GasChromatographySimulator.jl

INSTALLATION GUIDE

INTRODUCTION

GasChromatographySimulator.jl is a free Open Source Software for simulation, prediction and method development of GC-separations[1].

You can find the Software in the web:

https://github.com/JanLeppert/GasChromatographySimulator.jl

INSTALLATION JULIA AND PLUTO

GasChromatographySimulator.jl is released as a Package in programming language Julia. To use GasChromatographySimulator.jl follow the Steps:

1.) INSTALL JULIA

Go to https://julialang.org/downloads and download the current stable release, using the correct version for your operating system (Linux x86, Mac, Windows, etc).

2.) OPEN JULIA

Open Julia on your PC. Check that Julia is working by typing a simple command like

```
julia> 1+1
```

Julia will answer by solving the task.

3.) INSTALL PLUTO

Next, we will install Pluto console (https://github.com/fonsp/Pluto.jl) which we will use for the simulator. Pluto is a Julia programming environment and designed for interactivity and quick experiments.

Open **Julia**: This is the command-line interface to Julia, similar to the previous screenshot.

Here you can type commands and when you press "Enter", it will run, so you can see the result.

To install Pluto, we have to run a package manager command (Pkg). To switch from Julia mode to PKG mode, type "]" (closing square bracket):

```
julia> ]
```

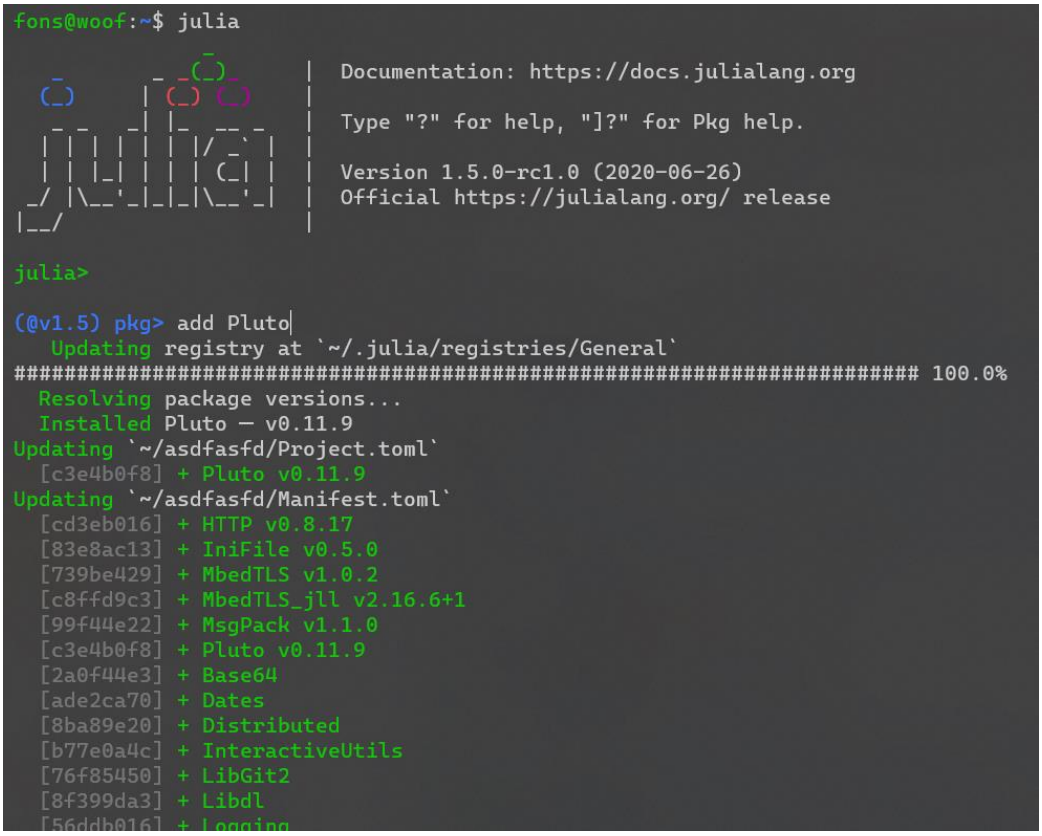
```
(@v1.6) pkg>
```

The line turns blue and the changes to pkg>, which tells you that you are now in the Pkg mode. This mode allows you to do operations on **packages** (also called libraries), like installation or updating.

