VSAS V1.0

Documentation

1. Introduction

VSAS is mainly used for fully automatic fitting of small Angle scattering curve, and at the same time, it can judge the matching degree between theoretical model and experimental data of the research object, and obtain quantitative information such as size, volume fraction, composition and distribution of nano-structure in accordance with the actual situation.

Small-angle scattering is mainly used to characterize nanostructures in materials, including the average size, particle size distribution, shape, specific surface area and interface fractal of nanostructures, so it can provide extremely useful 3D information in many fields. However, the existing small-angle scattering data processing software can not completely solve the problems such as required manual adjustment, low efficiency, cumbersome process, low accuracy, and subjectivity.

VSAS solves the problems of low data processing efficiency, tedious, low accuracy and complex operation of similar software. Based on the functions of similar software abroad and the requirements of common projects, a new fully automated method of small-angle scattering data fitting based on statistics is applied in VSAS. The specific model is selected based on the sample system to be processed, and the automatic fitting of data is realized while the manual fitting function is retained. The influence of subjectivity on data fitting is weakened and the objectivity and accuracy of fitting results are improved.

2. Hardware and software environment

CPU: Any Intel or AMD x86-64 processor

Hard disk: 2GB or more

Memory: 2GB or more

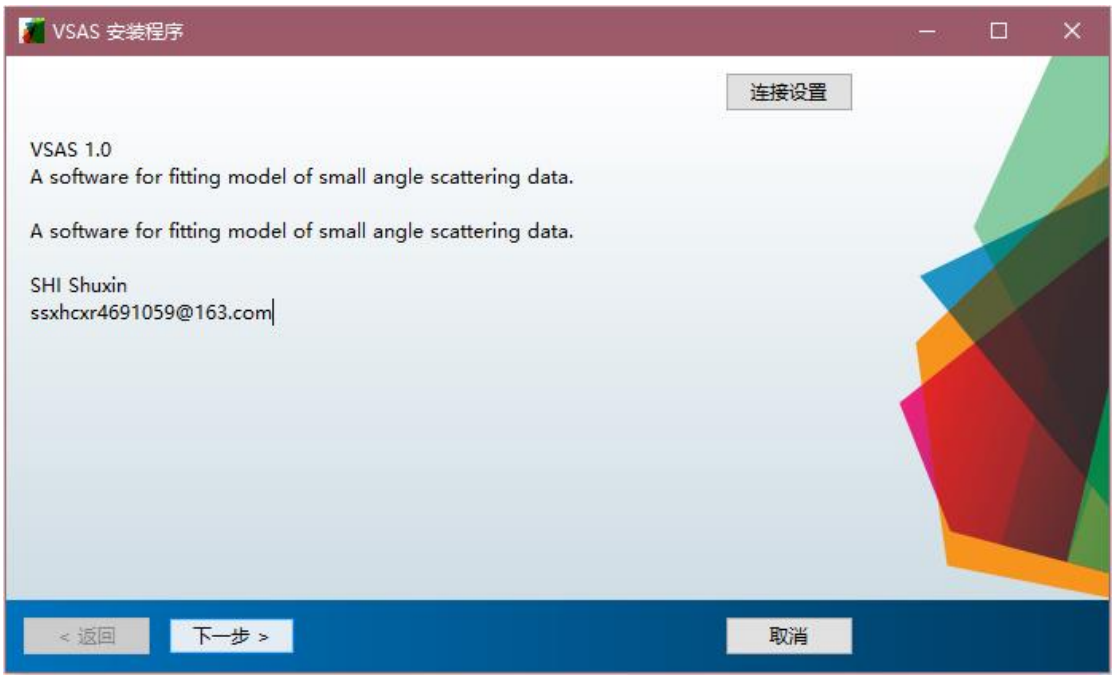
OS: Windows 10or higher version

Software: MATLAB Runtime 9.1 or higher version (included in installer)

