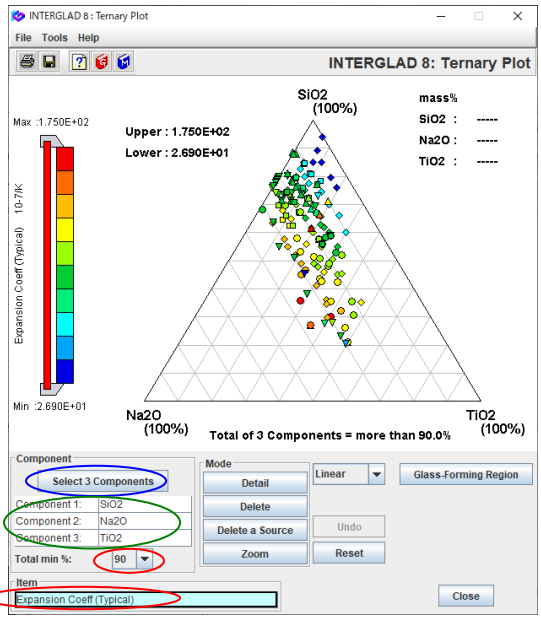
- Select '90' mass% as the minimum Total of Main Components, SiO_2, Na_2O and TiO_2.
- Select 'Expansion Coeff (Typical)' for the Specified of the [Property] column.

2) Search result ([Data List of Property] window)

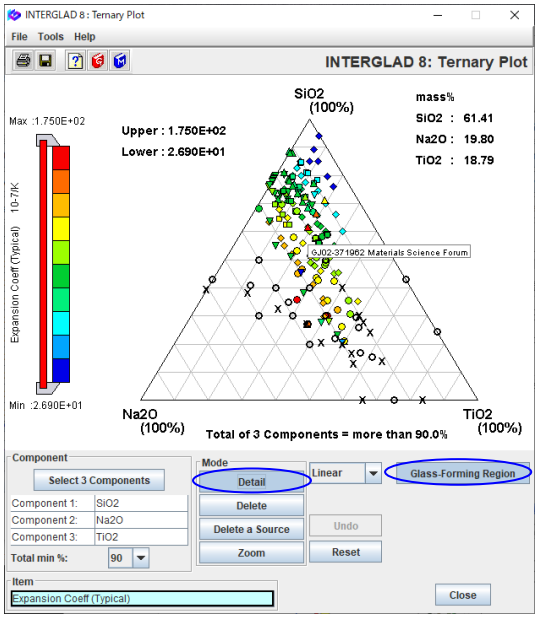


- 234 glasses are searched.

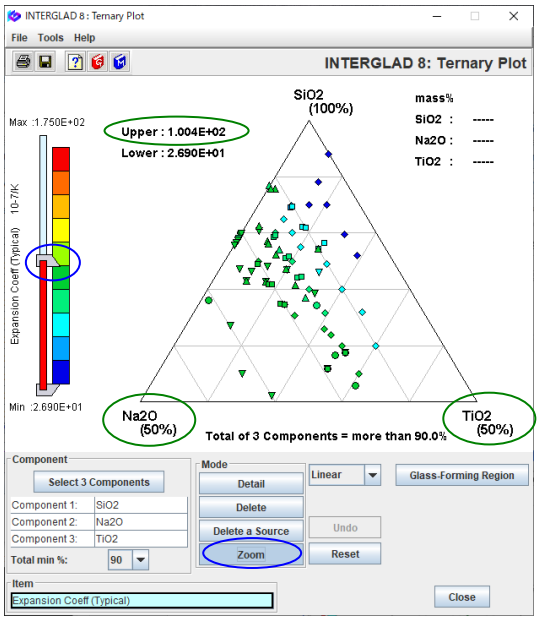
3) Ternary plot



- Open the [Ternary Plot] window by clicking the [Ternary Plot] icon. Select SiO_2, Na_2O and TiO_2 for the 3 Components, '90' for the Total min%, and 'Expansion Coeff (Typical)' for the Item.
- Value levels of thermal expansion coefficients can be overviewed by plot-points with ten steps of colors in the diagram. Thermal expansion coefficient is high in the center region and decreases as the position moves to the upper right (near to SiO_2 100%).



- The Glass No. and Data Source of each plot-point are indicated in a balloon by putting the mouse-pointer at a plot-point. The detailed data of each plot-point can be checked by clicking a plot-point with the [Detail] button active.
- The Glass-forming region data are shown by clicking the [Glass-Forming Region] button. ○ indicates Glass and × Non-Vitrified.
- Glass-forming region data in the database are those of glasses in which total of 3 components is 100%. Note that in the collected data of this example the total of 3 components is 90-100%.
- The state (glass or non-vitrified) of each plot-point can be checked by opening each [Detail Data of Property] window.
- The detailed data of glass-forming region also can be checked by clicking a mark or line with the [Detail] button active.



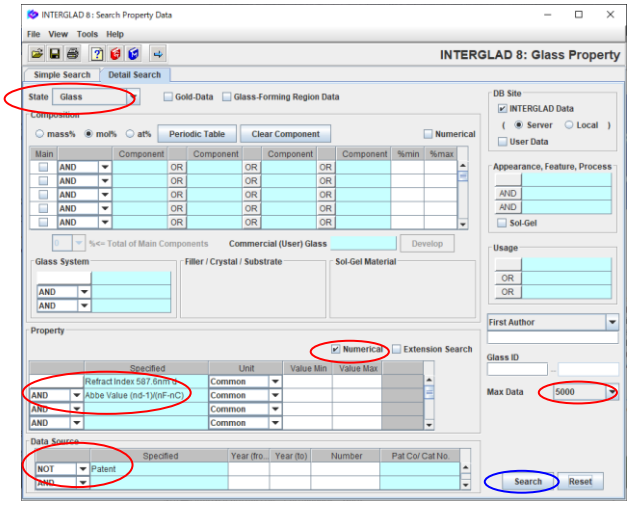
- By sliding the slider, property value range of glasses in the diagram can be changed. In the example of the left figure thermal expansion coefficient is limited to ≤ 100.4×10^{-7}/K, and the ternary diagram with SiO_2 (100%), Na_2O (50%), TiO_2 (50%) is shown by using the [Zoom] button.

3. XY plot analysis of properties – Refractive index vs. Abbe value

Investigate a relation between refractive index and Abbe value of glasses.

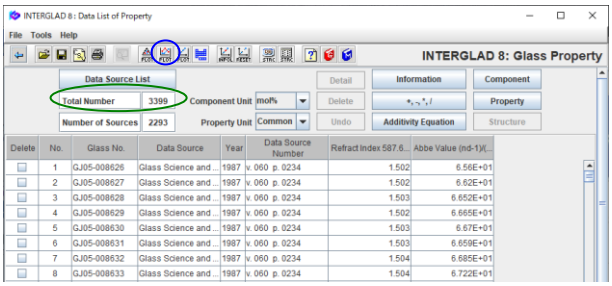
<Refer to B and C.2 of Chapter 3, and 2 and 3.2 of Chapter 4>

1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag) → Search



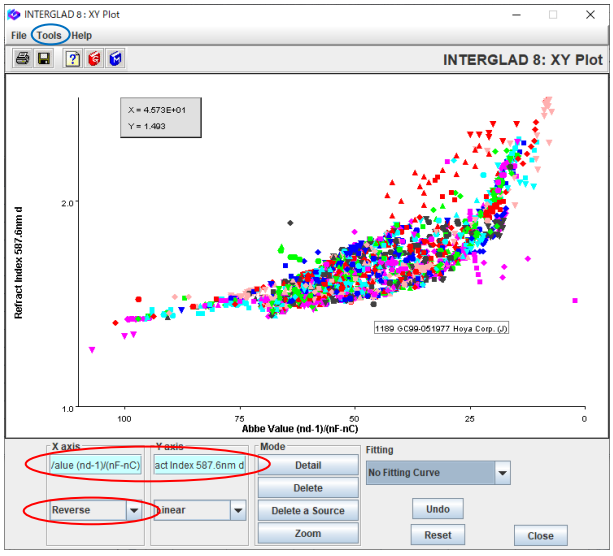
- Select 'Glass' in the [State] pulldown menu.
- As for refractive index, data measured by illuminants with various wavelengths are in the database. In this example, data by He d-line with 587.6nm are searched.
- Select '(nd-1)/(nF-nC)' for the Abbe value.
- Check in the [Numerical] checkbox.
- Select 'NOT Patent' in the [Data Source] column.
- Select '5000' in the [Max Data] pulldown menu.

2) Search result ([Data List of Property] window)



- 3399 glasses are listed.

3) XY Plot Analysis ([XY Plot] window)



- From the [XY Plot] icon, an XY plot (Abbe value vs. refractive index) is shown. The distribution of Abbe values and refractive indexes of 3399 glasses is visualized.
- In this example, the style of x-axis for Abbe value is set to 'Reverse', and the ranges and scales are changed from the [Tools/ Option] menu.

4. Search using data interpolation for high temperature properties

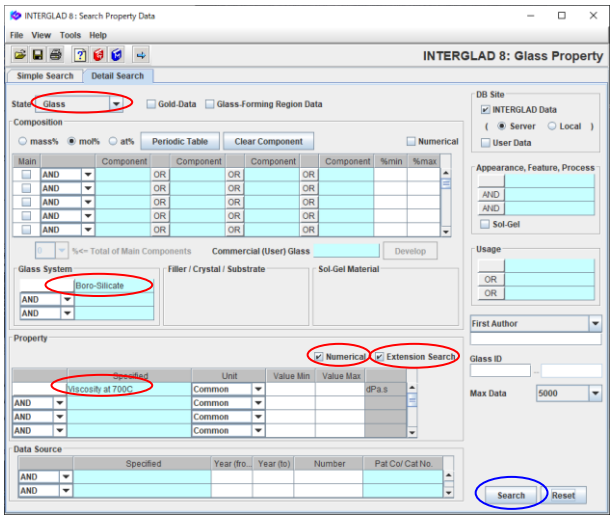
– Viscosity at high temperatures of boro-silicate glasses

Search viscosity data at 700°C of boro-silicate glasses using data interpolation or extrapolation.

<Refer to B and C.3 of Chapter 3, and 2 and 3.3 of Chapter 4>

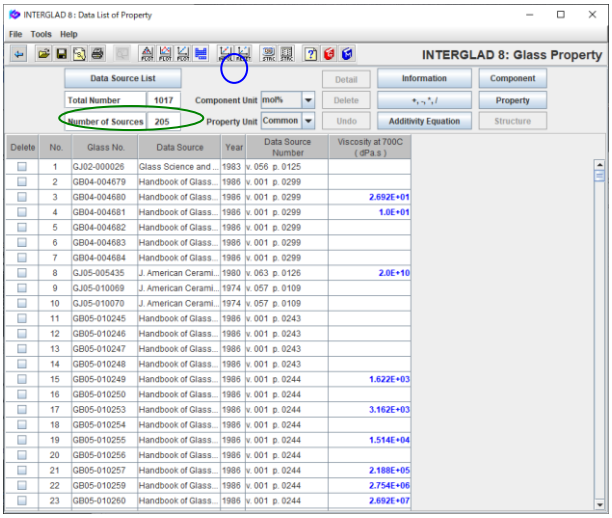
1) Specification of search conditions （[Search Property Data] window with [Detail Search] tag)

→ Search



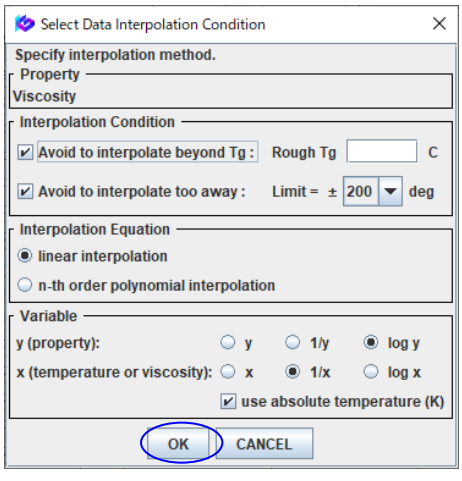
- Select 'Glass' for the State, and 'Boro-Silicate' for the Glass System.
- Select 'Viscosity 700C' for the Property, and check in the [Numerical] and the [Extension Search] checkboxes shown in the window example.