To install Pluto, run the following (case sensitive) command to **"add"** (install) the package to your system by downloading it from the internet. You should only need to do this once for each installation of Julia:

```
(@v1.6) pkg> add Pluto
```

This might take a couple of minutes, so you can go get yourself a cup of tea!



RUNNING GASCHROMATOGRAPHYSIMULATOR.JL

Repeat the following steps whenever you want to work on a project.

1.) START PLUTO

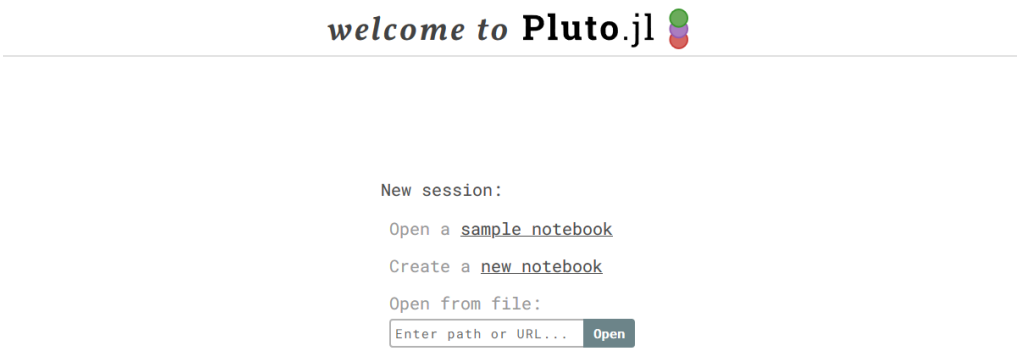
Start Julia, like you did during the setup. In the REPL, type:

```
julia> using Pluto
```

```
julia> Pluto.run()
```

The terminal tells us to go to http://localhost:1234/ (or a similar URL). Now Pluto automatically starts in your standard Browser.

If not: Let's open Firefox or Chrome and type http://localhost:1234/ into the address bar.



2.) RUN GASCHROMATOGRAPHYSIMULATOR.JL

The whole Simulation can be found in the Web:

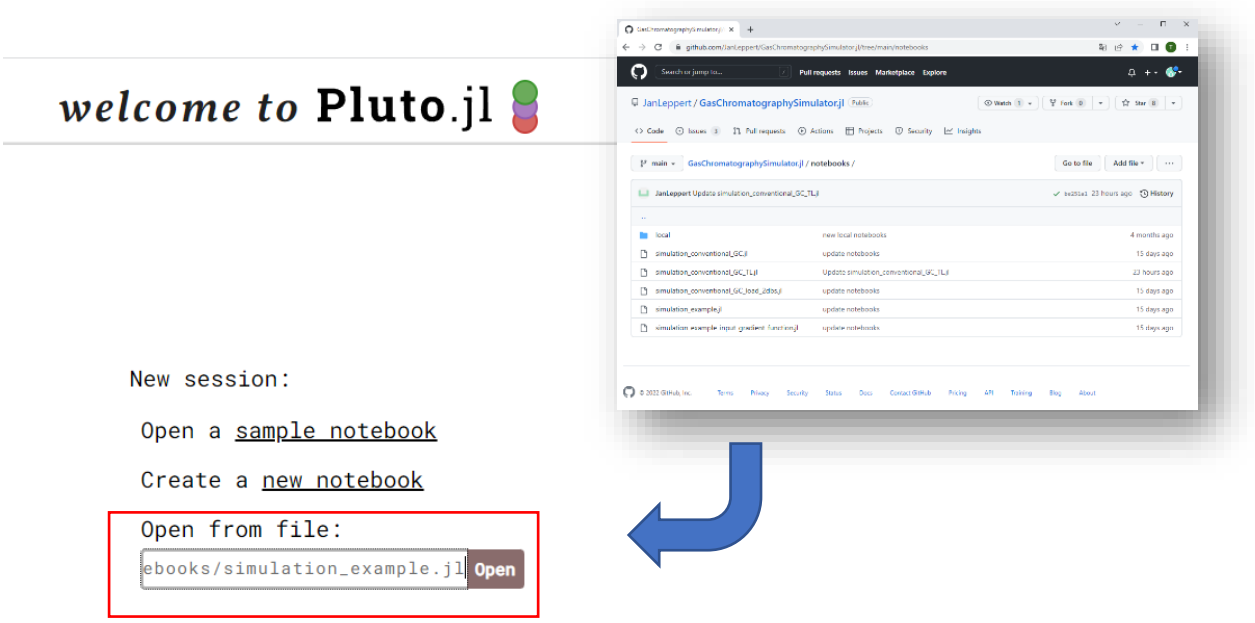
https://github.com/JanLeppert/GasChromatographySimulator.jl