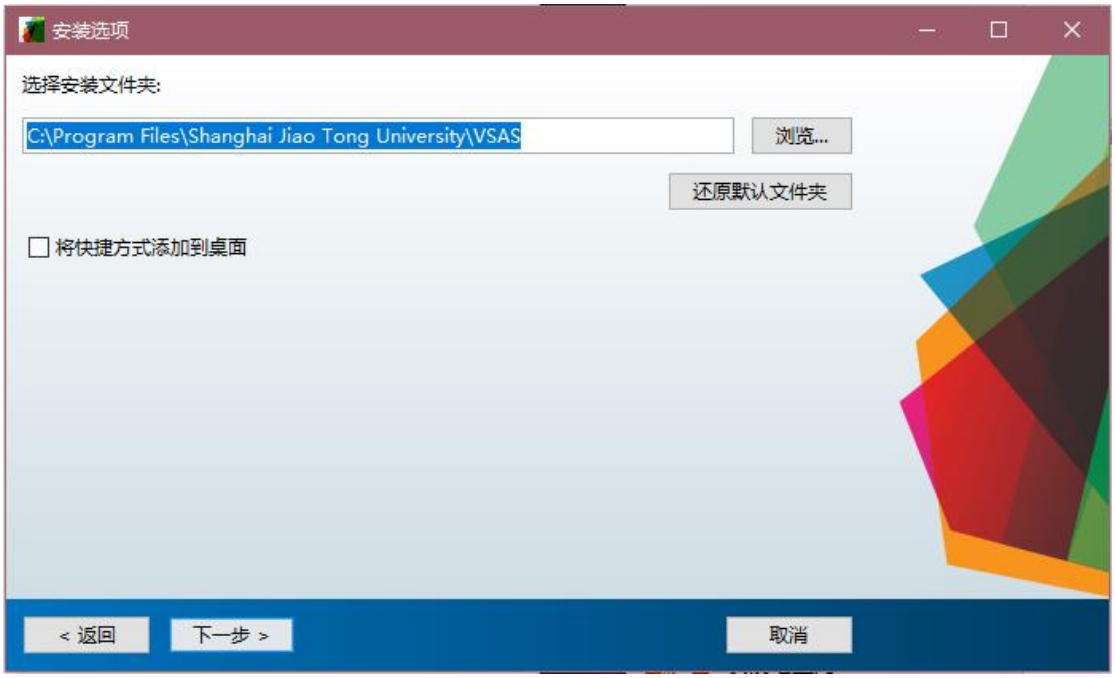
3. Installation

The installer of VSAS is available at https://na.sjtu.edu.cn/ for free. If the MATLAB Runtime has not been installed in your computer before, please select the option. The main steps of installation of VSAS are shown as following:

3.1 Start to install VSAS



3.2 Choose installation folder for VSAS



3.3 Choose installation folder for MATLAB Runtime (if needed)

4. Operation

4.1 Start

After the VSAS is launched, the users can double-click the VSAS shortcut on the desktop or run the VSAS.exe file in the installation directory to start the VSAS software. Enter the initial software startup interface as shown in Figure 4.1, and wait for the user to select the software mode and load the small-angle scattering data file. A dataset is provided for testing. Users can download the zip file from https://na.sjtu.edu.cn/.

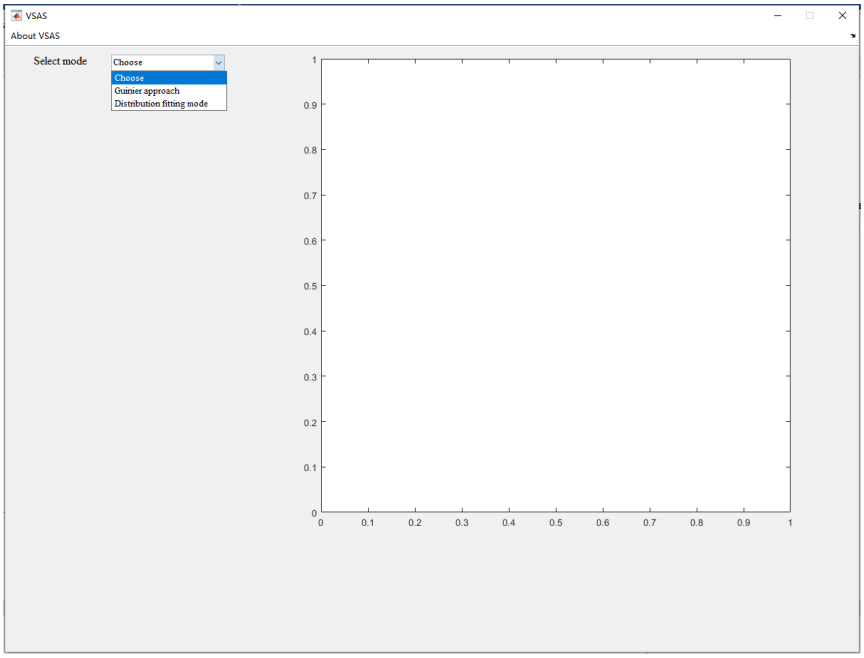


Figure 4.1 Initial startup interface of VSAS

4.2 Mode selection

Click the Select mode button, and choose the fitting mode as shown in Figure 4.1.

4.2.1. If choose “Guinier approach”, and click “Load” button, the “Select Data File” page pops up. Select the required fitting small-angle scattering data file, as shown in Fig 4.2.1(a). The data will be automatically loaded into the fitting software and

displayed on the right side of the interface.

