The subject proposed in the project concerns the separation of chemical compounds by column chromatography. A chromatographic column is a metal tube packed with granules of a highly porous substance (adsorbent). Molecules of chemical compounds (called analytes) can penetrate deep into the pores of the sorbent grains, and then bind with different strengths to the surface of the solid inside the pores. If a liquid (eluent) is passed through such a column, into which a small amount of analytes have been injected, then they will leave the column in the form of narrow signals (peaks), after different times of staying inside (retention times) - those more penetrating pores and stronger binding with the adsorbent surface will stay in the column longer, while the weaker ones - shorter.

This idea is used practically when analyzing the composition of mixtures, in testing the purity of chemical compounds, and also, if the column size is sufficient, for the production of chemical compounds. For this reason, adsorption and chromatography methods are intensively used, among others, in the pharmaceutical industry to analyze the purity of medicines. They are also an important stage in production processes (preparative or production scale chromatography).

Chromatographic processes require high-efficiency columns. Efficiency is the higher the peaks at the column outlet are narrower. The narrower the peaks (they do not overlap), the easier their separation can be made, and the more accurate is the analysis of the impurity composition or the higher column production efficiency – obtained fractions are cleaner.

Currently, the highest efficiency is achieved by using ultra-high-performance liquid-chromatography columns (UHPLC). UHPLC columns are filled with very fine sorbent grains (the order of 1 μm), which promotes the production of heat during fluid flow through the densely packed bed in the column and the formation of gradients of physicochemical parameters along and across the bed, which in turn adversely affects the efficiency of the column. A similar problem arises in preparative columns when a relatively large mass of separated compounds is injected into the column. Significant amounts of adsorption heat emitted at that time cause the formation of local temperature gradients that can significantly deform chromatographic peaks.

Retention times of strongly adsorbing analytes can be very long (even many hours). To avoid such problems, multi-component eluents are used, e.g. water (basic ingredient) and acetonitrile (modifier). By increasing the concentration of the modifier, the analysis time can be significantly reduced and chemical reagents can be saved. Chromatographic separation, in which the concentration of a modifier changes over time, is called gradient chromatography and is one of the most important methods of chromatographic separation. However, the right selection of parameters value of the gradient process is not an easy task, especially for UHPLC or for preparative columns. Many parameters influence the optimal conditions of separation: column sizes, properties of sorbent grains, eluent composition, eluent flow rate, temperature, pressure, and many others. It would be almost impossible to experimentally determine the conditions for achieving the effective separation of specific compounds, because of the extremely large amount of work, and, as a result very high cost of experiments. However, it is possible to accelerate the obtaining of the results and reduce costs by theoretical consideration and selection parameters that have the strongest impact. The most valuable tool to do it is the mathematical model of the process. It takes into account all phenomena, and, for this reason, can help select parameters having a significant influence on the investigated process.

The main objective of the project is to propose mathematical formulas allowing for reliable modeling of gradient chromatography under UHPLC conditions and gradient preparative chromatography under strong overload conditions. We will formulate a two-dimensional (2D) model of the chromatography column assuming axial symmetry. The model will be validated based on various laboratory tests. The ability to theoretically predict how the column will behave facilitates understanding of the phenomena taking place inside the column, enables quick analysis of the impact of certain parameters on the performance of the column, enables analysis of the retention process, and optimize the process.

Mathematical modeling is often limited by unacceptable large time of computations. This issue can be solved by the application of powerful computers (high-cost solution) or by reduction of the model complexity (low-cost solution). The CPU time expected for the numerical solution of the two-dimensional model is rather long compared with the one-dimensional (1D) model. The secondary goal will be to test if for some specific conditions the 2D model can be replaced by 1D model.