
batchcalculator Documentation

Release 0.3.0

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November 11, 2016

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Contents:

Installation

1.1 Dependencies

- Python 2.7.x
- wxPython
- ObjectListView,
- reportlab
- numpy
- jinja2
- SQLAlchemy

If you want to export your calculations to a [TeX](#) report and be able to automatically typeset the pdf you should have a TeX distribution installed. If you don't know what TeX is [TUG \(TeX Users Group\)](#) is a good place to start.

1.2 Installing from source

Currently the preferred way is to install the package from source and manually setup the link and/or shortcuts if you want an launcher on you desktop.

You can either download the code from the [repository](#) and run:

```
[sudo] pip install batchcalc-x.x.x.tgz
```

or:

```
[sudo] easy_install batchcalc-x.x.x.tgz
```

or clone the repository:

```
git clone https://github.com/lmmentel/batchcalculator.git
```

pull the latest version and update:

```
git pull
```

then *cd* to the package directory and run:

```
[sudo] python setup.py install
```

If the installation finishes without errors you should be able to start the GUI from the command line by typing:

```
$ zbc
```

Tutorial

To illustrate the usage of the **Batch Calculator** we will calculate the the amounts of reactants required to perform the synthesis of ZSM-22 described by Ernst et al.¹.

The batch composition is given as (p. 139 of ¹):

- 13 K₂O
- Al₂O₃
- 91 SiO₂
- 3670 H₂O
- 27 NH₂(CH₂)₆NH₂

The reactants used are:

- silica sol (40% silica; Ludox AS40, DuPont) was
- Al₂(SO₄)₃* 18H₂O
- KOH
- 1,6-diaminohexane (HMDA)
- water

The amounts of reactants used in the synthesis are presented in the table below for reference

Name	Amount [g]
KOH	7.8
Al ₂ (SO ₄) ₃	3.5
silica sol	72
water	301
HMDA	16.7

After starting the **Batch Calculator** the main window appears. As a first step we need to add the components by clicking on the **Add/Remove** button in the **Components** panel.

¹ Ernst, S., Weitkamp, J., Martens, J. A., & Jacobs, P. A. (1989). Synthesis and shape-selective properties of ZSM-22. *Applied Catalysis*, 48(1), 137–148. doi:10.1016/S0166-9834(00)80271-7

The screenshot shows the 'Zeolite Batch Calculator' application window. It has a menu bar with 'File', 'View', 'Calculation', 'Database', 'Syntheses', and 'Help'. The main interface is divided into three sections: 'Components', 'Chemicals', and 'Results'. The 'Components' section has a table with columns 'Label' and 'Moles' and a large text area saying 'Add Components'. The 'Chemicals' section has a table with columns 'Label' and 'Concentration' and a large text area saying 'Add Chemicals'. Both the 'Components' and 'Chemicals' sections have an 'Add/Remove' button below them. The 'Results' section has a table with columns 'Label', 'Mass [g]', and 'Volume [cm3]' and a large text area saying 'This list is empty'. To the right of the 'Results' table is a 'Scaling options' panel with four radio buttons: 'No scaling' (selected), 'Scale all', 'Scale to sample', and 'Scale to item'. A 'Calculate' button is located at the bottom right of the 'Results' section.

Components	
Label	Moles
Add Components	

Add/Remove

Chemicals	
Label	Concentration
Add Chemicals	

Add/Remove

Results		
Label	Mass [g]	Volume [cm3]
This list is empty		

Scaling options

- ☒ No scaling
- ☐ Scale all
- ☐ Scale to sample
- ☐ Scale to item

Calculate

A dialog window should appear with all the components that are currently available in the database.

Choose Zeolite Components...

	Name	Formula	Molecular Weight	Short name	Category
<input type="checkbox"/>	sodium oxide	Na ₂ O	61.9789		zeolite
<input type="checkbox"/>	potassium oxide	K ₂ O	94.1960		zeolite
<input type="checkbox"/>	aluminium oxide	Al ₂ O ₃	101.9613		zeolite
<input type="checkbox"/>	silicone dioxide	SiO ₂	60.0843		zeolite
<input type="checkbox"/>	water	H ₂ O	18.0152		zeolite
<input type="checkbox"/>	tetramethylammonium chloride	(CH ₃) ₄ NCl	109.5985	TMACl	template
<input type="checkbox"/>	tetramethylammonium hydro...	(CH ₃) ₄ N(OH)	91.1528	TMAOH	template
<input type="checkbox"/>	hexamethylenediamine	NH ₂ (CH ₂) ₆ NH ₂	116.2058	HMDA	template
<input type="checkbox"/>	choline chloride	(CH ₃) ₃ N(CH ₂) ₂ OHCl	139.6247		template
<input type="checkbox"/>	ethanol	C ₂ H ₅ OH	46.0688	EtOH	zgm
<input type="checkbox"/>	ethylene glycol	C ₂ H ₆ O ₂	62.0682	glycol	zgm
<input type="checkbox"/>	1-propanol	C ₃ H ₇ OH	60.0956	PrOH	zgm
<input type="checkbox"/>	2-propanol	C ₃ H ₇ OH	60.0956	iPrOH	zgm
<input type="checkbox"/>	glycerol	C ₃ H ₈ O ₃	92.0944		zgm
<input type="checkbox"/>	1-butanol	C ₄ H ₉ OH	74.1224	ButOH	zgm
<input type="checkbox"/>	sulfur trioxide	SO ₃	80.0582		byproduct

Cancel OK

We need to choose the appropriate components by ticking the correct boxes as shown below and click the **OK** button.