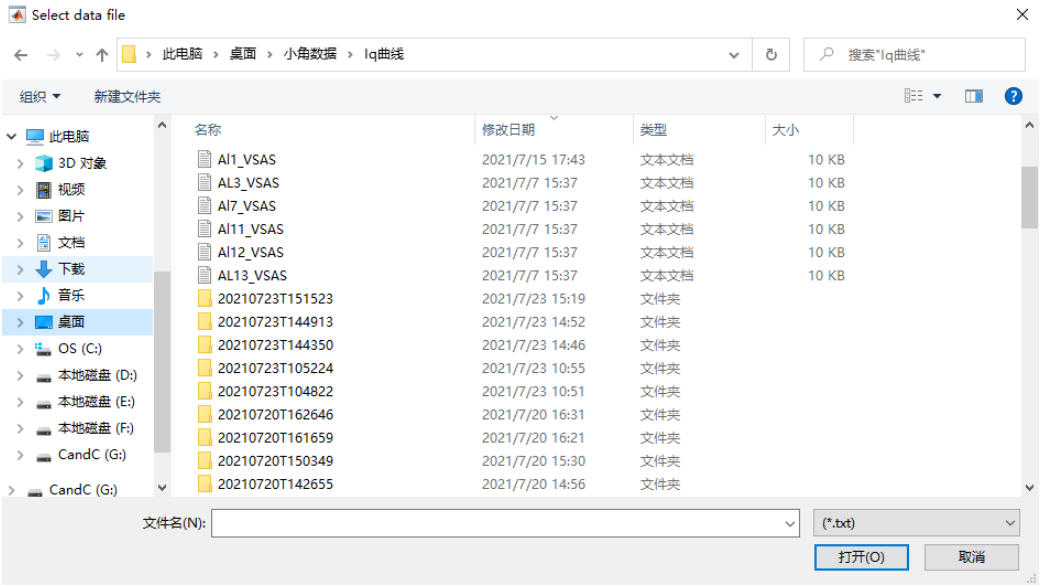


Figure 4.2.1(a) File loading interface of VSAS

a. Return to the main page, and the Porod fitting part can fit the small-angle scattering data according to the corresponding formula in Figure 4.2.1(b). Click "Help" button to obtain the specific meaning of each fitting parameter under Porod law.

b. Return to the main page, and Guinier fitting part can fit the small-angle scattering data according to the corresponding formula in Figure 4.2.1(b). Click "Help" button to obtain the specific meaning of each fitting parameter under Guinier's law.

Under the "Parameters" panel, the fractal dimension Parameters α, the minimum and maximum values of scattering vector q_{min}, and the q_{max} parts can be adjusted to fit the required range of scattering vector and the possible fractal dimension of the structure.

