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# Mathematical modeling, software simulation and directions of development for waste gas purification from $SO_2$

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The environment is still awaiting the development of better technologies, apparatus and equipment to reduce gas emissions in the atmosphere, where one of the most hazardous atmospheric air pollutants is sulfur dioxide. The aim of the present work is to study and evaluate the part of the mathematical modeling and software simulations for purification of waste gases from $SO_2$ in the scientific literature in recent years. For this purpose, the selected articles are grouped and analyzed according to the type of their content and directions of development in order to outline the current approaches to sulfur dioxide removal. Some future development guidelines are also highlighted. The innovative approaches for $SO_2$ purification of the Institute of Chemical Engineering, Bulgarian Academy of Sciences, are summarized too.

**Keywords:** $SO_2$ removal, desulfurization of waste gas, mathematical modeling, software simulation.

## INTRODUCTION

Prolonged global pollution with $SO_2$ is the cause of various respiratory diseases and is one of the main components of acid rain and urban smog. According to World Health Organization'2021 the average human exposure to $SO_2$ is 20 μg $m^{-3}$ per day or 500 μg $m^{-3}$ for 10 min [1]. Anthropogenic sources of $SO_2$ are fossil fuels with a substantial sulfur content and pyrometallurgical processes; another 30% of global $SO_2$ emissions are of natural origin in form of volcanic eruptions and sea contribution. The annual $SO_2$ loads from 2012 to 2015 over eastern China, Mexico and South Africa are given in [2]. Losses in Chinese agriculture and assessment of accumulated sulfur concentrations in pine needles as a criterion for $SO_2$ pollution were analyzed in [3] and [4], respectively.

Approaches to reduce $SO_2$ emissions aim at increasing the efficiency of standard or new technologies by optimizing related processes and environmental use of the raw materials, byproduct and disposal products. In many cases, determining better technology requires a detailed cost-effectiveness analysis.

Increasingly, mathematical modeling and software simulations are being used to generate an effective solution by optimizing existing technologies or predicting the success of innovations. Theoretical approaches are preferred due to low cost, fast results, reduced number of experiments and environmental safety. Some mathematical models of technological processes are so complex that only computer programs can solve them.

The aim of the present work is to study and evaluate the part of the of mathematical modeling and software simulations for $SO_2$ removal in terms of purification and desulfurization of waste or flue gas in the scientific literature in recent years. The scope of the study is focused on the scientific articles from the years 2020 and 2021. Demand has been extended until 2015, when some of the last limits of permissible harmful emissions into the atmosphere have been adopted. The selected articles are grouped in several sections and are analyzed according to the set criteria for content and direction of development. Some modern presentations of scientific results using software applications are also shown. The role of the Institute of Chemical Engineering, Bulgarian Academy of Sciences in the field of purification of gases from $SO_2$ is summarized too.

## RESULTS AND DISCUSSION

### *Report of the available literature on the topic*

The study began with a search for articles on $SO_2$ purification in the last 2021 and 2020, including mathematical modeling and software simulations. Most of the first significant articles are only experimental studies. Studies involving mathematical modeling and software simulations are less common, for the 200 articles reviewed, only 11. Then the keywords *modeling* and *simulation* were added to find more articles using theoretical approaches in 2020/2021 and as a result of the search 18 more articles were found. The same approach was implemented for the period down to 2014. As a result of this search, 43 more articles were collected.

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Some modern trends in the presentation of scientific results for $SO_2$ purification are also listed.

*Analyzes according to the type of content*

The articles are divided into those containing experiments, mathematical modeling, software simulation and their combinations, a total of six types, see Fig. 1. Fig. 1 shows that the articles are mainly experimental studies with mathematical models of the processes. Unfortunately, theoretical approaches are rarely discussed in reviews, and are found only in Dzhonova-Atanasova *et al*. [5] and Wang *et al.* [6].

