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APPLICATION OF GIS FOR INVENTORY POLLUTION SOURCES AND STORAGE SITES OF CARBON DIOXIDE

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Introduction. Performed analysis of Ukrainian stationary sources of carbon dioxide emissions (CO_2) into the atmosphere and the geology of eastern regions leads to a number of preliminary recommendations for further scientific and technological research to be carried out to provide process of implementation of CCS technologies in Ukraine.
Keywords: CO_2 emissions, carbon capture, geological storage, geographic information system, Eastern Ukraine.

The study was carried out in the framework of the Grant No. DCI/ENV 2010/243-865 “Low-Carbon Opportunities for Industrial Regions Of Ukraine (LCOIR-UA)”, which is implemented by the Donetsk National University (Ukraine) and funded by the European Union.

The potential of Sourses of CO_2 Emissions. Using the information of the 5 open databases: IEA, BELLONA, CARMA, DTEK and BIOMASS,- as well as new more data obtained directly from the thermal power plants, iron and steel, coke, cement, chemical plants and oil refineries, geographic information system(GIS) sources of CO_2 were established. The study covers five eastern regions of Ukraine (previously mentioned).

This GIS in the test mode is available on the LCOIR-UA project website and businesses can read this data about their emissions of CO_2, which are listed in network connections, and correct the data in accordance with the actual volumes of emissions of the enterprise.

Using this GIS, one can estimate the amount of CO_2 emissions from a particular company, as well as obtain data about its geographic location and other useful information about the company (5 variants of icon size of enterprises conform to the following gradation of enterprises in terms of emissions of CO_2: 1Mt/year or less, 1-4 Mt/year, 4-7 Mt/year, 7-10 Mt/year. 10 Mt/year or more).

Fig. 1. GIS of CO_2 sources of emissions in eastern Ukraine.

GIS makes it possible to simultaneously analyze all the enterprises of chosen industries of the Ukrainian economy (Fig.1), or consider only companies in selected industries: coal-fired power stations (as of 2011, the share of coal in the fuel thermal power plants is more than 97.5% vs 52.3% as shown in the CARMA) is currently represented in the GIS4 12 gas-fired plants-1; steel mills-13; coking plants-14; cement plants-8; various chemical plants (including oil)-3 [1].

It is planned to extend this database with data on CO_2 emissions from all enterprises which are the major air pollutants in these regions – the enterprises of housing and communal services of the city, houses in the private sector, as well as from road transport.

As this GIS is based on informal sources of information, the real value of the volume of CO_2 emissions from particular company may differ from the values presented in the GIS. In such cases, an enterprise may apply to the LCOIR-UA project website with a proposal to update the information on the volume of CO_2 emissions, to be in line with the official statistical reporting of the enterprise. Such regular updates on the amount of CO_2 emissions would indicate a commitment to a responsible attitude towards the problems of global climate change and an awareness of the role of a "carbon footprint" in the occurrence of these problems [2].

The potential of CO_2 Storage Reservoirs. Pumping of CO_2 in geological formations has more than thirty years of experience working to improve oil and gas recovery beds. In addition, in recent times numerous studies on the geological storage of CO_2 are held in various countries. As a long-term storage of CO_2, porous or fractured sedimentary rocks (collectors) are mainly considered, limited by the surrounding mountain environment and the earth's surface with low permeable or substantially impermeable rocks (confining or tires).

It should be noted that natural gas storage (including combustible ones) of natural genesis are reliable over hundreds of thousands or millions of years, leakage of these gases are negligible. There are three main types of formations where geological storage of CO_2 is possible: oil and gas basins which are depleted or are in some stage of depletion deep lying saline formations and have no commercial coal seams.

There are three main types of formations where geological storage of CO_2 is possible: oil and gas basins which are depleted or are in the stage of depletion, deep lying saline formations, and have no commercial coal seams. Among other possible geological formations basalt and shale oil are also considered, but their potential remains insufficiently studied.

The success of the method of the geological storage of CO_2 is confirmed by the results of experiments carried out at different times of the companies MRCSP, MGSC, SECARB, SWP, WESTCARB, BIG SKY, PCOR (USA), as well as in projects Weyburn, Fenn Big Valley (Canada), Sleipner (Norway), Yubari (Japan), Qinshui Basin (China), ets.

Search and selection of geological structures and horizons that can serveas long term storage of CO_2 in oil and gas basins is based, as a rule, on the results of the previous searching and exploration works, and the determination of the potential areas for CO_2 storage requires additional research.

In Ukraine, there are large oil and gas provinces with large amounts of productive horizons. One of the largest oil and gas regions- the Dnieper-Donets Basin is located within the boundaries of two large structures-the Dnieper-Donets Valley (DDV) and the Donets Coal Basin (Donbass). Gas presence of Dnieper-Donets basin is closely related to the clastic sedimentary rocks of the Middle and Upper Carboniferous and Lower Pernian. The Methane gas content of Donbass is also associated with the coal-bearing Carboniferous strata.