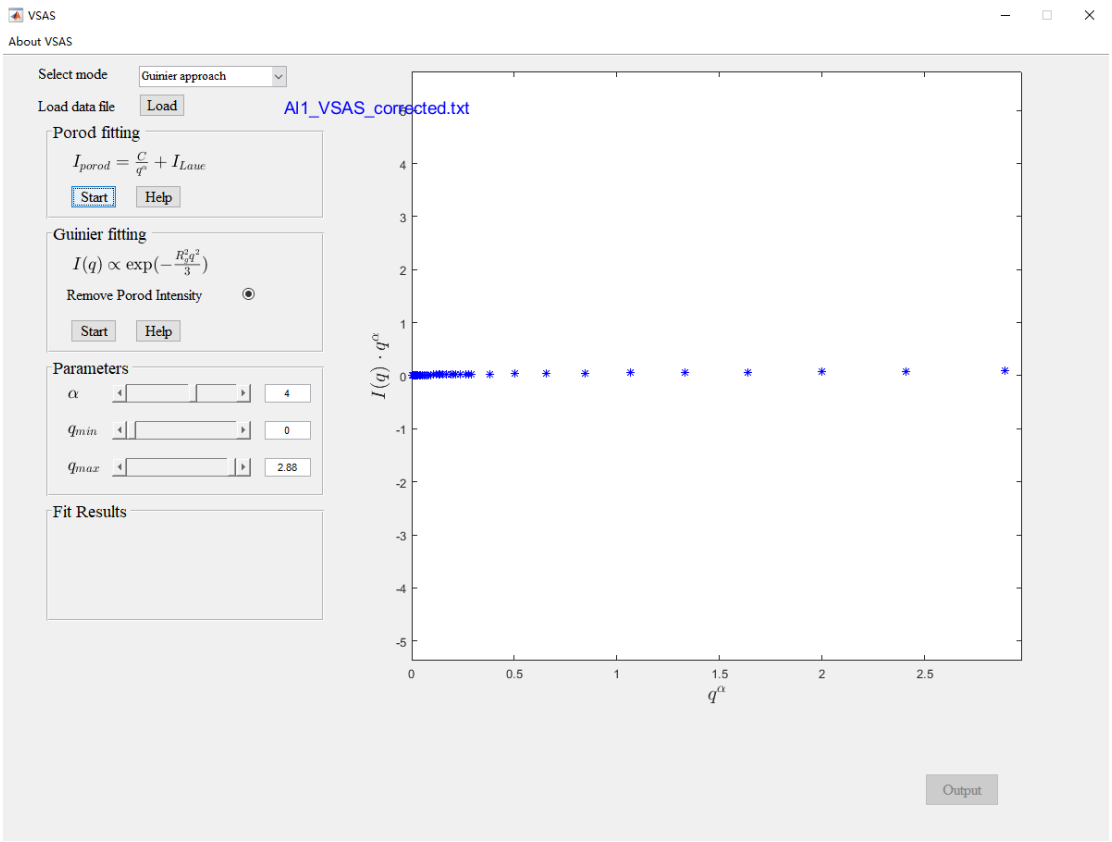


Figure 4.2.1(b) Fitting interface of Guinier approach mode

4.2.2. If you select "Distribution fitting Mode", click the "Load" button, and the "Select Data File" page will pop up. Select the required small-angle scattering data file, as shown in Figure 4.2.1(a). The data will be automatically loaded into the fitting software and displayed on the right side of the interface. Click the "Setting" option to manually set the fitting parameter range, model parameters, and algorithm super-parameters of Bayesian optimization and grid search method, as shown in Figure 4.2.2(a). Click "Help" button to obtain the specific meanings of each fitting parameter under this mode, as shown in Figure 4.4.2(b).