2) Search result ([Data List of Property] window)

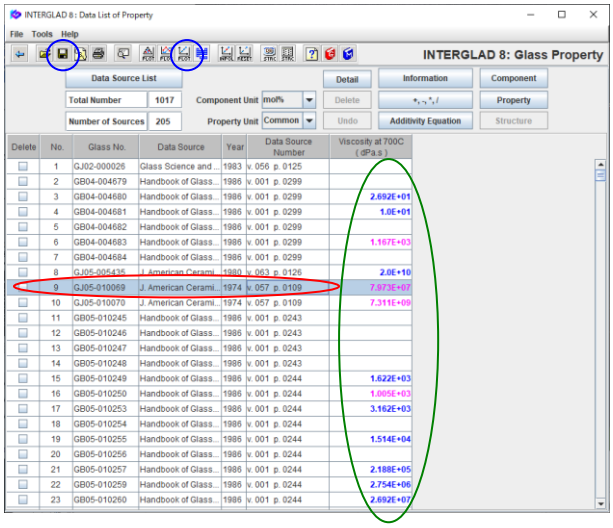


- As the search result, all the boro-silicate glasses which have registered viscosity data at high temperatures are listed. 1017 glasses appear.
- Search of viscosity data at 700°C can be performed, also when the user selects the bold type item 'Viscosity(100-1000C).' In this case, all the glasses which have one or more numerical data of viscosity at 100-1000°C are listed. 551 glasses appear.

3) Data interpolation or extrapolation

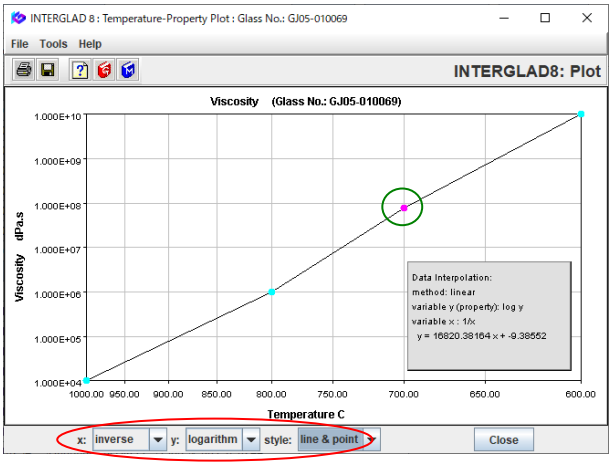


- Set conditions in the [Data Interpolation Condition] dialog box, which is opened by clicking the [Data Interpolation] icon. In this example the default of variable y (viscosity) is logy, and that of variable x (temperature) is 1/ (absolute temperature). Then click the [OK] button.



- The interpolated or extrapolated data at 700°C appear in red-purple color in the list.
- The glasses with no value are those which has only one value at another temperature, or which has no data in the range of 700 ± 200°C (default condition).
- When the user searches for 'Viscosity (100-1000C),' the calculation is done also for the other temperatures except 700°C.
- The interpolated or extrapolated values can be saved in the user's PC by clicking the [Save] icon. In case of the Internet edition, the save is unable.

4) Temperature-Property plot ([Temperature-Property Plot] window)



- Select a glass in the list, and by clicking the [Temperature-Property Plot] icon (the right [PLOT] icon), the [Temperature-Property Plot] window is shown.
- In the XY Plot, the interpolated or extrapolated plot-points appear in red-purple color. The style of plot-points and axis-scales can be changed by the pulldown menus on the bottom of the graph.

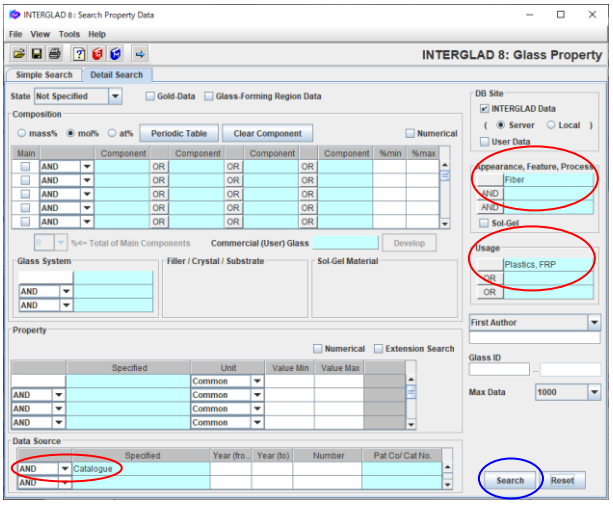
5. Search commercial glasses – High strength glass fibers for FRP

Investigate high strength glass fibers for FRP.

<Refer to B of Chapter 3, and 2 of Chapter 4>

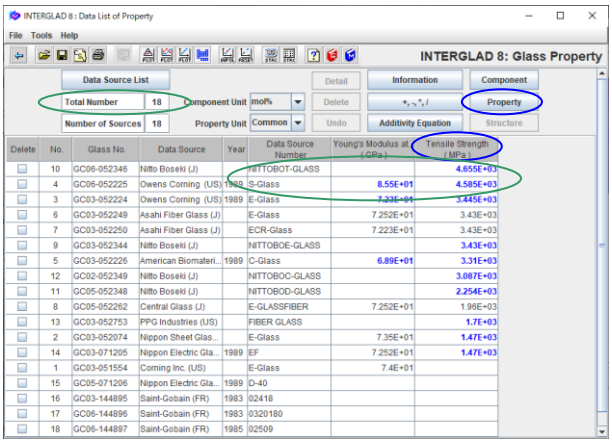
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

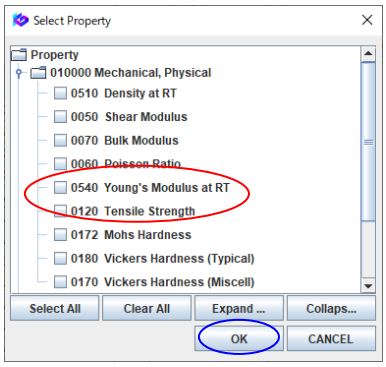
→ Search



- Select 'Fiber' after opening 'Appearance' →'Shape'→'Linear' in the [Appearance, Feature, Process] column. Or select 'Fiber' after inputting 'Fiber' in the [Keyword] column.
- Select 'Plastics, FRP' in 'Material' by clicking the [Usage] column. Or select 'FRP' after inputting 'FRP' in the [Keyword] column.
- Select 'Catalogue' for the [Data Source] column.

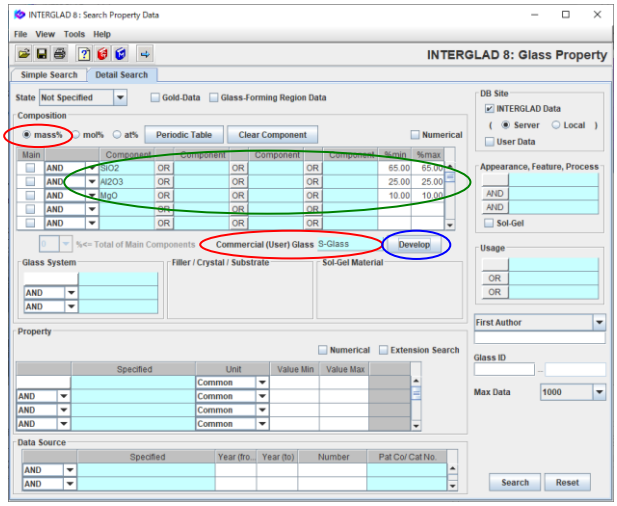
2) Search result ([Data List of Property] window)

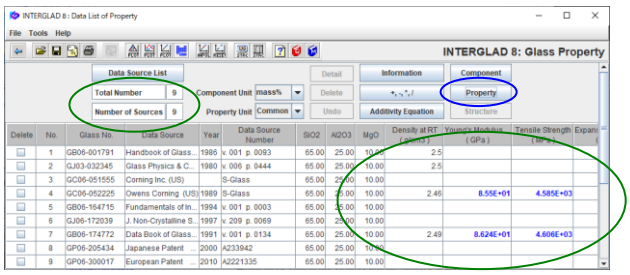




- 18 glasses are listed. These are found to be data of 10 manufacturers in the Data Source column.
- Open the [Select Property] dialog box by clicking the [Property] button.
- Check in the 'Tensile Strength' and 'Young's Modulus at RT' checkboxes, and both the data are shown. Tensile strength and Young's modulus are important properties for high strength glass fibers.
- By sorting the Tensile Strength column, glasses with high strength can be found. (NITTOBO T-Glass and S-Glass are the highest.)

3) Investigation of a searched glass

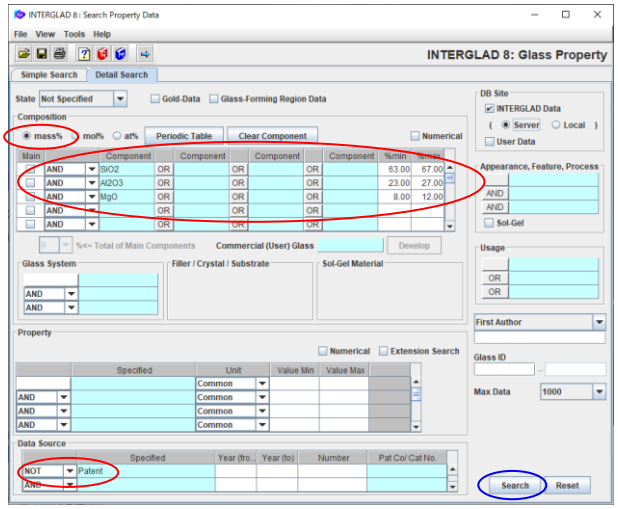




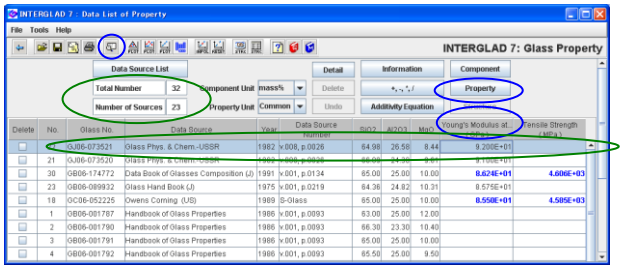
- Here S-glass with high tensile strength and high Young's modulus is investigated.
- Go back to the [Search Property Data] window, select 'S-Glass' in the [Commercial (User) Glass] column, and click the [Develop] button after selecting 'mass%' for the Unit. Not specify the Data Source.
- In this case values of %min and %max are the same, because the glass compositions registered have no difference.

- 9 glasses (9 data sources) are listed. When the search is performed without clicking the [Develop] button, only 3 glasses are listed. By developing the composition, it is found that data of Journals, etc. besides catalogues are also searched.
- By clicking the [Select All] button in the [Select Property] dialog box from the [Property] button, all the property data registered are shown in the list.

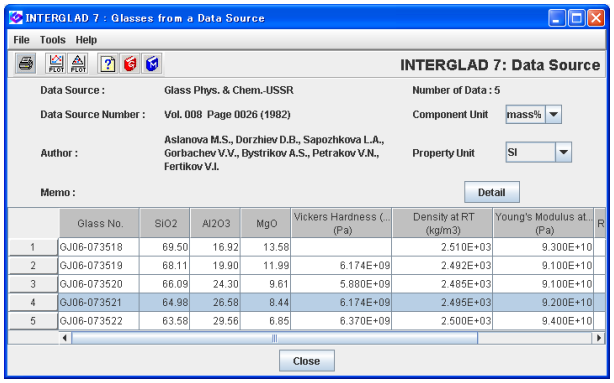
4) Investigation of data around S-Glass



- Information of glasses around S-Glass is collected.
- ±2% values of %min and %max are set as a search condition.
- Select 'NOT Patent' for the Data Source.



