

# EZGC Chromatogram Modeler Manual

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## Introduction

The EZGC Chromatogram Modeler by Restek allows you to learn about gas chromatography parameters as well as optimize them for an individual separation process. The software runs on the rules of solubility and a compound database of empirical data. It walks you through a method development process where you first enter a compound list, generate a basic model and refine the model before you apply it to a real chromatographic system.

## Interface

The EZGC interface basically consists of three tabs as shown in Figure 1. In the first one you can enter your compounds of interest and click “Solve”. A chromatogram and a list of all the peaks alongside with their retention times, resolution values, peak widths and peak temperatures will be displayed. By clicking on the magnifying glass, you can see more detailed information on the compound as well as its MS spectrum. The drop-down menu in the sidebar allows you to select a sufficient stationary phase. Most of the work is done within the conditions tab. Here all the chromatographic parameters are controlled. The chromatogram as well as the table of peaks will respond promptly to all modifications that are being made. A model can be saved by clicking the save button in the header menu. It can be loaded from the “My EZGC” tab at any time in the future.

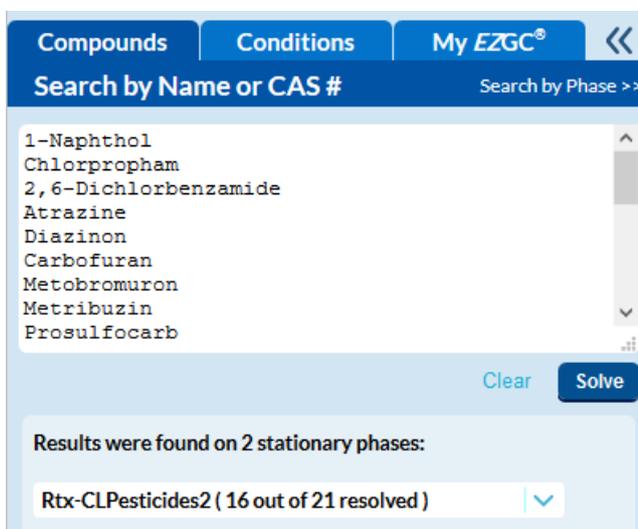


Figure 1: Menu to navigate through the three basic tabs of the modeler.

## Basic functions

To enter a compound list, you can type in the names or CAS numbers of your substances of interest. Hit “Solve” and choose a stationary phase from the drop-down menu that suits you well. Another approach would be to go to “Search by phase”, select the stationary phase you will be working with and search the assigned library for compounds.

Once you hit “Solve” you will get an initial model that needs to be adjusted to your specific chromatographic set-up in the conditions tab (Figure 2). Select the carrier gas you are working with and specify the parameters of your column. Hit the “Vacuum” button if you are using mass spectrometry for detection. The control method specifies how the flow and the linear velocity in the column or the head pressure are controlled by your GC system. This depends on the injector or detector you are using. Select one out of three options in the drop-down menu:

- Constant Flow: A constant outlet flow of carrier gas is maintained.
- Constant Pressure: The inlet pressure on the column is held constant.
- Constant Linear Velocity: The system maintains a constant linear velocity by programming pressure changes.

Under “Results” you can choose one of three modelling purposes:

- Efficiency: Fits the linear velocity to the column dimensions and oven conditions
- Speed: Finds the best separation conditions in the shortest amount of time
- Custom: Enables all fields to leave the modelling completely up to you

Under “Oven Program” you can determine the target resolution. Resolution values in the peak list marked orange or red are falling under this minimum. The default value is 1.50 which is baseline separations.

After modelling your chromatographic system, the temperature program needs to be optimized to these specific parameters. When clicking “Refine Oven Program”, the ramp rate, the temperature and the hold time will be adjusted. You might be able to execute this function several times before the button turns grey. Make sure to repeat this step after every single change that has been made to the conditions.

### Example showing further optimization

Table 1 shows a list of pesticides and their respective CAS numbers. Our laboratory is equipped with a GC-MS coupling. The system details are displayed in Table 2. Before running the first experiment, a model should be created on the EZGC to establish all parameters that guarantee an efficient separation. For this purpose, make sure that all compounds are being resolved and keep an eye on the total run time.

Table 1: List of pesticides with names and CAS numbers.