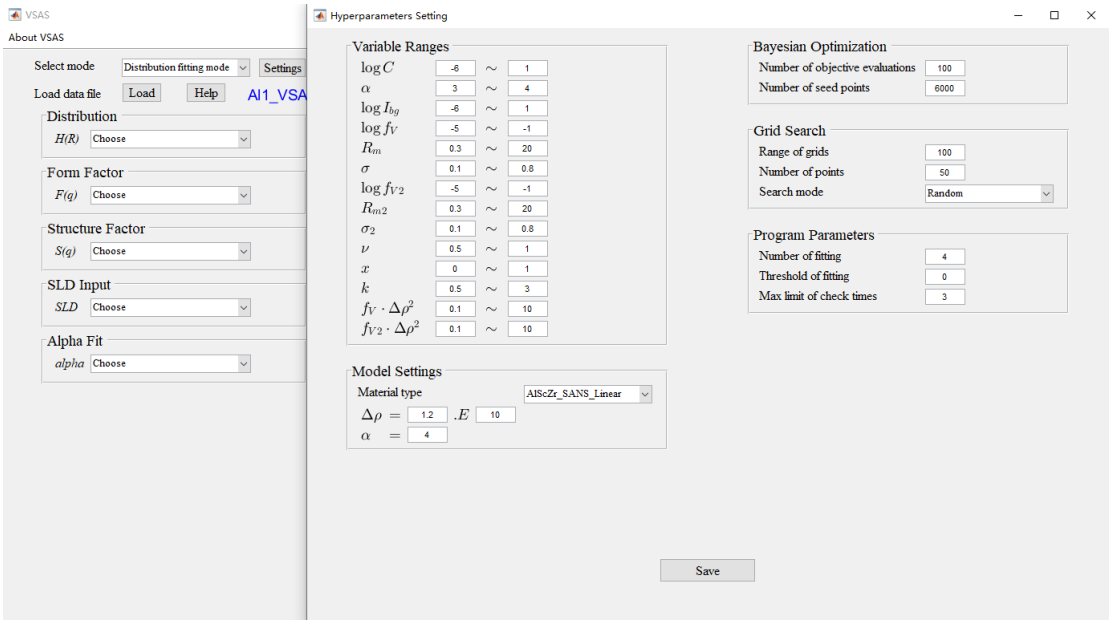


Figure 4.2.2(a) Setting menu

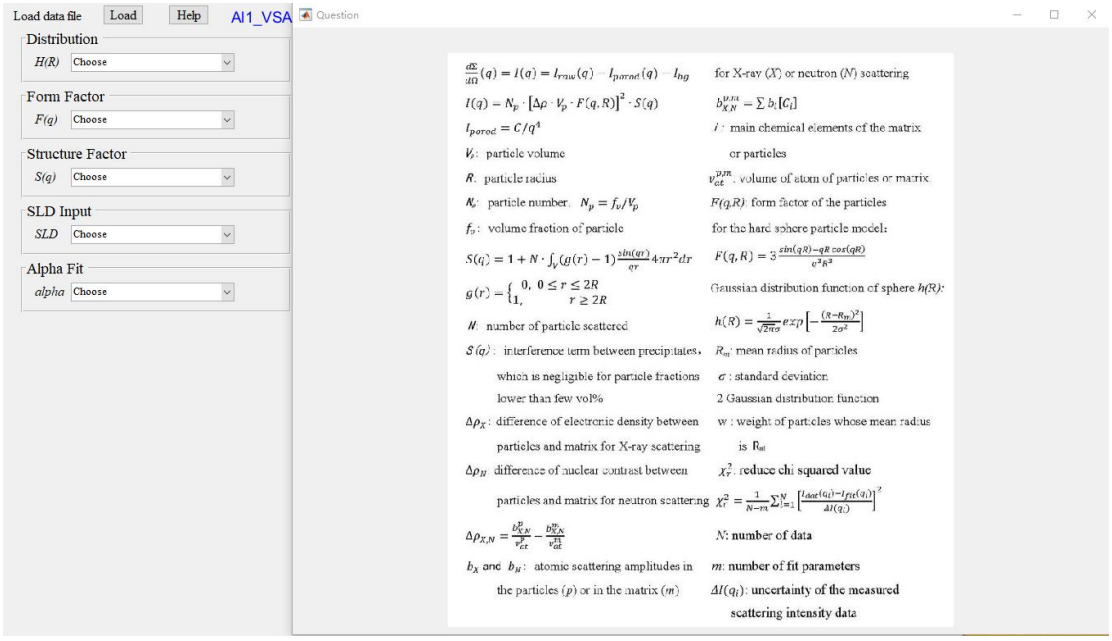


Figure 4.2.2(b) Help menu

4.3 Fitting parameter preset

Return to the main page and find the appropriate fitting model corresponding to the particle system in the "Distribution" section. In the "Form Factor" part, the users select appropriate corresponding particle morphology model, and the "Structure Factor" part depends on whether the particle system is sparse. If so, it should select "Dilute System S(Q)=1". In the "SLD Input" part,

the users can decide whether scattering intensity density can be selected as one of the fitting parameters. In the "Alpha Fit" part, the fractal dimension of large size particles can be selected as one of the fitting parameters. The "Parameters" part can be preset to adjust the desired fitting size, distribution, volume fraction and background signal strength, as shown in Figure 4.3.

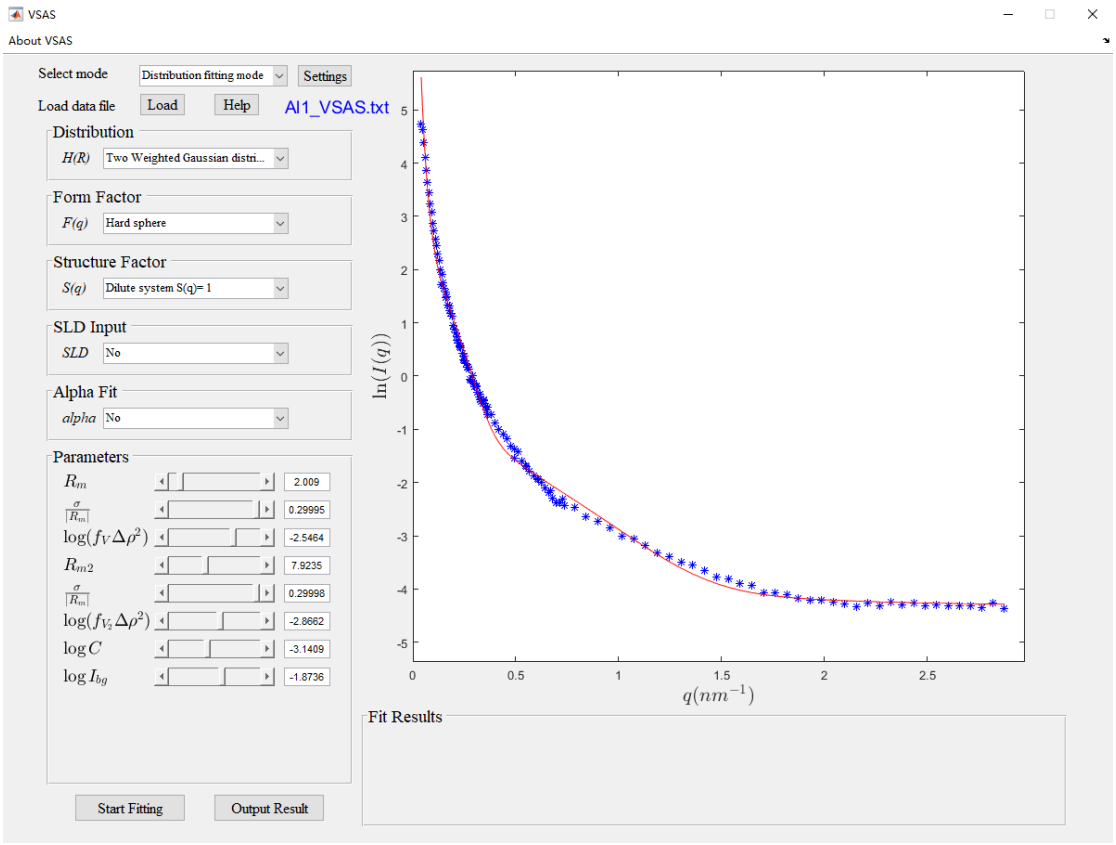


Figure 4.3 Fitting interface of Distribution fitting mode

4.4 Fitting process

Click "Start" or "Start Fitting" button to Start the Fitting process, as shown in Figure 4.4, the software interface will be locked, and a fitting progress bar will pop up to mark the completion progress of the fitting task, and users can manually cancel the Fitting process. After the fitting is completed, the fitting curve will be displayed on the right side of the software interface. For the "Guinier Approach" mode, the fitting results are displayed in the "Fit Results" section at the lower left of the software interface, as shown in Figure 4.4. For "Distribution Fitting Mode", the parameter in the left work bar will be replaced by the parameter value of the fitting

result of the program, and you can continue to manually optimize by adjusting the value. Goodness of fit Results are displayed in the "Fit Results" panel at the lower right of the software interface as shown in Figure 4.4.