To use the simulation, choose a notebook **online.** You can find the different notebooks for simulation at:

https://github.com/JanLeppert/GasChromatographySimulator.jl/tree/main/notebooks

Every notebook can simulate different kinds of GC separation. See short overview under 3.)

We will show you the simulation for example with the notebook simulation_conventional_GC.jl". So insert the URL of the notebook into the URL box and click “open”.



It may now take a few minutes to load the notebook. Meanwhile, a short introduction to the functions of the simulation follows. Let’s go!

Packages, simulation_conventional_GC.jl, for GasChromatographySimulator v0.3.11

GasChromatographySimulator.jl

A Simulation of a conventional Gas Chromatography (GC) System (without a thermal gradient).

Settings

Solute Database

Load own database: ☐

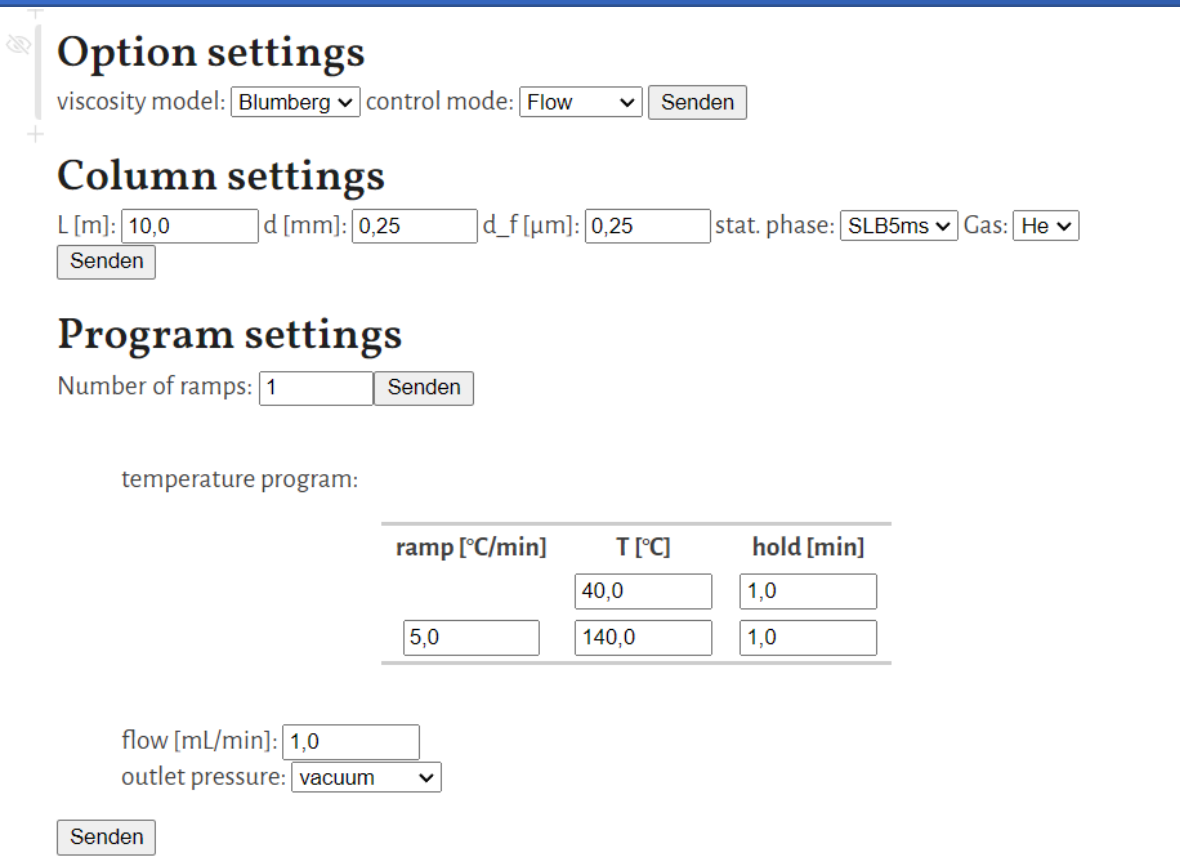
The simulation works with databases, which can look like the database below:

	Name	CAS	Phase	Tchar	thetachar	DeltaCp	phio	Sourc
1	"Heptane"	"142-82-5"	"SLB5ms"	44.738	25.519	60.91	0.001	"Blumberg
2	"Octane"	"111-65-9"	"SLB5ms"	67.346	26.779	66.363	0.001	"Blumberg
3	"Nonane"	"111-84-2"	"SLB5ms"	87.42	27.699	71.797	0.001	"Blumberg
4	"2-Octanone"	"111-13-7"	"SLB5ms"	105.29	28.876	81.294	0.001	"Blumberg
5	"Decane"	"124-18-5"	"SLB5ms"	106.44	28.588	76.602	0.001	"Blumberg
6	"2-Octanol"	"123-96-6"	"SLB5ms"	107.03	28.644	88.469	0.001	"Blumberg
7	"1-Octanol"	"111-87-5"	"SLB5ms"	119.5	29.317	92.778	0.001	"Blumberg
8	"5-Nonanol"	"623-93-8"	"SLB5ms"	122.92	29.571	90.768	0.001	"Blumberg
9	"Undecane"	"1120-21-4"	"SLB5ms"	124.75	29.628	83.819	0.001	"Blumberg
10	"2-Nonanol"	"628-99-9"	"SLB5ms"	124.84	29.561	93.722	0.001	"Blumberg
⋮	more							
51	"1-Nonanol"	"143-8-8"	"Wax"	169.04	33.106	102.05	0.001	"Blumberg

The Solute Database shows the available substances you can choose for your chromatography and its thermodynamic parameters. We need these parameters to calculate the simulation by the K-centric model.

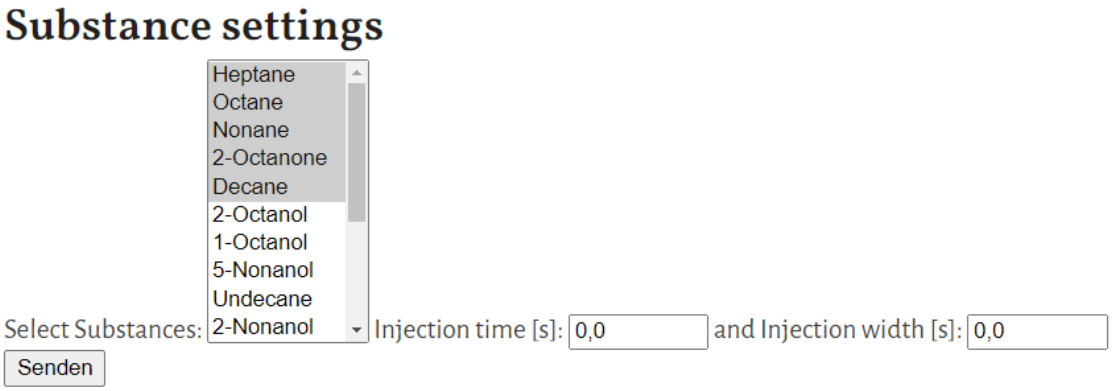
Detail information can be found in the literature[2,3], even to convert the data from other retention models (e.g. ABC-Model). If you want you can load your own database as CSV format.

When you don't find your stationary phase in the table, try the simulation with another but similar phase.