- 40 glasses of 26 data sources are listed. When patents are also included for the search condition, 119 glasses of 57 data sources are listed.
- List the values of 'Tensile Strength' and 'Young's Modulus at RT' from the [Property] button, and sort the Young's Modulus column. By this procedure the mechanical property of the glasses around the S-Glass composition are shown.



	Glass No.	SiO2	Al2O3	MgO	Vickers Hardness (... (Pa)	Density at RT (kg/m3)	Young's Modulus at... (Pa)
1	GJ06-073518	69.50	16.92	13.58		2.510E+03	9.300E+10
2	GJ06-073519	68.11	19.90	11.99	6.174E+09	2.492E+03	9.100E+10
3	GJ06-073520	66.09	24.30	9.61	5.880E+09	2.485E+03	9.100E+10
4	GJ06-073521	64.98	26.58	8.44	6.174E+09	2.495E+03	9.200E+10
5	GJ06-073522	63.58	29.56	6.85	6.370E+09	2.500E+03	9.400E+10

- Clicking the [Glasses from a Data Source] icon after selecting the glass 'GJ06-073521' with the highest Young's modulus opens the [Glasses from a Data Source] window of the glasses. All the data (5 glasses) in this data source can be checked.

[Glasses from a Data Source] window

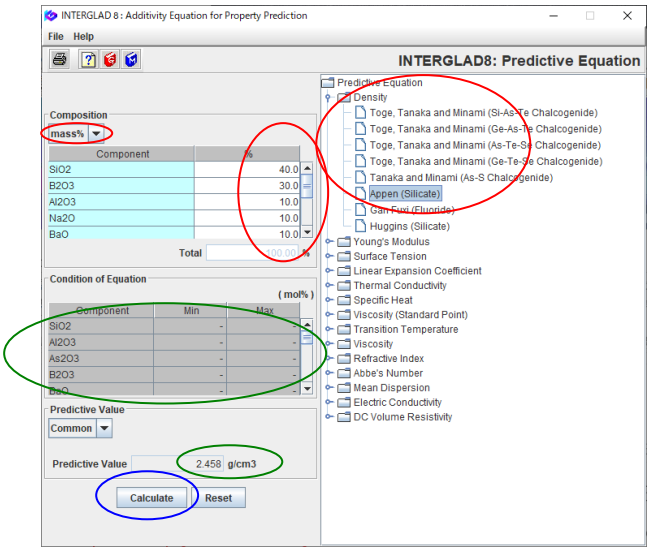
Property Prediction by Additivity Equations

6. Property prediction of glasses with a specified composition – Boro-silicate glasses

Predict density, thermal expansion coefficient and refractive index of a boro-silicate glass with SiO_2 40%, B_2O_3 30%, Al_2O_3 10%, Na_2O 10% and BaO 10% (mass%).

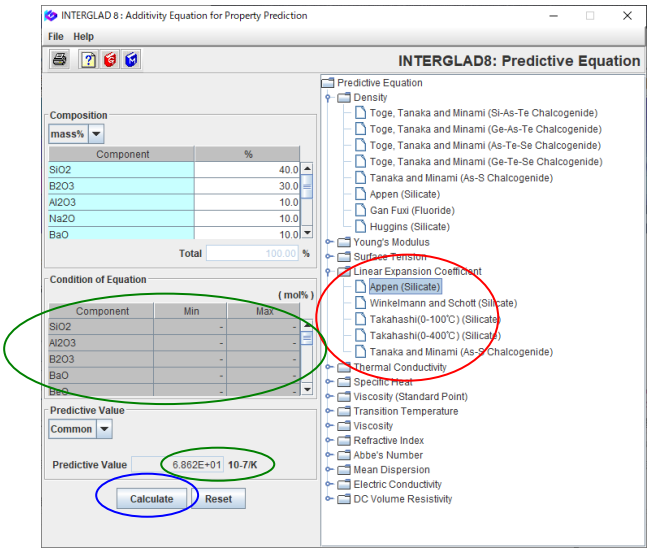
<Refer to D.1 of Chapter 3, 4.1 of Chapter 4, and 1 of Chapter 6>

1) Prediction of density ([Additivity Equation for Property Prediction] window)



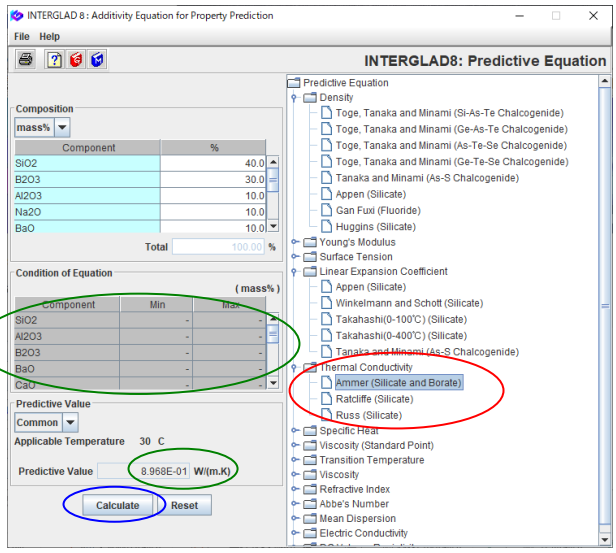
- Open the [Additivity Equation for Property Prediction] window by clicking the [Property Prediction] button in the [Main] window and [Additivity Equation for Property] button. Select 'Appen (Silicate)' after developing 'Density' in the [Predictive Equation] menu on the right-hand part of the window.
- The Condition of Equation appears on the left-hand part. Check if the values of the components of glasses to be predicted are included in the condition.
- Select components required for the property prediction, and enter each value in the [Component %] column. In this example the component unit is mass%.
- After clicking the [Calculate] button, the predictive value 2.458 g/cm^3 appears in the [Predictive Value] column.

2) Prediction of thermal expansion coefficient



- In case of prediction of the other properties for the same composition, property prediction can be performed only by reselecting the property equation.
- Select 'Appen(Silicate)' after developing 'Linear Expansion Coefficient' in the [Predictive Equation] menu.
- Clicking the [Calculate] button shows the predictive value 68.62 × 10^{-7} /K in the [Predictive Value] column.

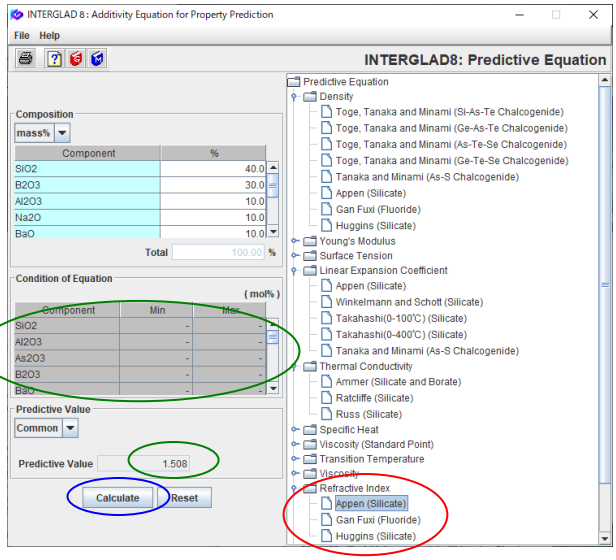
3) Prediction of thermal conductivity



- Select 'Ammer (Silicate and Borate)' after developing 'Thermal Conductivity' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 0.8968 W/(mK) (30°C) appears in the [Predictive Value] column.

- In this example, equations of 'Ratcliffe (Silicate)' and 'Russ (Silicate)' are also available, and 0.8349 W/(mK) (0°C) and 0.9256 W/(mK) (0°C) are obtained respectively. The user can compare the results by the difference of additivity equations.

4) Prediction of refractive index



- Select 'Appen (Silicate)' after developing 'Refractive Index' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 1.508 appears in the [Predictive Value] column.

- Predictive values of various properties can be calculated for a composition as described above, but in many cases calculations are not possible owing to various composition limitation of equations.

＜Refer to 1 of Chapter 6＞

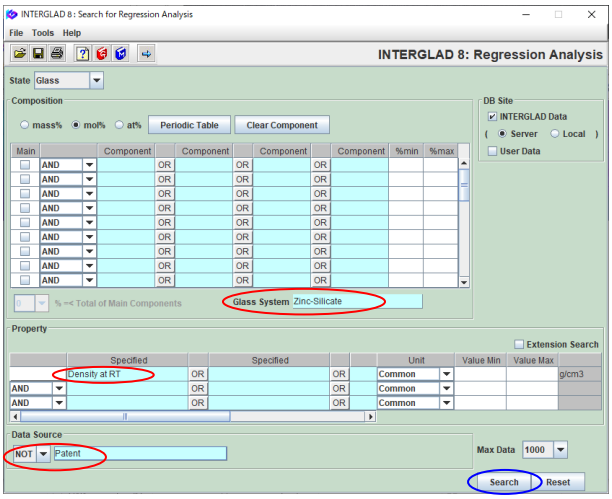
Property Prediction & Material Designing (Composition Optimization) by Multiple Regression Analysis

7. Obtaining an additivity equation of a property — Density of zinc-silicate glasses

Obtain a multiple regression equation of density at RT for zinc-silicate glasses.

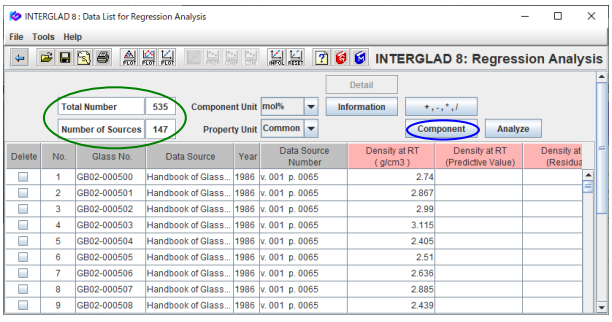
<Refer to D.2 of Chapter 3, 4.2-4.5 of Chapter 4>

1) Specification of search conditions ([Search for Regression Analysis] window) → Search

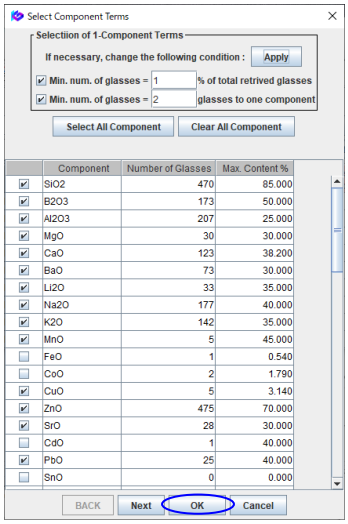


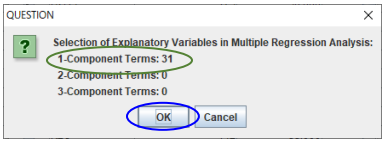
- Open the [Search for Regression Analysis] window by clicking the [Property Prediction] button and then the [Multiple Regression Analysis] button in the [Main] window.
- Select 'Glass' (default) for the State.
- Select 'Zinc-Silicate' for the Glass System, 'Density at RT' for the Property, and 'NOT Patent' for the Data Source.