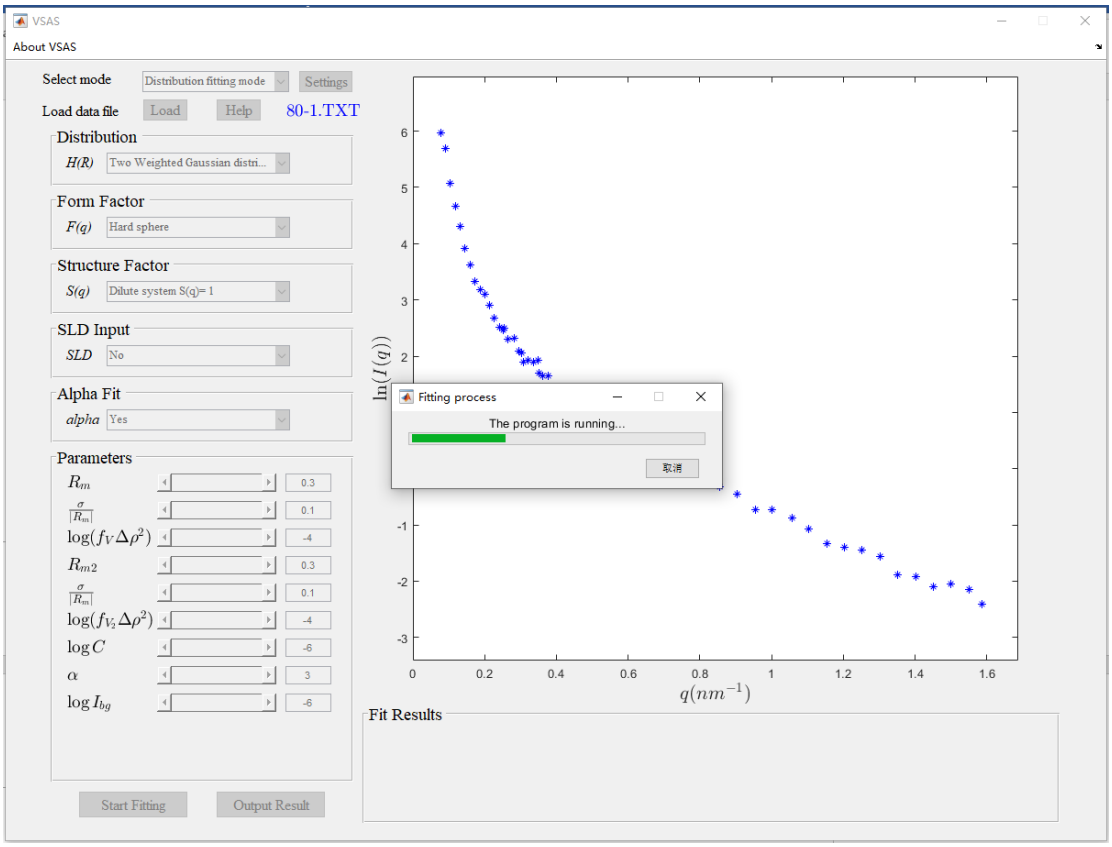


图 10：拟合任务界面

4.5 Fitting result output

Click "Output Result", the path inquiry dialog box will pop up, and the parameters and images of the fitting results can be exported as local files and saved to the specified path, as shown in Figure 4.5.