Choose Zeolite Components...

	Name	Formula	Molecular Weight	Short name	Category
<input type="checkbox"/>	sodium oxide	Na ₂ O	61.9789		zeolite
<input checked="" type="checkbox"/>	potassium oxide	K ₂ O	94.1960		zeolite
<input checked="" type="checkbox"/>	aluminium oxide	Al ₂ O ₃	101.9613		zeolite
<input checked="" type="checkbox"/>	silicone dioxide	SiO ₂	60.0843		zeolite
<input checked="" type="checkbox"/>	water	H ₂ O	18.0152		zeolite
<input type="checkbox"/>	tetramethylammonium chloride	(CH ₃) ₄ NCl	109.5985	TMACl	template
<input type="checkbox"/>	tetramethylammonium hydro...	(CH ₃) ₄ N(OH)	91.1528	TMAOH	template
<input checked="" type="checkbox"/>	hexamethylenediamine	NH ₂ (CH ₂) ₆ NH ₂	116.2058	HMDA	template
<input type="checkbox"/>	choline chloride	(CH ₃) ₃ N(CH ₂) ₂ OHCl	139.6247		template
<input type="checkbox"/>	ethanol	C ₂ H ₅ OH	46.0688	EtOH	zgm
<input type="checkbox"/>	ethylene glycol	C ₂ H ₆ O ₂	62.0682	glycol	zgm
<input type="checkbox"/>	1-propanol	C ₃ H ₇ OH	60.0956	PrOH	zgm
<input type="checkbox"/>	2-propanol	C ₃ H ₇ OH	60.0956	iPrOH	zgm
<input type="checkbox"/>	glycerol	C ₃ H ₈ O ₃	92.0944		zgm
<input type="checkbox"/>	1-butanol	C ₄ H ₉ OH	74.1224	ButOH	zgm
<input type="checkbox"/>	sulfur trioxide	SO ₃	80.0582		byproduct

Cancel OK

By doing that the selected components are now shown in the main window with the default amounts equal to 1.

Zeolite Batch Calculator

File View Calculation Database Syntheses Help

Components		Chemicals	
Label	Moles	Label	Concentration
potassium oxide	1.0000	Add Chemicals	
aluminium oxide	1.0000		
silicone dioxide	1.0000		
water	1.0000		
HMDA	1.0000		

Add/Remove

Add/Remove

Results		
Label	Mass [g]	Volume [cm3]
This list is empty		

Scaling options

- ☒ No scaling
- ☐ Scale all
- ☐ Scale to sample
- ☐ Scale to item

Calculate

To adjust the amount double click on the appropriate number and enter the correct amount, in our case the amounts are:

Zeolite Batch Calculator

File View Calculation Database Syntheses Help

Components

Label	Moles
potassium oxide	13.0000
aluminium oxide	1.0000
silicone dioxide	91.0000
water	3670.0000
HMDA	27.0000

