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Regression and soft computing models to estimate young's modulus of CO_2 saturated coals

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ABSTRACT

Young's modulus of coal is a very important deformational property which dictates how the material will behave in presence of sub- and super-critical carbon dioxide during sequestration. But this is also a difficult property to measure due to the extensive instrumental requirements, and wide compositional and structural heterogeneity of the coal. Therefore, an indirect method to measure the saturated Young's modulus of coals has been developed in the present research using artificial neural network (ANN) and adaptive neuro-fuzzy inference system (ANFIS). Low and high rank specimens from three different basins of India and Australia have been used for the analysis. Saturation pressure and the compressive strength (UCS) of the coal specimens have been used as the input parameters to build the models. The performance of the models were evaluated against the multivariate regression model using four different types of statistical parameters such as root mean square error (RMSE), coefficient of determination (R2), mean absolute error percentage (MAPE), and variables accounted for (VAF). Results show that ANFIS model is the best performing one with the least RMSE and MAPE, and highest VAF and R^2. This research demonstrates that it is possible to develop soft computing models that can successfully estimate some of the critical rock mechanics parameters essential for the technical evaluation of the sequestration projects on coal. This generalized model is also excellent in incorporating the possible effect of heterogeneity in specimens and performs well for samples that show similar data distribution. If applied, this can potentially reduce the requirement of extensive, complex and expensive instruments that are required for similar investigations.

1. Introduction

Rapidly increasing greenhouse gases such as CO_2 of the atmosphere are considered as the main drivers of climate change and global warming. Carbon dioxide sequestration in the geological medium has been proposed as an effective way to mitigate such changes. But calculations show that trillions of tons of CO_2 must be sequestered at the end of this century to maintain a safe level of CO_2 in the atmosphere [1–3]. Therefore, multiple geological mediums have been evaluated as potential targets for sequestration: (a) depleted oil and gas reservoirs (b) unminable deep coal seams (c) saline aquifers, and (d) basalts. Among them, coal-seams have been identified as one of the most promising options as it can absorb large amount of CO_2 due to large surface area, has reduced chance of leakage, and CO_2 injection can be coupled with coal bed methane (CBM) recovery to reduce the cost of operations [4–6].

Although advantageous, but carbon dioxide sequestration in coal seams causes abrupt changes in the physico-mechanical and chemical properties of the host rock. Larsen [7] has argued that under ambient condition, dry coal behaves as glassy, strained, and cross-linked macromolecular system. Because of higher intermolecular strength, the molecules cannot undergo large deformation. They are only allowed small-scale rotation and can be considered as 'frozen' in time. It causes the overall mass to behave in a brittle manner. But if heated to a certain temperature named 'glass transition temperature', the molecules become relatively free, can undergo large movement and the system becomes viscous [8]. At this stage only the cross-linking remains intact and maintains the overall shape of this rubbery material. Similarly, evidences show that CO_2 saturation also brings the 'glass transition temperature' down. The dissolved CO_2 molecules can easily rearrange the internal structure of the coal [9]. Due to the porous structure of the coal, under high confining pressure, a large amount of CO_2 get absorbed on the surface as well as get dissolved into the micro-structure [9]. This slow diffusion of the gas in the coal causes extensive swelling and creation of large volumetric strain of the material. Research showed that such swelling has large negative effect on the coal permeability and

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overall strength [10,11].

Experiments on multiple low and high rank Indian and Australian coals [10,12,13] have confirmed decreasing Young's modulus and compressive strength with increasing saturation pressure. From unconfined to up to 3 MPa saturation pressure, 2–17% reduction in compressive strength, and 15–27% decrease in Young's modulus are observed in these cases. Additionally, the phase of the CO_2, which is being sequestered also has tremendous control on the swelling amount and reduction of strength of coal. Perera et al. [14] reported that in naturally fractured black coal, swelling increases significantly as the CO_2 turns from subcritical to super-critical phase. An investigation by Perera et al. [15] on the bituminous coal of Southern Sydney Basin showed that, between 6 and 8 MPa, where CO_2 phase changes from sub-critical to supercritical, a sharp decrease (from 40 to 50% to 70–80%) in the strength values are registered. Apart from this 'transition region', they have farther divided the 'supercritical region' into a 'near-critical' and a 'far-critical' parts. Similarly, Ranathunga et al. [16] also reported 20% to 40–60% decrease in the strength of the brown coal in this 'transition region', which they have termed 'transfer region'. It is understood that greater adsorption potential of the super-critical CO_2 causes the organic compounds to be polymerized, resulting in the plasticization, enhanced ductility, and sharp reduction in the strength of the coal during sequestration [16,17].

While detailed investigation on the control of the coal rank, phase of the saturating CO_2, seam depth, and cleat orientations have revealed highly detailed and very important information regarding the sequestration potential of the coal seams, but they are not easy to conduct. As reported in all the previous studies, any such experimental investigation requires highly sophisticated, complex, sensitive and expensive instrumental setup [18,19]. Also, such instruments needed to be customized as per the intended purpose of the study and each of the experiments run for multiple weeks and months. In such experiments, sensitive parameters such as Young's modulus turns out to be difficult to measure at very high saturation pressures. Due to such constraints, these studies are limited to the places where massive financial support, technological expertise, and man power exists.