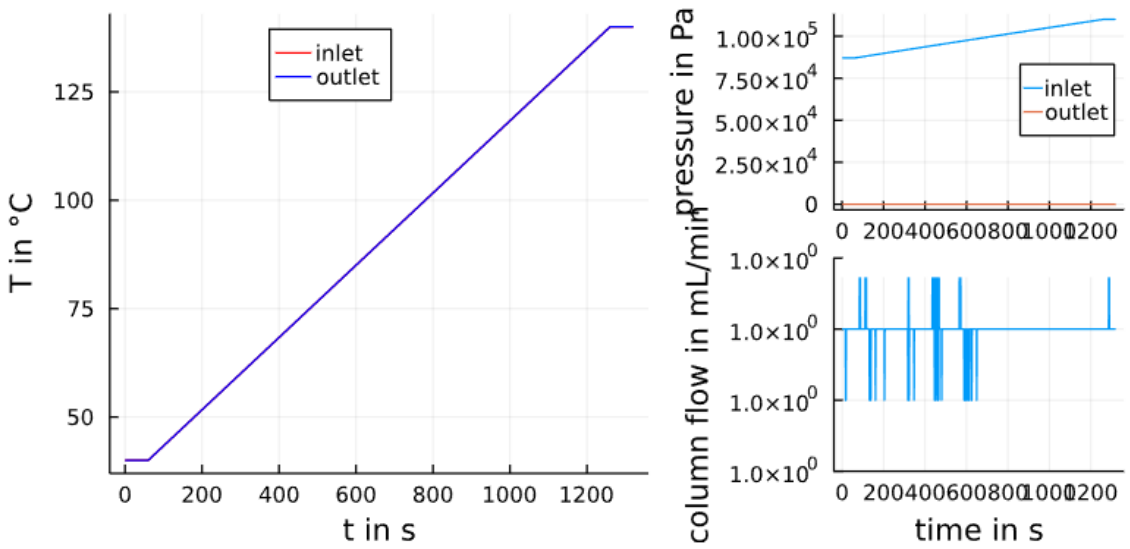
You can choose the GC settings: diameter and length of the GC column, constant pressure vs. constant flow and isothermal versus temperature programmed GC. To confirm your settings, press the **"send"** button.

Choose the substances you want to simulate:



Then the simulation starts working. Scroll down to see the results.

Plot of the program



The simulation shows you an overview of the GC settings and the plot of the temperature program, such as in your GC software in the laboratory.

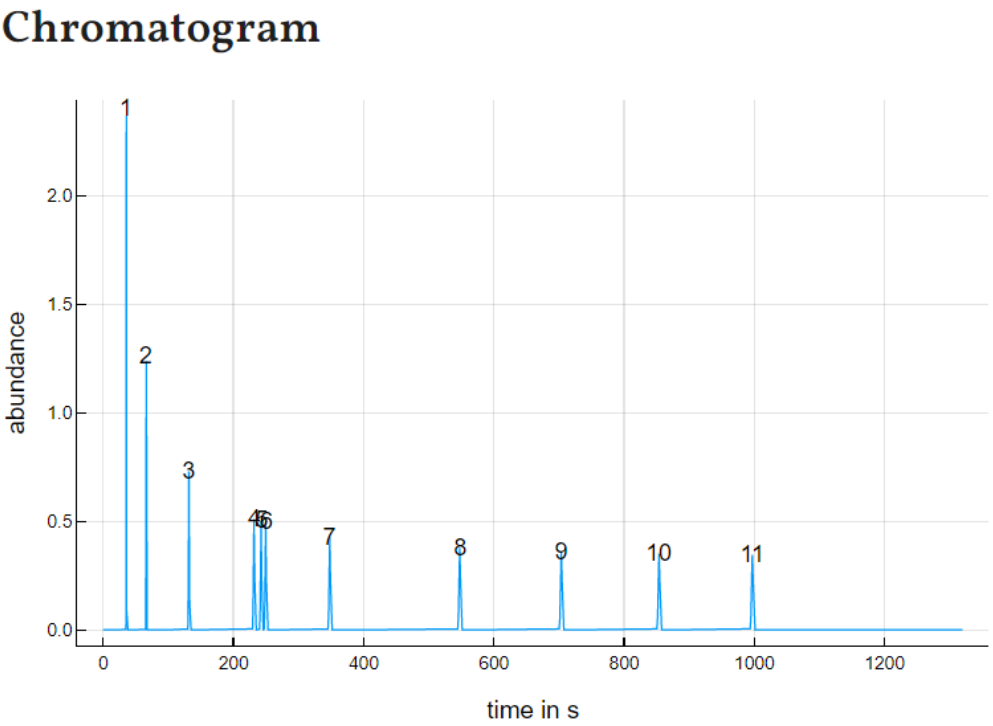
The simulation calculates the retention parameters e.g. retention time, peak width, retention factor or the resolution.