Add/Remove

Chemicals

Add Chemicals

Add/Remove

Results

Label	Mass [g]	Volume [cm3]
This list is empty		

Scaling options

- ☒ No scaling
- ☐ Scale all
- ☐ Scale to sample
- ☐ Scale to item

Calculate

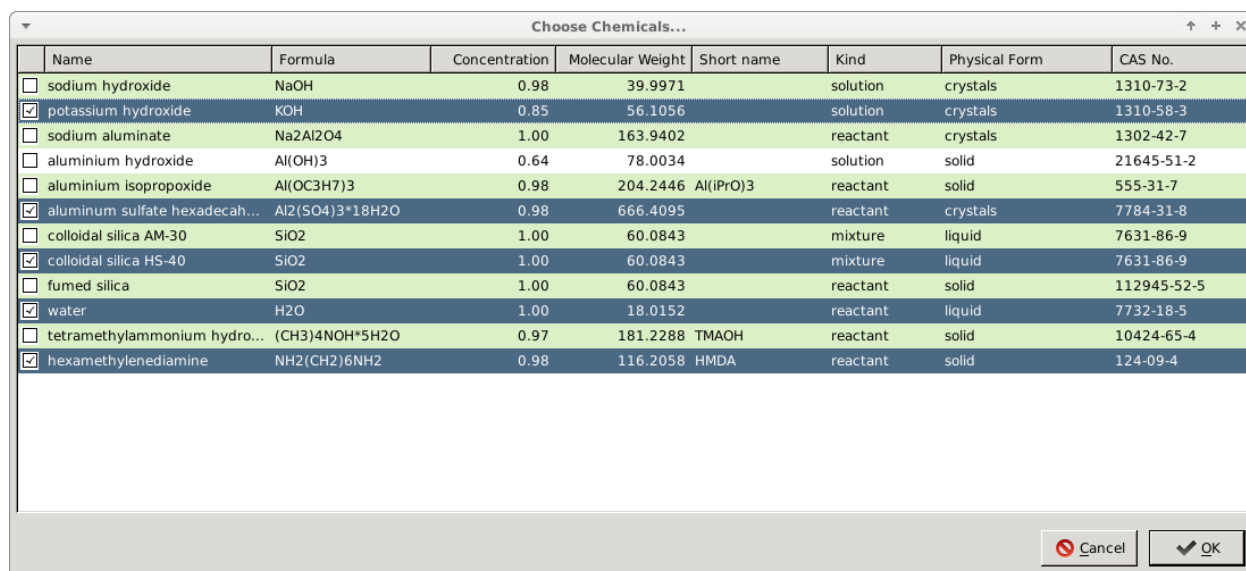
Now we need to add the chemicals by clicking the **Add/Remove** button in the **Chemicals** panel to open the dialog with all the chemicals in the database that are potential sources for the selected components

Choose Chemicals...

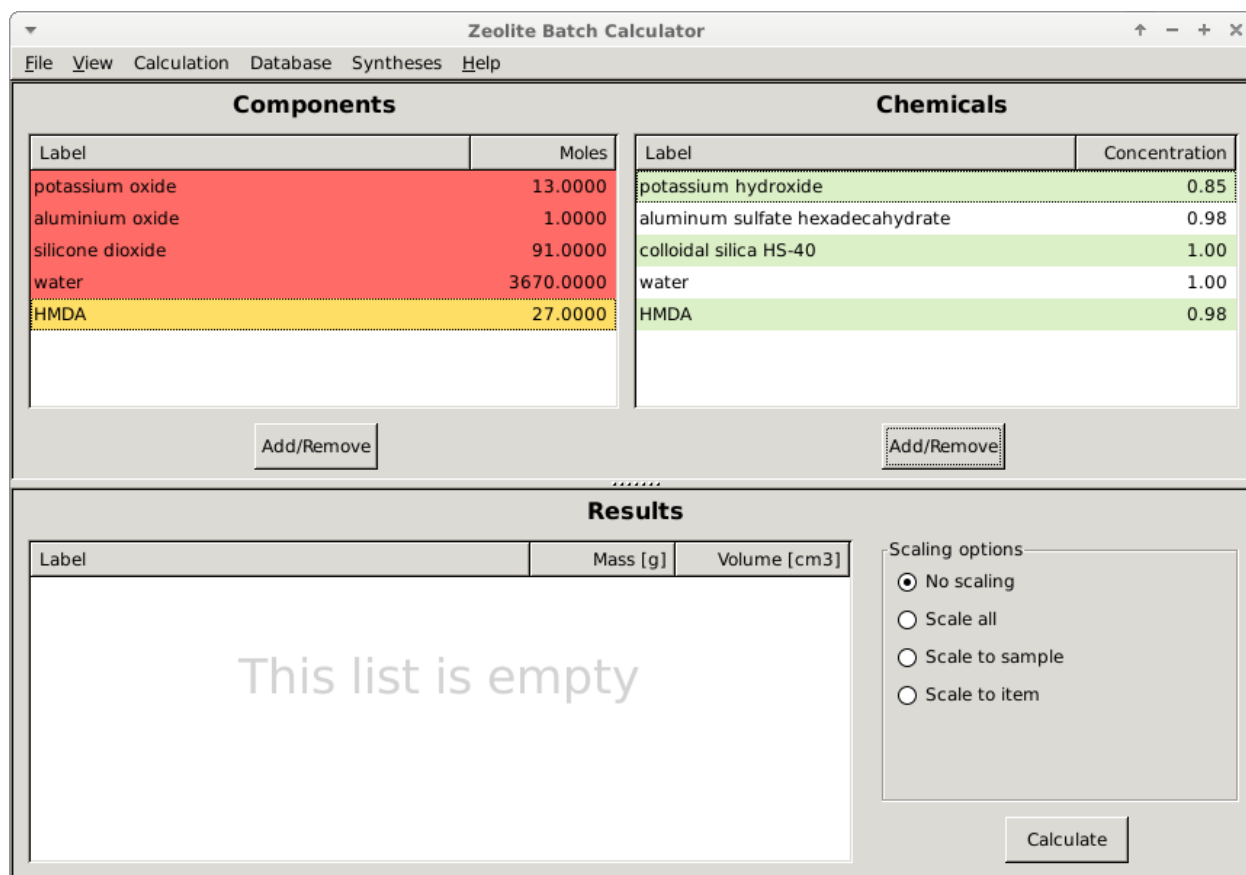
	Name	Formula	Concentration	Molecular Weight	Short name	Kind	Physical Form	CAS No.
<input type="checkbox"/>	sodium hydroxide	NaOH	0.98	39.9971		solution	crystals	1310-73-2
<input type="checkbox"/>	potassium hydroxide	KOH	0.85	56.1056		solution	crystals	1310-58-3
<input type="checkbox"/>	sodium aluminate	Na ₂ Al ₂ O ₄	1.00	163.9402		reactant	crystals	1302-42-7
<input type="checkbox"/>	aluminium hydroxide	Al(OH) ₃	0.64	78.0034		solution	solid	21645-51-2
<input type="checkbox"/>	aluminium isopropoxide	Al(OC ₃ H ₇) ₃	0.98	204.2446	Al(iPrO) ₃	reactant	solid	555-31-7
<input type="checkbox"/>	aluminum sulfate hexadecahydrate	Al ₂ (SO ₄) ₃ ·18H ₂ O	0.98	666.4095		reactant	crystals	7784-31-8
<input type="checkbox"/>	colloidal silica AM-30	SiO ₂	1.00	60.0843		mixture	liquid	7631-86-9
<input type="checkbox"/>	colloidal silica HS-40	SiO ₂	1.00	60.0843		mixture	liquid	7631-86-9
<input type="checkbox"/>	fumed silica	SiO ₂	1.00	60.0843		reactant	solid	112945-52-5
<input type="checkbox"/>	water	H ₂ O	1.00	18.0152		reactant	liquid	7732-18-5
<input type="checkbox"/>	tetramethylammonium hydroxide	(CH ₃) ₄ NOH·5H ₂ O	0.97	181.2288	TMAOH	reactant	solid	10424-65-4
<input type="checkbox"/>	hexamethylenediamine	NH ₂ (CH ₂) ₆ NH ₂	0.98	116.2058	HMDA	reactant	solid	124-09-4