The results of previous exploration works has shown that the geological conditions of DDV and Donbass one of the most promising gas-bearing areas are the areas with the stored hydro chemical sediments of Permian age. The important role of hydro-chemical sediments of

Permian age. The important role of hydro-chemical deposits in their good insulating properties (alternating-tight oil and gas layers of rock salt, gypsum and anhydrite dense). The location of hydro chemical sediments in the upper part of a large cycle of sedimentation where lithofacies composition is dominated by rocks with good reservoir properties is also important [3].

These factors combined with high power gas permeable sedimentary rocks, have creted favorable conditions for the free migration of hydrocarbons and their concentration under an impenetrable veil oh hydro-chemical sediments. In the Donbas Lower Permian hydro-chemical formations are developed in the north-western part within Bakhmutskaya and Kalmius Toretskoy-basins. The structure Bakhmutskaya and Kalmius-Toretskoy basins contains three floors: the Paleozoic, Mesozoic and Cenozoic. Mesozoic and Cenozoic structural floors are unpromising in terms of the geological storage of CO_2.

The results of analysis on the possible areas of geological storage of CO_2 have been merged into a single GIS of storage of CO_2 (fig. 2), which is available on the project website and shows the following: Devonian salt stocks, Permian salt bearing sediments, Carboniferous coal-bearing deposits, Devonian boundary saline aquifers horizons, the border of the Paleozoic sediments, the Dnieper-Donets gas-and oil-bearing basin and the Donetsk coal basin, as well as the location of the main sources of CO_2-energy enterprises and steel sectors.

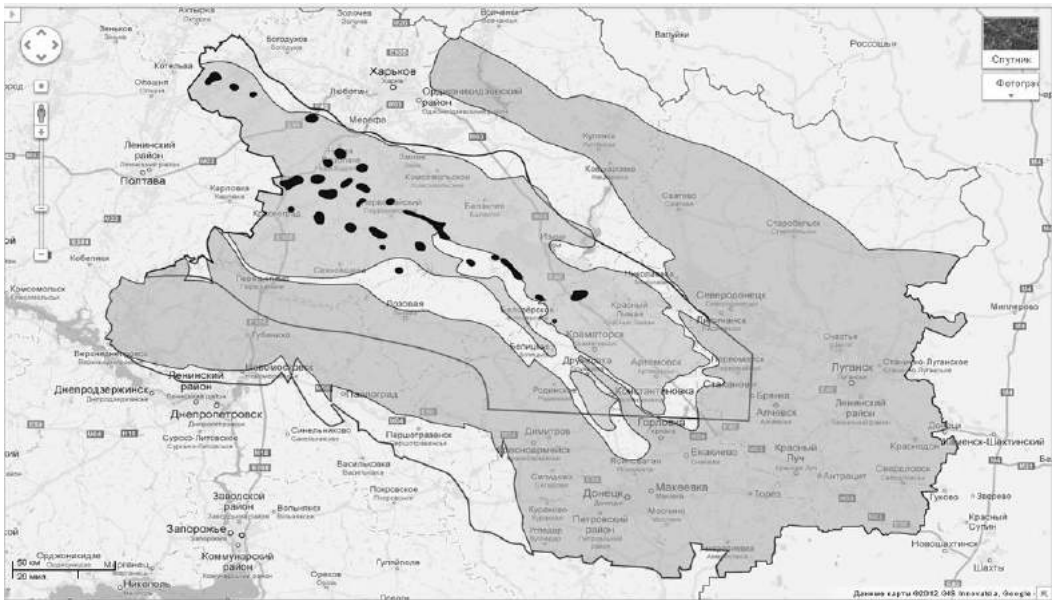

Fig. 2. GIS of CO_2 storage areas in the Ukrainian target regions.

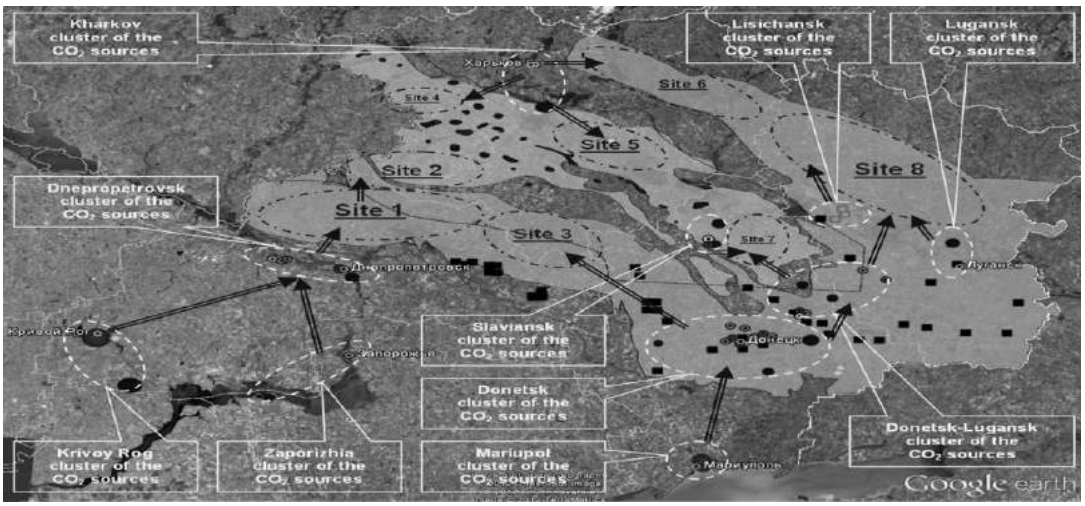

Fig. 3. Geographic location scheme of clusters of sources of CO_2 emissions, possible sites for the geological storage of CO_2 and the direction of transport of CO_2 from emission sources to the geological storage sates.