2) Search result ([Data List for Regression Analysis] window) → Selection of explanatory variables ([Select Component Terms] dialog boxes)

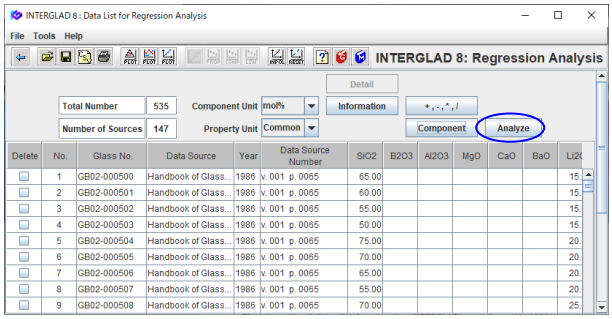


- 535 glasses (147 data sources) are listed.
- Open the [Select Component Terms] dialog boxes by clicking the [Component] button, and specify component terms for a multiple regression equation.
- In this example, click the [OK] button in the [Select Component Terms] dialog box for the Selection of 1-component Terms at the default setting.
- By this command the explanatory variables are limited to 1-component terms. Check the number of the component terms in the [Question] dialog box.



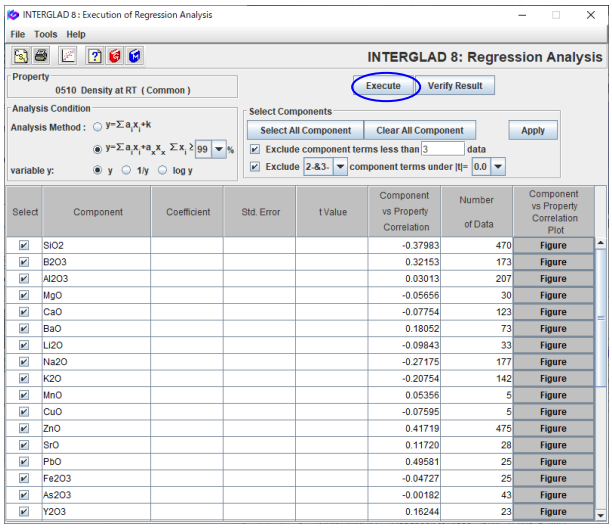


1-Component Terms: 31.

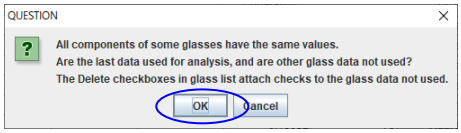


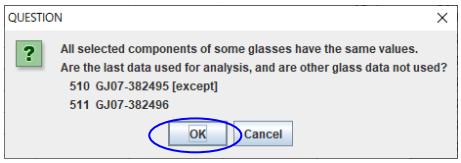
- By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens.

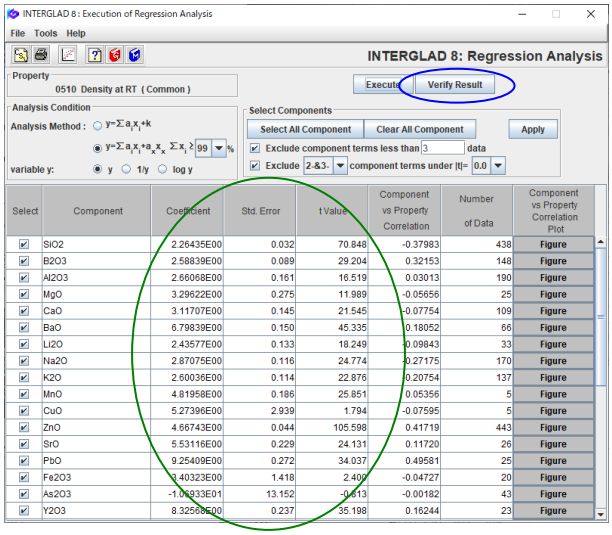
3) Execution of multiple regression analysis ([Execution of Regression Analysis] window)



- Execute the multiple regression analysis at the default setting by clicking the [Execute] button.
- [Question] dialog boxes appear one after one. Check the dialog, and click the [OK] button for them.

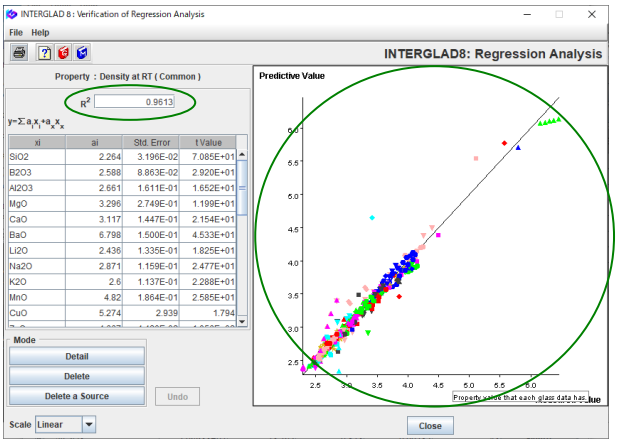






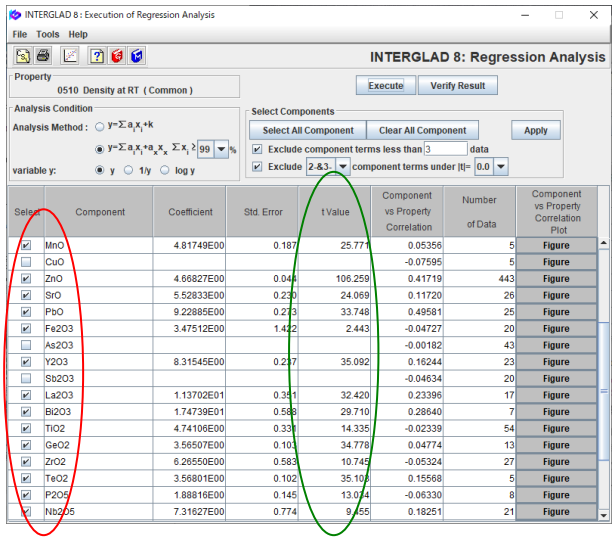
- The regression coefficients, the standard errors and t values appear in the table after the calculation.
- By clicking the [Verify Result] button, open the [Verification of Regression Analysis] window.

4) Verification of regression analysis ([Verification of regression analysis] window)

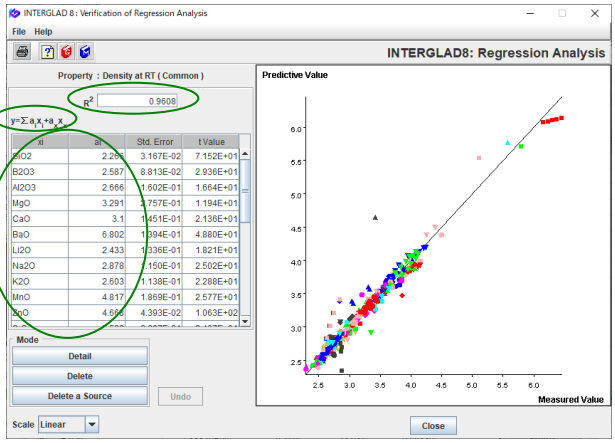


- In this example a high contribution rate R^2 (0.9613) is obtained. The scattering of the plot-points is relatively small from the linear line y=x on the XY plot of the measured values vs. the predictive values. R^2 value of ≥0.8 is recommended.

5) t value check → Recalculation



- Return to the [Execution of Regression Analysis] window, and check if the absolute value of t for each component term is low <2 or not. |t| value is recommended to be ≥2 (1).
- In this example, |t| of CuO, As_2O_3, Sb_2O_3 and Ho_2O_3 are <2. First, delete ✓ in the checkboxes of As_2O_3, Sb_2O_3 and Ho_2O_3 with |t|<1, and recalculate by clicking the [Execute] button. Second, delete ✓ of CuO with |t|<2, and recalculate. By these procedures the component terms with |t|<2 are removed from the multiple regression equation.



- Verification of the multiple regression analysis is performed again. R^2 decreases a little, but it is still high (0.9068).

6) Completion of an additivity equation (multiple regression equation)

- The equation and the coefficients of its component terms are shown in the [Execution of Regression Analysis] window and the [Verification of Regression Analysis] window.
- The obtained equation:

Density at RT (g/cm³) = 2.266×(SiO_2) + 2.587×(B_2O_3) + 2.666×(Al_2O_3) + ·····

(SiO_2), (B_2O_3) ,…… : mole ratio of each component （27 components except others）

- The analysis results can be saved in the user's PC from the [Save] icon in the [Data List for Regression Analysis] window. The save is available in the cases of Standard edition and CD Full Function edition, but not Internet edition.

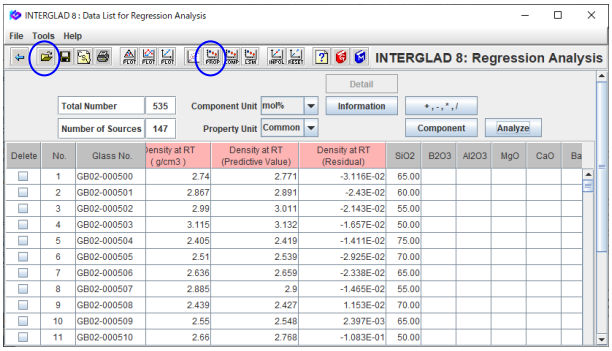
8. Property prediction — Density of zinc-silicate glasses

Predict density at RT of a glass with SiO_2 60%, Li_2O 20% and ZnO 20% (mol%).

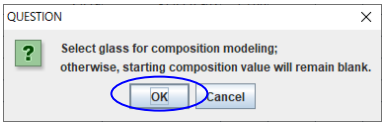
<Refer to D.2 of Chapter 3, 4.6 of Chapter 4>

The multiple regression equation for the zinc-silicate glass system obtained in Example 7 is used.

1) Regression analysis result → Transit to the [Property Prediction] window

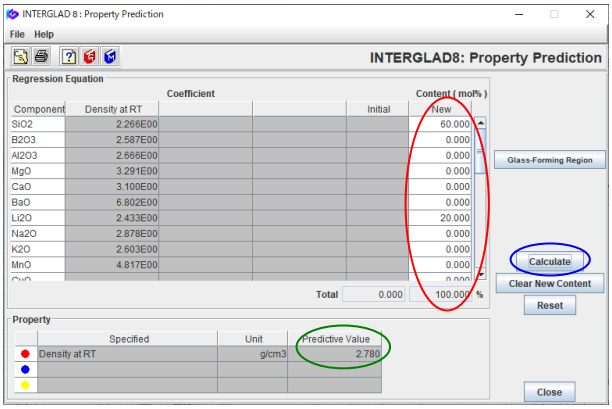


- Open a [Data List for Regression Analysis] window, and by clicking the [Open] icon open the [Data List for Regression Analysis] window of the result of 3.1 saved in the folder of the user's PC.



- Here do not select any glass row. By clicking the [PROP] icon, a [Question] dialog box appears. Click the [OK] button, and the [Property Prediction] window opens.

2) Calculation of a property value



- Enter the specified component values of the composition value in the [New] cells of the [Content] column to predict a property. By clicking the [Calculate] button, the calculated value appears in the [Predictive Value] cell of the [Property] column.
- The predicted density: 2.780 g/cm^3.

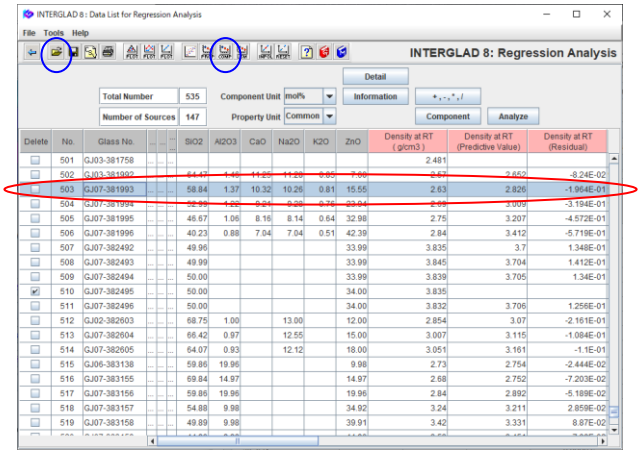
9. Composition optimization — Zinc-silicate glass with a specified density

Obtain a composition of zinc-silicate glass with density of 2.6 g/cm³ at RT. The components of the glass are SiO_2, Al_2O_3, CaO, Na_2O, K_2O and ZnO.