Cancel OK

We can now select the appropriate chemicals by ticking the boxes in the first column and click **OK**.



We can see that the chemical we successfully added to the main window with their default concentration/purities depending on the kind of chemical. The concentrations/purities can be adjusted in the same way as the amounts of components by double clicking the fields and entering the desired values.



By clicking the **Calculate** button, the calculation will be performed and the result will appear in the **Results** panel.

Zeolite Batch Calculator

File View Calculation Database Syntheses Help

Components		Chemicals	
Label	Moles	Label	Concentration
potassium oxide	13.0000	potassium hydroxide	0.85
aluminium oxide	1.0000	aluminum sulfate hexadecahydrate	0.98
silicone dioxide	91.0000	colloidal silica HS-40	1.00
water	3670.0000	water	1.00
HMDA	27.0000	HMDA	0.98

Add/Remove

Add/Remove

Results		
Label	Mass [g]	Volume [cm3]
potassium hydroxide	1716.1713	
aluminum sulfate hexadecahydrate	680.0097	
colloidal silica HS-40	13669.1782	10555.350
water	57098.3802	57270.191
HMDA	3201.5884	

Scaling options

☒ No scaling

☐ Scale all

☐ Scale to sample

☐ Scale to item

Calculate

On the right hand side of the **Results** panel are the scaling options to adjust the batch size. In order to compare our results to the ones used in the paper we will rescale all the masses to the 16.7 g of HMDA using the **Scale to item** option.

Zeolite Batch Calculator

File View Calculation Database Syntheses Help

Components		Chemicals	
Label	Moles	Label	Concentration
potassium oxide	13.0000	potassium hydroxide	0.85
aluminium oxide	1.0000	aluminum sulfate hexadecahydrate	0.98
silicone dioxide	91.0000	colloidal silica HS-40	1.00
water	3670.0000	water	1.00
HMDA	27.0000	HMDA	0.98
Add/Remove		Add/Remove	

Results

Label	Mass [g]	Volume [cm3]
potassium hydroxide	1716.1713	
aluminum sulfate hexadecahydrate	680.0097	
colloidal silica HS-40	13669.1782	10555.350
water	57098.3802	57270.191
HMDA	3201.5884	

Scaling options

☐ No scaling

☐ Scale all

☐ Scale to sample

☒ Scale to item

Calculate

After selecting that option and clicking **Calculate** again a dialog will appear where we will select **HMDA** and enter a value of **16.7** to scale all the masses (and volumes) to 16.7 g of **HMDA** and click **OK**.

Choose chemical and desired mass

	Label	Mass [g]
<input type="checkbox"/>	potassium hydroxide	1716.1713
<input type="checkbox"/>	aluminum sulfate hexadecahydrate	680.0097
<input type="checkbox"/>	colloidal silica HS-40	13669.1782
<input type="checkbox"/>	water	57098.3802
<input checked="" type="checkbox"/>	HMDA	3201.5884

Amount:

The updated masses are now shown in the **Results** panel instead of the initial results.