Recommendations on the allocation of plots of CO_2 storage. Operation proceeds to the step, which includes analytical studies of reservoir properties of each layer at different depths, mineralogical and spectrographic analyzes of rocks that form the horizon, the study of hydrodynamic, hydro-geological and structural-tectonic features of the entire thickness to the depth of the proposed store. Based an these data collector capacitance can be calculated.

Only when the full complex of studies will be carried out, the conclusions about the suitability of the selected horizons for long term storage of CO_2 will be made, and most importantly – the conclusion of the environmental services of process safety injection and storage of CO_2 to the environment and people, it will be possible to proceed to the stage of preparation of experimental studies. Based on the results of foreign geological storage of CO_2 and features of the geological structure of the Donets Basin Districts (Novomoskovskiy, Petrikovskiy, Lozovskaya, Starobelsky and North-western outskirts of the Donbass) are proposed for further study of their potential geological storage of CO_2.

Summarizing the results of these preliminary studies, which are based on open sourse information, the geographical location scheme of clusters of seurces of CO_2 emissins, possible sites for the geological storage of CO_2 and the approximate direction of transport of CO_2 from emission sources to storage tanks was built, where conventional sources of CO_2 clusters are marked with yellow hatched ovals, from which the blue arrows indicate the approximate direction of transport of CO_2 to the alleged sites of storage – brown dash-dotted ovals (fig. 3). Furthermore, black squares show the location of existing coal mines near which reservoirs for CO_2 storage fundamentally cannot be placed [4].

The Figure 3 shows the location of exploration wells from which the samples were taken in order to determine the porosity of rocks by means of computerized tomography on the synchrotron.Hereinafter 5 samples have been studied in the software avizofire with 2-times and 10-times enlargement. Obtained porosity value is about 3, which allows us to make a preliminary conclusion of the promising use of Donbas sedimentary deposits for long-term CO_2 storage [5].

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MP2 ТА DFT ДОСЛІДЖЕННЯ ВНУТРІШНЬОМОЛЕКУЛЯРНОЇ ДИНАМІКИ 2-ПІРІДИН-2-ІЛ-1Н-БЕНЗІМІДАЗОЛА

К. В. Рульова., О. В. Ракша

Резюме. У роботі представлені результати DFT і MP2 теоретичних досліджень внутрішньої динаміки 2-(піридин-2-іл)-1Н-бензімідазолу. В наближенні даних методів розраховані структурні параметри для конформерів 2-(піридин-2-іл)-1Н-бензоімідазолу, оцінені значення внутрішніх бар'єрів обертання, розраховані хімічні зсуви ядер ^{1}H і ^{13}C. Виконано порівняльний аналіз розрахованих та експериментальних величин.

Ключові слова. 2-пірідин-2-іл-1Н-бензімідазол, DFT, MP2, молекулярне моделювання, внутрішньомолекулярна динаміка, конформери.

Вступ

Похідні бензімідазолу – перспективні сполуки-лідери в дизайні лікарських препаратів, що мають антимікробну, противірусну та протиракову активність [1]. Введення в структуру бензімідазолу піридинового фрагмента забезпечує додатковий координаційний центр і відкриває широкі можливості для створення на основі такої структури біоміметичних каталітичних і сенсорних систем. Ефективність і селективність таких систем буде залежати від конформаційних властивостей піридиніл-бензімідазольного фрагмента.

Похідні бензімідазолу, як відомо, мають цікаві фотохімічні і фотофізичні властивості [2-6]. У роботах [7-12] 2-пірідин-2-іл-1Н-бензімідазол пропонується як модельна сполука для вивчення вмісту води у мембранах паливних елементів. Молекула існує як монокатіон, дікатіон або у нейтральній формі в основному стані, залежно від кислотності середовища і зазнає збудженого стану при внутрішньомолекулярному перенесенні протона з утворенням таутомерної формі у збудженому стані [10]. Цей процес відбувається через водний місток, що складається з однієї молекули води, або шляхом передачі атома водню з азоту імідазолу в азот піридину [10-13].

Метою даної роботи є вивчення внутрішньомолекулярної динаміки 2-пірідин-2-іл-1Н-бензімідазолу та параметрів його ЯМР ^{1}H і ^{13}C спектрів методами комп'ютерної хімії.

Експериментальна частина

Експериментальні спектроскопічні ЯМР ^{1}H і ^{13}C дослідження 2-пірідин-2-іл-1Н-бензімідазолу (PBI) виконані на пристрої Bruker Avance II 400 (400 МГц для ядер ^{1}H і