<Refer to D.3 of Chapter 3, 4.7 of Chapter 4>

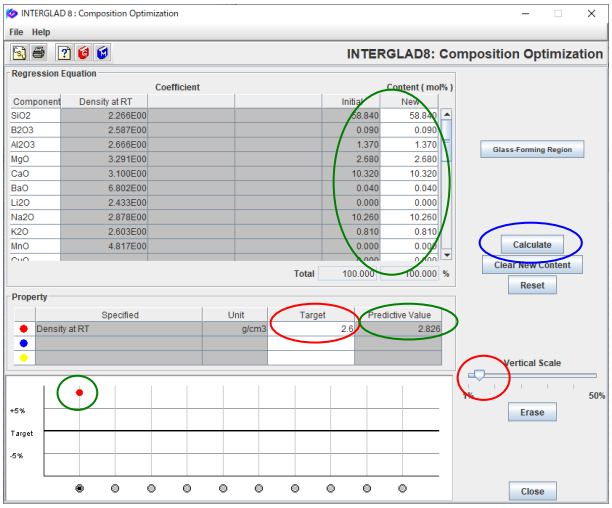
The multiple regression equation obtained in Example 7 is used because of the same zinc-silicate glass system.

1) Regression analysis result → Transit to the [Composition Optimization] window

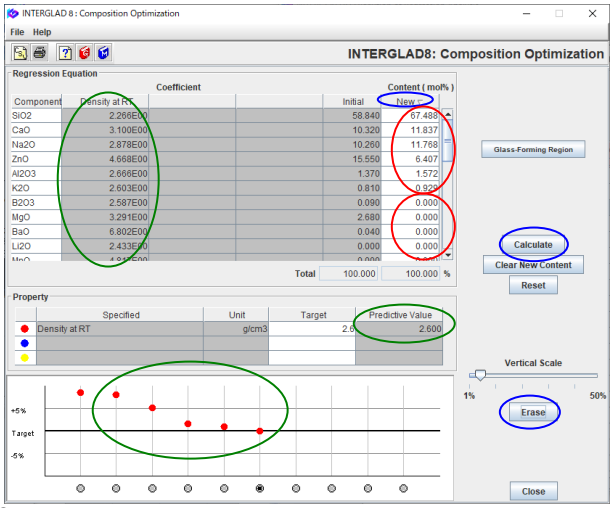


- Open the [Data List for Regression Analysis] window, and by clicking the [Open] icon open that of the result of 3.1 saved in the folder of the user's PC.
- Select a model glass which has a near density value to the target and which contains components of the target glass as possible by clicking the glass row. In this example sort the [Density at RT] column in the ascending order, and select a glass, No. 503(GJ07-381993) with density of 2.83 g/cm³ as a model.
- By clicking the [COMP] icon, the [Composition Optimization] window opens.

2) Composition optimization



- Enter the target value 2.6 in the [Target] cell of the [Property] column, and click the [Calculate] button. The calculated value appears in the [Predictive Value] cell. In the graph on the bottom part of the window, the difference(%) between the value of the model glass and the target is shown as a point in red color. Drag the slider of the [Vertical Scale] to the left (minimun 1%), and the difference is magnified for easy visualization.



- Next sort the content values in the [New] column, and correct the values of B2O3, MgO, BaO and Fe3O3, which are not included in the target composition with 6 components, to 0.
- By clicking the [Calculate] button, the property value is calculated after the proportional conversion of total values of components to 100%, and it appears in the [Predictive Value] cell. At the same time a new red point appears also in the graph, and the difference between the calculated value and the target value can be checked.

- Next correct the values in the [New] column, and recalculate. Repeat these procedures to bring the calculated value close to the target value. When the red point becomes apart from the target, click the [Erase] button to cancel the predictive value, and the red point and the composition return to the previous state. Component terms with a higher absolute value of regression coefficient have higher effect on the increase or decrease of the property value. In this example, decrease the content of ZnO with a high coefficient little by little.
- In final the Density at RT becomes 2.600 g/cm^3 in case of the following composition.
  The composition: SiO_2 67.49 mol%, Al_2O_3 1.57%, CaO 11.84%, Na_2O 11.77%, K_2O 0.93%, ZnO 6.41%.
- The composition with the target property is not only one. Therfore calculate changing the other components also, and optimize the composition.

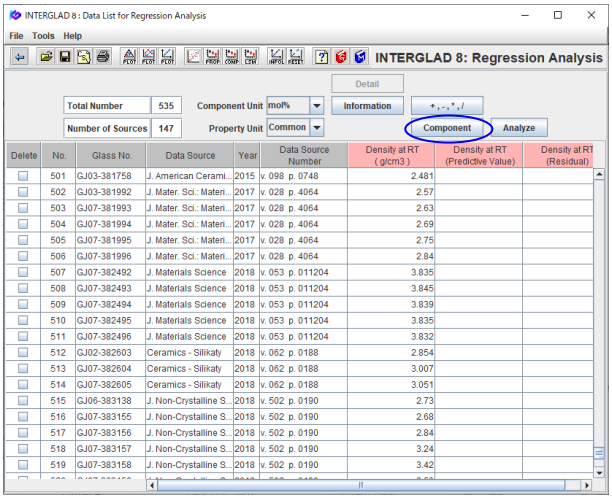
10. Composition optimization (Automatic calculation)— Zinc-silicate glass with a specified density

In the same example as 3.3, obtain a composition of zinc-silicate glass with density of 2.6 g/cm^3 at RT. The components of the glass are SiO_2, Al_2O_3, CaO, Na_2O, K_2O and ZnO.

<Refer to D.4 of Chapter 3, and 4.8, 4.9 of Chapter 4>

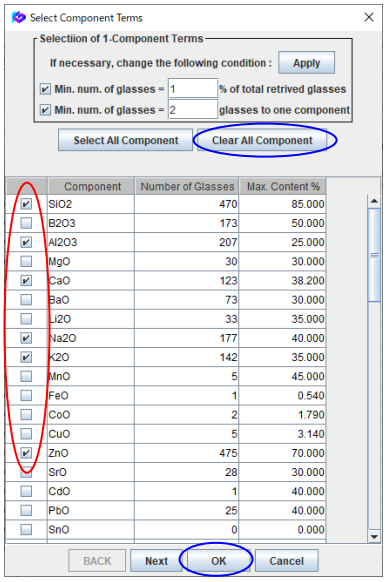
Composition optimization is performed by the least squares method using a new multiple regression equation from the search result in Example 7.

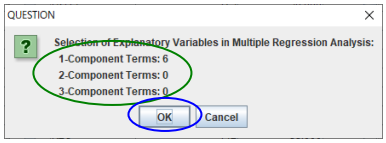
1) Search result ([Data List for Regression Analysis] window) → Selection of explanatory variables ([Select Component Terms] dialog boxes)



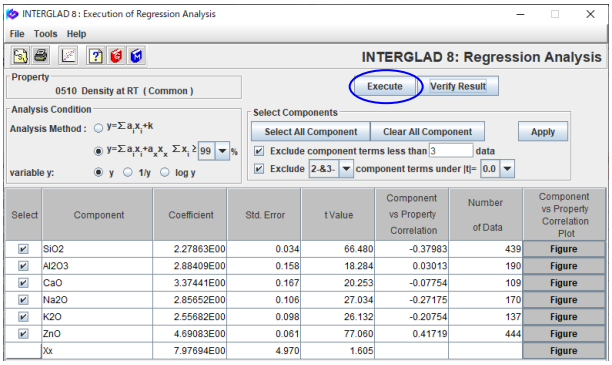
- Open the [Selection of 1 Component Terms] dialog box by clicking the [Component] button, and specify component terms for a multiple regression equation.
- In this example, first click the [Clear All Component] button in the [Select Component Terms] dialog box for the Selection of 1-Component Terms, and check the 6 checkboxes of SiO_2, Al_2O_3, CaO, Na_2O, K_2O and ZnO. Click the [OK] button.
- Check the number of the component terms in the [Question] dialog box.

  1-Component Terms: 6.
- Click the [Analyze] button.

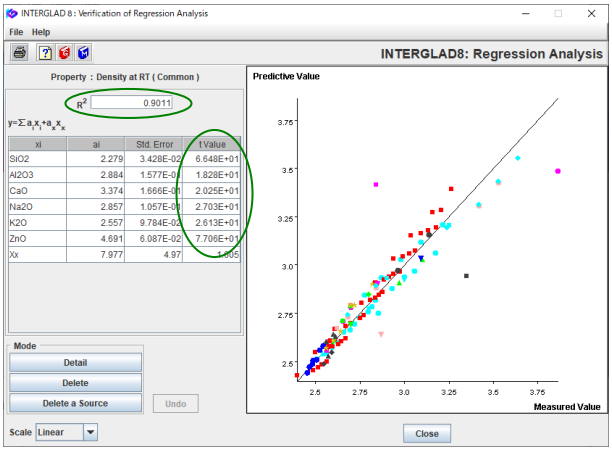




2) Execution of multiple regression analysis ([Execution of Regression Analysis] window)

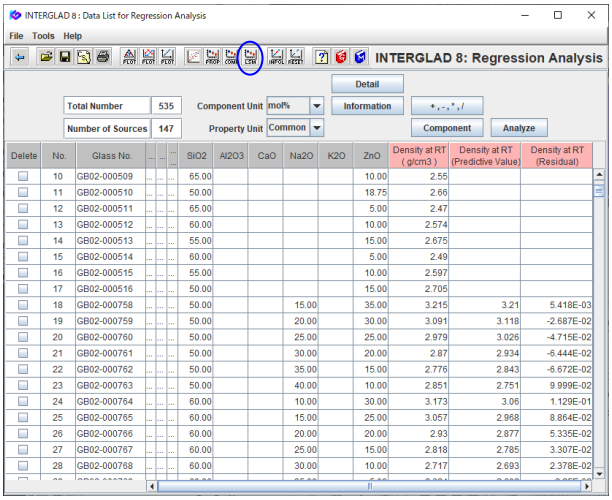


- Execute the multiple regression analysis with the default setting by clicking the [Execute] button.
- A [Question] dialog box appears. Check the dialog, and click the [OK] button.

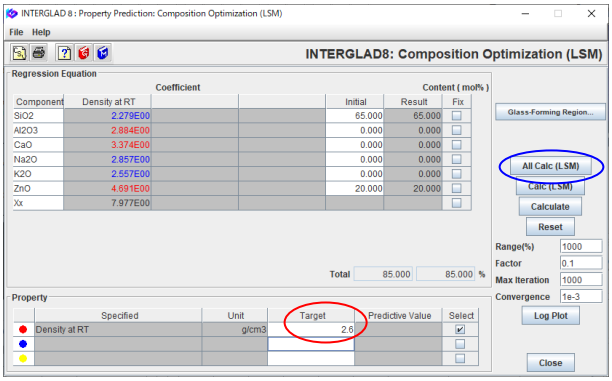


- The regression coefficients, the standard errors and t values appear in the table after the calculation.
- By clicking the [Verify Result] button, open the [Verification of Regression Analysis] window. Confirm R^2=0.9091 and t value≥18.3.