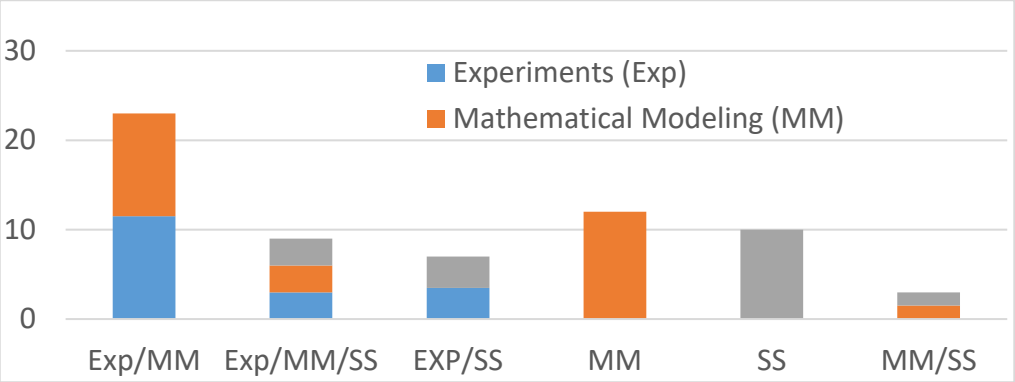



**Fig. 1.** All chosen articles on $SO_2$ purification during the years 2015 - 2021 in the study.

Scientific papers presenting only a theoretical approach to new technology, the choice of apparatus and the optimization of equipment for the purification of waste gas from $SO_2$ and applications of byproduct also occupy a significant part of the considered articles.

There is a tendency to derive mathematical models for each specific process, which allows accurate predicting of future innovative proposals. Valera *et al.* created a neural network to predict the efficiency of $SO_2$ removal in a spray tower [7]. Models obtained by Vermeulen and an improved linear driving force rate equation were studied for the adsorption of $SO_2$ on activated carbon particles of different sizes [8].

Mathematical modeling studies are published independently and usually much later after the experiments as the second stage of the research, for example, the proposal of Guo *et al.* for accurate modeling method to predict outlet concentration of wet flue gas desulfurization (FGD) and comprehensive cost model for real - time operational cost estimation [9]. Also in the work of Boyadjiev *et al*. a new approach of the convection-diffusion type model in column apparatuses for gas purification at a low $SO_2$ concentration in the thermal power plants is proposed. The convection-diffusion type of models allows to create models of average concentration and to give a quantitative description of the absorption processes [10-13]. The team of the Institute of Chemical Engineering, Bulgarian Academy of Sciences, has been working on innovative approaches for $SO_2$ purification since +1965, leading to many patents and utility models, some of which have been industrially applied, e.g. in the copper mining plant, Elisejna, Bulgaria [14-21]. A waste-free technology for waste gases purification from $SO_2$ has also been developed by means of regenerable absorbent and adsorbent [22, 23].

Wang *et al.* summarized that compared to the experimental method, the numerical simulation method is more convenient, cheaper and easier to evaluate the overall performances of the tower for $SO_2$ purification [24]. Abdulrasheed *et al*. clearly state that for further development and understanding of adsorption or cost optimization, computational tools are necessary such as density functional theory, grand canonical Monte Carlo and reactive force field and conductor [25].

The least represented are articles with combinations using software simulation. The reason is that software simulation studies have a rich database of independent operation and reliability of results as using literature data for verification. ASPEN Plus is used for detailed reactor simulations of CuO+CaO supported on inert SiC for coal combustion and separation of the streams of $CO_2$ and $SO_2$ and thermodynamic analysis of the process [26]. The energy-minimized structure models of boron nitride nanoflake for hazardous $SO_2$ capturing are created by a Gaussian program [27]. A disadvantage of the current software simulation is that it is still difficult to insert the established mathematical dependencies for the specific processes in practice, review of the CFD applications [28]. CFD simulations are used when measurements are difficult, relying mainly on generalized equations as analyzing only part of the process. An example for

this is the study by Tomanović *et al.* where the gas phase is modeled in Eulerian field, while the particles are tracked in Lagrangian field to predict a boiler unit efficiency [29]. The population balance model combined with CFD is used to characterize the behavior of droplets in the venture scrubber [30].

*Analyzes according to the directions of development*

The available technologies for $SO_2$ removal can be divided into two main categories: non-regenerable and regenerable processes. The predominant process for flue gas desulfurization is wet scrubbing using a lime or a limestone slurry. This process can provide 90%-99% sulfur dioxide removal using cheaper raw materials and marketable byproducts ($NH_3$, gypsum, $H_2$, $N_2O$, $N_2$). The disadvantages are the high cost of installation and large quantities of waste water. Where lower removal efficiencies can be tolerated, spray drying and dry injection processes are more economical. Some improvements with a rare commercial application are the combined removal processes of $SO_2/NO_X/CO_2$/VOC. The disadvantages of the available technologies are the regeneration of catalysts or scrubbing solutions, clogging, corrosion and the accumulation of other pollutants.