Therefore, it is essential to develop alternate indirect methods to measure the strength of the coal samples at different saturation pressures. At least, partial replacement of the experimental procedure with the indirect method can reduce the required instrumental complexities and expedite the analysis. This will also help to conduct studies more easily and effectively in previously unexplored basins. Here, in the present paper, we have tried to develop a soft computing model to estimate the Young's modulus of the coal blocks from the CO_2 saturation pressure and the compressive strength. There are at least three major advantages of this process: (a) it circumnavigates the requirement of sensitive instruments to measure the Young's modulus at elevated pressure; (b) this generalized model is built by considering data from a variety of basins. Therefore, it can be confidently applied to new study areas where limited data are available; (c) this model considers saturation data from both sub-critical and super-critical tests. Therefore, the model is applicable to a wide variety of scenario and depth. Further, application of soft computing in CO_2 sequestration also remained a relatively unexplored territory.

2. Study areas

The data for the present analysis were collected from the following sources: Viete and Ranjith [10] Perera et al. [12,15] Vishal et al. [13], Ranathunga et al. [16]. The specimens belong to the Jharia coal field (India), Latrobe Valley (south-east Victoria, Australia), and Southern Sydney Basin (Australia) and they include both the high (bituminous) and low rank (lignite) coals. The geological maps of the respective basins are shown in Fig. 1 [20–22]. Jharia coal field is Indi's most important coal field. This sickle shaped field has major boundary faults in its southern part. Stratigraphically, at the bottom it has metamorphic rock, followed by Talchir formation, Barakar formation, Barren measures, and Raniganj formations. Among them, Barakar and Raniganj formations are coal bearing [20]. The brown coals of Latrobe Valley group belongs to the Tertiary age and is an important part of onshore Gippsland basin. Traralgon formation (Middle to Late Eocene), is the

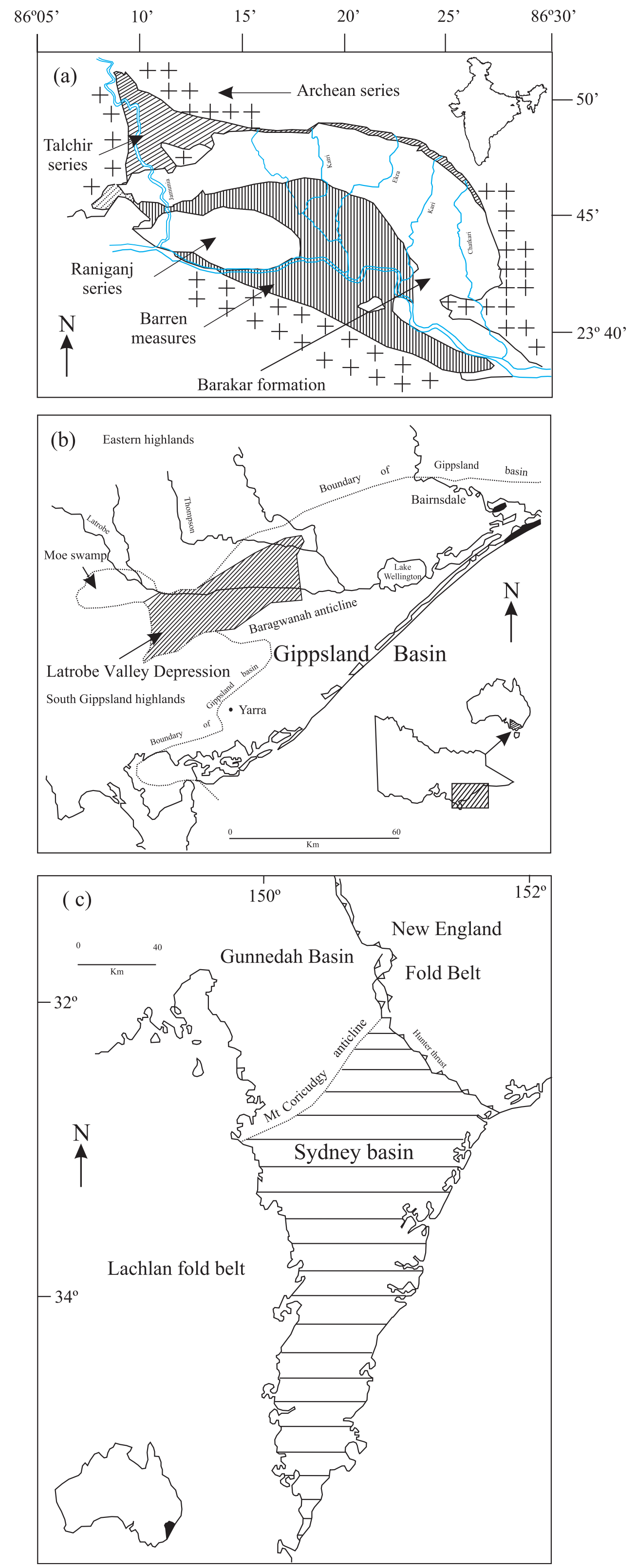

Fig. 1. (a) Jharia coal field, India [20] (b) Latrobe valley, Australia [21] (c) Sydney basin, Australia, [22].