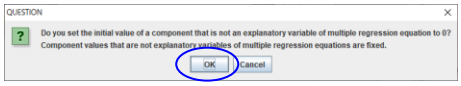
3) Composition optimization by automatic calculation

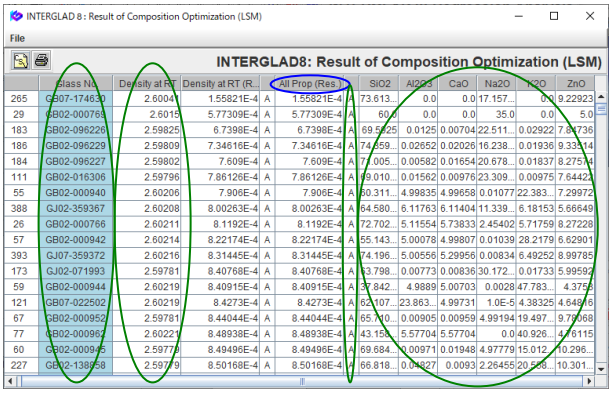


- Go back to the [Data List for Regression [Analysis] window, and by clicking the [LSM] icon open the [Composition Optimization (LSM)] window.



- Input the target value in the [Target] column (in this example, Density at RT=2.6 g/cm^3).
- Click the [All Calc (LSM)] button. The [Question] dialog box, 'Do you set the initial value of a component that is not an explanatory variable of multiple regression equation to 0?' opens, and click the [OK] button.





- After calculation, the [Result of Composition Optimization (LSM)] window opens. In the table, sort the [All Prop (Res.)] values in ascending order by clicking the title column, All Prop (Res.). In this example 153 glasses with density values lower than 0.1% to the target value are obtained. They are marked as A and their background color of Glass No. is blue. Each composition is indicated in the component columns in the right-hand side of the table.
- One of examples of composition optimized is as follows. In case of No. 388 (The model glass, GJ02-359367), SiO_2 64.58 mol%, Al_2O_3 6.12%, CaO 6.11%, Na_2O 11.34%, K_2O 6.18% and ZnO 5.67%. Its density at RT is 2.602 g/cm^3.
- The user can use also the multiple regression equation obtained in Example 7. for automatic calculation. In

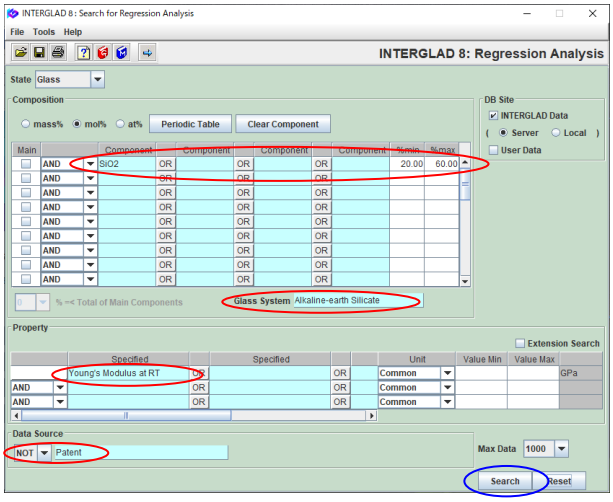
this case, compositions with 27 components as the explanatory variables are obtained.

11. Property prediction by a linear equation — Young' s modulus of alkaline-earth silicate glasses

Predict Young's modulus at RT of an alkaline-earth silicate glass with the composition of SiO_2 45%, Al_2O_3 12%, MgO 13%, CaO 20%, Y_2O_3 7% and TiO_2 3% (mol%).

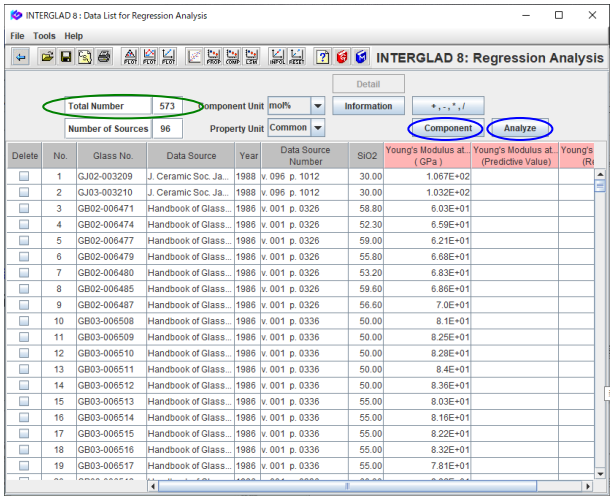
<Refer to D.2 of Chapter 3, 4.2-4.6 of Chapter 4>

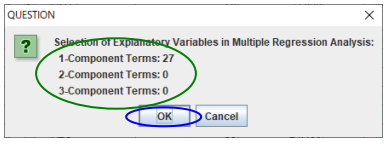
1) Specification of search conditions ([Search for Regression Analysis] window) → Search



- Specify $20 \leq SiO_2 \leq 80$ mol% for the Composition. Select 'Alkaline-earth Silicate' for the Glass System, 'Young' Modulus at RT' for the Property, and 'NOT Patent' for the Data Source. Various search conditions for the composition are available in this example. Here a simple composition condition by which many data can be collected is selected.

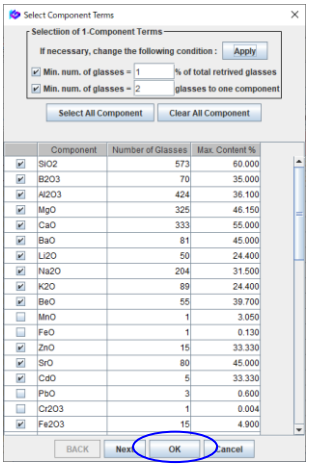
2) Search result ([Data List for Regression Analysis] window) → Selection of explanatory variables ([Selection of 1, 2, 3-Component Terms] dialog boxes)



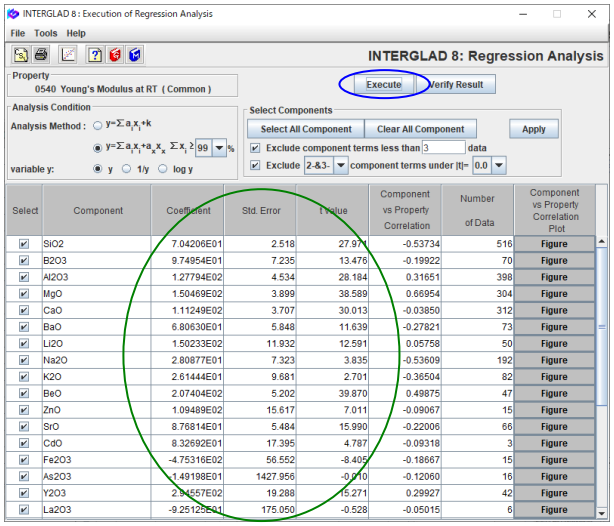


- 573 glasses are listed.
- After clicking the [Component] button, specify only 1-component terms for explanatory variables at the default setting.

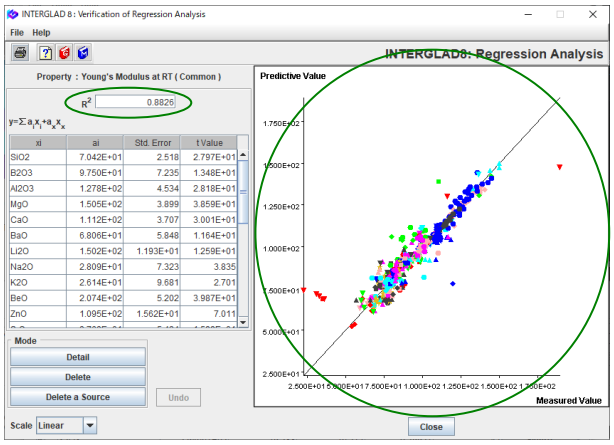
  1-componet terms: 27.



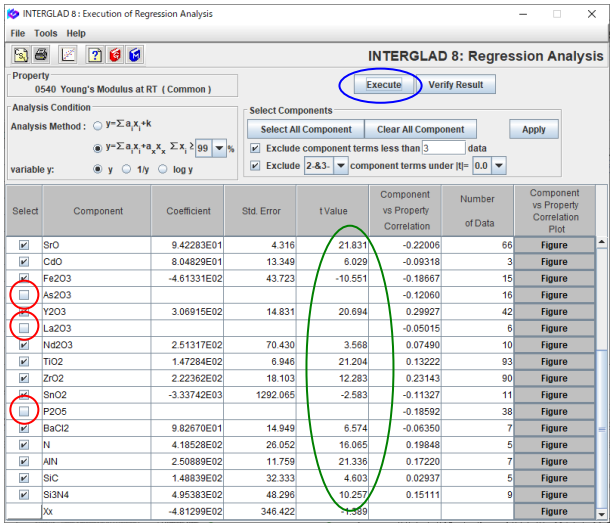
3) Execution of regression analysis ([Execution of Regression Analysis] window → [Verification of Regression Analysis] window)



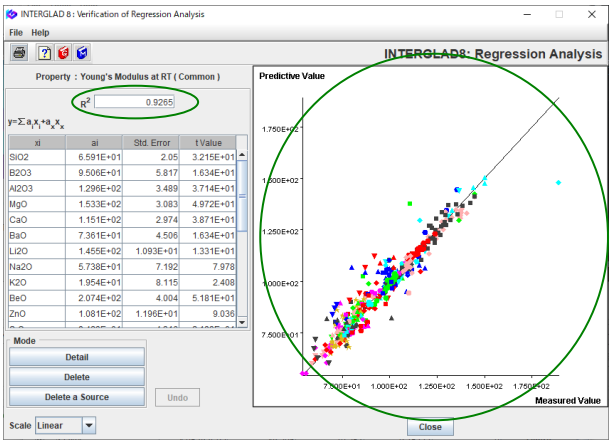
- By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens. Click the [Execute] button, and click the [OK] button in each [Question] dialog box which appears one after another. Finally the regression coefficients, etc. are shown.



- Open the [Verification of Regression analysis] window by clicking the [Verify Result] button. The contribution rate R^2 is 0.8826. A lot of plot-points concentrate near a line of y = x. If recalculation is performed after deleting separate plot-points, R^2 will increase, but the effect on the regression equation would be small. In this example a simple prediction is performed without such a data deletion.

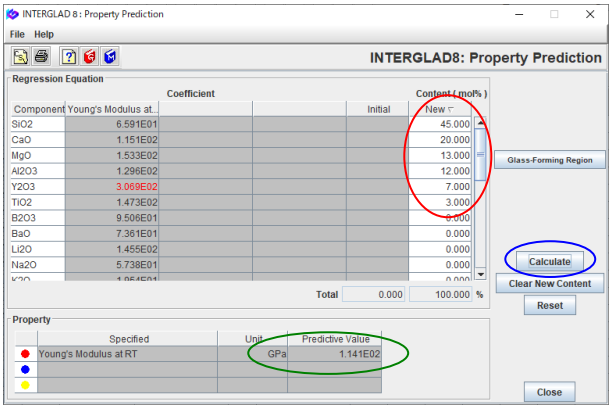


- $|t|$ values of As_2O_3, La_2O_3 and P_2O_5 are <2. Delete ✓ in the 3 checkboxes, and click the [Execute] button again.



- In this case R^2 is 0.9265 ($\geq$ 0.8).
- $|t|$ value of each component term becomes $\geq$ 2. The multiple regression equation is completed.

4) Property prediction ([Property Prediction] window)



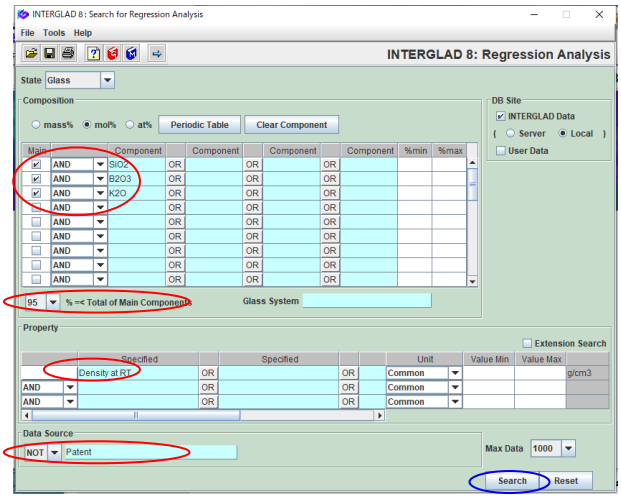
- Return to the [Data List for Regression Analysis] window, and without selecting any glass, click the [PROP] icon. In the opened [Question] dialog box, click the [OK] button, and the [Property Prediction] window opens.
- Enter the specified component values (SiO_2 45 mol%, Al_2O_3 12%, MgO 13%, CaO 20%, Y_2O_3 7%, TiO_2 3%) in the [New] cells, and click the [Calculate] button.
- 114.1 GPa for Young's modulus appears in the [Predictive Value] cell of the [Property] column.