Zeolite Batch Calculator

File View Calculation Database Syntheses Help

Components		Chemicals	
Label	Moles	Label	Concentration
potassium oxide	13.0000	potassium hydroxide	0.85
aluminium oxide	1.0000	aluminum sulfate hexadecahydrate	0.98
silicone dioxide	91.0000	colloidal silica HS-40	1.00
water	3670.0000	water	1.00
HMDA	27.0000	HMDA	0.98

Add/Remove

.....

Results		
Label	Mass [g]	Volume [cm3]
potassium hydroxide	8.9518	
aluminum sulfate hexadecahydrate	3.5470	
colloidal silica HS-40	71.3006	55.058
water	297.8343	298.731
HMDA	16.7000	

Scaling options

☐ No scaling
☐ Scale all
☐ Scale to sample
☒ Scale to item 16.70

Calculate

The result can be stored internally for further reference or modification by clicking the **Add current** option from the **Syntheses** drop down menu

Show All

Add current

A dialog will be opened with an option to provide additional information about the synthesis of the material

Save a Synthesis Record

Save a Synthesis Record

Name

Target Material

Laborant

Reference

Temperature

Crystallization Time

Stirring

Description

Components

Label	Moles
potassium oxide	13.0000
aluminium oxide	1.0000
silicone dioxide	91.0000
water	3670.0000
HMDA	27.0000

Chemicals

Label	Mass [g]
potassium hydr...	1716.1713
aluminum sulfat...	680.0097
colloidal silica H...	13669.1782
water	57098.3802
HMDA	3201.5884

Add

Cancel

16

Chapter 2. Tutorial

After filling in the form we can click the **Add** button that will store the information in the internal database.

Save a Synthesis Record

Save a Synthesis Record

Name

ZSM-22 by Ernst

Target Material

ZSM-22

Laborant

The Scientist

Reference

Ernst, S., Weitkamp, J., Martens, J. A., & Jacobs, P. A.

Temperature

433

Crystallization Time

48

Stirring

50 rpm

Description

The autoclaves were filled with this gel and rotated at 50 rpm in a furnace heated at 433 K. After 2 days the autoclaves were quenched in cold water and the white powder was recovered by filtering and washing with deionized water.

Components

Label	Moles
potassium oxide	13.0000
aluminium oxide	1.0000
silicone dioxide	91.0000
water	3670.0000
HMDA	27.0000

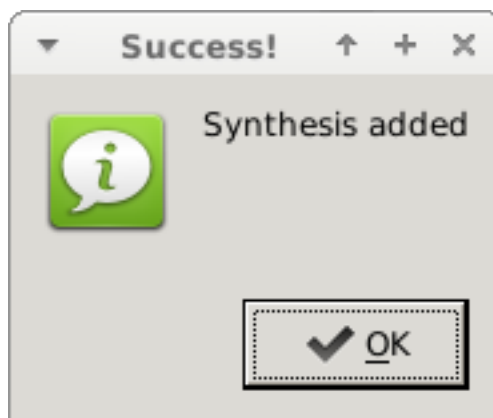
Chemicals

Label	Mass [g]
potassium hydr...	1716.1713
aluminum sulfat...	680.0097
colloidal silica H...	13669.1782
water	57098.3802
HMDA	3201.5884