Simulation

Peaklist

	Name	tR	τR	TR	σR	uR	kR	Res	Δs
1	"Heptane"	35.4781	0.165839	40.0	Inf	Inf	1.20841	31.8549	131.
2	"Octane"	66.1953	0.316305	40.5163	Inf	Inf	3.05026	37.9602	155.
3	"Nonane"	131.636	0.545658	45.9697	Inf	Inf	5.80038	37.6342	152.
4	"2-Octanone"	231.531	0.781528	54.2943	Inf	Inf	8.5729	3.45976	13.8
5	"Decane"	242.427	0.793076	55.2022	Inf	Inf	8.79054	2.21662	8.86
6	"2-Octanol"	249.518	0.806583	55.7932	Inf	Inf	8.88558	28.2953	113.
7	"1-Octanol"	347.893	0.931769	63.991	Inf	Inf	10.3979	50.2278	201.
8	"Dodecane"	547.529	1.05554	80.6274	Inf	Inf	12.0706	36.1366	144.
9	"Tridecane"	703.519	1.1028	93.6266	Inf	Inf	12.7165	33.5855	134.
10	"Tetradecane"	853.665	1.13249	106.139	Inf	Inf	13.1488	31.3195	125.
11	"Pentadecane"	996.921	1.15451	118.077	Inf	Inf	13.4845	NaN	NaN

Most important is the simulation of the chromatogram, if you wish so you can also add measured data to compare the measurement with the simulated data.



You can even investigate dependencies of the retention parameters to each other. E.g. you can observe the velocity of the analytes during the time or the position of the analyte in the GC column.

To export the simulated chromatogram and the data, you can push the **“download”** button. The exported data can be found in the download order.

3.) AVAILABLE NOTEBOOKS

To use the simulation, choose a notebook and insert the URL of the notebook into the URL – Box

CONVENTIONAL GC

URL:
https://github.com/JanLeppert/GasChromatographySimulator.jl/blob/main/notebooks/simulation_conventional_GC.jl

Simulation of a conventional GC Setup. With one separation column, isothermal or temperature programmed GC, different outlet pressures (e.g. for FID or MS). Good tool for method developers.

CONVENTIONAL GC WITH TRANSFER LINE

URL:
https://github.com/JanLeppert/GasChromatographySimulator.jl/blob/main/notebooks/simulation_conventional_GC_TL.jl

Simulation of a conventional GC Setup. With one separation column, isothermal or temperature programmed GC, different outlet pressures (e.g. for FID or MS). You can even vary the length of a transfer line (e.g. to MS).

GC WITH THERMAL GRADIENT

URL:
https://github.com/JanLeppert/GasChromatographySimulator.jl/blob/main/notebooks/simulation_example.jl

Simulation of a GC Setup with or without a spatial thermal gradient along the separation column. With one separation column, isothermal or temperature programmed GC, different outlet pressures (e.g. for FID or MS).

URL:

https://github.com/JanLeppert/GasChromatographySimulator.jl/blob/main/notebooks/simulation_example_input_gradient_function.jl

Simulation of a GC Setup with or without a spatial thermal gradient along the separation column. A function (with two parameters) for the spatial thermal gradient can be defined by the user. With one separation column, isothermal or temperature programmed GC, different outlet pressures (e.g. for FID or MS).

REFERENCES

(1) Leppert, Jan (2022): GasChromatographySimulator.jl. In: *JOSS* 7 (76), S. 4565. DOI: 10.21105/joss.04565.

(2) Blumberg, Leonid M. (2017): Distribution-centric 3-parameter thermodynamic models of partition gas chromatography. In: *Journal of chromatography. A* 1491, S. 159–170. DOI: 10.1016/j.chroma.2017.02.047.

(3) Leppert, Jan; Müller, Peter J.; Chopra, Miriam D.; Blumberg, Leonid M.; Boeker, Peter (2020b): Simulation of spatial thermal gradient gas chromatography. In: *Journal of chromatography. A* 1620, S. 460985. DOI: 10.1016/j.chroma.2020.460985.