12. Property prediction by a cubic equation — Density of boro-silicate glasses

Predict density at RT of a glass of SiO_2-B_2O_3-K_2O system with the following composition. SiO_2 40%, B_2O_3 30%, K_2O 26%, CaO 3%, Al_2O_3 1% (mol%).

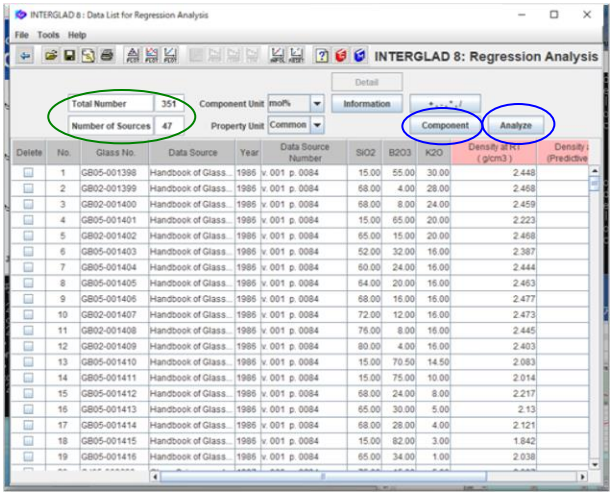
<Refer to D.2 of Chapter 3, 4.2-4.6 of Chapter 4>

1) Specification of search conditions ([Search for Regression Analysis] window) → Search



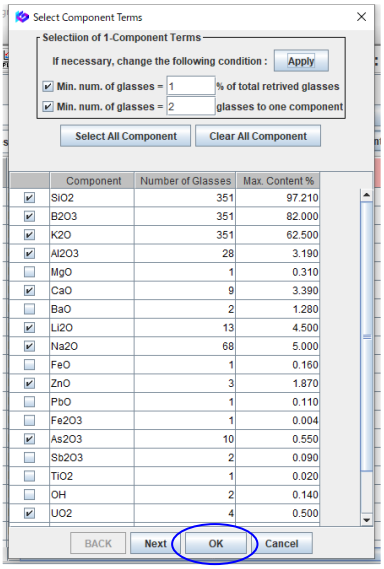
- Specify the following condition of composition. SiO_2 + B_2O_3 + $K_2O \geq 95$ mol%
- Select 'Density at RT' for the Property and 'NOT Patent' for the Data Source.

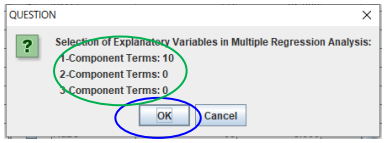
2) Search result ([Data List for Regression Analysis] window)



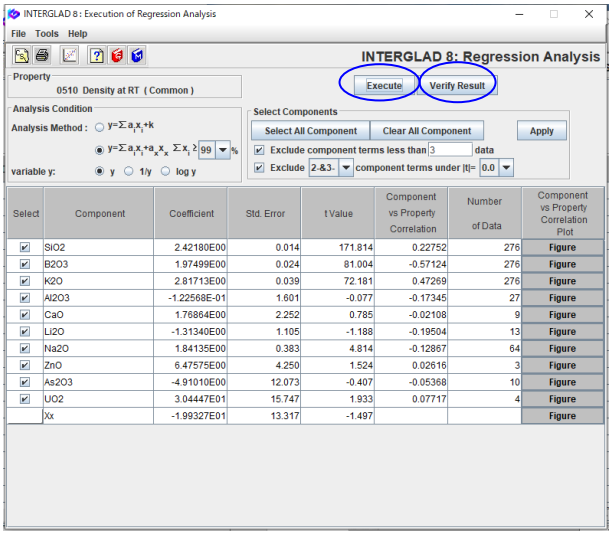
- 351 glasses are listed.
- First, regression analysis by a linear equation is carried out for comparison.

3) Regression analysis by a linear equation

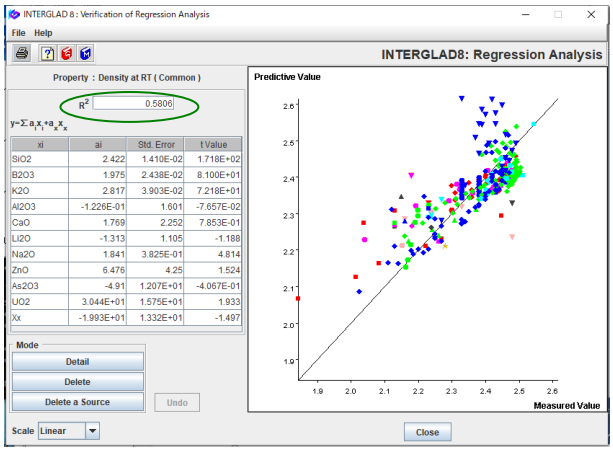




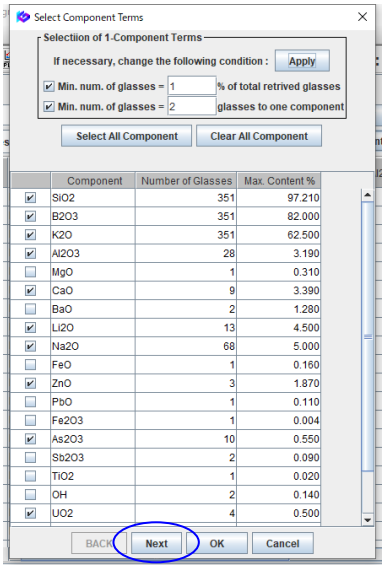
- After clicking the [Component] button, specify only 1-component terms for explanatory variables at the default setting.
  10 component terms for 1-componet terms are selected.

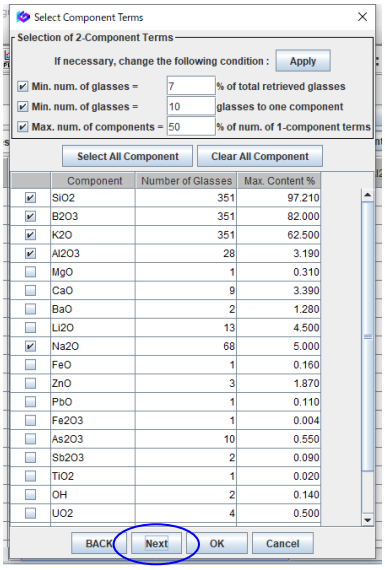


- By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens. Click the [Execute] button and the [Verify Result] button. The contribution rate R^2 is relatively low, 0.5806.

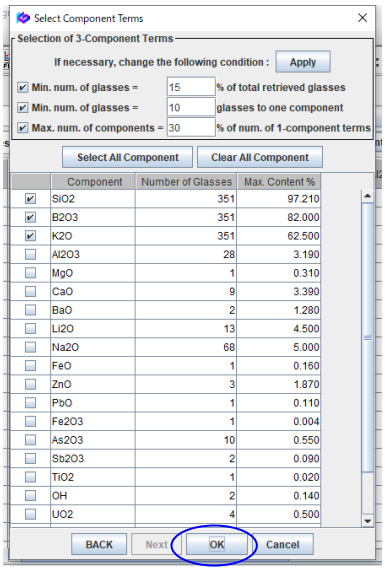


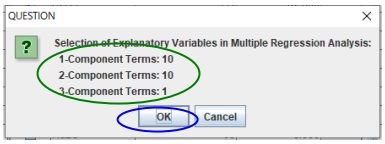
4) Regression analysis by a cubic equation

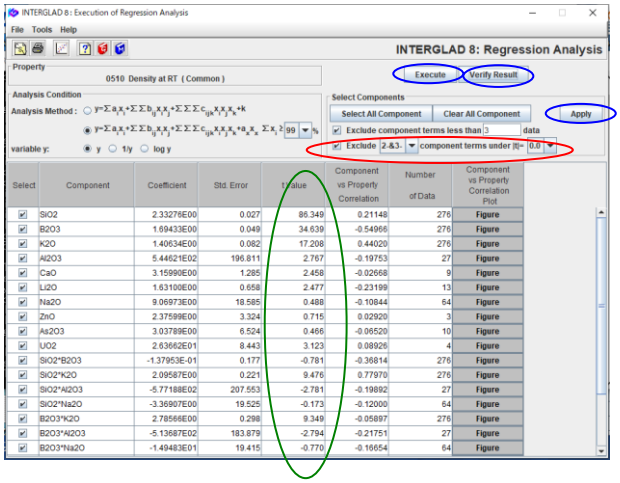


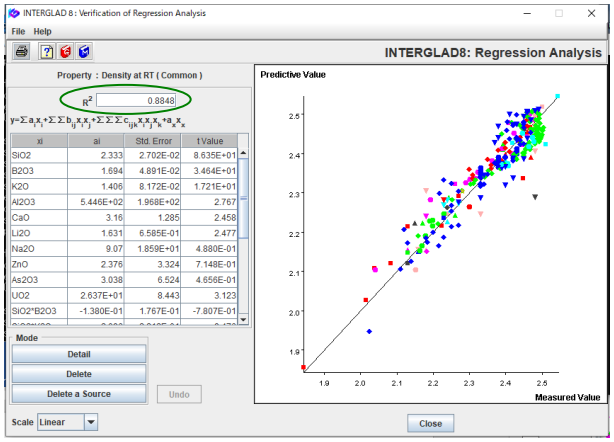


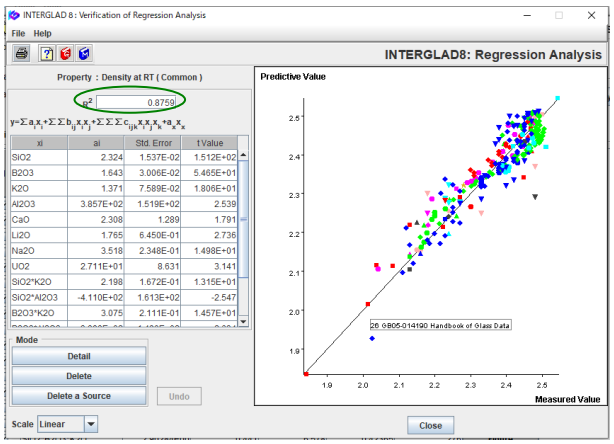
- Return to the [Data List for Regression Analysis] window, and select the 1, 2, 3-component terms at the default settings. The numbers of the selected component terms are shown in the [Question] dialog







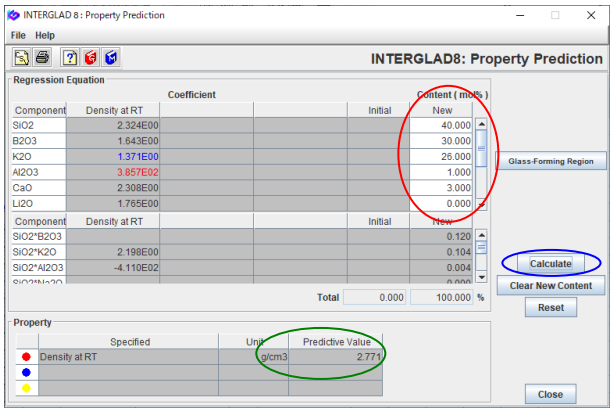




- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. R^2 is found to be 0.8848, a good result.
- Check t values in the [Execution of Regression Analysis] window. Component terms with $|t|<1$ are 7 (1-component 1terms: 3, 2-component terms: 4, 3-component terms: 0).
- In the third row of the [Select Components] column in the [Regression Analysis] window, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button, and click the [Execute] button. Exclude not in one time, step by step as follows.
  1) Exclude '2 & 3' component terms under $|t|$ = '1.0.'
  2) Exclude 'all' component terms under $|t|$ = '1.0.'
  3) Exclude 'all' component terms under $|t|$ = '1.0' again.