Compound name	CAS number
1-Naphthol	90-15-3
Chlorpropham	101-21-3
2,6-Dichlorobenzamide	2008-58-4
Atrazine	1912-24-9
Diazinon	333-41-5
Carbofuran	1563-66-2
Metobromuron	3060-89-7
Metribuzin	21087-64-9

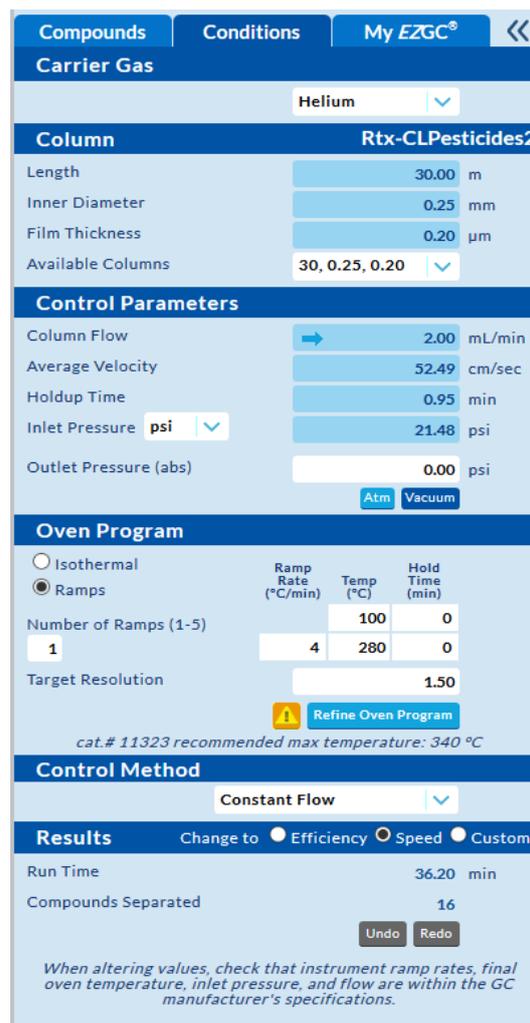


Figure 2: The conditions tab where all chromatographic parameters can be controlled.

When altering values, check that instrument ramp rates, final oven temperature, inlet pressure, and flow are within the GC manufacturer's specifications.

Prosulfocarb	52888-80-9
Monuron	150-68-5
Alachlor	15972-60-8
Linuron	330-55-2
Metolachlor	51218-45-2
Malathion	121-75-5
Chlorotoluron	15545-48-9
Metazachlor	67129-08-2
Chlorfenvinphos	470-90-6
Picoxystrobin	117428-22-5
Carboxin	5234-68-4
Quinoxifen	124495-18-7
Oxadixyl	77732-09-3
Flurtamone	96525-23-4

### Create an initial model:

Enter all compounds from Table 1 and choose a stationary phase after you hit “Solve”. As explained under “Basic functions”, fill in the chromatographic frame settings from Table 2 in the conditions tab. After refining the oven program, you will look at your first chromatogram with the according peak list.

*Table 2: Parameter settings for your exemplary chromatographic setup*

Parameter	Value
Carrier Gas	Nitrogen
Column length	20 m
Inner Diameter	0.18 mm
Film Thickness	0.18 µm
Outlet Pressure	0.00 psi
Control Method	Constant Linear Velocity
Results	Efficiency

### Refine your model:

You might notice that there are still some coeluting substances, marked orange or red in your peak list. In the following a set of tools are presented, that could help you to achieve adequate resolutions. You probably still want to save your initial model, since these measures do not necessarily lead to improvements.

1. Check the MS spectra of the poorly resolved compounds for overlapping ions. To do so, find the set of substances marked orange or red in your peak list. Open the spectrum of a middle coeluter and click the “Show coelutions” button.
2. Especially when working with MS, lowering the global resolution constraint down to ~ 1.00 – 1.20 might still be sufficient and often decreases run times.
3. Relaxing its specific resolution constraint, may help pulling a compound away from a bundle of coeluters. At first, go back to the compound tab and target the compound you want to resolve by typing two exclamation marks right behind its name. Then, hit “Solve” again and the substance you just marked should be highlighted in light green in your peak list. If you now change the target resolution, it is no longer a global constraint but specific to the

targeted substance. Refresh the “Refine Oven Program” button to adjust the temperature program. You can add as many compound specific resolution constraints as you wish. But keep in mind that by assigning compound specific values, the resolution of other compounds may be sacrificed.

4. If you still want to improve the resolution between multiple compounds, you can add up to four oven ramps to split the run. Just increase the number of ramps and the corresponding fields will appear. Tailor the temperature limits of the new ramps around the peak temperatures of the coeluting compounds. If you are changing the ramp rate, make sure to stay within the ramp limits of your instrument!

Now that you know all the tools, try to model an efficient separation within a reasonable run time.