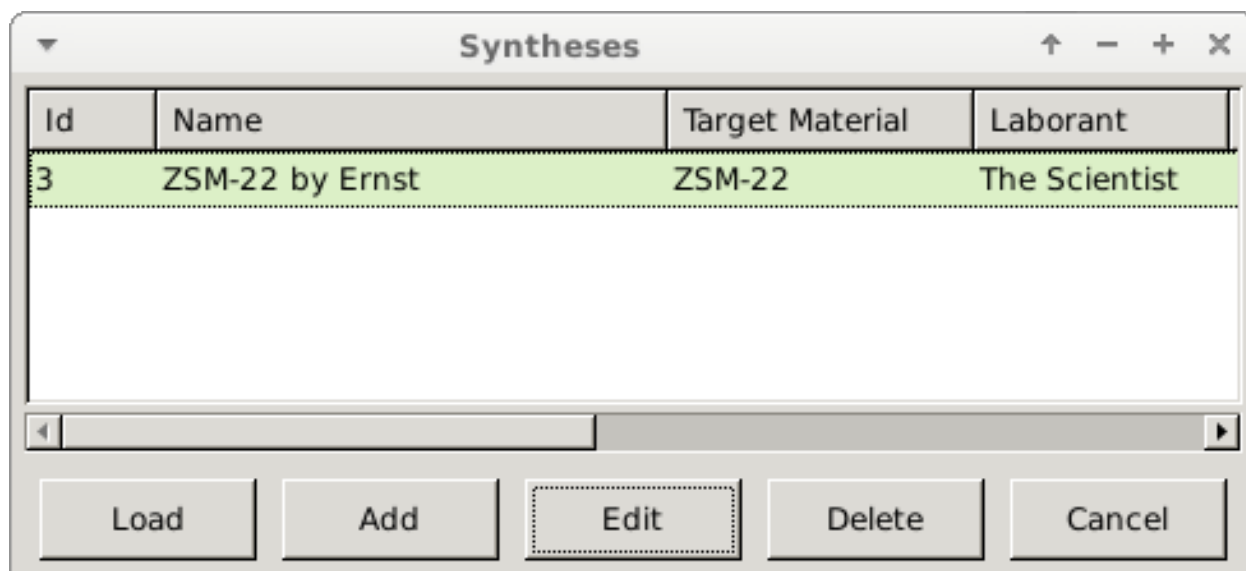
Add

Cancel

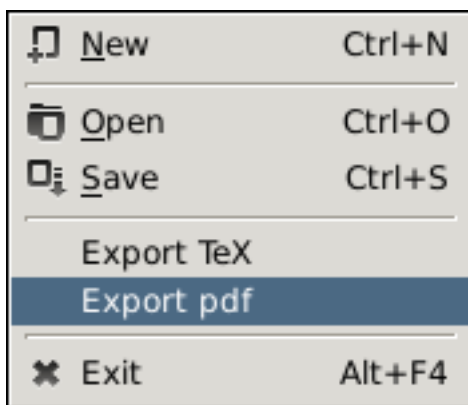
The dialog confirming the success of the modification should be displayed.



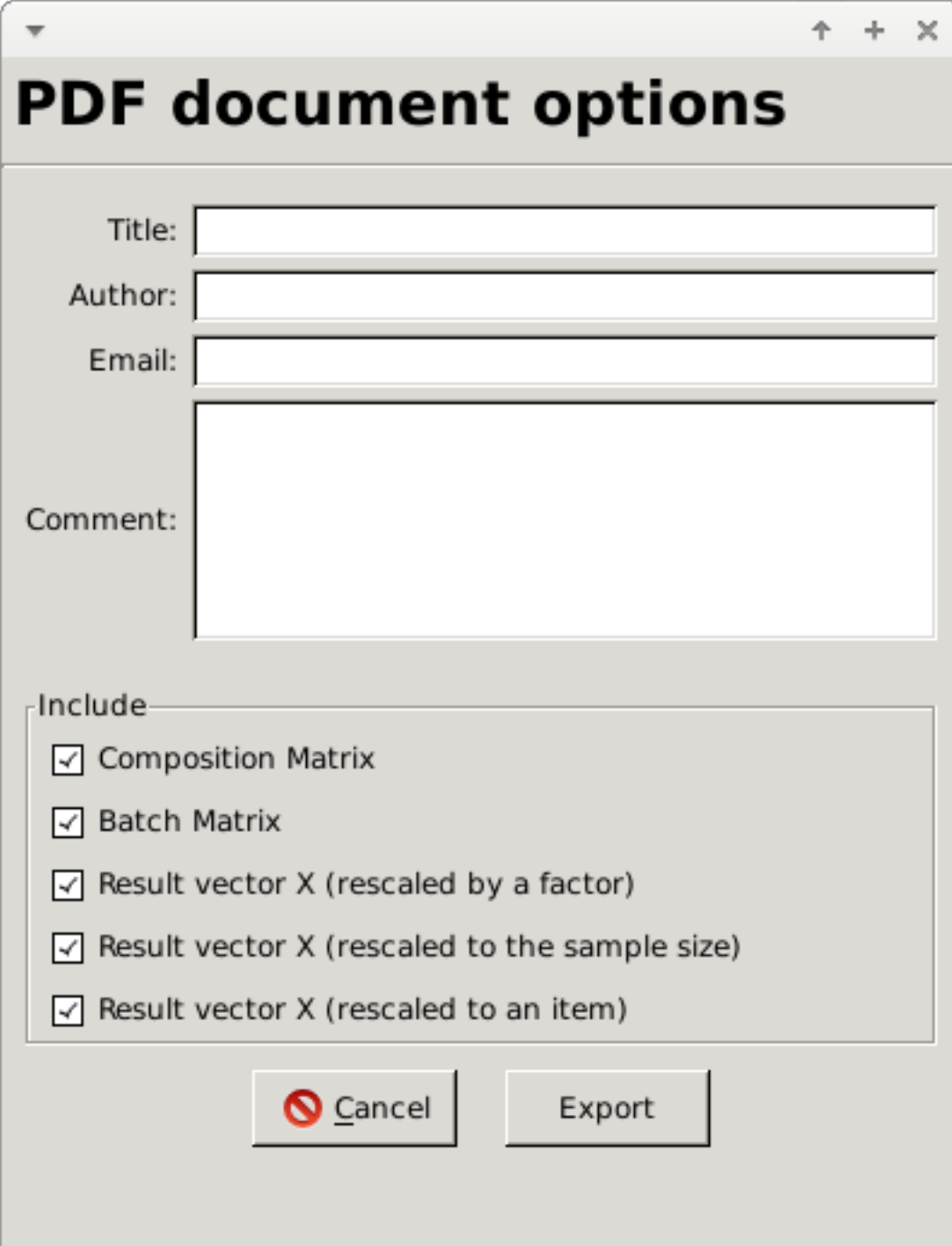
To verify or access the stored syntheses go to the **Syntheses** menu and select **Show All** which will open up a dialog with the stored records. From here the syntheses can be loaded back into the *Batch Calculator* deleted or modified.