The considered articles using theoretical approaches for purification of waste gases from sulfur dioxide are presented in five directions of development (DD), see Fig. 2 and Table 1: DD_1. Innovation absorbents, adsorbents, membranes - types, effective interface surface area, characteristic, quantities; DD_2. Operating conditions - flow rate, pressure drop, inlet and outlet sulfur dioxide concentrations, pH, t, removal efficiency; DD_3. Construction - ease and time of installation, operating and maintenance labor and material, space and sparing requirements; DD_4. New *vs*. retrofit method/ technology/ constructions; DD_5. Cost material and Energy *vs.* Ecological risk. What happens with disposal and byproducts after gas purification?

The efforts of scientists are mainly focused on the use of activated carbon as a proposal for renewable engineering solutions [8, 25] and combined removal processes of $SO_2$/ $NO_X$/ $CO_2$/ VOC [31-39]. The found studies using seawater are for hybrid technologies combined electron beam [9] and wet scrubber to control $SO_2$ and NOx from a diesel generator [40]. Ionic liquids are characterized by excellent chemical and thermal stability, low vapor pressure and environmental properties. The conclusions are that the costs of some kinds of ionic liquids are extremely high and are still limited [41-43]. Xin *et al*. present a membrane contactor technology as a promising alternative technology for capturing $SO_2$ using liquid absorbent [44]. Fig. 2 and Table 1 show that mathematical modeling and software simulation regarding operating conditions at waste gas purification from $SO_2$ are used more frequently. From the distribution of the selected articles by type of content and directions of development it can be seen that only mathematical modeling for innovation material is not found, Table 1.

Our study shows that it is not a small part of the scientific papers using mathematical modeling and software simulation presenting an optimization of the auxiliary equipment, cost material and energy through environmentally friendly solutions.

*Future directions of development on the topic*

Future development guidelines suggest to use the solar energy in the hybrid systems, as well as the sustainable green conversion of waste into valuable products in order to protect the environment. Koralegedara *et al.* have summarized applications using waste construction materials [80] as a raw material for flue gas desulfurization.

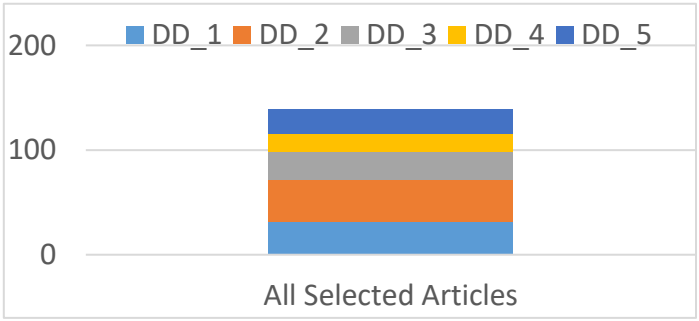
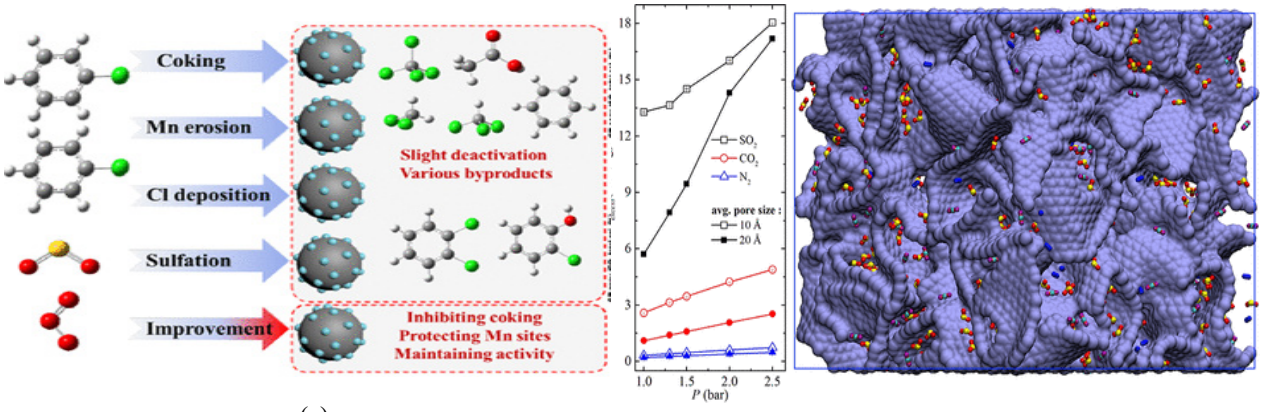