  Finally all the $|t|$ values become ≥1.0, and R^2=0.8759. A cubic multiple regression equation is complete.

5) Property prediction ([Property Prediction] window)



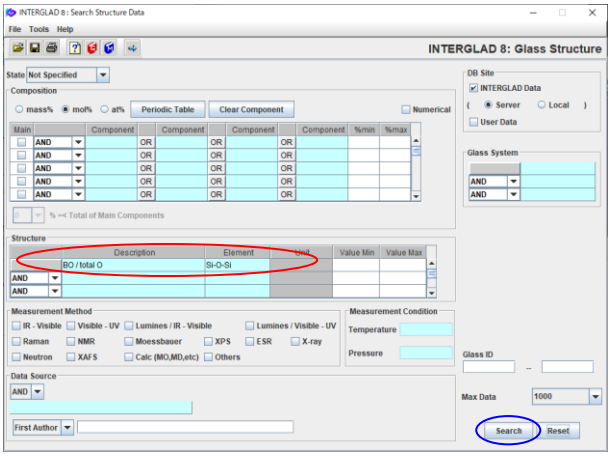
- Return to the [Data List for Regression Analysis] window, and open the [Property Prediction] window from the [PROP] icon.
- Input component values (SiO_2 40 mol%, B_2O_3 30%, K_2O 26%, CaO 3%, Al_2O_3 1%) in the [New] cells of the [Regression Equation/ Content] column, and click the [Calculate] button.
- 2.771 g/cm^3 for the calculated density appears in the [Predictive Value] cell of the [Property] column.

Search and Analysis of Structure Data

13. Investigation of correlation between composition and structure — Bridging oxygen fraction vs. SiO_2 content

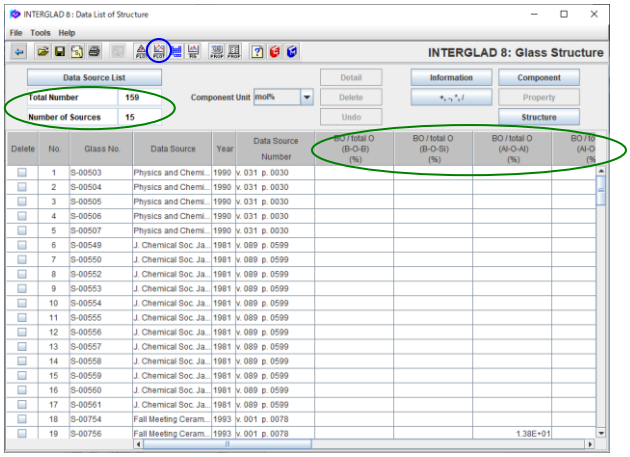
<Refer to E of Chapter 3, and 5 of Chapter 4>

1) Specification of search conditions ([Search Structure Data] window) → Search



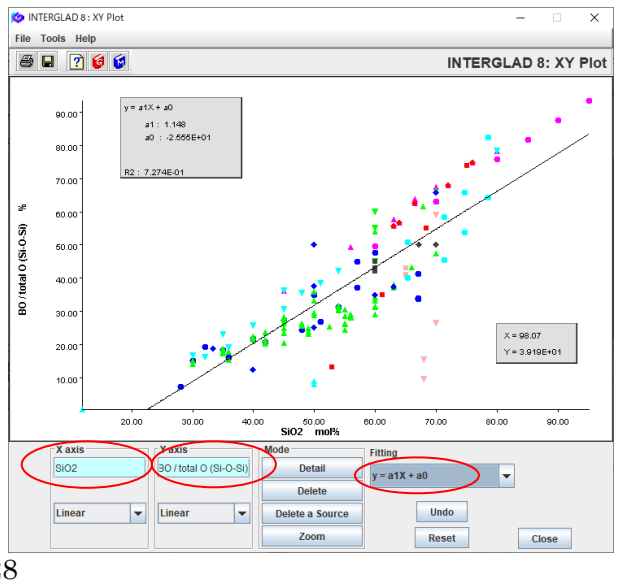
- Specify 'BO/ [totalO]' for the Description and 'Si-O-Si' for the Element in the [Structure] column. 'BO/ [totalO] (Si-O-Si)' means fraction of Bridging Oxygen bonding with Si to the total oxygen.

2) Search result ([Data List of Structure] window)



- 159 glasses of 15 data sources are listed.
- BO/[totalO] data of not only Si-O-Si but also Al-O-Al, Si-O-B, Si-O-Al etc. appear in the list.

3) Utilization of search result ([XY Plot] window)

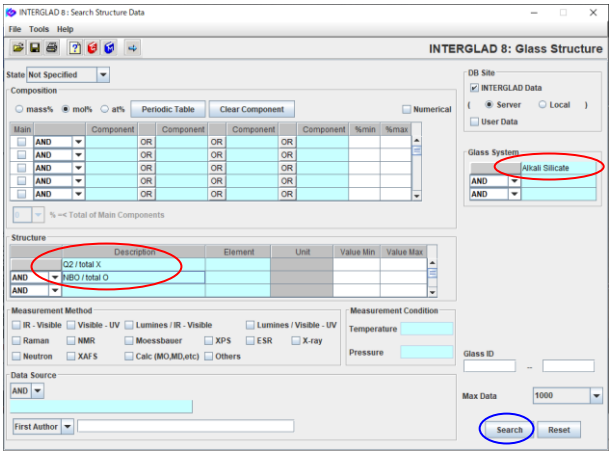


- An XY plot of SiO_2 content vs. BO/[total O] (Si-O-Si) is shown. In this example, the linear equation is selected as a fitting curve.
- In this example, as composition is not specified in the search condition, various components are contained. It is found that the bridging oxygen (Si-O-Si) increases with increasing SiO_2 content.

14. Investigation of correlation between structure factors — Q^2 vs. non-bridging oxygen fraction of alkali-silicate glasses

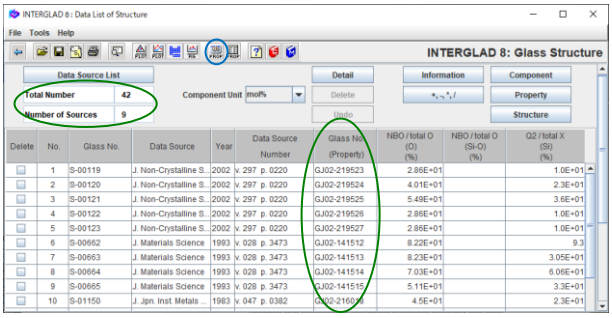
<Refer to E of Chapter 3, and 5 of Chapter 4>

1) Specification of search conditions ([Search Structure Data] window) → Search



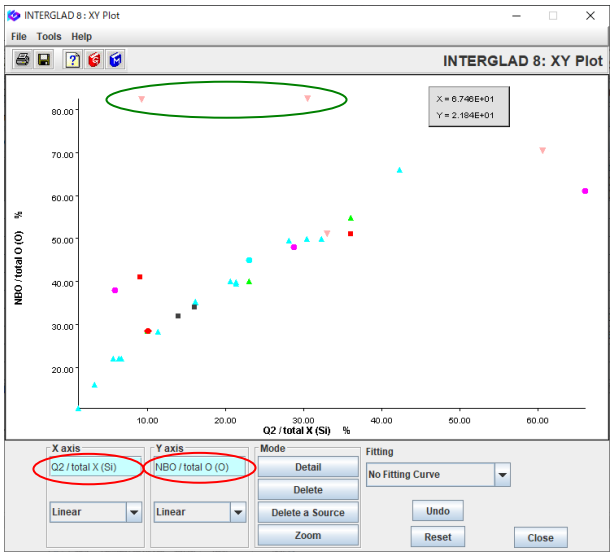
- Specify 'Alkali Silicate' for the Glass System.
  Select 'Q2/totalX' of the 'Qn Distribution' and 'NBO/ [totalO]' both in the 'Bridging Oxygen Information' for the Description of the [Structure] column. 'Q2/totalX' means Q^2 fraction in tetrahedra XO_4. 'NBO/ [totalO]' means fraction of non-bridging oxygen to the total oxygen.

2) Search result ([Data List of Structure] window)

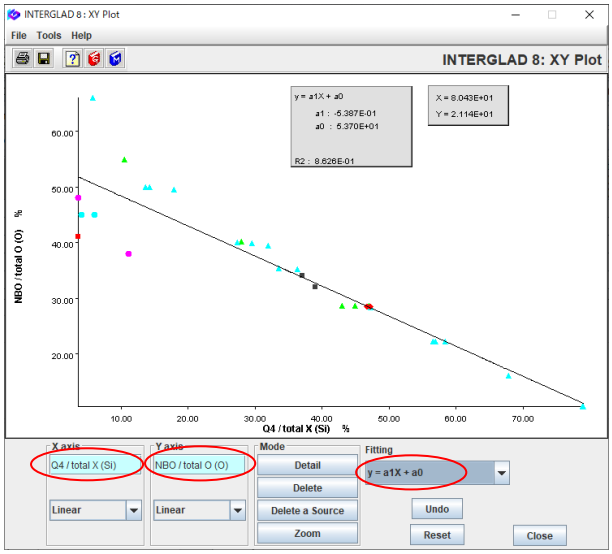


- 42 glasses of 9 data sources are listed.
- By clicking the [Search Property DB] icon, the Glass Numbers of the corresponding glasses in the Property Database appear in the list.

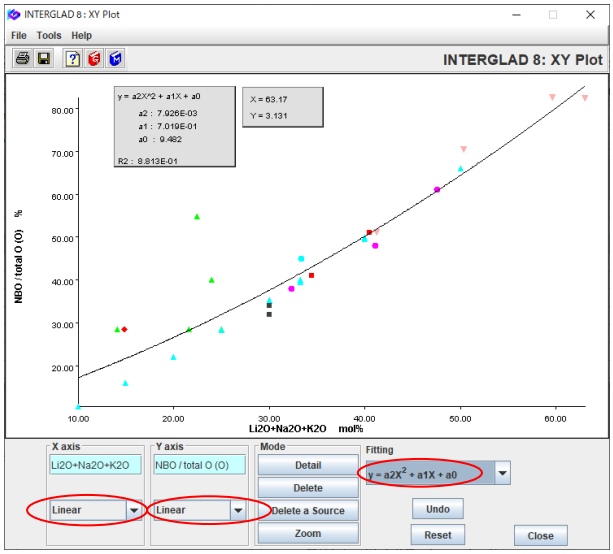
3) Correlation between Q^2 and NBO ([XY Plot] window)



- An XY Plot of Q2/totalX (Si) vs. NBO/ [totalO] (O) is shown.
- With increasing Q^2, NBO fraction increases almost proportionally. If the 2 glasses at separated positions from the others are checked in the [Detail Data of Property] windows of the corresponding Glass No. (Property), it is found that they are both rapid-quenched glasses. This could be the reason why the plot-points are separated from the others.



- For comparison, an XY Plot of Q4/totalX(Si) vs. NBO/ [totalO](O) is shown.
- The figure shows a reasonable tendency that NBO fraction decreases with increasing Q^4.



- All the searched glasses in this example contain alkali components. Relation between content of alkali oxides and fraction of non-bridging oxygen is checked in this XY Plot of content of $Li_2O+Na_2O+K_2O$ vs. NBO/ [total O] (O). It is found that the NBO fraction increases proportionally with increasing the alkali content.

(October 26, 2022)