To finalize we can export a lab report for this synthesis by selecting the **Export to pdf** option from the **File** menu



Another dialog appears with additional options for the report, where also the sections of the report can be chosen



A screenshot of a software dialog box titled "PDF document options". The dialog has a standard window header with a close button (X) and two other icons. The main area contains several input fields: "Title:", "Author:", "Email:", and a larger "Comment:" field. Below these is a section titled "Include" containing five checked checkboxes: "Composition Matrix", "Batch Matrix", "Result vector X (rescaled by a factor)", "Result vector X (rescaled to the sample size)", and "Result vector X (rescaled to an item)". At the bottom are two buttons: "Cancel" (with a red prohibition icon) and "Export".

PDF document options

Title:



Author:

Email:

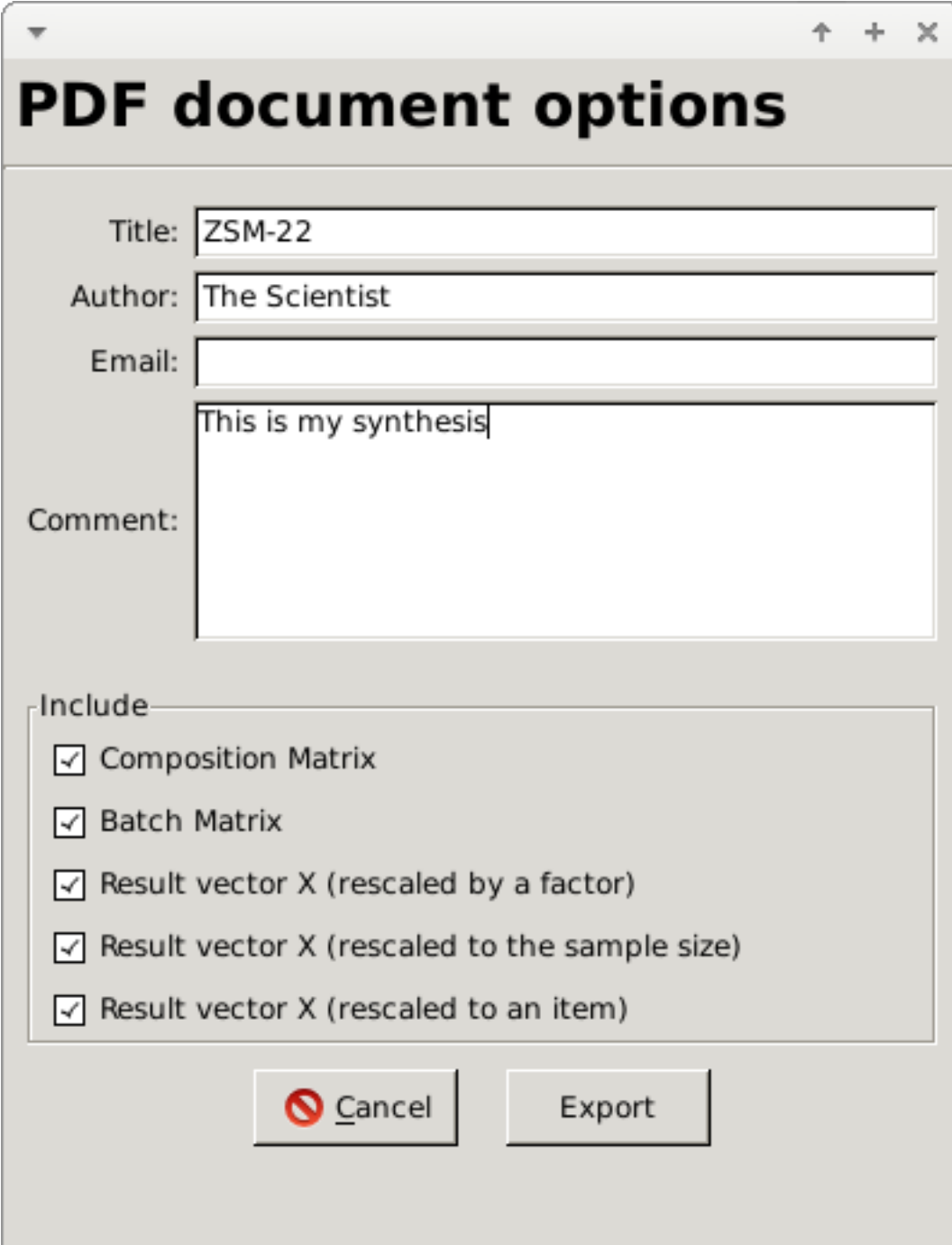
Comment:

Include

- ☒ Composition Matrix
- ☒ Batch Matrix
- ☒ Result vector X (rescaled by a factor)
- ☒ Result vector X (rescaled to the sample size)
- ☒ Result vector X (rescaled to an item)