**Fig. 2.** All selected articles on $SO_2$ purification during the years 2015 - 2021 by the directions of development. DD_1 Innovation materials; DD_2 Operating conditions; DD_3 Construction adjustment; DD_4 New *vs*. retrofit; DD_5 Cost material and Energy *vs*. Ecological risk.

**Table 1.** All selected articles on $SO_2$ purification during the years 2015 - 2021 distributed by the directions of development and the content.

| | DD_1 | DD_2 | DD_3 | DD_4 | DD_5 |
|---|---|---|---|---|---|
| Exp/MM | 8, 32, 35, 36, 42, 43, 47, 57, 58, 63, 65, 66, 80 | 7, 8, 31, 32, 33, 34, 35, 36 40, 43, 45, 47 53, 57, 63, 64, 65, 66 | 7, 8, 33, 34 35, 36, 40, 43, 45, 47, 57, 65 | 8, 33, 40, 43, 47, 54 | 8, 33, 43, 45, 47, 63 |
| Exp/MM/SS | 29, 30, 38, 51, 55, 60, 72, 73 | 29, 30, 38, 50, 55, 72, 73 | 30, 50, 73 | 30 | 29, 30, 38, 51 |
| Exp/SS | 5, 48, 49, 78 | 5, 39 | 5, 39, 56 | 5, 39, 56 | 5, 56 |
| MM | no | 9, 67, 75, 76, 77 | 10, 11 | 10, 11, 61 | 6, 9, 61, 74, 75, 76 |
| SS | 24, 27, 59, 70, 71 | 24, 46, 59, 68, 69, 70, 71 | 24, 26, 46, 68, 69 | 46, 62, 69 | 26, 46, 62, 69 |
| MM/SS | 37 | 37, 52 | 37 | 28, 52 | 28 |




(a) (b)

**Fig. 3.** Presentation of innovation materials (a) Adsorption mechanism by Grand canonical Monte Carlo simulations of a 3D graphene sponge for flue gas stream, Maurya *et al.* [70]; (b) Results and 3D graphics of chlorobenzene oxidation by oxygen and ozone over a simple $Mn/Al_2O_3$ catalyst, Tseng and Li [82].

Some new applications in the field are for fertilizer and soil amendment in agriculture and water treatment. The bioscrubbers are proposed as an environmentally friendly and economical alternative for flue gas purification. Advanced oxidation processes (AOPs) as with ozone, UV, hydrogen peroxide are the alternative that is looking for its place for a wider application in $SO_2$ adsorption. Our team is trying to contribute to the development of a waste gas purification process through a technology using an integrated absorption-adsorption process for waste-free decontamination of gas containing $SO_2$ [81].

Some modern trends in presentation of scientific results for $SO_2$ purification for adsorption mechanism using computational tools are shown in Fig. 3. The graphs are characterized by a good visualization of the topic of studies and the corresponding results.

## CONCLUSIONS

Analysis was made of articles using mathematical modeling and software simulations as approaches to study of purification of waste gases from $SO_2$ in the scientific literature in recent years. The significance of mathematical modeling and software simulations in terms of the type of content and field of research are discussed and the results are presented graphically and tabular. It seems that among the first articles for sulfur dioxide removal there are rarely articles using mathematical modeling and software simulation, including reviews. Studies still rarely rely on mathematical modeling and software simulations, although they save time and materials for experiments. When laboratory tests cannot be performed, theoretical approaches are used for larger and more difficult objects and tasks.

Our review of modern trends in science in the field of purification of waste gases from $SO_2$ using mathematical modeling and software simulations provides opportunities to gather ideas and applications. The main problems about the considered multi-stage recycling system are: the need for recovery of the materials after $SO_2$ removal processes and the difficulty in finding practical realization of the byproducts.

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