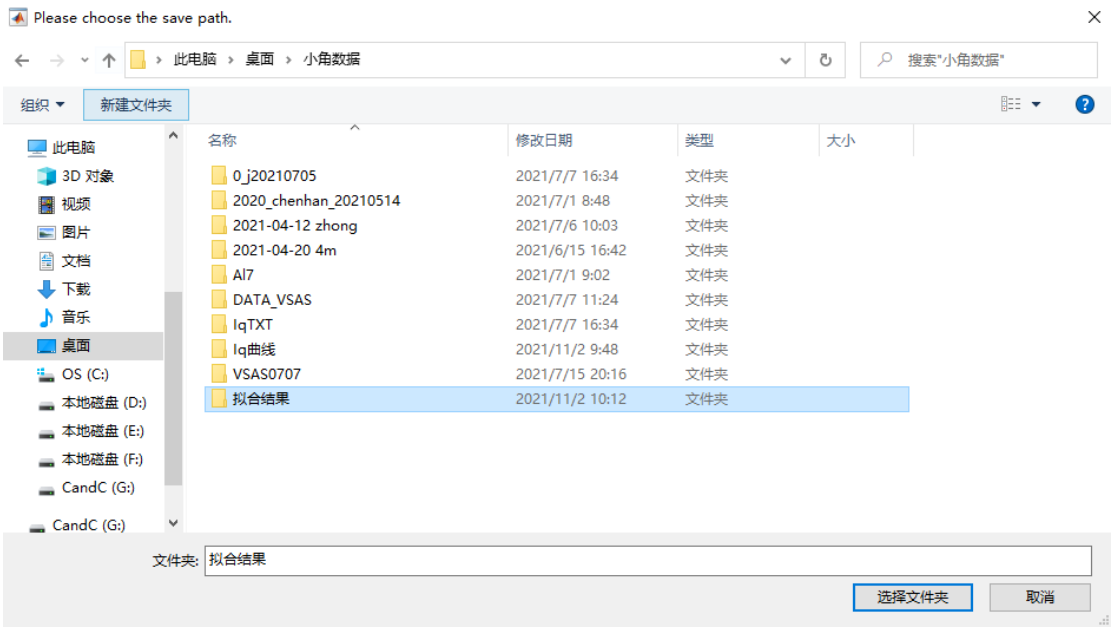


Figure 4.5 The saving interface of fitting results in VSAS

There are 5 parts in the saved small-angle scattering fitting results:

a. The image file of fitting curve, as shown in Figure 4.5(a)

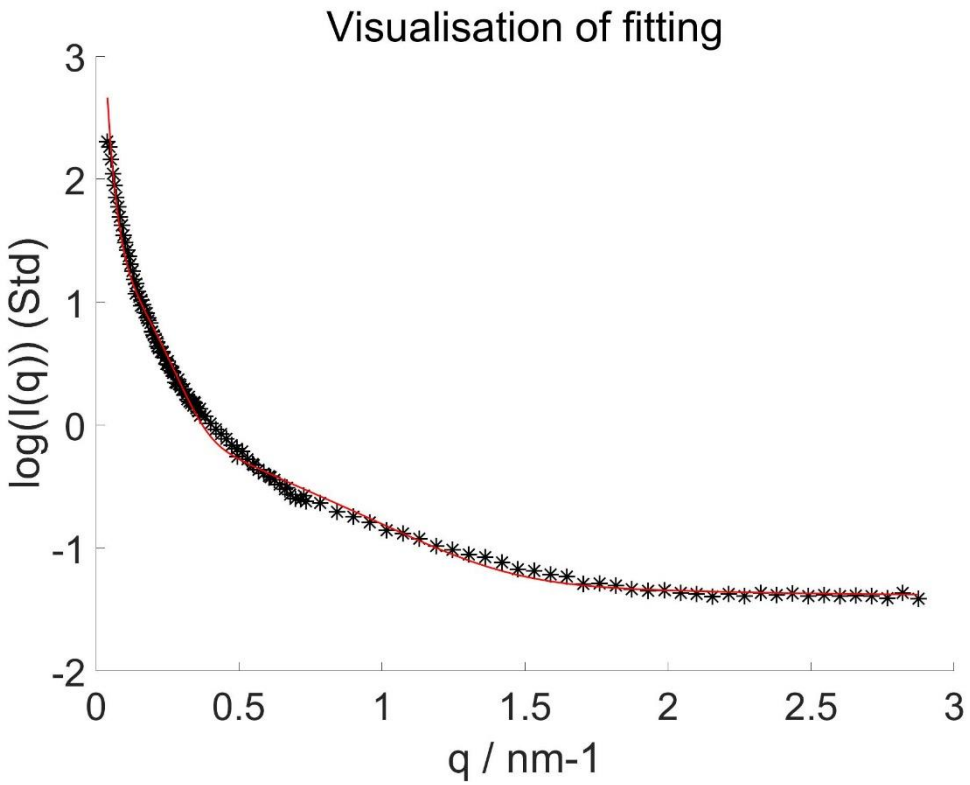


Figure 4.5(a) The image file of fitting curve

b. The image file of CorMap, which can help the users to judge the matching degree between theoretical model and experimental data visually without experimental

error. When CorMap has obvious regions, the model fitting is biased, as shown in the left figure in Figure 4.5(b). On the contrary, when CorMap has a random pattern, the model and data match well, as shown on the right in Figure 4.5(b).

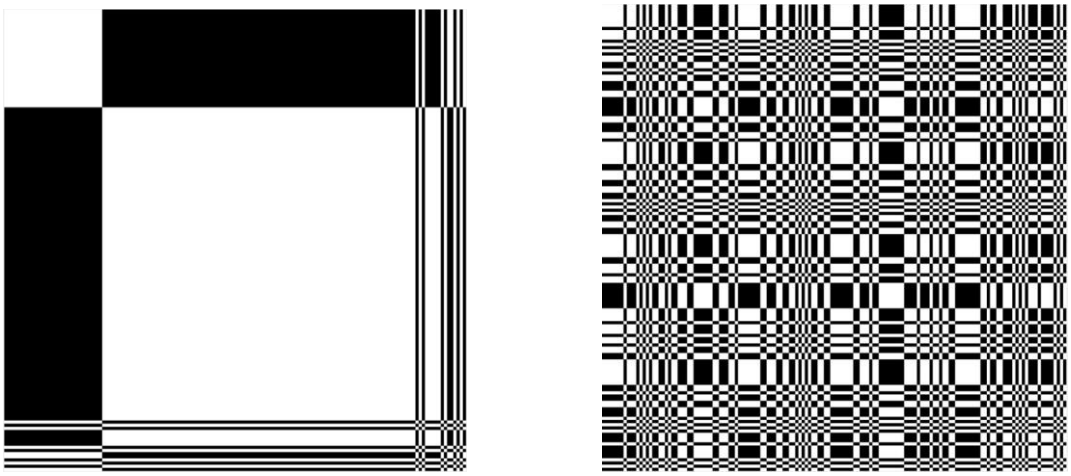


Figure 4.5(b) The image file of CorMap of the fitting results

c. The MATLAB file of fitting results, including the radius, distribution, volume fraction, and the background signal of the sample system, as shown in Figure 4.5(c).