 **Cancel**  **Export**

After filling out the details and clicking **Export**



A screenshot of a software dialog box titled "PDF document options". The dialog has a title bar with standard window controls (minimize, maximize, close). The main area contains several input fields: "Title:" with the value "ZSM-22", "Author:" with the value "The Scientist", "Email:" (empty), and a larger "Comment:" text area containing the text "This is my synthesis". Below these fields is a section titled "Include" which contains five checked checkboxes: "Composition Matrix", "Batch Matrix", "Result vector X (rescaled by a factor)", "Result vector X (rescaled to the sample size)", and "Result vector X (rescaled to an item)". At the bottom of the dialog are two buttons: "Cancel" (with a red prohibition icon) and "Export".

PDF document options

Title: ZSM-22


Author: The Scientist

Email:

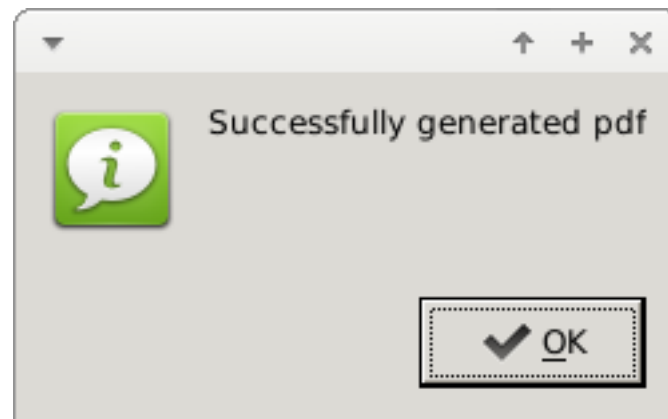
Comment: This is my synthesis

Include

- ☒ Composition Matrix
- ☒ Batch Matrix
- ☒ Result vector X (rescaled by a factor)
- ☒ Result vector X (rescaled to the sample size)
- ☒ Result vector X (rescaled to an item)

 Cancel **Export**

a dialog will appear to choose the file name and finally a message should appear that the pdf was successfully generated.



The report should like similar to the one below

19:56:25 04.09.2016

ZSM-22

$$13.0\text{K}_2\text{O}:1.0\text{Al}_2\text{O}_3:91.0\text{SiO}_2:3670.0\text{H}_2\text{O}:27.0\text{HMDA}$$

The Scientist

Composition Matrix [C]

Compound	K2O	Al2O3	SiO2	H2O	NH2(CH2)6NH2
Mole ratio	13.000	1.000	91.000	3670.000	27.000
Weight [g]	1224.548	101.961	5467.671	66115.784	3137.557
Mol. wt. [g/mol]	94.196	101.961	60.084	18.015	116.206

Batch Matrix [B]

Compound	K2O	Al2O3	SiO2	H2O	NH2(CH2)6NH2
KOH (85.00%)	0.7135	0.0000	0.0000	0.2865	0.0000
Al2(SO4)3*18H2O (98.00%)	0.0000	0.1530	0.0000	0.4866	0.0000
SiO2 (100.00%)	0.0000	0.0000	0.4000	0.6000	0.0000
H2O (100.00%)	0.0000	0.0000	0.0000	1.0000	0.0000
NH2(CH2)6NH2 (98.00%)	0.0000	0.0000	0.0000	0.0000	1.0000

Results [X] (SF=100.0000)

Substance	Formula	Mass [g]	Volume [cm3]	Weighted Mass [g]
potassium hydroxide	KOH	17.1617		
aluminum sulfate hexadecahydrate	Al2(SO4)3*18H2O	6.8001		
colloidal silica HS-40	SiO2	136.6918	105.5535	
water	H2O	570.9838	572.7019	
HMDA	NH2(CH2)6NH2	32.0159		
Sum		763.6533	678.2554	

Results [X] (SF= 1.0000)

Substance	Formula	Mass [g]	Volume [cm3]	Weighted Mass [g]
potassium hydroxide	KOH	1716.1713		
aluminum sulfate hexadecahydrate	Al2(SO4)3*18H2O	680.0097		
colloidal silica HS-40	SiO2	13669.1782	10555.3500	
water	H2O	57098.3802	57270.1907	
HMDA	NH2(CH2)6NH2	3201.5884		
Sum		76365.3277	67825.5407	

Results [X] (SF=191.7119)

Substance	Formula	Mass [g]	Volume [cm3]	Weighted Mass [g]
potassium hydroxide	KOH	8.9518	55.0584	
aluminum sulfate hexadecahydrate	Al2(SO4)3*18H2O	3.5470		
colloidal silica HS-40	SiO2	71.3006		
water	H2O	297.8343	298.7305	
HMDA	NH2(CH2)6NH2	16.7000		
Sum		398.3338	353.7889	

Comments

This is my synthesis

Indices and tables

- `genindex`
- `modindex`
- `search`