Final_report

1x19 table

	1 No	2 Rm1	3 sigma1	4 fV1rho2	5 Rm2	6 sigma2	7 fV2rho2	8 C	9 Ibg	10 Chi2	11 CorMap	12 MaxPatch	13 PValue	14 Fit_Times	15 Total_Time	16 Mean_Time	17 Form_Type	18 Dis_Mode	19 Dis_Type
1	'Al1_VSAS'	2.0090	0.3000	-2.5464	7.9235	0.3000	-2.8662	7.2290e-04	0.0134	0.0045	26.1062	26	3.8743e-07	4	257.9800	64.5000	'Sphere'	'Double'	'LogNormal'

Figure 4.5(c) The MATLAB file of fitting results

d. The excel file of fitting results, including the radius, distribution, volume fraction, and the background signal of the sample system, as shown in Figure 4.5(d).

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	No	Rm1	sigma1	fV1rho2	Rm2	sigma2	fV2rho2	C	Ibg	Chi2	CorMap	MaxPatch	PValue	Fit_Times	Total_Time	Mean_Time	Form_Type	Dis_Mode	Dis_Type
2	Al1_VSAS	2.0089762	0.2999521	-2.546379	7.9235331	0.2999838	-2.86618	0.0007229	0.0133781	0.0044683	26.106172	26	3.874E-07	4	257.98	64.5	Sphere	Double	LogNormal

Figure 4.5(d) The excel file of fitting results

e. The image file of particle size distribution curve, showing particle size distribution and corresponding volume fraction in the sample, as shown in Figure 4.5(e).

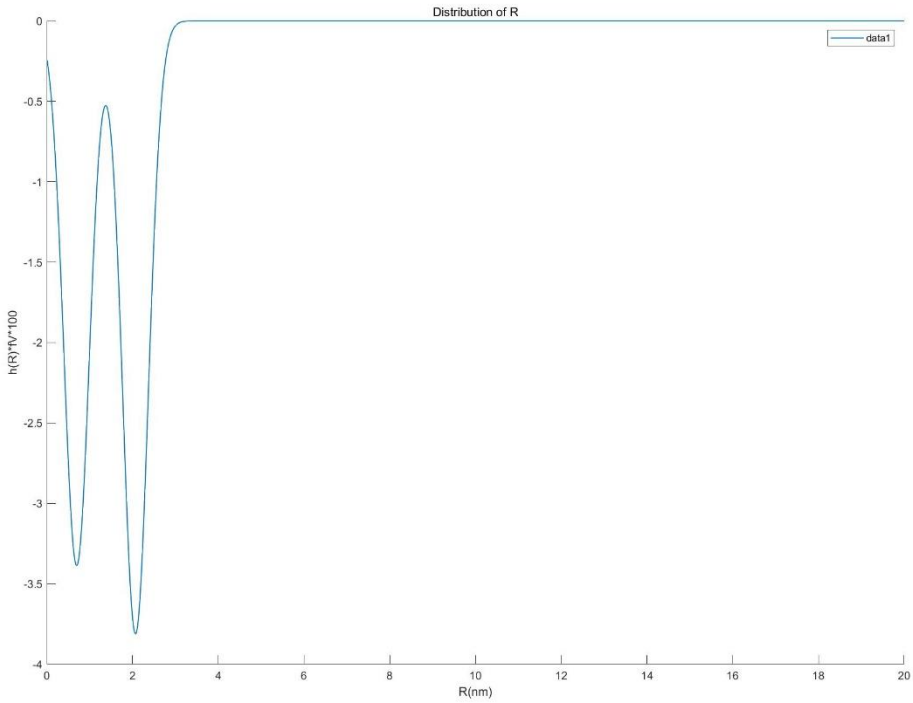


Figure 4.5(e) The image file of particle size distribution curve

4.6 Exit

After completing the entire operation, click the "X" button on the upper right of the interface to exit and close the software.

5. Authors

Shengyi ZHONG

SJTU - ParisTech Elite Institute of Technology

SJTU - School of Materials Science and Engineering

E-mail: shengyi.zhong@sjtu.edu.cn

Shuxin SHI

SJTU - ParisTech Elite Institute of Technology

E-mail: ssxhcxr2008 @sjtu.edu.cn

Yifei TANG

SJTU - School of Materials Science and Engineering

E-mail: yftang@sjtu.edu.cn